



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:54 AM UTC

PDB ID : 7VTQ / pdb\_00007vtq  
EMDB ID : EMD-32120  
Title : Cryo-EM structure of mouse NLRP3 (full-length) dodecamer  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2021-10-30  
Resolution : 3.55 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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

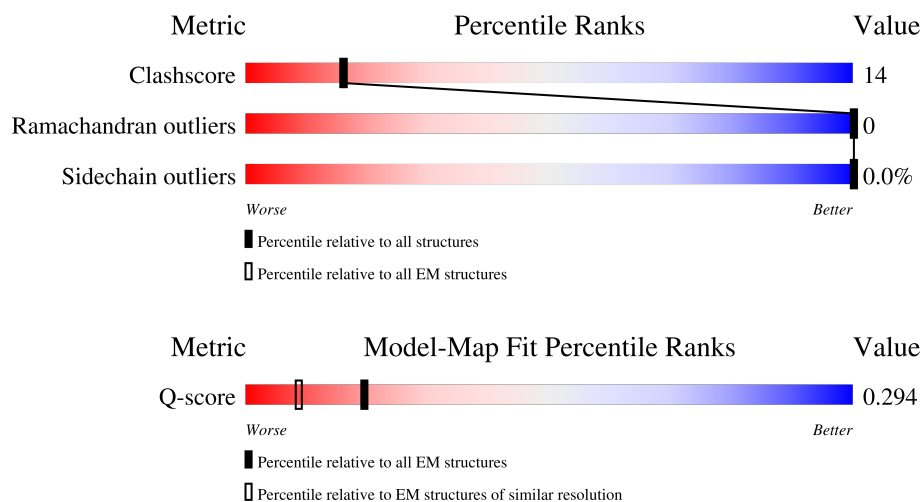
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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.



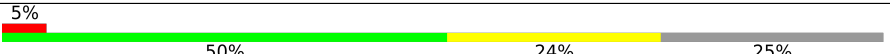
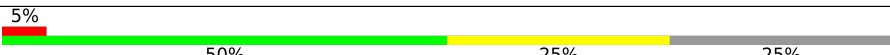
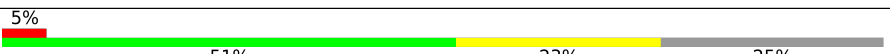
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 12819 ( 3.05 - 4.05 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1057   |                  |
| 1   | B     | 1057   |                  |
| 1   | C     | 1057   |                  |
| 1   | D     | 1057   |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | E     | 1057   |  |
| 1   | F     | 1057   |  |
| 1   | G     | 1057   |  |
| 1   | H     | 1057   |  |
| 1   | I     | 1057   |  |
| 1   | J     | 1057   |  |
| 1   | K     | 1057   |  |
| 1   | L     | 1057   |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 76572 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 NACHT, LRR and PYD domains-containing protein 3.

| Mol | Chain | Residues | Atoms         |           |           |           |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|---------|-------|
| 1   | A     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | B     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | C     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | D     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | E     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | F     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | G     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | H     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | I     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | J     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | K     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |
| 1   | L     | 789      | Total<br>6326 | C<br>4047 | N<br>1081 | O<br>1146 | S<br>52 | 0       | 0     |

There are 288 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| A     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| A     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| A     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| A     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| A     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| A     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| A     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| A     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| A     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| A     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| A     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| A     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| A     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| A     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| A     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| A     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| A     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| A     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| A     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| A     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| A     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| A     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| B     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| B     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| B     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| B     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| B     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| B     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| B     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| B     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| B     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| B     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| B     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| B     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| B     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| B     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| B     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| B     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| B     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| B     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| B     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| C     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| C     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| C     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| C     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| C     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| C     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| C     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| C     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| C     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| C     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| C     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| C     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| C     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| C     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| C     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| C     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| C     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| C     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| D     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| D     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| D     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| D     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| D     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
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| D     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| D     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| D     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| D     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
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| D     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| D     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| D     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| D     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| D     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| D     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| D     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| D     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| D     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| D     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| D     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| D     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| E     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| E     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| E     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
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| E     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| E     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| E     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| E     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| E     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| E     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| E     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| E     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| E     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| E     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| E     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| E     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| E     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| E     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| E     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| E     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| E     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| E     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| E     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| F     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
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| F     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| F     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| F     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| F     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| F     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| F     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| F     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| F     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| F     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| F     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| F     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| F     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| F     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| F     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
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| F     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| F     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| F     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| G     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| G     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| G     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| G     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| G     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| G     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| G     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| G     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| G     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| G     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| G     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| G     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| G     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| G     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| G     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| G     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| G     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| G     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| G     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| H     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| H     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| H     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| H     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| H     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| H     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| H     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| H     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
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| H     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| H     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
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| H     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| H     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| H     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| H     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| H     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| H     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| H     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| H     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| H     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| H     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| H     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| I     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| I     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| I     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| I     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| I     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| I     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| I     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| I     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| I     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| I     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| I     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| I     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| I     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| I     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| I     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| I     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| I     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| I     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| I     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |

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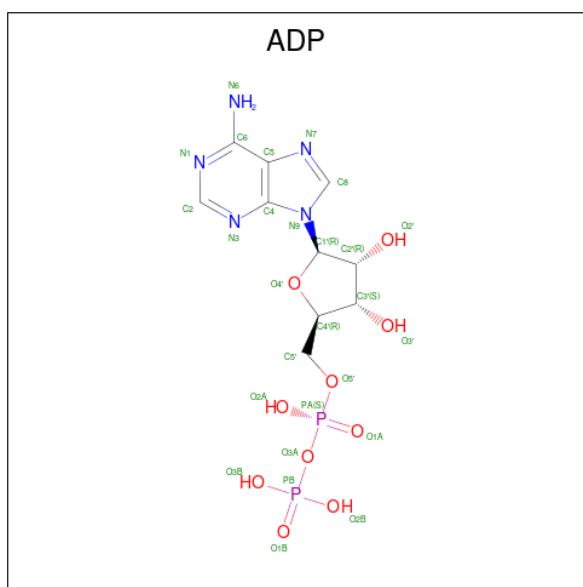
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
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| J     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| J     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| J     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| J     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| J     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| J     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| J     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| J     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| J     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| J     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| J     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| J     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| J     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| J     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| J     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| J     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| J     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| J     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| J     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| J     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| J     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| J     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| J     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| K     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| K     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| K     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| K     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| K     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| K     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| K     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| K     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| K     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| K     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| K     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| K     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| K     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |

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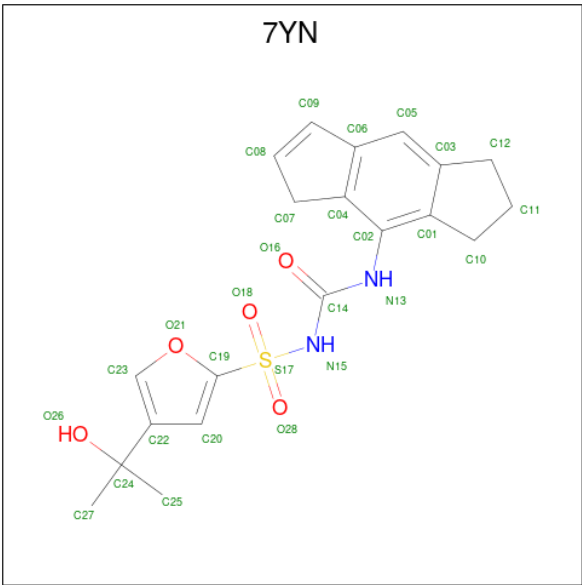
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|-------|---------|----------|--------|----------------|------------|
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| K     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| K     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| K     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| K     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| K     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |
| L     | -23     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -22     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -21     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -20     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -19     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -18     | HIS      | -      | expression tag | UNP Q8R4B8 |
| L     | -17     | ASP      | -      | expression tag | UNP Q8R4B8 |
| L     | -16     | TYR      | -      | expression tag | UNP Q8R4B8 |
| L     | -15     | LYS      | -      | expression tag | UNP Q8R4B8 |
| L     | -14     | ASP      | -      | expression tag | UNP Q8R4B8 |
| L     | -13     | ASP      | -      | expression tag | UNP Q8R4B8 |
| L     | -12     | ASP      | -      | expression tag | UNP Q8R4B8 |
| L     | -11     | ASP      | -      | expression tag | UNP Q8R4B8 |
| L     | -10     | LYS      | -      | expression tag | UNP Q8R4B8 |
| L     | -9      | LEU      | -      | expression tag | UNP Q8R4B8 |
| L     | -8      | GLU      | -      | expression tag | UNP Q8R4B8 |
| L     | -7      | VAL      | -      | expression tag | UNP Q8R4B8 |
| L     | -6      | LEU      | -      | expression tag | UNP Q8R4B8 |
| L     | -5      | PHE      | -      | expression tag | UNP Q8R4B8 |
| L     | -4      | GLN      | -      | expression tag | UNP Q8R4B8 |
| L     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| L     | -2      | PRO      | -      | expression tag | UNP Q8R4B8 |
| L     | -1      | GLU      | -      | expression tag | UNP Q8R4B8 |
| L     | 0       | PHE      | -      | expression tag | UNP Q8R4B8 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



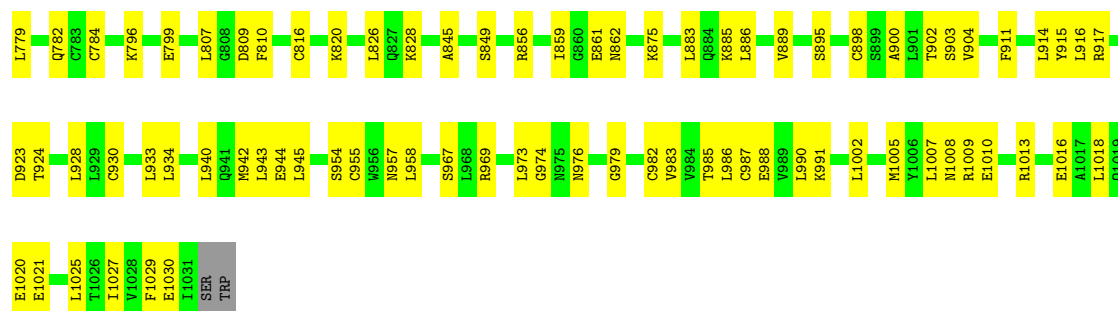
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 3 is 1-[4-(2-oxidanylpropan-2-yl)furan-2-yl]sulfonyl-3-(1,2,3,5-tetrahydro-s-indacen-4-yl)urea (CCD ID: 7YN) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>2</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).

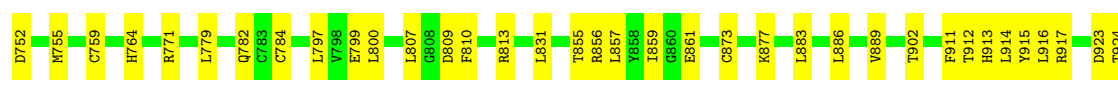
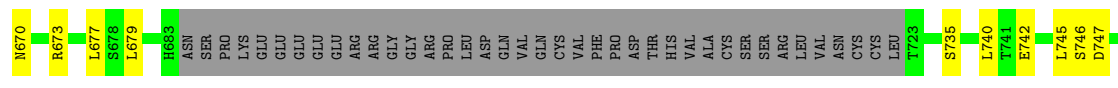
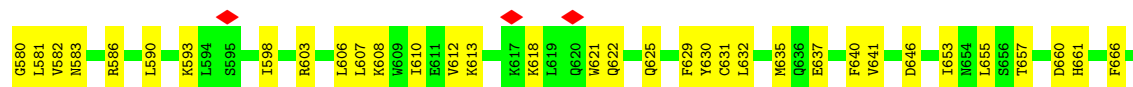
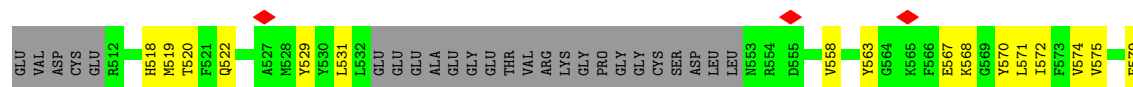
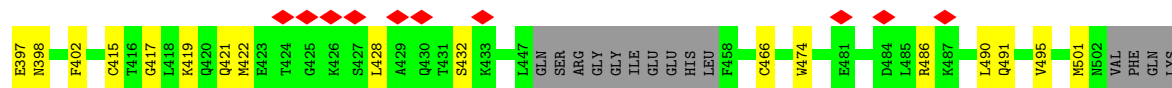
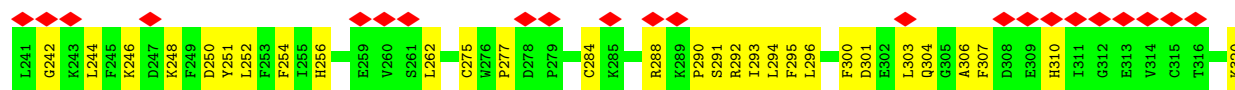
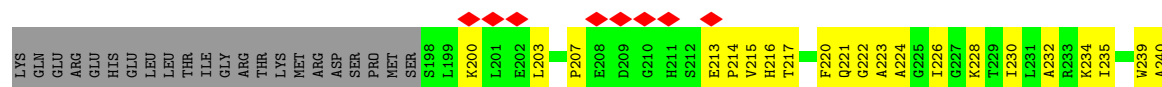
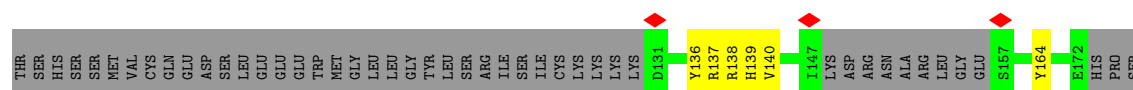
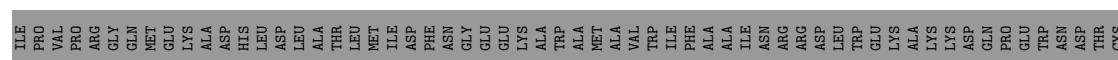
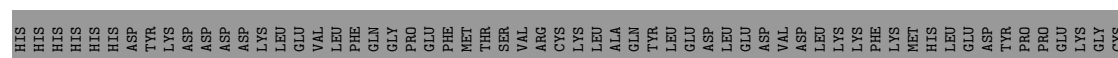


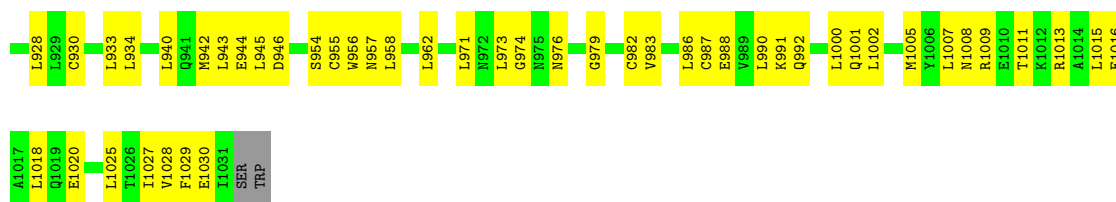
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | G     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | H     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | I     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | J     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | K     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |
| 3   | L     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 28    | 20 | 2 | 5 | 1 |         |



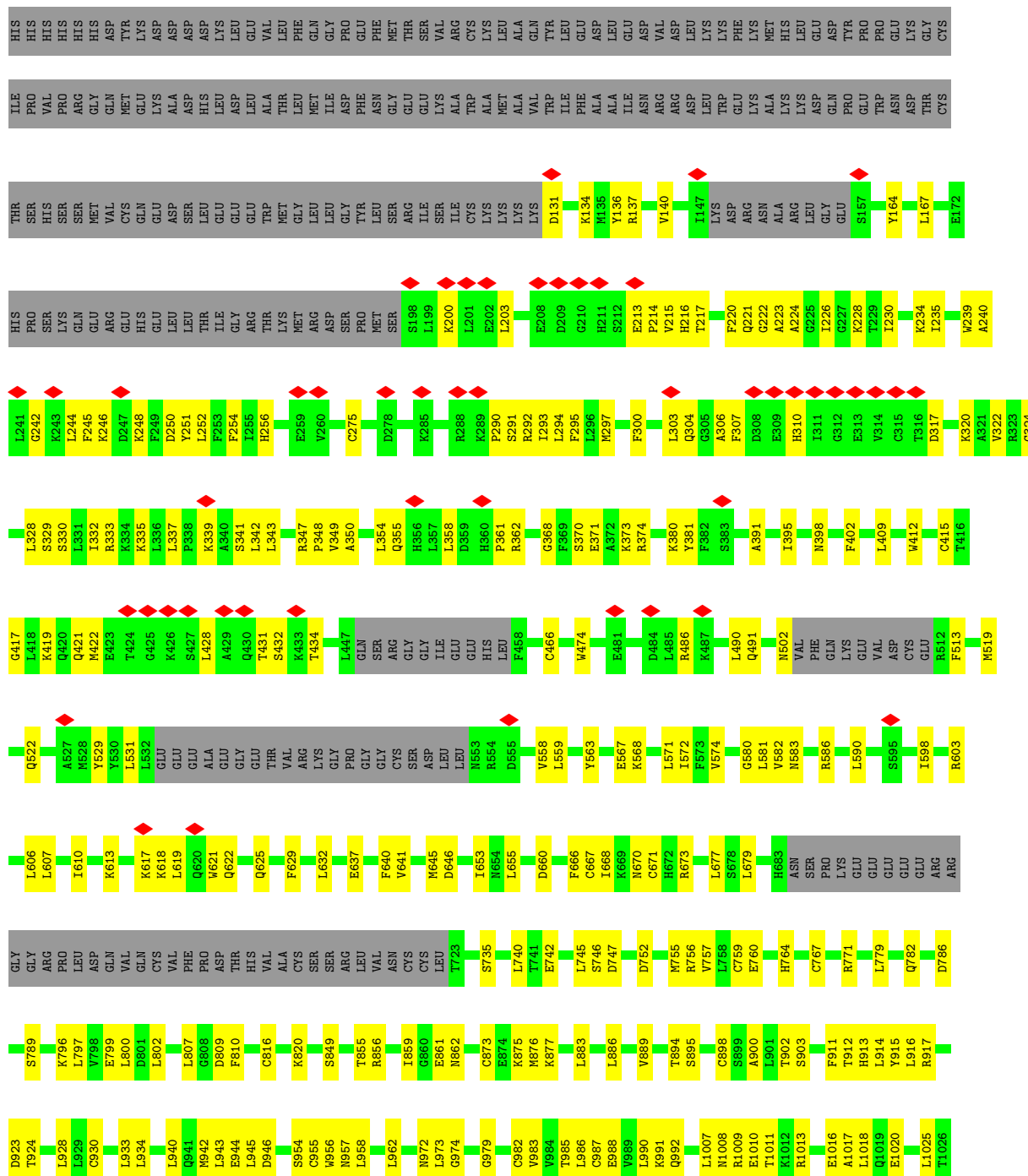


- Molecule 1: NACHT, LRR and PYD domains-containing protein 3





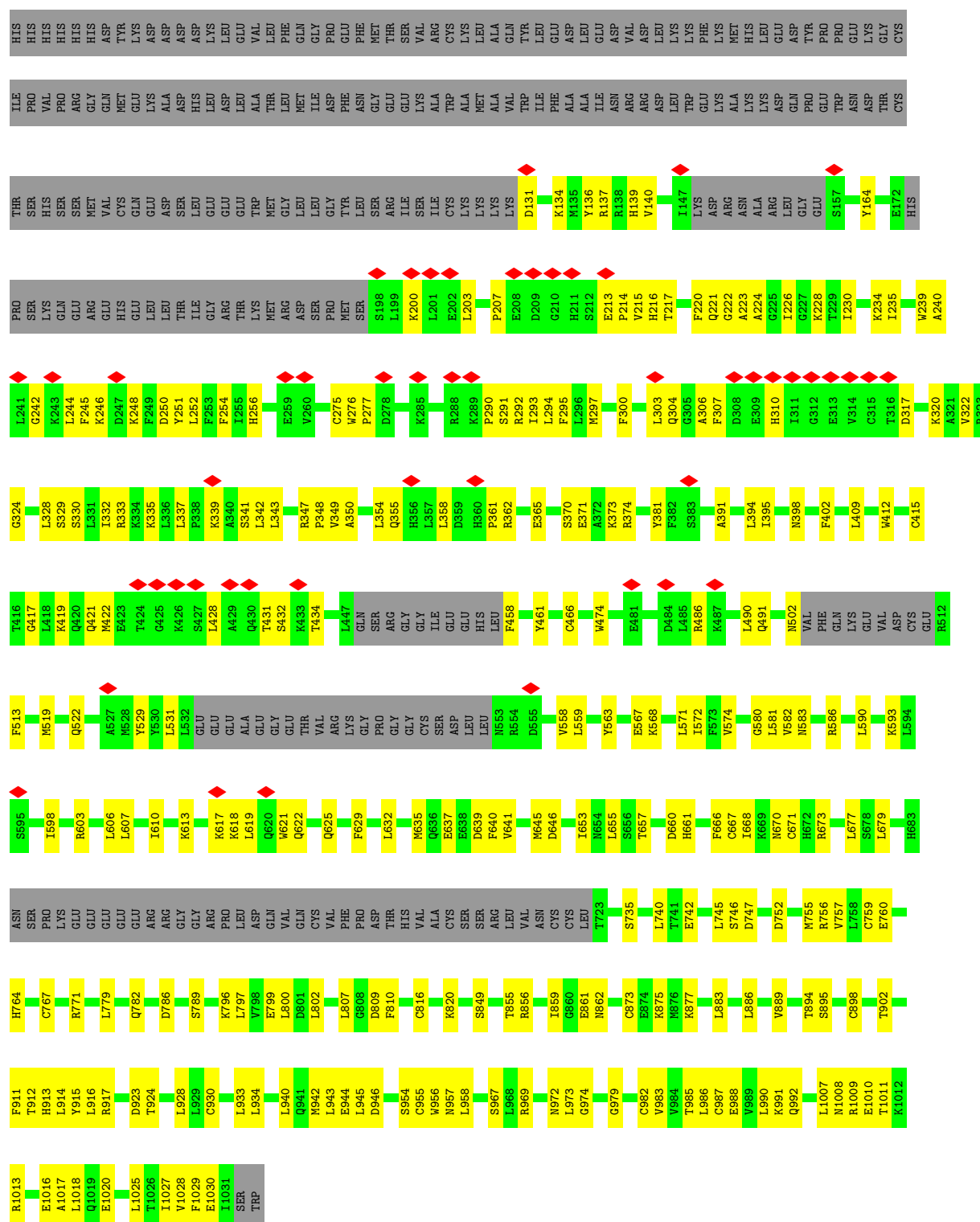
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



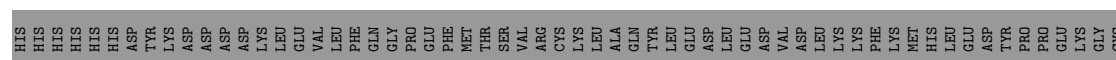


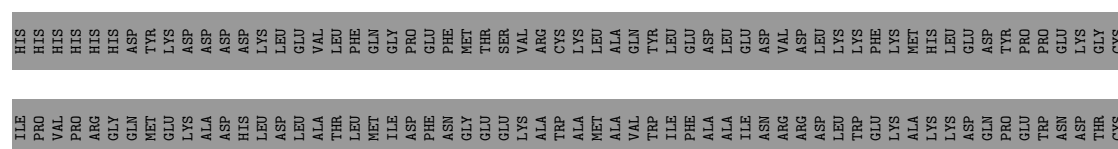
Chain E: 

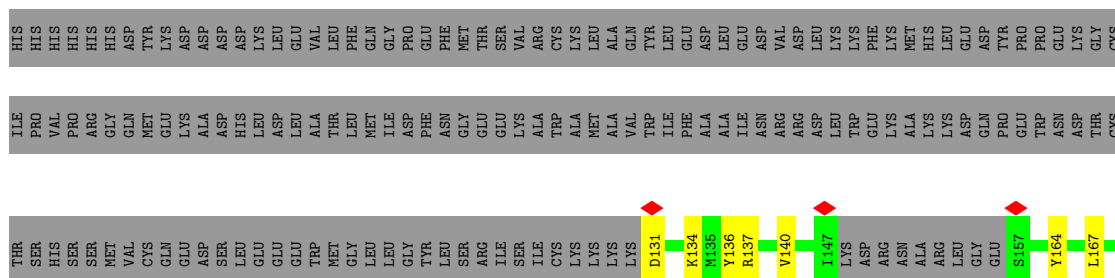




- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



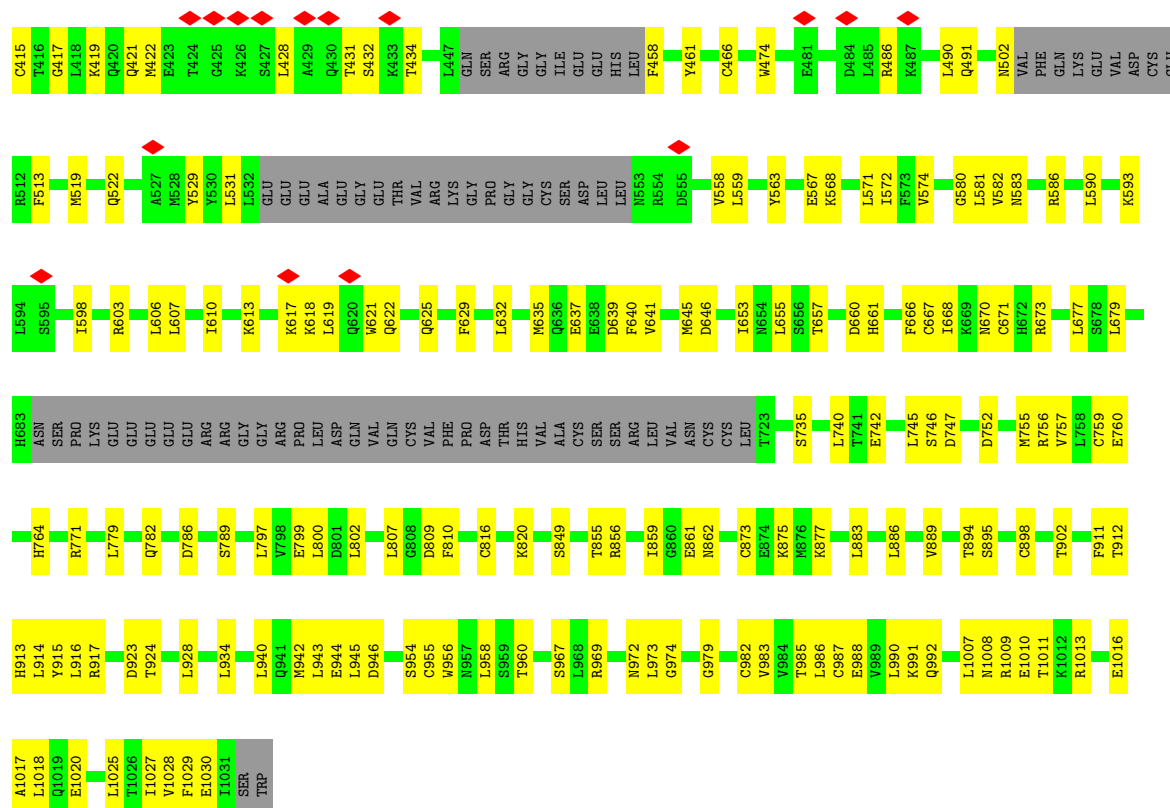












## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, D6           | Depositor |
| Number of particles used             | 73930               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 68                  | Depositor |
| Minimum defocus (nm)                 | Not provided        |           |
| Maximum defocus (nm)                 | Not provided        |           |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.047               | Depositor |
| Minimum map value                    | -0.017              | Depositor |
| Average map value                    | 0.000               | Depositor |
| Map value standard deviation         | 0.004               | Depositor |
| Recommended contour level            | 0.01                | Depositor |
| Map size ( $\text{\AA}$ )            | 298.8, 298.8, 298.8 | wwPDB     |
| Map dimensions                       | 240, 240, 240       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.245, 1.245, 1.245 | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 7YN, ADP

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | B     | 0.13         | 0/6444      | 0.33        | 0/8685      |
| 1   | C     | 0.13         | 0/6444      | 0.33        | 0/8685      |
| 1   | D     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | E     | 0.13         | 0/6444      | 0.33        | 0/8685      |
| 1   | F     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | G     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | H     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | I     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | J     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| 1   | K     | 0.14         | 0/6444      | 0.33        | 0/8685      |
| 1   | L     | 0.13         | 0/6444      | 0.34        | 0/8685      |
| All | All   | 0.13         | 0/77328     | 0.34        | 0/104220    |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6326  | 0        | 6409     | 182     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 6326  | 0        | 6409     | 188     | 0            |
| 1   | C     | 6326  | 0        | 6409     | 184     | 0            |
| 1   | D     | 6326  | 0        | 6409     | 180     | 0            |
| 1   | E     | 6326  | 0        | 6409     | 187     | 0            |
| 1   | F     | 6326  | 0        | 6409     | 191     | 0            |
| 1   | G     | 6326  | 0        | 6409     | 186     | 0            |
| 1   | H     | 6326  | 0        | 6409     | 183     | 0            |
| 1   | I     | 6326  | 0        | 6409     | 192     | 0            |
| 1   | J     | 6326  | 0        | 6409     | 181     | 0            |
| 1   | K     | 6326  | 0        | 6409     | 184     | 0            |
| 1   | L     | 6326  | 0        | 6409     | 185     | 0            |
| 2   | A     | 27    | 0        | 12       | 4       | 0            |
| 2   | B     | 27    | 0        | 12       | 3       | 0            |
| 2   | C     | 27    | 0        | 12       | 4       | 0            |
| 2   | D     | 27    | 0        | 12       | 4       | 0            |
| 2   | E     | 27    | 0        | 12       | 3       | 0            |
| 2   | F     | 27    | 0        | 12       | 4       | 0            |
| 2   | G     | 27    | 0        | 12       | 4       | 0            |
| 2   | H     | 27    | 0        | 12       | 3       | 0            |
| 2   | I     | 27    | 0        | 12       | 4       | 0            |
| 2   | J     | 27    | 0        | 12       | 4       | 0            |
| 2   | K     | 27    | 0        | 12       | 3       | 0            |
| 2   | L     | 27    | 0        | 12       | 4       | 0            |
| 3   | A     | 28    | 0        | 0        | 1       | 0            |
| 3   | B     | 28    | 0        | 0        | 1       | 0            |
| 3   | C     | 28    | 0        | 0        | 1       | 0            |
| 3   | D     | 28    | 0        | 0        | 0       | 0            |
| 3   | E     | 28    | 0        | 0        | 1       | 0            |
| 3   | F     | 28    | 0        | 0        | 1       | 0            |
| 3   | G     | 28    | 0        | 0        | 1       | 0            |
| 3   | H     | 28    | 0        | 0        | 1       | 0            |
| 3   | I     | 28    | 0        | 0        | 1       | 0            |
| 3   | J     | 28    | 0        | 0        | 1       | 0            |
| 3   | K     | 28    | 0        | 0        | 1       | 0            |
| 3   | L     | 28    | 0        | 0        | 1       | 0            |
| All | All   | 76572 | 0        | 77052    | 2195    | 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 14.

All (2195) 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:I:645:MET:HE1   | 1:I:667:CYS:HB3  | 1.55                     | 0.88              |
| 1:C:645:MET:HE1   | 1:C:667:CYS:HB3  | 1.56                     | 0.88              |
| 1:F:645:MET:HE1   | 1:F:667:CYS:HB3  | 1.55                     | 0.88              |
| 1:L:645:MET:HE1   | 1:L:667:CYS:HB3  | 1.55                     | 0.88              |
| 1:J:645:MET:HE1   | 1:J:667:CYS:HB3  | 1.57                     | 0.87              |
| 1:D:645:MET:HE1   | 1:D:667:CYS:HB3  | 1.57                     | 0.86              |
| 1:G:645:MET:HE1   | 1:G:667:CYS:HB3  | 1.57                     | 0.85              |
| 1:A:645:MET:HE1   | 1:A:667:CYS:HB3  | 1.57                     | 0.85              |
| 1:A:1009:ARG:HH12 | 1:A:1013:ARG:HB2 | 1.43                     | 0.83              |
| 1:G:1009:ARG:HH12 | 1:G:1013:ARG:HB2 | 1.43                     | 0.83              |
| 1:F:635:MET:HE3   | 1:F:637:GLU:HB3  | 1.62                     | 0.82              |
| 1:L:635:MET:HE3   | 1:L:637:GLU:HB3  | 1.62                     | 0.82              |
| 1:I:635:MET:HE3   | 1:I:637:GLU:HB3  | 1.61                     | 0.82              |
| 1:D:1009:ARG:HH12 | 1:D:1013:ARG:HB2 | 1.43                     | 0.82              |
| 1:I:1009:ARG:HH12 | 1:I:1013:ARG:HB2 | 1.45                     | 0.81              |
| 1:J:1009:ARG:HH12 | 1:J:1013:ARG:HB2 | 1.43                     | 0.81              |
| 1:C:1009:ARG:HH12 | 1:C:1013:ARG:HB2 | 1.45                     | 0.81              |
| 1:F:1009:ARG:HH12 | 1:F:1013:ARG:HB2 | 1.44                     | 0.80              |
| 1:L:1009:ARG:HH12 | 1:L:1013:ARG:HB2 | 1.45                     | 0.80              |
| 1:H:579:PHE:HD2   | 1:H:631:CYS:HB3  | 1.48                     | 0.78              |
| 1:B:419:LYS:HA    | 1:B:422:MET:HE2  | 1.65                     | 0.78              |
| 1:H:419:LYS:HA    | 1:H:422:MET:HE2  | 1.65                     | 0.78              |
| 1:L:419:LYS:HA    | 1:L:422:MET:HE2  | 1.65                     | 0.78              |
| 1:D:635:MET:HE3   | 1:D:637:GLU:HB3  | 1.65                     | 0.77              |
| 1:J:635:MET:HE3   | 1:J:637:GLU:HB3  | 1.65                     | 0.77              |
| 1:C:419:LYS:HA    | 1:C:422:MET:HE2  | 1.65                     | 0.77              |
| 1:A:215:VAL:HA    | 1:A:362:ARG:HH12 | 1.50                     | 0.77              |
| 1:G:215:VAL:HA    | 1:G:362:ARG:HH12 | 1.49                     | 0.77              |
| 1:K:419:LYS:HA    | 1:K:422:MET:HE2  | 1.65                     | 0.77              |
| 1:E:419:LYS:HA    | 1:E:422:MET:HE2  | 1.65                     | 0.77              |
| 1:J:215:VAL:HA    | 1:J:362:ARG:HH12 | 1.49                     | 0.77              |
| 1:F:419:LYS:HA    | 1:F:422:MET:HE2  | 1.65                     | 0.77              |
| 1:B:579:PHE:HD2   | 1:B:631:CYS:HB3  | 1.49                     | 0.77              |
| 1:I:419:LYS:HA    | 1:I:422:MET:HE2  | 1.65                     | 0.77              |
| 1:D:215:VAL:HA    | 1:D:362:ARG:HH12 | 1.50                     | 0.77              |
| 1:G:635:MET:HE3   | 1:G:637:GLU:HB3  | 1.65                     | 0.76              |
| 1:A:635:MET:HE3   | 1:A:637:GLU:HB3  | 1.65                     | 0.76              |
| 1:E:215:VAL:HA    | 1:E:362:ARG:HH12 | 1.51                     | 0.76              |
| 1:K:579:PHE:HD2   | 1:K:631:CYS:HB3  | 1.48                     | 0.76              |
| 1:K:215:VAL:HA    | 1:K:362:ARG:HH12 | 1.51                     | 0.76              |
| 1:E:579:PHE:HD2   | 1:E:631:CYS:HB3  | 1.48                     | 0.76              |
| 1:B:215:VAL:HA    | 1:B:362:ARG:HH12 | 1.51                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:215:VAL:HA   | 1:H:362:ARG:HH12  | 1.51                     | 0.74              |
| 1:B:474:TRP:HE1  | 1:B:558:VAL:HG21  | 1.54                     | 0.72              |
| 1:H:474:TRP:HE1  | 1:H:558:VAL:HG21  | 1.54                     | 0.72              |
| 1:E:495:VAL:HG13 | 1:E:501:MET:HE3   | 1.71                     | 0.72              |
| 1:F:239:TRP:O    | 1:F:246:LYS:NZ    | 2.23                     | 0.72              |
| 1:L:239:TRP:O    | 1:L:246:LYS:NZ    | 2.23                     | 0.72              |
| 1:B:495:VAL:HG13 | 1:B:501:MET:HE3   | 1.71                     | 0.72              |
| 1:C:883:LEU:HD21 | 1:C:886:LEU:HB2   | 1.73                     | 0.71              |
| 1:L:883:LEU:HD21 | 1:L:886:LEU:HB2   | 1.72                     | 0.71              |
| 1:F:883:LEU:HD21 | 1:F:886:LEU:HB2   | 1.72                     | 0.71              |
| 1:I:883:LEU:HD21 | 1:I:886:LEU:HB2   | 1.73                     | 0.71              |
| 1:A:845:ALA:HB1  | 1:A:875:LYS:HG2   | 1.72                     | 0.71              |
| 1:G:845:ALA:HB1  | 1:G:875:LYS:HG2   | 1.71                     | 0.71              |
| 1:D:845:ALA:HB1  | 1:D:875:LYS:HG2   | 1.71                     | 0.71              |
| 1:F:894:THR:HG22 | 1:F:895:SER:H     | 1.55                     | 0.71              |
| 1:L:894:THR:HG22 | 1:L:895:SER:H     | 1.55                     | 0.71              |
| 1:K:474:TRP:HE1  | 1:K:558:VAL:HG21  | 1.54                     | 0.71              |
| 1:H:239:TRP:O    | 1:H:246:LYS:NZ    | 2.24                     | 0.70              |
| 1:J:845:ALA:HB1  | 1:J:875:LYS:HG2   | 1.72                     | 0.70              |
| 1:B:239:TRP:O    | 1:B:246:LYS:NZ    | 2.24                     | 0.70              |
| 1:E:474:TRP:HE1  | 1:E:558:VAL:HG21  | 1.54                     | 0.70              |
| 1:E:635:MET:HE3  | 1:E:637:GLU:HB3   | 1.74                     | 0.70              |
| 1:K:217:THR:O    | 1:K:361:PRO:HA    | 1.91                     | 0.70              |
| 1:K:635:MET:HE3  | 1:K:637:GLU:HB3   | 1.74                     | 0.70              |
| 1:G:138:ARG:NH2  | 1:G:240:ALA:O     | 2.25                     | 0.70              |
| 1:I:894:THR:HG22 | 1:I:895:SER:H     | 1.55                     | 0.70              |
| 1:J:466:CYS:HB3  | 1:J:529:TYR:HB2   | 1.74                     | 0.70              |
| 1:C:894:THR:HG22 | 1:C:895:SER:H     | 1.55                     | 0.70              |
| 1:A:138:ARG:NH2  | 1:A:240:ALA:O     | 2.25                     | 0.69              |
| 1:D:466:CYS:HB3  | 1:D:529:TYR:HB2   | 1.74                     | 0.69              |
| 1:D:641:VAL:O    | 1:D:645:MET:HB2   | 1.92                     | 0.69              |
| 1:D:883:LEU:HD21 | 1:D:886:LEU:HB2   | 1.74                     | 0.69              |
| 1:I:466:CYS:HB3  | 1:I:529:TYR:HB2   | 1.73                     | 0.69              |
| 1:J:641:VAL:O    | 1:J:645:MET:HB2   | 1.92                     | 0.69              |
| 1:C:239:TRP:O    | 1:C:246:LYS:NZ    | 2.23                     | 0.69              |
| 1:E:217:THR:O    | 1:E:361:PRO:HA    | 1.92                     | 0.69              |
| 1:E:666:PHE:O    | 1:E:670:ASN:ND2   | 2.26                     | 0.69              |
| 1:F:1010:GLU:HG3 | 1:F:1013:ARG:HH22 | 1.57                     | 0.69              |
| 1:J:883:LEU:HD21 | 1:J:886:LEU:HB2   | 1.74                     | 0.69              |
| 1:A:666:PHE:O    | 1:A:670:ASN:ND2   | 2.26                     | 0.69              |
| 1:D:138:ARG:NH2  | 1:D:240:ALA:O     | 2.25                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:666:PHE:O    | 1:G:670:ASN:ND2   | 2.26                     | 0.69              |
| 1:G:883:LEU:HD21 | 1:G:886:LEU:HB2   | 1.74                     | 0.69              |
| 1:J:666:PHE:O    | 1:J:670:ASN:ND2   | 2.26                     | 0.69              |
| 1:K:666:PHE:O    | 1:K:670:ASN:ND2   | 2.26                     | 0.69              |
| 1:L:1010:GLU:HG3 | 1:L:1013:ARG:HH22 | 1.57                     | 0.69              |
| 1:A:883:LEU:HD21 | 1:A:886:LEU:HB2   | 1.74                     | 0.69              |
| 1:D:666:PHE:O    | 1:D:670:ASN:ND2   | 2.25                     | 0.69              |
| 1:J:138:ARG:NH2  | 1:J:240:ALA:O     | 2.25                     | 0.69              |
| 1:B:217:THR:O    | 1:B:361:PRO:HA    | 1.91                     | 0.69              |
| 1:I:239:TRP:O    | 1:I:246:LYS:NZ    | 2.23                     | 0.69              |
| 1:K:466:CYS:HB3  | 1:K:529:TYR:HB2   | 1.73                     | 0.69              |
| 1:G:641:VAL:O    | 1:G:645:MET:HB2   | 1.92                     | 0.69              |
| 1:H:466:CYS:HB3  | 1:H:529:TYR:HB2   | 1.74                     | 0.69              |
| 1:E:466:CYS:HB3  | 1:E:529:TYR:HB2   | 1.74                     | 0.69              |
| 1:F:466:CYS:HB3  | 1:F:529:TYR:HB2   | 1.73                     | 0.69              |
| 1:A:239:TRP:O    | 1:A:246:LYS:NZ    | 2.24                     | 0.69              |
| 1:A:641:VAL:O    | 1:A:645:MET:HB2   | 1.92                     | 0.69              |
| 1:L:466:CYS:HB3  | 1:L:529:TYR:HB2   | 1.73                     | 0.69              |
| 1:L:474:TRP:HE1  | 1:L:558:VAL:HG21  | 1.57                     | 0.69              |
| 1:A:131:ASP:HB3  | 1:A:134:LYS:HG3   | 1.75                     | 0.69              |
| 1:C:466:CYS:HB3  | 1:C:529:TYR:HB2   | 1.73                     | 0.69              |
| 1:G:131:ASP:HB3  | 1:G:134:LYS:HG3   | 1.75                     | 0.69              |
| 1:G:239:TRP:O    | 1:G:246:LYS:NZ    | 2.24                     | 0.69              |
| 1:I:1010:GLU:HG3 | 1:I:1013:ARG:HH22 | 1.57                     | 0.69              |
| 1:E:216:HIS:HB3  | 1:E:341:SER:HA    | 1.75                     | 0.68              |
| 1:F:474:TRP:HE1  | 1:F:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:H:217:THR:O    | 1:H:361:PRO:HA    | 1.92                     | 0.68              |
| 1:L:666:PHE:O    | 1:L:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:B:666:PHE:O    | 1:B:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:D:131:ASP:HB3  | 1:D:134:LYS:HG3   | 1.75                     | 0.68              |
| 1:J:131:ASP:HB3  | 1:J:134:LYS:HG3   | 1.75                     | 0.68              |
| 1:B:216:HIS:HB3  | 1:B:341:SER:HA    | 1.75                     | 0.68              |
| 1:C:666:PHE:O    | 1:C:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:D:474:TRP:HE1  | 1:D:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:F:666:PHE:O    | 1:F:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:J:474:TRP:HE1  | 1:J:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:K:216:HIS:HB3  | 1:K:341:SER:HA    | 1.76                     | 0.68              |
| 1:A:217:THR:O    | 1:A:361:PRO:HA    | 1.94                     | 0.68              |
| 1:I:666:PHE:O    | 1:I:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:C:1010:GLU:HG3 | 1:C:1013:ARG:HH22 | 1.57                     | 0.68              |
| 1:D:239:TRP:O    | 1:D:246:LYS:NZ    | 2.24                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:221:GLN:HB3  | 1:G:348:PRO:HG3   | 1.75                     | 0.68              |
| 1:G:474:TRP:HE1  | 1:G:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:H:216:HIS:HB3  | 1:H:341:SER:HA    | 1.76                     | 0.68              |
| 1:A:221:GLN:HB3  | 1:A:348:PRO:HG3   | 1.76                     | 0.68              |
| 1:A:1010:GLU:HG3 | 1:A:1013:ARG:HH22 | 1.59                     | 0.68              |
| 1:G:217:THR:O    | 1:G:361:PRO:HA    | 1.94                     | 0.68              |
| 1:G:1010:GLU:HG3 | 1:G:1013:ARG:HH22 | 1.59                     | 0.68              |
| 1:H:138:ARG:NH2  | 1:H:240:ALA:O     | 2.27                     | 0.68              |
| 1:L:221:GLN:HB3  | 1:L:348:PRO:HG3   | 1.75                     | 0.68              |
| 1:A:474:TRP:HE1  | 1:A:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:B:375:LYS:HA   | 1:B:392:PHE:CE1   | 2.29                     | 0.68              |
| 1:E:221:GLN:HB3  | 1:E:348:PRO:HG3   | 1.76                     | 0.68              |
| 1:H:635:MET:HE3  | 1:H:637:GLU:HB3   | 1.74                     | 0.68              |
| 1:B:138:ARG:NH2  | 1:B:240:ALA:O     | 2.27                     | 0.68              |
| 1:J:239:TRP:O    | 1:J:246:LYS:NZ    | 2.24                     | 0.68              |
| 1:K:221:GLN:HB3  | 1:K:348:PRO:HG3   | 1.76                     | 0.68              |
| 1:B:635:MET:HE3  | 1:B:637:GLU:HB3   | 1.74                     | 0.68              |
| 1:C:474:TRP:HE1  | 1:C:558:VAL:HG21  | 1.58                     | 0.68              |
| 1:D:217:THR:O    | 1:D:361:PRO:HA    | 1.94                     | 0.68              |
| 1:H:666:PHE:O    | 1:H:670:ASN:ND2   | 2.26                     | 0.68              |
| 1:A:466:CYS:HB3  | 1:A:529:TYR:HB2   | 1.74                     | 0.67              |
| 1:G:466:CYS:HB3  | 1:G:529:TYR:HB2   | 1.74                     | 0.67              |
| 1:H:883:LEU:HD21 | 1:H:886:LEU:HB2   | 1.76                     | 0.67              |
| 1:B:466:CYS:HB3  | 1:B:529:TYR:HB2   | 1.74                     | 0.67              |
| 1:B:136:TYR:OH   | 1:B:275:CYS:SG    | 2.53                     | 0.67              |
| 1:B:883:LEU:HD21 | 1:B:886:LEU:HB2   | 1.76                     | 0.67              |
| 1:J:221:GLN:HB3  | 1:J:348:PRO:HG3   | 1.75                     | 0.67              |
| 1:H:136:TYR:OH   | 1:H:275:CYS:SG    | 2.53                     | 0.67              |
| 1:H:579:PHE:CD2  | 1:H:631:CYS:HB3   | 2.30                     | 0.67              |
| 1:H:375:LYS:HA   | 1:H:392:PHE:CE1   | 2.30                     | 0.67              |
| 1:J:217:THR:O    | 1:J:361:PRO:HA    | 1.94                     | 0.67              |
| 1:D:221:GLN:HB3  | 1:D:348:PRO:HG3   | 1.76                     | 0.67              |
| 1:E:375:LYS:HA   | 1:E:392:PHE:CE1   | 2.29                     | 0.67              |
| 1:E:138:ARG:NH2  | 1:E:240:ALA:O     | 2.27                     | 0.67              |
| 1:E:239:TRP:O    | 1:E:246:LYS:NZ    | 2.24                     | 0.67              |
| 1:K:239:TRP:O    | 1:K:246:LYS:NZ    | 2.24                     | 0.67              |
| 1:C:221:GLN:HB3  | 1:C:348:PRO:HG3   | 1.76                     | 0.67              |
| 1:K:138:ARG:NH2  | 1:K:240:ALA:O     | 2.27                     | 0.67              |
| 1:K:375:LYS:HA   | 1:K:392:PHE:CE1   | 2.29                     | 0.67              |
| 1:J:1009:ARG:NH1 | 1:J:1009:ARG:O    | 2.27                     | 0.67              |
| 1:K:883:LEU:HD21 | 1:K:886:LEU:HB2   | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1009:ARG:NH1  | 1:D:1009:ARG:O    | 2.27                     | 0.67              |
| 1:E:883:LEU:HD21  | 1:E:886:LEU:HB2   | 1.76                     | 0.66              |
| 1:A:486:ARG:NH2   | 1:A:491:GLN:OE1   | 2.28                     | 0.66              |
| 1:B:221:GLN:HB3   | 1:B:348:PRO:HG3   | 1.76                     | 0.66              |
| 1:G:486:ARG:NH2   | 1:G:491:GLN:OE1   | 2.28                     | 0.66              |
| 1:I:474:TRP:HE1   | 1:I:558:VAL:HG21  | 1.59                     | 0.66              |
| 1:E:1009:ARG:HH12 | 1:E:1013:ARG:HB2  | 1.59                     | 0.66              |
| 1:D:1010:GLU:HG3  | 1:D:1013:ARG:HH22 | 1.59                     | 0.66              |
| 1:J:1010:GLU:HG3  | 1:J:1013:ARG:HH22 | 1.59                     | 0.66              |
| 1:H:1009:ARG:HH12 | 1:H:1013:ARG:HB2  | 1.59                     | 0.66              |
| 1:A:1009:ARG:NH1  | 1:A:1009:ARG:O    | 2.27                     | 0.66              |
| 1:F:221:GLN:HB3   | 1:F:348:PRO:HG3   | 1.78                     | 0.66              |
| 1:G:1009:ARG:NH1  | 1:G:1009:ARG:O    | 2.27                     | 0.66              |
| 1:I:221:GLN:HB3   | 1:I:348:PRO:HG3   | 1.77                     | 0.66              |
| 1:K:1009:ARG:HH12 | 1:K:1013:ARG:HB2  | 1.60                     | 0.66              |
| 1:A:301:ASP:O     | 1:A:570:TYR:OH    | 2.14                     | 0.66              |
| 1:E:136:TYR:OH    | 1:E:275:CYS:SG    | 2.52                     | 0.66              |
| 1:G:301:ASP:O     | 1:G:570:TYR:OH    | 2.14                     | 0.66              |
| 1:H:221:GLN:HB3   | 1:H:348:PRO:HG3   | 1.77                     | 0.66              |
| 1:G:486:ARG:NH2   | 1:G:490:LEU:O     | 2.29                     | 0.66              |
| 1:A:486:ARG:NH2   | 1:A:490:LEU:O     | 2.29                     | 0.66              |
| 1:B:1009:ARG:HH12 | 1:B:1013:ARG:HB2  | 1.60                     | 0.66              |
| 1:K:136:TYR:OH    | 1:K:275:CYS:SG    | 2.52                     | 0.66              |
| 1:B:607:LEU:HD12  | 1:B:640:PHE:HE2   | 1.61                     | 0.65              |
| 1:D:486:ARG:NH2   | 1:D:490:LEU:O     | 2.29                     | 0.65              |
| 1:D:486:ARG:NH2   | 1:D:491:GLN:OE1   | 2.28                     | 0.65              |
| 1:E:301:ASP:O     | 1:E:570:TYR:OH    | 2.14                     | 0.65              |
| 1:J:486:ARG:NH2   | 1:J:490:LEU:O     | 2.29                     | 0.65              |
| 1:K:607:LEU:HD12  | 1:K:640:PHE:HE2   | 1.61                     | 0.65              |
| 1:B:1009:ARG:NH1  | 1:B:1009:ARG:O    | 2.29                     | 0.65              |
| 1:H:389:ARG:HA    | 1:H:392:PHE:HD2   | 1.62                     | 0.65              |
| 1:H:1009:ARG:NH1  | 1:H:1009:ARG:O    | 2.30                     | 0.65              |
| 1:J:301:ASP:O     | 1:J:570:TYR:OH    | 2.14                     | 0.65              |
| 1:J:486:ARG:NH2   | 1:J:491:GLN:OE1   | 2.28                     | 0.65              |
| 1:K:301:ASP:O     | 1:K:570:TYR:OH    | 2.14                     | 0.65              |
| 1:D:301:ASP:O     | 1:D:570:TYR:OH    | 2.14                     | 0.65              |
| 1:E:607:LEU:HD12  | 1:E:640:PHE:HE2   | 1.61                     | 0.65              |
| 1:H:607:LEU:HD12  | 1:H:640:PHE:HE2   | 1.61                     | 0.65              |
| 1:K:917:ARG:NE    | 1:K:944:GLU:OE2   | 2.30                     | 0.65              |
| 1:E:917:ARG:NE    | 1:E:944:GLU:OE2   | 2.30                     | 0.65              |
| 1:C:486:ARG:NH2   | 1:C:490:LEU:O     | 2.31                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:422:MET:HB3  | 1:E:428:LEU:HD21 | 1.77                     | 0.64              |
| 1:H:333:ARG:HB2  | 1:H:335:LYS:HZ2  | 1.62                     | 0.64              |
| 1:I:216:HIS:ND1  | 1:I:341:SER:OG   | 2.30                     | 0.64              |
| 1:I:333:ARG:HB2  | 1:I:335:LYS:HZ2  | 1.62                     | 0.64              |
| 1:K:422:MET:HB3  | 1:K:428:LEU:HD21 | 1.77                     | 0.64              |
| 1:K:579:PHE:CD2  | 1:K:631:CYS:HB3  | 2.31                     | 0.64              |
| 1:C:333:ARG:HB2  | 1:C:335:LYS:HZ2  | 1.62                     | 0.64              |
| 1:E:579:PHE:CD2  | 1:E:631:CYS:HB3  | 2.31                     | 0.64              |
| 1:H:375:LYS:HA   | 1:H:392:PHE:HE1  | 1.63                     | 0.64              |
| 1:H:301:ASP:O    | 1:H:570:TYR:OH   | 2.14                     | 0.64              |
| 1:I:486:ARG:NH2  | 1:I:490:LEU:O    | 2.31                     | 0.64              |
| 1:B:486:ARG:NH2  | 1:B:490:LEU:O    | 2.31                     | 0.64              |
| 1:F:486:ARG:NH2  | 1:F:490:LEU:O    | 2.31                     | 0.64              |
| 1:L:486:ARG:NH2  | 1:L:490:LEU:O    | 2.31                     | 0.64              |
| 1:E:486:ARG:NH2  | 1:E:490:LEU:O    | 2.31                     | 0.64              |
| 1:H:486:ARG:NH2  | 1:H:490:LEU:O    | 2.31                     | 0.64              |
| 1:K:486:ARG:NH2  | 1:K:490:LEU:O    | 2.31                     | 0.64              |
| 1:B:422:MET:HB3  | 1:B:428:LEU:HD21 | 1.78                     | 0.64              |
| 1:H:422:MET:HB3  | 1:H:428:LEU:HD21 | 1.78                     | 0.64              |
| 1:B:375:LYS:HA   | 1:B:392:PHE:HE1  | 1.64                     | 0.63              |
| 1:B:389:ARG:HA   | 1:B:392:PHE:HD2  | 1.63                     | 0.63              |
| 1:B:579:PHE:CD2  | 1:B:631:CYS:HB3  | 2.32                     | 0.63              |
| 1:C:222:GLY:HA3  | 1:C:226:ILE:HG21 | 1.80                     | 0.63              |
| 1:E:333:ARG:HB2  | 1:E:335:LYS:HZ2  | 1.63                     | 0.63              |
| 1:K:375:LYS:HA   | 1:K:392:PHE:HE1  | 1.64                     | 0.63              |
| 1:B:333:ARG:HB2  | 1:B:335:LYS:HZ2  | 1.63                     | 0.63              |
| 1:E:375:LYS:HA   | 1:E:392:PHE:HE1  | 1.64                     | 0.63              |
| 1:K:389:ARG:HA   | 1:K:392:PHE:HD2  | 1.63                     | 0.62              |
| 1:I:222:GLY:HA3  | 1:I:226:ILE:HG21 | 1.81                     | 0.62              |
| 1:A:486:ARG:HH22 | 1:A:491:GLN:HA   | 1.64                     | 0.62              |
| 1:E:389:ARG:HA   | 1:E:392:PHE:HD2  | 1.63                     | 0.62              |
| 1:G:486:ARG:HH22 | 1:G:491:GLN:HA   | 1.64                     | 0.62              |
| 1:K:333:ARG:HB2  | 1:K:335:LYS:HZ2  | 1.64                     | 0.62              |
| 1:B:301:ASP:O    | 1:B:570:TYR:OH   | 2.14                     | 0.62              |
| 1:C:131:ASP:HB3  | 1:C:134:LYS:HG3  | 1.81                     | 0.62              |
| 1:L:222:GLY:HA3  | 1:L:226:ILE:HG21 | 1.80                     | 0.62              |
| 1:G:917:ARG:NE   | 1:G:944:GLU:OE2  | 2.32                     | 0.62              |
| 1:L:235:ILE:HD11 | 1:L:244:LEU:HD23 | 1.82                     | 0.62              |
| 1:A:917:ARG:NE   | 1:A:944:GLU:OE2  | 2.32                     | 0.62              |
| 1:E:235:ILE:HD11 | 1:E:244:LEU:HD23 | 1.81                     | 0.62              |
| 1:H:917:ARG:NE   | 1:H:944:GLU:OE2  | 2.30                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:1009:ARG:NH1 | 1:L:1009:ARG:O   | 2.31                     | 0.62              |
| 1:E:746:SER:OG   | 1:E:747:ASP:OD1  | 2.18                     | 0.61              |
| 1:F:222:GLY:HA3  | 1:F:226:ILE:HG21 | 1.82                     | 0.61              |
| 1:B:235:ILE:HD11 | 1:B:244:LEU:HD23 | 1.81                     | 0.61              |
| 1:K:235:ILE:HD11 | 1:K:244:LEU:HD23 | 1.81                     | 0.61              |
| 1:F:1009:ARG:NH1 | 1:F:1009:ARG:O   | 2.31                     | 0.61              |
| 1:B:917:ARG:NE   | 1:B:944:GLU:OE2  | 2.30                     | 0.61              |
| 1:A:235:ILE:HD11 | 1:A:244:LEU:HD23 | 1.83                     | 0.61              |
| 1:B:486:ARG:NH2  | 1:B:491:GLN:OE1  | 2.31                     | 0.61              |
| 1:G:235:ILE:HD11 | 1:G:244:LEU:HD23 | 1.83                     | 0.61              |
| 1:C:245:PHE:HD1  | 1:C:252:LEU:HD11 | 1.65                     | 0.61              |
| 1:I:131:ASP:HB3  | 1:I:134:LYS:HG3  | 1.82                     | 0.61              |
| 1:K:746:SER:OG   | 1:K:747:ASP:OD1  | 2.18                     | 0.61              |
| 1:H:519:MET:O    | 1:H:522:GLN:HG3  | 2.01                     | 0.61              |
| 1:I:245:PHE:HD1  | 1:I:252:LEU:HD11 | 1.65                     | 0.61              |
| 1:E:486:ARG:NH2  | 1:E:491:GLN:OE1  | 2.31                     | 0.61              |
| 1:H:235:ILE:HD11 | 1:H:244:LEU:HD23 | 1.81                     | 0.61              |
| 1:E:1009:ARG:NH1 | 1:E:1009:ARG:O   | 2.30                     | 0.61              |
| 1:F:131:ASP:HB3  | 1:F:134:LYS:HG3  | 1.83                     | 0.61              |
| 1:K:1009:ARG:NH1 | 1:K:1009:ARG:O   | 2.30                     | 0.61              |
| 1:L:245:PHE:HD1  | 1:L:252:LEU:HD11 | 1.66                     | 0.61              |
| 1:A:333:ARG:HB2  | 1:A:335:LYS:HZ2  | 1.66                     | 0.60              |
| 1:A:659:MET:HE2  | 1:A:659:MET:HA   | 1.82                     | 0.60              |
| 1:D:222:GLY:HA3  | 1:D:226:ILE:HG21 | 1.83                     | 0.60              |
| 1:F:245:PHE:HD1  | 1:F:252:LEU:HD11 | 1.65                     | 0.60              |
| 1:G:659:MET:HE2  | 1:G:659:MET:HA   | 1.82                     | 0.60              |
| 1:H:486:ARG:NH2  | 1:H:491:GLN:OE1  | 2.31                     | 0.60              |
| 1:J:222:GLY:HA3  | 1:J:226:ILE:HG21 | 1.83                     | 0.60              |
| 1:G:646:ASP:O    | 1:G:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:L:131:ASP:HB3  | 1:L:134:LYS:HG3  | 1.82                     | 0.60              |
| 1:A:216:HIS:HB3  | 1:A:341:SER:HA   | 1.83                     | 0.60              |
| 1:A:646:ASP:O    | 1:A:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:D:374:ARG:NH1  | 1:D:402:PHE:O    | 2.35                     | 0.60              |
| 1:G:216:HIS:HB3  | 1:G:341:SER:HA   | 1.83                     | 0.60              |
| 1:C:235:ILE:HD11 | 1:C:244:LEU:HD23 | 1.82                     | 0.60              |
| 1:D:486:ARG:HH22 | 1:D:491:GLN:HA   | 1.64                     | 0.60              |
| 1:I:1009:ARG:NH1 | 1:I:1009:ARG:O   | 2.31                     | 0.60              |
| 1:C:1009:ARG:NH1 | 1:C:1009:ARG:O   | 2.31                     | 0.60              |
| 1:F:646:ASP:O    | 1:F:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:J:374:ARG:NH1  | 1:J:402:PHE:O    | 2.35                     | 0.60              |
| 1:J:486:ARG:HH22 | 1:J:491:GLN:HA   | 1.64                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:646:ASP:O    | 1:L:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:C:646:ASP:O    | 1:C:673:ARG:NH2  | 2.34                     | 0.60              |
| 1:J:136:TYR:OH   | 1:J:275:CYS:SG   | 2.59                     | 0.60              |
| 1:A:374:ARG:NH1  | 1:A:402:PHE:O    | 2.35                     | 0.60              |
| 1:D:136:TYR:OH   | 1:D:275:CYS:SG   | 2.59                     | 0.60              |
| 1:K:486:ARG:NH2  | 1:K:491:GLN:OE1  | 2.31                     | 0.60              |
| 1:D:646:ASP:O    | 1:D:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:G:374:ARG:NH1  | 1:G:402:PHE:O    | 2.35                     | 0.60              |
| 1:J:646:ASP:O    | 1:J:673:ARG:NH2  | 2.35                     | 0.60              |
| 1:J:917:ARG:NE   | 1:J:944:GLU:OE2  | 2.32                     | 0.60              |
| 1:B:519:MET:O    | 1:B:522:GLN:HG3  | 2.02                     | 0.60              |
| 1:D:216:HIS:HB3  | 1:D:341:SER:HA   | 1.83                     | 0.60              |
| 1:I:235:ILE:HD11 | 1:I:244:LEU:HD23 | 1.82                     | 0.60              |
| 1:F:486:ARG:NH2  | 1:F:491:GLN:OE1  | 2.34                     | 0.59              |
| 1:J:216:HIS:HB3  | 1:J:341:SER:HA   | 1.83                     | 0.59              |
| 1:J:235:ILE:HD11 | 1:J:244:LEU:HD23 | 1.83                     | 0.59              |
| 1:L:486:ARG:NH2  | 1:L:491:GLN:OE1  | 2.34                     | 0.59              |
| 1:D:235:ILE:HD11 | 1:D:244:LEU:HD23 | 1.83                     | 0.59              |
| 1:D:917:ARG:NE   | 1:D:944:GLU:OE2  | 2.32                     | 0.59              |
| 1:A:136:TYR:OH   | 1:A:275:CYS:SG   | 2.59                     | 0.59              |
| 1:I:646:ASP:O    | 1:I:673:ARG:NH2  | 2.35                     | 0.59              |
| 1:L:519:MET:O    | 1:L:522:GLN:HG3  | 2.03                     | 0.59              |
| 1:C:217:THR:O    | 1:C:361:PRO:HA   | 2.02                     | 0.59              |
| 1:F:519:MET:O    | 1:F:522:GLN:HG3  | 2.03                     | 0.59              |
| 1:G:136:TYR:OH   | 1:G:275:CYS:SG   | 2.59                     | 0.59              |
| 1:J:659:MET:HA   | 1:J:659:MET:HE2  | 1.82                     | 0.59              |
| 1:F:235:ILE:HD11 | 1:F:244:LEU:HD23 | 1.85                     | 0.59              |
| 1:H:222:GLY:HA3  | 1:H:226:ILE:HG21 | 1.85                     | 0.59              |
| 1:B:746:SER:OG   | 1:B:747:ASP:OD1  | 2.18                     | 0.59              |
| 1:B:607:LEU:HD12 | 1:B:640:PHE:CE2  | 2.38                     | 0.59              |
| 1:C:618:LYS:HD3  | 1:C:621:TRP:HE1  | 1.68                     | 0.59              |
| 1:D:659:MET:HE2  | 1:D:659:MET:HA   | 1.82                     | 0.59              |
| 1:K:519:MET:O    | 1:K:522:GLN:HG3  | 2.02                     | 0.59              |
| 1:C:917:ARG:NE   | 1:C:944:GLU:OE2  | 2.35                     | 0.59              |
| 1:E:519:MET:O    | 1:E:522:GLN:HG3  | 2.02                     | 0.59              |
| 1:F:333:ARG:HB2  | 1:F:335:LYS:HZ2  | 1.68                     | 0.59              |
| 1:I:398:ASN:ND2  | 1:I:432:SER:O    | 2.36                     | 0.59              |
| 1:I:917:ARG:NE   | 1:I:944:GLU:OE2  | 2.35                     | 0.59              |
| 1:L:398:ASN:ND2  | 1:L:432:SER:O    | 2.36                     | 0.59              |
| 1:H:607:LEU:HD12 | 1:H:640:PHE:CE2  | 2.38                     | 0.59              |
| 1:L:220:PHE:HE2  | 1:L:343:LEU:HD22 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:618:LYS:HD3   | 1:I:621:TRP:HE1  | 1.68                     | 0.58              |
| 1:B:646:ASP:O     | 1:B:673:ARG:NH2  | 2.36                     | 0.58              |
| 1:D:607:LEU:HD12  | 1:D:640:PHE:HE2  | 1.68                     | 0.58              |
| 1:H:646:ASP:O     | 1:H:673:ARG:NH2  | 2.36                     | 0.58              |
| 1:I:519:MET:O     | 1:I:522:GLN:HG3  | 2.03                     | 0.58              |
| 1:J:607:LEU:HD12  | 1:J:640:PHE:HE2  | 1.68                     | 0.58              |
| 1:A:222:GLY:HA3   | 1:A:226:ILE:HG21 | 1.83                     | 0.58              |
| 1:F:618:LYS:HD3   | 1:F:621:TRP:HE1  | 1.68                     | 0.58              |
| 1:G:222:GLY:HA3   | 1:G:226:ILE:HG21 | 1.83                     | 0.58              |
| 1:E:607:LEU:HD12  | 1:E:640:PHE:CE2  | 2.38                     | 0.58              |
| 1:K:607:LEU:HD12  | 1:K:640:PHE:CE2  | 2.38                     | 0.58              |
| 1:K:646:ASP:O     | 1:K:673:ARG:NH2  | 2.36                     | 0.58              |
| 1:K:502:ASN:HB2   | 1:K:513:PHE:HB2  | 1.85                     | 0.58              |
| 1:B:222:GLY:HA3   | 1:B:226:ILE:HG21 | 1.86                     | 0.58              |
| 1:C:519:MET:O     | 1:C:522:GLN:HG3  | 2.03                     | 0.58              |
| 1:D:1027:ILE:HG22 | 1:D:1029:PHE:H   | 1.68                     | 0.58              |
| 1:F:1027:ILE:HG22 | 1:F:1029:PHE:H   | 1.69                     | 0.58              |
| 1:L:618:LYS:HD3   | 1:L:621:TRP:HE1  | 1.68                     | 0.58              |
| 1:C:220:PHE:HE2   | 1:C:343:LEU:HD22 | 1.68                     | 0.58              |
| 1:C:755:MET:HE3   | 1:C:759:CYS:SG   | 2.44                     | 0.58              |
| 1:E:646:ASP:O     | 1:E:673:ARG:NH2  | 2.36                     | 0.58              |
| 1:I:755:MET:HE3   | 1:I:759:CYS:SG   | 2.44                     | 0.58              |
| 1:J:1027:ILE:HG22 | 1:J:1029:PHE:H   | 1.68                     | 0.58              |
| 1:A:1027:ILE:HG22 | 1:A:1029:PHE:H   | 1.68                     | 0.58              |
| 1:G:1027:ILE:HG22 | 1:G:1029:PHE:H   | 1.68                     | 0.58              |
| 1:L:217:THR:O     | 1:L:361:PRO:HA   | 2.03                     | 0.58              |
| 1:L:917:ARG:NE    | 1:L:944:GLU:OE2  | 2.35                     | 0.58              |
| 1:L:1027:ILE:HG22 | 1:L:1029:PHE:H   | 1.69                     | 0.58              |
| 1:K:632:LEU:HD12  | 1:K:641:VAL:HG22 | 1.86                     | 0.58              |
| 1:C:486:ARG:HH22  | 1:C:491:GLN:HA   | 1.67                     | 0.57              |
| 1:E:632:LEU:HD12  | 1:E:641:VAL:HG22 | 1.86                     | 0.57              |
| 1:F:422:MET:HB3   | 1:F:428:LEU:HD21 | 1.86                     | 0.57              |
| 1:F:531:LEU:HB3   | 1:F:598:ILE:HG23 | 1.86                     | 0.57              |
| 1:F:917:ARG:NE    | 1:F:944:GLU:OE2  | 2.35                     | 0.57              |
| 1:B:295:PHE:HB2   | 1:B:342:LEU:HD23 | 1.86                     | 0.57              |
| 1:B:374:ARG:NH1   | 1:B:402:PHE:O    | 2.37                     | 0.57              |
| 1:B:632:LEU:HD12  | 1:B:641:VAL:HG22 | 1.86                     | 0.57              |
| 1:H:502:ASN:HB2   | 1:H:513:PHE:HB2  | 1.86                     | 0.57              |
| 1:I:531:LEU:HB3   | 1:I:598:ILE:HG23 | 1.86                     | 0.57              |
| 1:A:607:LEU:HD12  | 1:A:640:PHE:HE2  | 1.68                     | 0.57              |
| 1:F:755:MET:HE3   | 1:F:759:CYS:SG   | 2.44                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:333:ARG:HB2   | 1:G:335:LYS:HZ2   | 1.70                     | 0.57              |
| 1:H:632:LEU:HD12  | 1:H:641:VAL:HG22  | 1.86                     | 0.57              |
| 1:J:333:ARG:HB2   | 1:J:335:LYS:HZ2   | 1.70                     | 0.57              |
| 1:L:755:MET:HE3   | 1:L:759:CYS:SG    | 2.44                     | 0.57              |
| 1:B:955:CYS:HA    | 1:B:958:LEU:HD13  | 1.87                     | 0.57              |
| 1:C:531:LEU:HB3   | 1:C:598:ILE:HG23  | 1.86                     | 0.57              |
| 1:D:333:ARG:HB2   | 1:D:335:LYS:HZ2   | 1.70                     | 0.57              |
| 1:G:802:LEU:HD13  | 1:G:807:LEU:HD11  | 1.85                     | 0.57              |
| 1:K:398:ASN:ND2   | 1:K:432:SER:O     | 2.38                     | 0.57              |
| 1:L:531:LEU:HB3   | 1:L:598:ILE:HG23  | 1.87                     | 0.57              |
| 1:C:215:VAL:HG12  | 1:C:362:ARG:HH22  | 1.70                     | 0.57              |
| 1:F:216:HIS:HB3   | 1:F:341:SER:HA    | 1.87                     | 0.57              |
| 1:H:746:SER:OG    | 1:H:747:ASP:OD1   | 2.18                     | 0.57              |
| 1:H:955:CYS:HA    | 1:H:958:LEU:HD13  | 1.87                     | 0.57              |
| 1:I:215:VAL:HG12  | 1:I:362:ARG:HH22  | 1.70                     | 0.57              |
| 1:I:217:THR:O     | 1:I:361:PRO:HA    | 2.04                     | 0.57              |
| 1:E:398:ASN:ND2   | 1:E:432:SER:O     | 2.38                     | 0.57              |
| 1:G:607:LEU:HD12  | 1:G:640:PHE:HE2   | 1.68                     | 0.57              |
| 1:B:911:PHE:HZ    | 1:B:914:LEU:HD13  | 1.69                     | 0.57              |
| 1:C:1027:ILE:HG22 | 1:C:1029:PHE:H    | 1.69                     | 0.57              |
| 1:F:217:THR:O     | 1:F:361:PRO:HA    | 2.04                     | 0.57              |
| 1:K:295:PHE:HB2   | 1:K:342:LEU:HD23  | 1.86                     | 0.57              |
| 1:D:531:LEU:HB3   | 1:D:598:ILE:HG23  | 1.87                     | 0.57              |
| 1:I:645:MET:HE2   | 1:I:671:CYS:SG    | 2.45                     | 0.57              |
| 1:I:1027:ILE:HG22 | 1:I:1029:PHE:H    | 1.69                     | 0.57              |
| 1:K:374:ARG:NH1   | 1:K:402:PHE:O     | 2.37                     | 0.57              |
| 1:L:215:VAL:HG12  | 1:L:362:ARG:HH22  | 1.70                     | 0.57              |
| 1:L:216:HIS:HB3   | 1:L:341:SER:HA    | 1.87                     | 0.57              |
| 1:F:486:ARG:HH22  | 1:F:491:GLN:HA    | 1.69                     | 0.57              |
| 1:H:911:PHE:HZ    | 1:H:914:LEU:HD13  | 1.69                     | 0.57              |
| 1:I:220:PHE:HE2   | 1:I:343:LEU:HD22  | 1.70                     | 0.57              |
| 1:J:531:LEU:HB3   | 1:J:598:ILE:HG23  | 1.87                     | 0.57              |
| 1:A:531:LEU:HB3   | 1:A:598:ILE:HG23  | 1.87                     | 0.56              |
| 1:D:1005:MET:HG3  | 1:D:1007:LEU:HD21 | 1.87                     | 0.56              |
| 1:F:220:PHE:HE2   | 1:F:343:LEU:HD22  | 1.68                     | 0.56              |
| 1:G:531:LEU:HB3   | 1:G:598:ILE:HG23  | 1.87                     | 0.56              |
| 1:H:295:PHE:HB2   | 1:H:342:LEU:HD23  | 1.86                     | 0.56              |
| 1:E:295:PHE:HB2   | 1:E:342:LEU:HD23  | 1.86                     | 0.56              |
| 1:E:955:CYS:HA    | 1:E:958:LEU:HD13  | 1.86                     | 0.56              |
| 1:J:1005:MET:HG3  | 1:J:1007:LEU:HD21 | 1.87                     | 0.56              |
| 1:C:911:PHE:HZ    | 1:C:914:LEU:HD13  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:215:VAL:HG12 | 1:F:362:ARG:HH22 | 1.70                     | 0.56              |
| 1:F:629:PHE:HE1  | 1:F:645:MET:HE3  | 1.69                     | 0.56              |
| 1:L:422:MET:HB3  | 1:L:428:LEU:HD21 | 1.87                     | 0.56              |
| 1:L:486:ARG:HH22 | 1:L:491:GLN:HA   | 1.69                     | 0.56              |
| 1:L:629:PHE:HE1  | 1:L:645:MET:HE3  | 1.70                     | 0.56              |
| 1:C:216:HIS:HB3  | 1:C:341:SER:HA   | 1.86                     | 0.56              |
| 1:E:374:ARG:NH1  | 1:E:402:PHE:O    | 2.38                     | 0.56              |
| 1:G:606:LEU:O    | 1:G:610:ILE:HG12 | 2.06                     | 0.56              |
| 1:I:629:PHE:HE1  | 1:I:645:MET:HE3  | 1.70                     | 0.56              |
| 1:K:531:LEU:HB3  | 1:K:598:ILE:HG23 | 1.88                     | 0.56              |
| 1:A:606:LEU:O    | 1:A:610:ILE:HG12 | 2.06                     | 0.56              |
| 1:D:295:PHE:HB2  | 1:D:342:LEU:HD23 | 1.88                     | 0.56              |
| 1:F:911:PHE:HZ   | 1:F:914:LEU:HD13 | 1.70                     | 0.56              |
| 1:G:583:ASN:HB3  | 1:G:586:ARG:HB2  | 1.88                     | 0.56              |
| 1:H:324:GLY:O    | 1:H:328:LEU:HG   | 2.04                     | 0.56              |
| 1:I:486:ARG:HH22 | 1:I:491:GLN:HA   | 1.69                     | 0.56              |
| 1:L:645:MET:HE2  | 1:L:671:CYS:SG   | 2.45                     | 0.56              |
| 1:A:583:ASN:HB3  | 1:A:586:ARG:HB2  | 1.88                     | 0.56              |
| 1:E:531:LEU:HB3  | 1:E:598:ILE:HG23 | 1.88                     | 0.56              |
| 1:F:645:MET:HE2  | 1:F:671:CYS:SG   | 2.45                     | 0.56              |
| 1:J:295:PHE:HB2  | 1:J:342:LEU:HD23 | 1.88                     | 0.56              |
| 1:K:911:PHE:HZ   | 1:K:914:LEU:HD13 | 1.69                     | 0.56              |
| 1:A:136:TYR:HH   | 1:A:275:CYS:HG   | 1.52                     | 0.56              |
| 1:A:295:PHE:HB2  | 1:A:342:LEU:HD23 | 1.88                     | 0.56              |
| 1:C:645:MET:HE2  | 1:C:671:CYS:SG   | 2.46                     | 0.56              |
| 1:K:242:GLY:H    | 1:K:246:LYS:HZ2  | 1.53                     | 0.56              |
| 1:A:220:PHE:HE2  | 1:A:343:LEU:HD22 | 1.71                     | 0.56              |
| 1:G:295:PHE:HB2  | 1:G:342:LEU:HD23 | 1.88                     | 0.56              |
| 1:H:374:ARG:NH1  | 1:H:402:PHE:O    | 2.39                     | 0.56              |
| 1:D:606:LEU:O    | 1:D:610:ILE:HG12 | 2.06                     | 0.56              |
| 1:E:911:PHE:HZ   | 1:E:914:LEU:HD13 | 1.69                     | 0.56              |
| 1:F:398:ASN:ND2  | 1:F:432:SER:O    | 2.36                     | 0.56              |
| 1:G:220:PHE:HE2  | 1:G:343:LEU:HD22 | 1.71                     | 0.56              |
| 1:I:216:HIS:HB3  | 1:I:341:SER:HA   | 1.87                     | 0.56              |
| 1:I:422:MET:HB3  | 1:I:428:LEU:HD21 | 1.86                     | 0.56              |
| 1:I:911:PHE:HZ   | 1:I:914:LEU:HD13 | 1.71                     | 0.56              |
| 1:L:911:PHE:HZ   | 1:L:914:LEU:HD13 | 1.71                     | 0.56              |
| 1:D:297:MET:HE2  | 1:D:344:ILE:HG12 | 1.88                     | 0.56              |
| 1:G:136:TYR:HH   | 1:G:275:CYS:HG   | 1.52                     | 0.56              |
| 1:J:297:MET:HE2  | 1:J:344:ILE:HG12 | 1.88                     | 0.56              |
| 1:J:606:LEU:O    | 1:J:610:ILE:HG12 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:607:LEU:HD12 | 1:D:640:PHE:CE2   | 2.41                     | 0.55              |
| 1:D:755:MET:HE3  | 1:D:759:CYS:SG    | 2.46                     | 0.55              |
| 1:J:607:LEU:HD12 | 1:J:640:PHE:CE2   | 2.41                     | 0.55              |
| 1:J:755:MET:HE3  | 1:J:759:CYS:SG    | 2.46                     | 0.55              |
| 1:A:607:LEU:HD12 | 1:A:640:PHE:CE2   | 2.41                     | 0.55              |
| 1:A:645:MET:HE1  | 1:A:667:CYS:CB    | 2.34                     | 0.55              |
| 1:C:398:ASN:ND2  | 1:C:432:SER:O     | 2.36                     | 0.55              |
| 1:H:606:LEU:O    | 1:H:610:ILE:HG12  | 2.07                     | 0.55              |
| 1:B:242:GLY:H    | 1:B:246:LYS:HZ1   | 1.54                     | 0.55              |
| 1:C:641:VAL:O    | 1:C:645:MET:HB2   | 2.06                     | 0.55              |
| 1:G:607:LEU:HD12 | 1:G:640:PHE:CE2   | 2.41                     | 0.55              |
| 1:G:645:MET:HE1  | 1:G:667:CYS:CB    | 2.34                     | 0.55              |
| 1:A:1005:MET:HG3 | 1:A:1007:LEU:HD21 | 1.87                     | 0.55              |
| 1:B:220:PHE:HE2  | 1:B:343:LEU:HD22  | 1.71                     | 0.55              |
| 1:B:606:LEU:O    | 1:B:610:ILE:HG12  | 2.07                     | 0.55              |
| 1:J:982:CYS:O    | 1:J:986:LEU:HD23  | 2.07                     | 0.55              |
| 1:K:606:LEU:O    | 1:K:610:ILE:HG12  | 2.07                     | 0.55              |
| 1:A:755:MET:HE3  | 1:A:759:CYS:SG    | 2.46                     | 0.55              |
| 1:B:398:ASN:ND2  | 1:B:432:SER:O     | 2.38                     | 0.55              |
| 1:B:755:MET:HE3  | 1:B:759:CYS:SG    | 2.47                     | 0.55              |
| 1:C:629:PHE:HE1  | 1:C:645:MET:HE3   | 1.71                     | 0.55              |
| 1:D:982:CYS:O    | 1:D:986:LEU:HD23  | 2.07                     | 0.55              |
| 1:E:606:LEU:O    | 1:E:610:ILE:HG12  | 2.07                     | 0.55              |
| 1:F:802:LEU:HD13 | 1:F:807:LEU:HD11  | 1.88                     | 0.55              |
| 1:G:1005:MET:HG3 | 1:G:1007:LEU:HD21 | 1.87                     | 0.55              |
| 1:H:755:MET:HE3  | 1:H:759:CYS:SG    | 2.47                     | 0.55              |
| 1:I:771:ARG:HG3  | 1:I:799:GLU:HG2   | 1.89                     | 0.55              |
| 1:K:222:GLY:HA3  | 1:K:226:ILE:HG21  | 1.87                     | 0.55              |
| 1:B:990:LEU:HD22 | 1:B:1025:LEU:HD11 | 1.88                     | 0.55              |
| 1:C:583:ASN:HB3  | 1:C:586:ARG:HB2   | 1.87                     | 0.55              |
| 1:L:802:LEU:HD13 | 1:L:807:LEU:HD11  | 1.89                     | 0.55              |
| 1:A:982:CYS:O    | 1:A:986:LEU:HD23  | 2.07                     | 0.55              |
| 1:C:771:ARG:HG3  | 1:C:799:GLU:HG2   | 1.89                     | 0.55              |
| 1:E:990:LEU:HD22 | 1:E:1025:LEU:HD11 | 1.89                     | 0.55              |
| 1:G:755:MET:HE3  | 1:G:759:CYS:SG    | 2.46                     | 0.55              |
| 1:G:982:CYS:O    | 1:G:986:LEU:HD23  | 2.07                     | 0.55              |
| 1:K:755:MET:HE3  | 1:K:759:CYS:SG    | 2.47                     | 0.55              |
| 1:B:531:LEU:HB3  | 1:B:598:ILE:HG23  | 1.88                     | 0.55              |
| 1:C:617:LYS:HE2  | 1:L:956:TRP:HE3   | 1.72                     | 0.55              |
| 1:E:220:PHE:HE2  | 1:E:343:LEU:HD22  | 1.71                     | 0.55              |
| 1:E:755:MET:HE3  | 1:E:759:CYS:SG    | 2.47                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:583:ASN:HB3  | 1:F:586:ARG:HB2   | 1.89                     | 0.55              |
| 1:H:990:LEU:HD22 | 1:H:1025:LEU:HD11 | 1.88                     | 0.55              |
| 1:D:291:SER:HB3  | 1:D:339:LYS:HD3   | 1.89                     | 0.55              |
| 1:H:398:ASN:ND2  | 1:H:432:SER:O     | 2.38                     | 0.55              |
| 1:J:291:SER:HB3  | 1:J:339:LYS:HD3   | 1.89                     | 0.55              |
| 1:K:990:LEU:HD22 | 1:K:1025:LEU:HD11 | 1.89                     | 0.55              |
| 1:L:583:ASN:HB3  | 1:L:586:ARG:HB2   | 1.89                     | 0.55              |
| 1:A:618:LYS:HD3  | 1:A:621:TRP:HE1   | 1.70                     | 0.55              |
| 1:C:216:HIS:ND1  | 1:C:341:SER:OG    | 2.30                     | 0.55              |
| 1:E:222:GLY:HA3  | 1:E:226:ILE:HG21  | 1.88                     | 0.55              |
| 1:J:911:PHE:HZ   | 1:J:914:LEU:HD13  | 1.71                     | 0.55              |
| 1:L:531:LEU:HB3  | 1:L:598:ILE:HD12  | 1.89                     | 0.55              |
| 1:A:582:VAL:HB   | 1:A:603:ARG:HG2   | 1.90                     | 0.54              |
| 1:B:618:LYS:HD3  | 1:B:621:TRP:HE1   | 1.71                     | 0.54              |
| 1:C:422:MET:HB3  | 1:C:428:LEU:HD21  | 1.87                     | 0.54              |
| 1:D:220:PHE:HE2  | 1:D:343:LEU:HD22  | 1.71                     | 0.54              |
| 1:E:290:PRO:HB3  | 1:E:337:LEU:HD22  | 1.89                     | 0.54              |
| 1:G:618:LYS:HD3  | 1:G:621:TRP:HE1   | 1.70                     | 0.54              |
| 1:H:583:ASN:HB3  | 1:H:586:ARG:HB2   | 1.88                     | 0.54              |
| 1:J:220:PHE:HE2  | 1:J:343:LEU:HD22  | 1.71                     | 0.54              |
| 1:L:333:ARG:HB2  | 1:L:335:LYS:HZ2   | 1.72                     | 0.54              |
| 1:C:136:TYR:OH   | 1:C:275:CYS:SG    | 2.54                     | 0.54              |
| 1:C:486:ARG:NH2  | 1:C:491:GLN:OE1   | 2.34                     | 0.54              |
| 1:G:582:VAL:HB   | 1:G:603:ARG:HG2   | 1.90                     | 0.54              |
| 1:H:618:LYS:HD3  | 1:H:621:TRP:HE1   | 1.71                     | 0.54              |
| 1:J:618:LYS:HD3  | 1:J:621:TRP:HE1   | 1.70                     | 0.54              |
| 1:K:291:SER:HB3  | 1:K:339:LYS:HD3   | 1.89                     | 0.54              |
| 1:K:618:LYS:HD3  | 1:K:621:TRP:HE1   | 1.71                     | 0.54              |
| 1:L:606:LEU:O    | 1:L:610:ILE:HG12  | 2.08                     | 0.54              |
| 1:D:911:PHE:HZ   | 1:D:914:LEU:HD13  | 1.71                     | 0.54              |
| 1:E:618:LYS:HD3  | 1:E:621:TRP:HE1   | 1.71                     | 0.54              |
| 1:F:606:LEU:O    | 1:F:610:ILE:HG12  | 2.08                     | 0.54              |
| 1:G:911:PHE:HZ   | 1:G:914:LEU:HD13  | 1.71                     | 0.54              |
| 1:A:911:PHE:HZ   | 1:A:914:LEU:HD13  | 1.71                     | 0.54              |
| 1:G:297:MET:HE2  | 1:G:344:ILE:HG12  | 1.88                     | 0.54              |
| 1:H:220:PHE:HE2  | 1:H:343:LEU:HD22  | 1.72                     | 0.54              |
| 1:I:486:ARG:NH2  | 1:I:491:GLN:OE1   | 2.34                     | 0.54              |
| 1:I:607:LEU:HD12 | 1:I:640:PHE:CE1   | 2.42                     | 0.54              |
| 1:A:297:MET:HE2  | 1:A:344:ILE:HG12  | 1.88                     | 0.54              |
| 1:A:856:ARG:HD3  | 1:A:885:LYS:HD3   | 1.90                     | 0.54              |
| 1:D:618:LYS:HD3  | 1:D:621:TRP:HE1   | 1.70                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:856:ARG:HD3  | 1:G:885:LYS:HD3  | 1.90                     | 0.54              |
| 1:B:291:SER:HB3  | 1:B:339:LYS:HD3  | 1.89                     | 0.54              |
| 1:F:956:TRP:HE3  | 1:I:617:LYS:HE2  | 1.73                     | 0.54              |
| 1:I:802:LEU:HD13 | 1:I:807:LEU:HD11 | 1.89                     | 0.54              |
| 1:K:291:SER:H    | 1:K:339:LYS:HZ2  | 1.56                     | 0.54              |
| 1:D:583:ASN:HB3  | 1:D:586:ARG:HB2  | 1.88                     | 0.54              |
| 1:J:583:ASN:HB3  | 1:J:586:ARG:HB2  | 1.88                     | 0.54              |
| 1:A:617:LYS:HE2  | 1:H:956:TRP:HE3  | 1.73                     | 0.54              |
| 1:B:956:TRP:HE3  | 1:G:617:LYS:HE2  | 1.73                     | 0.54              |
| 1:D:582:VAL:HB   | 1:D:603:ARG:HG2  | 1.90                     | 0.54              |
| 1:F:531:LEU:HB3  | 1:F:598:ILE:HD12 | 1.90                     | 0.54              |
| 1:F:607:LEU:HD12 | 1:F:640:PHE:CE1  | 2.42                     | 0.54              |
| 1:I:607:LEU:HD12 | 1:I:640:PHE:HE1  | 1.72                     | 0.54              |
| 1:I:635:MET:HE2  | 1:I:641:VAL:HG23 | 1.89                     | 0.54              |
| 1:L:607:LEU:HD12 | 1:L:640:PHE:CE1  | 2.42                     | 0.54              |
| 1:C:291:SER:HB3  | 1:C:339:LYS:HD3  | 1.90                     | 0.54              |
| 1:C:374:ARG:NH1  | 1:C:402:PHE:O    | 2.41                     | 0.54              |
| 1:C:802:LEU:HD13 | 1:C:807:LEU:HD11 | 1.89                     | 0.54              |
| 1:L:374:ARG:NH1  | 1:L:402:PHE:O    | 2.41                     | 0.54              |
| 1:A:419:LYS:HA   | 1:A:422:MET:HE2  | 1.90                     | 0.54              |
| 1:E:571:LEU:O    | 1:E:574:VAL:HB   | 2.09                     | 0.54              |
| 1:J:582:VAL:HB   | 1:J:603:ARG:HG2  | 1.90                     | 0.54              |
| 1:B:531:LEU:HB3  | 1:B:598:ILE:HD12 | 1.91                     | 0.53              |
| 1:E:291:SER:HB3  | 1:E:339:LYS:HD3  | 1.90                     | 0.53              |
| 1:G:419:LYS:HA   | 1:G:422:MET:HE2  | 1.90                     | 0.53              |
| 1:I:583:ASN:HB3  | 1:I:586:ARG:HB2  | 1.89                     | 0.53              |
| 1:K:232:ALA:HB1  | 1:K:296:LEU:HD11 | 1.89                     | 0.53              |
| 1:K:571:LEU:O    | 1:K:574:VAL:HB   | 2.08                     | 0.53              |
| 1:F:617:LYS:HE2  | 1:I:956:TRP:HE3  | 1.72                     | 0.53              |
| 1:H:290:PRO:HB3  | 1:H:337:LEU:HD22 | 1.89                     | 0.53              |
| 1:H:291:SER:HB3  | 1:H:339:LYS:HD3  | 1.89                     | 0.53              |
| 1:K:220:PHE:HE2  | 1:K:343:LEU:HD22 | 1.72                     | 0.53              |
| 1:C:894:THR:HG22 | 1:C:895:SER:N    | 2.24                     | 0.53              |
| 1:C:956:TRP:HE3  | 1:L:617:LYS:HE2  | 1.72                     | 0.53              |
| 1:F:771:ARG:HG3  | 1:F:799:GLU:HG2  | 1.89                     | 0.53              |
| 1:H:242:GLY:H    | 1:H:246:LYS:HZ1  | 1.57                     | 0.53              |
| 1:I:136:TYR:OH   | 1:I:275:CYS:SG   | 2.55                     | 0.53              |
| 1:I:374:ARG:NH1  | 1:I:402:PHE:O    | 2.41                     | 0.53              |
| 1:I:531:LEU:HB3  | 1:I:598:ILE:HD12 | 1.90                     | 0.53              |
| 1:I:894:THR:HG22 | 1:I:895:SER:N    | 2.24                     | 0.53              |
| 1:C:955:CYS:HA   | 1:C:958:LEU:HD13 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:583:ASN:HB3  | 1:E:586:ARG:HB2  | 1.89                     | 0.53              |
| 1:I:291:SER:HB3  | 1:I:339:LYS:HD3  | 1.90                     | 0.53              |
| 1:D:571:LEU:O    | 1:D:574:VAL:HB   | 2.09                     | 0.53              |
| 1:F:607:LEU:HD12 | 1:F:640:PHE:HE1  | 1.72                     | 0.53              |
| 1:G:531:LEU:HB3  | 1:G:598:ILE:HD12 | 1.91                     | 0.53              |
| 1:G:571:LEU:O    | 1:G:574:VAL:HB   | 2.09                     | 0.53              |
| 1:I:295:PHE:HB2  | 1:I:342:LEU:HD23 | 1.91                     | 0.53              |
| 1:J:571:LEU:O    | 1:J:574:VAL:HB   | 2.09                     | 0.53              |
| 1:L:607:LEU:HD12 | 1:L:640:PHE:HE1  | 1.72                     | 0.53              |
| 1:L:771:ARG:HG3  | 1:L:799:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:531:LEU:HB3  | 1:A:598:ILE:HD12 | 1.91                     | 0.53              |
| 1:A:571:LEU:O    | 1:A:574:VAL:HB   | 2.09                     | 0.53              |
| 1:G:291:SER:HB3  | 1:G:339:LYS:HD3  | 1.89                     | 0.53              |
| 1:I:955:CYS:HA   | 1:I:958:LEU:HD13 | 1.91                     | 0.53              |
| 1:L:955:CYS:HA   | 1:L:958:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:291:SER:HB3  | 1:A:339:LYS:HD3  | 1.89                     | 0.53              |
| 1:C:242:GLY:H    | 1:C:246:LYS:HZ2  | 1.56                     | 0.53              |
| 1:F:374:ARG:NH1  | 1:F:402:PHE:O    | 2.42                     | 0.53              |
| 1:I:606:LEU:O    | 1:I:610:ILE:HG12 | 2.08                     | 0.53              |
| 1:B:571:LEU:O    | 1:B:574:VAL:HB   | 2.09                     | 0.53              |
| 1:C:531:LEU:HB3  | 1:C:598:ILE:HD12 | 1.90                     | 0.53              |
| 1:F:746:SER:OG   | 1:F:747:ASP:OD1  | 2.26                     | 0.53              |
| 1:H:486:ARG:HH22 | 1:H:491:GLN:HA   | 1.72                     | 0.53              |
| 1:I:679:LEU:HD12 | 1:I:745:LEU:HD21 | 1.91                     | 0.53              |
| 1:K:217:THR:HG22 | 1:K:361:PRO:HB3  | 1.91                     | 0.53              |
| 1:C:752:ASP:OD2  | 1:C:782:GLN:HB2  | 2.09                     | 0.53              |
| 1:D:617:LYS:HE2  | 1:K:956:TRP:HE3  | 1.73                     | 0.53              |
| 1:D:955:CYS:HA   | 1:D:958:LEU:HD13 | 1.91                     | 0.53              |
| 1:E:217:THR:HG22 | 1:E:361:PRO:HB3  | 1.91                     | 0.53              |
| 1:E:242:GLY:H    | 1:E:246:LYS:HZ2  | 1.56                     | 0.53              |
| 1:E:956:TRP:HE3  | 1:J:617:LYS:HE2  | 1.73                     | 0.53              |
| 1:F:290:PRO:HB3  | 1:F:337:LEU:HD22 | 1.90                     | 0.53              |
| 1:H:531:LEU:HB3  | 1:H:598:ILE:HD12 | 1.91                     | 0.53              |
| 1:I:752:ASP:OD2  | 1:I:782:GLN:HB2  | 2.09                     | 0.53              |
| 1:D:333:ARG:HB2  | 1:D:335:LYS:NZ   | 2.24                     | 0.53              |
| 1:J:333:ARG:HB2  | 1:J:335:LYS:NZ   | 2.24                     | 0.53              |
| 1:J:955:CYS:HA   | 1:J:958:LEU:HD13 | 1.91                     | 0.53              |
| 1:K:486:ARG:HH22 | 1:K:491:GLN:HA   | 1.73                     | 0.53              |
| 1:K:930:CYS:HA   | 1:K:933:LEU:HB2  | 1.91                     | 0.53              |
| 1:L:746:SER:OG   | 1:L:747:ASP:OD1  | 2.26                     | 0.53              |
| 1:F:955:CYS:HA   | 1:F:958:LEU:HD13 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:290:PRO:HB3  | 1:L:337:LEU:HD22 | 1.90                     | 0.52              |
| 1:B:982:CYS:O    | 1:B:986:LEU:HD23 | 2.09                     | 0.52              |
| 1:C:290:PRO:HB3  | 1:C:337:LEU:HD22 | 1.90                     | 0.52              |
| 1:F:582:VAL:HB   | 1:F:603:ARG:HG2  | 1.90                     | 0.52              |
| 1:G:752:ASP:OD2  | 1:G:782:GLN:HB2  | 2.09                     | 0.52              |
| 1:G:955:CYS:HA   | 1:G:958:LEU:HD13 | 1.91                     | 0.52              |
| 1:J:242:GLY:H    | 1:J:246:LYS:HZ2  | 1.57                     | 0.52              |
| 1:K:583:ASN:HB3  | 1:K:586:ARG:HB2  | 1.90                     | 0.52              |
| 1:K:982:CYS:O    | 1:K:986:LEU:HD23 | 2.09                     | 0.52              |
| 1:L:291:SER:HB3  | 1:L:339:LYS:HD3  | 1.90                     | 0.52              |
| 1:A:242:GLY:H    | 1:A:246:LYS:HZ2  | 1.57                     | 0.52              |
| 1:A:955:CYS:HA   | 1:A:958:LEU:HD13 | 1.91                     | 0.52              |
| 1:D:645:MET:HE1  | 1:D:667:CYS:CB   | 2.34                     | 0.52              |
| 1:E:531:LEU:HB3  | 1:E:598:ILE:HD12 | 1.91                     | 0.52              |
| 1:F:291:SER:HB3  | 1:F:339:LYS:HD3  | 1.90                     | 0.52              |
| 1:G:248:LYS:O    | 1:G:292:ARG:NE   | 2.43                     | 0.52              |
| 1:H:982:CYS:O    | 1:H:986:LEU:HD23 | 2.09                     | 0.52              |
| 1:J:771:ARG:HG3  | 1:J:799:GLU:HG2  | 1.91                     | 0.52              |
| 1:A:248:LYS:O    | 1:A:292:ARG:NE   | 2.43                     | 0.52              |
| 1:B:583:ASN:HB3  | 1:B:586:ARG:HB2  | 1.90                     | 0.52              |
| 1:C:248:LYS:O    | 1:C:292:ARG:NE   | 2.42                     | 0.52              |
| 1:C:679:LEU:HD12 | 1:C:745:LEU:HD21 | 1.92                     | 0.52              |
| 1:E:291:SER:H    | 1:E:339:LYS:HZ2  | 1.58                     | 0.52              |
| 1:E:333:ARG:HB2  | 1:E:335:LYS:NZ   | 2.24                     | 0.52              |
| 1:E:982:CYS:O    | 1:E:986:LEU:HD23 | 2.09                     | 0.52              |
| 1:G:350:ALA:HB3  | 1:G:568:LYS:HG3  | 1.91                     | 0.52              |
| 1:I:248:LYS:O    | 1:I:292:ARG:NE   | 2.42                     | 0.52              |
| 1:J:531:LEU:HB3  | 1:J:598:ILE:HD12 | 1.91                     | 0.52              |
| 1:K:333:ARG:HB2  | 1:K:335:LYS:NZ   | 2.24                     | 0.52              |
| 1:A:350:ALA:HB3  | 1:A:568:LYS:HG3  | 1.92                     | 0.52              |
| 1:D:531:LEU:HB3  | 1:D:598:ILE:HD12 | 1.91                     | 0.52              |
| 1:D:771:ARG:HG3  | 1:D:799:GLU:HG2  | 1.91                     | 0.52              |
| 1:D:856:ARG:HD3  | 1:D:885:LYS:HD3  | 1.90                     | 0.52              |
| 1:F:248:LYS:O    | 1:F:292:ARG:NE   | 2.42                     | 0.52              |
| 1:I:290:PRO:HB3  | 1:I:337:LEU:HD22 | 1.90                     | 0.52              |
| 1:K:290:PRO:HB3  | 1:K:337:LEU:HD22 | 1.92                     | 0.52              |
| 1:L:333:ARG:HB2  | 1:L:335:LYS:NZ   | 2.24                     | 0.52              |
| 1:A:752:ASP:OD2  | 1:A:782:GLN:HB2  | 2.09                     | 0.52              |
| 1:B:752:ASP:OD2  | 1:B:782:GLN:HB2  | 2.10                     | 0.52              |
| 1:D:242:GLY:H    | 1:D:246:LYS:HZ2  | 1.57                     | 0.52              |
| 1:D:248:LYS:O    | 1:D:292:ARG:NE   | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:486:ARG:HH22 | 1:E:491:GLN:HA   | 1.73                     | 0.52              |
| 1:F:752:ASP:OD2  | 1:F:782:GLN:HB2  | 2.09                     | 0.52              |
| 1:H:378:PHE:HE1  | 1:H:395:ILE:HG13 | 1.73                     | 0.52              |
| 1:H:752:ASP:OD2  | 1:H:782:GLN:HB2  | 2.10                     | 0.52              |
| 1:J:248:LYS:O    | 1:J:292:ARG:NE   | 2.43                     | 0.52              |
| 1:J:645:MET:HE1  | 1:J:667:CYS:CB   | 2.34                     | 0.52              |
| 1:A:784:CYS:SG   | 1:A:807:LEU:HD22 | 2.50                     | 0.52              |
| 1:F:295:PHE:HB2  | 1:F:342:LEU:HD23 | 1.91                     | 0.52              |
| 1:J:856:ARG:HD3  | 1:J:885:LYS:HD3  | 1.90                     | 0.52              |
| 1:K:531:LEU:HB3  | 1:K:598:ILE:HD12 | 1.91                     | 0.52              |
| 1:L:248:LYS:O    | 1:L:292:ARG:NE   | 2.42                     | 0.52              |
| 1:L:752:ASP:OD2  | 1:L:782:GLN:HB2  | 2.09                     | 0.52              |
| 1:A:974:GLY:O    | 1:A:976:ASN:ND2  | 2.43                     | 0.52              |
| 1:B:771:ARG:HG3  | 1:B:799:GLU:HG2  | 1.92                     | 0.52              |
| 1:D:419:LYS:HA   | 1:D:422:MET:HE2  | 1.90                     | 0.52              |
| 1:F:291:SER:H    | 1:F:339:LYS:HZ2  | 1.58                     | 0.52              |
| 1:F:333:ARG:HB2  | 1:F:335:LYS:NZ   | 2.24                     | 0.52              |
| 1:G:974:GLY:O    | 1:G:976:ASN:ND2  | 2.43                     | 0.52              |
| 1:H:771:ARG:HG3  | 1:H:799:GLU:HG2  | 1.92                     | 0.52              |
| 1:I:582:VAL:HB   | 1:I:603:ARG:HG2  | 1.90                     | 0.52              |
| 1:J:679:LEU:HD12 | 1:J:745:LEU:HD21 | 1.92                     | 0.52              |
| 1:L:295:PHE:HB2  | 1:L:342:LEU:HD23 | 1.91                     | 0.52              |
| 1:L:582:VAL:HB   | 1:L:603:ARG:HG2  | 1.91                     | 0.52              |
| 1:A:1008:ASN:OD1 | 1:A:1009:ARG:N   | 2.43                     | 0.52              |
| 1:F:221:GLN:HB2  | 1:F:365:GLU:HG2  | 1.91                     | 0.52              |
| 1:G:242:GLY:H    | 1:G:246:LYS:HZ2  | 1.57                     | 0.52              |
| 1:G:1008:ASN:OD1 | 1:G:1009:ARG:N   | 2.43                     | 0.52              |
| 1:H:579:PHE:HE1  | 1:H:606:LEU:HD22 | 1.75                     | 0.52              |
| 1:J:419:LYS:HA   | 1:J:422:MET:HE2  | 1.90                     | 0.52              |
| 1:J:422:MET:HB3  | 1:J:428:LEU:HD21 | 1.92                     | 0.52              |
| 1:B:613:LYS:HE3  | 1:B:622:GLN:HB3  | 1.92                     | 0.52              |
| 1:D:581:LEU:HD22 | 1:D:590:LEU:HD22 | 1.92                     | 0.52              |
| 1:D:679:LEU:HD12 | 1:D:745:LEU:HD21 | 1.92                     | 0.52              |
| 1:D:1008:ASN:OD1 | 1:D:1009:ARG:N   | 2.43                     | 0.52              |
| 1:E:232:ALA:HB1  | 1:E:296:LEU:HD11 | 1.91                     | 0.52              |
| 1:H:613:LYS:HE3  | 1:H:622:GLN:HB3  | 1.92                     | 0.52              |
| 1:I:224:ALA:HB2  | 1:I:347:ARG:HH21 | 1.75                     | 0.52              |
| 1:J:350:ALA:HB3  | 1:J:568:LYS:HG3  | 1.91                     | 0.52              |
| 1:B:486:ARG:HH22 | 1:B:491:GLN:HA   | 1.73                     | 0.51              |
| 1:D:422:MET:HB3  | 1:D:428:LEU:HD21 | 1.92                     | 0.51              |
| 1:H:232:ALA:HB1  | 1:H:296:LEU:HD11 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:581:LEU:HD22 | 1:J:590:LEU:HD22 | 1.93                     | 0.51              |
| 1:J:655:LEU:HG   | 1:J:660:ASP:HB3  | 1.92                     | 0.51              |
| 1:J:752:ASP:OD2  | 1:J:782:GLN:HB2  | 2.09                     | 0.51              |
| 1:J:1008:ASN:OD1 | 1:J:1009:ARG:N   | 2.43                     | 0.51              |
| 1:B:248:LYS:O    | 1:B:292:ARG:NE   | 2.43                     | 0.51              |
| 1:C:333:ARG:HB2  | 1:C:335:LYS:NZ   | 2.24                     | 0.51              |
| 1:H:248:LYS:O    | 1:H:292:ARG:NE   | 2.43                     | 0.51              |
| 1:A:1030:GLU:HG2 | 1:H:917:ARG:HH22 | 1.74                     | 0.51              |
| 1:B:232:ALA:HB1  | 1:B:296:LEU:HD11 | 1.91                     | 0.51              |
| 1:D:350:ALA:HB3  | 1:D:568:LYS:HG3  | 1.92                     | 0.51              |
| 1:D:655:LEU:HG   | 1:D:660:ASP:HB3  | 1.92                     | 0.51              |
| 1:D:742:GLU:HG2  | 1:D:771:ARG:HD2  | 1.93                     | 0.51              |
| 1:D:752:ASP:OD2  | 1:D:782:GLN:HB2  | 2.09                     | 0.51              |
| 1:G:655:LEU:HG   | 1:G:660:ASP:HB3  | 1.92                     | 0.51              |
| 1:I:242:GLY:H    | 1:I:246:LYS:HZ2  | 1.57                     | 0.51              |
| 1:J:742:GLU:HG2  | 1:J:771:ARG:HD2  | 1.93                     | 0.51              |
| 1:J:923:ASP:HB2  | 1:J:954:SER:HB2  | 1.92                     | 0.51              |
| 1:L:635:MET:HE2  | 1:L:641:VAL:HG23 | 1.90                     | 0.51              |
| 1:A:655:LEU:HG   | 1:A:660:ASP:HB3  | 1.92                     | 0.51              |
| 1:D:923:ASP:HB2  | 1:D:954:SER:HB2  | 1.92                     | 0.51              |
| 1:E:613:LYS:HE3  | 1:E:622:GLN:HB3  | 1.92                     | 0.51              |
| 1:E:752:ASP:OD2  | 1:E:782:GLN:HB2  | 2.10                     | 0.51              |
| 1:E:917:ARG:HH22 | 1:J:1030:GLU:HG2 | 1.74                     | 0.51              |
| 1:I:333:ARG:HB2  | 1:I:335:LYS:NZ   | 2.24                     | 0.51              |
| 1:K:248:LYS:O    | 1:K:292:ARG:NE   | 2.43                     | 0.51              |
| 1:L:571:LEU:O    | 1:L:574:VAL:HB   | 2.11                     | 0.51              |
| 1:A:422:MET:HB3  | 1:A:428:LEU:HD21 | 1.92                     | 0.51              |
| 1:C:982:CYS:O    | 1:C:986:LEU:HD23 | 2.10                     | 0.51              |
| 1:D:974:GLY:O    | 1:D:976:ASN:ND2  | 2.43                     | 0.51              |
| 1:E:248:LYS:O    | 1:E:292:ARG:NE   | 2.43                     | 0.51              |
| 1:F:635:MET:HE2  | 1:F:641:VAL:HG23 | 1.90                     | 0.51              |
| 1:F:1008:ASN:OD1 | 1:F:1009:ARG:N   | 2.43                     | 0.51              |
| 1:G:422:MET:HB3  | 1:G:428:LEU:HD21 | 1.92                     | 0.51              |
| 1:H:518:HIS:HB3  | 1:H:521:PHE:CE1  | 2.45                     | 0.51              |
| 1:I:982:CYS:O    | 1:I:986:LEU:HD23 | 2.10                     | 0.51              |
| 1:K:613:LYS:HE3  | 1:K:622:GLN:HB3  | 1.92                     | 0.51              |
| 1:K:955:CYS:HA   | 1:K:958:LEU:HD13 | 1.93                     | 0.51              |
| 1:L:242:GLY:H    | 1:L:246:LYS:HZ1  | 1.59                     | 0.51              |
| 1:L:1008:ASN:OD1 | 1:L:1009:ARG:N   | 2.43                     | 0.51              |
| 1:A:771:ARG:HG3  | 1:A:799:GLU:HG2  | 1.91                     | 0.51              |
| 1:B:917:ARG:HH22 | 1:G:1030:GLU:HG2 | 1.74                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:242:GLY:H    | 1:F:246:LYS:HZ2  | 1.59                     | 0.51              |
| 1:F:571:LEU:O    | 1:F:574:VAL:HB   | 2.11                     | 0.51              |
| 1:G:771:ARG:HG3  | 1:G:799:GLU:HG2  | 1.91                     | 0.51              |
| 1:H:333:ARG:HB2  | 1:H:335:LYS:NZ   | 2.24                     | 0.51              |
| 1:I:641:VAL:O    | 1:I:645:MET:HB2  | 2.10                     | 0.51              |
| 1:J:974:GLY:O    | 1:J:976:ASN:ND2  | 2.43                     | 0.51              |
| 1:K:752:ASP:OD2  | 1:K:782:GLN:HB2  | 2.10                     | 0.51              |
| 1:K:946:ASP:OD1  | 1:K:974:GLY:N    | 2.38                     | 0.51              |
| 1:K:1008:ASN:OD1 | 1:K:1009:ARG:N   | 2.42                     | 0.51              |
| 1:L:200:LYS:HB2  | 1:L:203:LEU:HG   | 1.92                     | 0.51              |
| 1:L:894:THR:HG22 | 1:L:895:SER:N    | 2.24                     | 0.51              |
| 1:A:333:ARG:HB2  | 1:A:335:LYS:NZ   | 2.24                     | 0.51              |
| 1:A:653:ILE:HD12 | 1:A:655:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:217:THR:HG22 | 1:B:361:PRO:HB3  | 1.91                     | 0.51              |
| 1:D:784:CYS:SG   | 1:D:807:LEU:HD22 | 2.50                     | 0.51              |
| 1:F:679:LEU:HD12 | 1:F:745:LEU:HD21 | 1.91                     | 0.51              |
| 1:F:940:LEU:HD21 | 1:F:943:LEU:HB2  | 1.93                     | 0.51              |
| 1:G:333:ARG:HB2  | 1:G:335:LYS:NZ   | 2.24                     | 0.51              |
| 1:G:653:ILE:HD12 | 1:G:655:LEU:HD11 | 1.93                     | 0.51              |
| 1:G:742:GLU:HG2  | 1:G:771:ARG:HD2  | 1.93                     | 0.51              |
| 1:H:217:THR:HG22 | 1:H:361:PRO:HB3  | 1.91                     | 0.51              |
| 1:J:784:CYS:SG   | 1:J:807:LEU:HD22 | 2.50                     | 0.51              |
| 1:K:771:ARG:HG3  | 1:K:799:GLU:HG2  | 1.92                     | 0.51              |
| 1:L:982:CYS:O    | 1:L:986:LEU:HD23 | 2.10                     | 0.51              |
| 1:B:290:PRO:HB3  | 1:B:337:LEU:HD22 | 1.91                     | 0.51              |
| 1:C:571:LEU:O    | 1:C:574:VAL:HB   | 2.11                     | 0.51              |
| 1:E:771:ARG:HG3  | 1:E:799:GLU:HG2  | 1.92                     | 0.51              |
| 1:F:894:THR:HG22 | 1:F:895:SER:N    | 2.24                     | 0.51              |
| 1:A:742:GLU:HG2  | 1:A:771:ARG:HD2  | 1.93                     | 0.51              |
| 1:E:1008:ASN:OD1 | 1:E:1009:ARG:N   | 2.42                     | 0.51              |
| 1:F:982:CYS:O    | 1:F:986:LEU:HD23 | 2.10                     | 0.51              |
| 1:H:304:GLN:HG2  | 1:H:307:PHE:CD2  | 2.46                     | 0.51              |
| 1:I:571:LEU:O    | 1:I:574:VAL:HB   | 2.11                     | 0.51              |
| 1:L:291:SER:H    | 1:L:339:LYS:HZ2  | 1.59                     | 0.51              |
| 1:A:581:LEU:HD22 | 1:A:590:LEU:HD22 | 1.92                     | 0.50              |
| 1:A:746:SER:OG   | 1:A:747:ASP:OD1  | 2.25                     | 0.50              |
| 1:C:224:ALA:HB2  | 1:C:347:ARG:HH21 | 1.76                     | 0.50              |
| 1:C:606:LEU:O    | 1:C:610:ILE:HG12 | 2.10                     | 0.50              |
| 1:D:1030:GLU:HG2 | 1:K:917:ARG:HH22 | 1.75                     | 0.50              |
| 1:E:378:PHE:HB2  | 1:E:392:PHE:CZ   | 2.47                     | 0.50              |
| 1:K:378:PHE:HB2  | 1:K:392:PHE:CZ   | 2.47                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:641:VAL:O     | 1:L:645:MET:HB2  | 2.11                     | 0.50              |
| 1:B:1008:ASN:OD1  | 1:B:1009:ARG:N   | 2.42                     | 0.50              |
| 1:E:946:ASP:OD1   | 1:E:974:GLY:N    | 2.39                     | 0.50              |
| 1:G:679:LEU:HD12  | 1:G:745:LEU:HD21 | 1.92                     | 0.50              |
| 1:K:582:VAL:HB    | 1:K:603:ARG:HG2  | 1.93                     | 0.50              |
| 1:L:679:LEU:HD12  | 1:L:745:LEU:HD21 | 1.92                     | 0.50              |
| 1:A:679:LEU:HD12  | 1:A:745:LEU:HD21 | 1.92                     | 0.50              |
| 1:D:653:ILE:HD12  | 1:D:655:LEU:HD11 | 1.93                     | 0.50              |
| 1:E:635:MET:HE1   | 1:E:640:PHE:CD1  | 2.47                     | 0.50              |
| 1:F:641:VAL:O     | 1:F:645:MET:HB2  | 2.11                     | 0.50              |
| 1:G:581:LEU:HD22  | 1:G:590:LEU:HD22 | 1.93                     | 0.50              |
| 1:H:1008:ASN:OD1  | 1:H:1009:ARG:N   | 2.42                     | 0.50              |
| 1:J:290:PRO:HB3   | 1:J:337:LEU:HD22 | 1.94                     | 0.50              |
| 1:K:579:PHE:HE1   | 1:K:606:LEU:HD22 | 1.77                     | 0.50              |
| 1:L:224:ALA:HB2   | 1:L:347:ARG:HH21 | 1.77                     | 0.50              |
| 1:B:333:ARG:HB2   | 1:B:335:LYS:NZ   | 2.24                     | 0.50              |
| 1:B:861:GLU:N     | 1:B:889:VAL:O    | 2.36                     | 0.50              |
| 1:D:290:PRO:HB3   | 1:D:337:LEU:HD22 | 1.94                     | 0.50              |
| 1:H:571:LEU:O     | 1:H:574:VAL:HB   | 2.11                     | 0.50              |
| 1:J:653:ILE:HD12  | 1:J:655:LEU:HD11 | 1.93                     | 0.50              |
| 1:K:635:MET:HE1   | 1:K:640:PHE:CD1  | 2.47                     | 0.50              |
| 1:K:1027:ILE:HG22 | 1:K:1029:PHE:H   | 1.76                     | 0.50              |
| 1:A:304:GLN:HG2   | 1:A:307:PHE:CD2  | 2.46                     | 0.50              |
| 1:B:304:GLN:HG2   | 1:B:307:PHE:CD2  | 2.47                     | 0.50              |
| 1:B:350:ALA:HB3   | 1:B:568:LYS:HG3  | 1.93                     | 0.50              |
| 1:E:579:PHE:HE1   | 1:E:606:LEU:HD22 | 1.77                     | 0.50              |
| 1:F:200:LYS:HB2   | 1:F:203:LEU:HG   | 1.93                     | 0.50              |
| 1:F:324:GLY:O     | 1:F:328:LEU:HG   | 2.12                     | 0.50              |
| 1:G:304:GLN:HG2   | 1:G:307:PHE:CD2  | 2.46                     | 0.50              |
| 1:K:304:GLN:HG2   | 1:K:307:PHE:CD2  | 2.46                     | 0.50              |
| 1:L:940:LEU:HD21  | 1:L:943:LEU:HB2  | 1.94                     | 0.50              |
| 1:A:239:TRP:CD1   | 1:A:252:LEU:HD13 | 2.47                     | 0.50              |
| 1:C:200:LYS:HB2   | 1:C:203:LEU:HG   | 1.93                     | 0.50              |
| 1:C:297:MET:HE1   | 1:C:342:LEU:HD22 | 1.94                     | 0.50              |
| 1:E:393:ARG:O     | 1:E:397:GLU:HG3  | 2.12                     | 0.50              |
| 1:E:582:VAL:HB    | 1:E:603:ARG:HG2  | 1.94                     | 0.50              |
| 1:E:1027:ILE:HG22 | 1:E:1029:PHE:H   | 1.76                     | 0.50              |
| 1:G:200:LYS:HB2   | 1:G:203:LEU:HG   | 1.93                     | 0.50              |
| 1:I:940:LEU:HD21  | 1:I:943:LEU:HB2  | 1.93                     | 0.50              |
| 1:J:200:LYS:HB2   | 1:J:203:LEU:HG   | 1.93                     | 0.50              |
| 1:E:304:GLN:HG2   | 1:E:307:PHE:CD2  | 2.46                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:239:TRP:CD1   | 1:G:252:LEU:HD13 | 2.47                     | 0.50              |
| 1:H:393:ARG:O     | 1:H:397:GLU:HG3  | 2.11                     | 0.50              |
| 1:I:324:GLY:O     | 1:I:328:LEU:HG   | 2.12                     | 0.50              |
| 1:J:799:GLU:HB2   | 1:J:828:LYS:HB2  | 1.94                     | 0.50              |
| 1:K:912:THR:OG1   | 1:K:913:HIS:ND1  | 2.33                     | 0.50              |
| 1:A:200:LYS:HB2   | 1:A:203:LEU:HG   | 1.93                     | 0.50              |
| 1:B:635:MET:HE1   | 1:B:640:PHE:CD1  | 2.47                     | 0.50              |
| 1:D:200:LYS:HB2   | 1:D:203:LEU:HG   | 1.93                     | 0.50              |
| 1:I:200:LYS:HB2   | 1:I:203:LEU:HG   | 1.93                     | 0.50              |
| 1:C:324:GLY:O     | 1:C:328:LEU:HG   | 2.12                     | 0.49              |
| 1:C:940:LEU:HD21  | 1:C:943:LEU:HB2  | 1.93                     | 0.49              |
| 1:D:799:GLU:HB2   | 1:D:828:LYS:HB2  | 1.94                     | 0.49              |
| 1:H:635:MET:HE1   | 1:H:640:PHE:CD1  | 2.47                     | 0.49              |
| 1:K:393:ARG:O     | 1:K:397:GLU:HG3  | 2.12                     | 0.49              |
| 1:A:371:GLU:HG3   | 1:A:402:PHE:CZ   | 2.47                     | 0.49              |
| 1:B:393:ARG:O     | 1:B:397:GLU:HG3  | 2.12                     | 0.49              |
| 1:B:582:VAL:HB    | 1:B:603:ARG:HG2  | 1.93                     | 0.49              |
| 1:B:1027:ILE:HG22 | 1:B:1029:PHE:H   | 1.76                     | 0.49              |
| 1:H:300:PHE:CD1   | 1:H:303:LEU:HD12 | 2.48                     | 0.49              |
| 1:H:371:GLU:O     | 1:H:375:LYS:HG2  | 2.12                     | 0.49              |
| 1:K:923:ASP:HB2   | 1:K:954:SER:HB2  | 1.94                     | 0.49              |
| 1:B:304:GLN:HB2   | 1:B:567:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:371:GLU:O     | 1:B:375:LYS:HG2  | 2.12                     | 0.49              |
| 1:B:857:LEU:HG    | 1:B:859:ILE:HG23 | 1.95                     | 0.49              |
| 1:E:912:THR:OG1   | 1:E:913:HIS:ND1  | 2.33                     | 0.49              |
| 1:F:224:ALA:HB2   | 1:F:347:ARG:HH21 | 1.78                     | 0.49              |
| 1:G:371:GLU:HG3   | 1:G:402:PHE:CZ   | 2.47                     | 0.49              |
| 1:I:581:LEU:HD22  | 1:I:590:LEU:HD22 | 1.95                     | 0.49              |
| 1:J:940:LEU:HD21  | 1:J:943:LEU:HB2  | 1.93                     | 0.49              |
| 1:L:324:GLY:O     | 1:L:328:LEU:HG   | 2.12                     | 0.49              |
| 1:B:378:PHE:HB2   | 1:B:392:PHE:CZ   | 2.47                     | 0.49              |
| 1:B:946:ASP:OD1   | 1:B:974:GLY:N    | 2.39                     | 0.49              |
| 1:C:295:PHE:HB2   | 1:C:342:LEU:HD23 | 1.95                     | 0.49              |
| 1:D:239:TRP:CD1   | 1:D:252:LEU:HD13 | 2.47                     | 0.49              |
| 1:H:350:ALA:HB3   | 1:H:568:LYS:HG3  | 1.94                     | 0.49              |
| 1:H:857:LEU:HG    | 1:H:859:ILE:HG23 | 1.95                     | 0.49              |
| 1:H:1027:ILE:HG22 | 1:H:1029:PHE:H   | 1.76                     | 0.49              |
| 1:I:1008:ASN:OD1  | 1:I:1009:ARG:N   | 2.43                     | 0.49              |
| 1:B:378:PHE:HB2   | 1:B:392:PHE:CE1  | 2.47                     | 0.49              |
| 1:D:613:LYS:HE3   | 1:D:622:GLN:HB3  | 1.94                     | 0.49              |
| 1:D:902:THR:OG1   | 1:D:928:LEU:O    | 2.30                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:940:LEU:HD21 | 1:D:943:LEU:HB2  | 1.94                     | 0.49              |
| 1:F:1010:GLU:HG3 | 1:F:1013:ARG:NH2 | 2.27                     | 0.49              |
| 1:J:304:GLN:HG2  | 1:J:307:PHE:CD2  | 2.46                     | 0.49              |
| 1:L:1010:GLU:HG3 | 1:L:1013:ARG:NH2 | 2.27                     | 0.49              |
| 1:C:581:LEU:HD22 | 1:C:590:LEU:HD22 | 1.95                     | 0.49              |
| 1:C:582:VAL:HB   | 1:C:603:ARG:HG2  | 1.93                     | 0.49              |
| 1:C:1008:ASN:OD1 | 1:C:1009:ARG:N   | 2.43                     | 0.49              |
| 1:D:217:THR:HG22 | 1:D:361:PRO:HB3  | 1.94                     | 0.49              |
| 1:E:371:GLU:O    | 1:E:375:LYS:HG2  | 2.12                     | 0.49              |
| 1:F:137:ARG:HH21 | 1:F:239:TRP:NE1  | 2.11                     | 0.49              |
| 1:G:613:LYS:HE3  | 1:G:622:GLN:HB3  | 1.94                     | 0.49              |
| 1:J:239:TRP:CD1  | 1:J:252:LEU:HD13 | 2.47                     | 0.49              |
| 1:J:613:LYS:HE3  | 1:J:622:GLN:HB3  | 1.94                     | 0.49              |
| 1:K:857:LEU:HG   | 1:K:859:ILE:HG23 | 1.95                     | 0.49              |
| 1:D:304:GLN:HG2  | 1:D:307:PHE:CD2  | 2.46                     | 0.49              |
| 1:E:304:GLN:HB2  | 1:E:567:GLU:OE1  | 2.12                     | 0.49              |
| 1:E:378:PHE:HB2  | 1:E:392:PHE:CE1  | 2.47                     | 0.49              |
| 1:F:371:GLU:HG3  | 1:F:402:PHE:CZ   | 2.47                     | 0.49              |
| 1:H:946:ASP:OD1  | 1:H:974:GLY:N    | 2.39                     | 0.49              |
| 1:L:923:ASP:HB2  | 1:L:954:SER:HB2  | 1.94                     | 0.49              |
| 1:A:613:LYS:HE3  | 1:A:622:GLN:HB3  | 1.94                     | 0.49              |
| 1:A:635:MET:HE1  | 1:A:640:PHE:CD1  | 2.48                     | 0.49              |
| 1:G:635:MET:HE1  | 1:G:640:PHE:CD1  | 2.48                     | 0.49              |
| 1:H:942:MET:SD   | 1:H:943:LEU:N    | 2.86                     | 0.49              |
| 1:I:653:ILE:HD12 | 1:I:655:LEU:HD11 | 1.94                     | 0.49              |
| 1:K:304:GLN:HB2  | 1:K:567:GLU:OE1  | 2.12                     | 0.49              |
| 1:L:137:ARG:HH21 | 1:L:239:TRP:NE1  | 2.11                     | 0.49              |
| 1:A:635:MET:HE1  | 1:A:640:PHE:HD1  | 1.77                     | 0.49              |
| 1:C:519:MET:SD   | 1:C:519:MET:N    | 2.86                     | 0.49              |
| 1:D:251:TYR:HB2  | 1:D:293:ILE:HG12 | 1.95                     | 0.49              |
| 1:E:857:LEU:HG   | 1:E:859:ILE:HG23 | 1.95                     | 0.49              |
| 1:F:304:GLN:HG2  | 1:F:307:PHE:CD2  | 2.48                     | 0.49              |
| 1:G:290:PRO:HB3  | 1:G:337:LEU:HD22 | 1.94                     | 0.49              |
| 1:G:923:ASP:HB2  | 1:G:954:SER:HB2  | 1.94                     | 0.49              |
| 1:H:531:LEU:HB3  | 1:H:598:ILE:HG23 | 1.93                     | 0.49              |
| 1:I:519:MET:SD   | 1:I:519:MET:N    | 2.86                     | 0.49              |
| 1:I:902:THR:OG1  | 1:I:928:LEU:O    | 2.29                     | 0.49              |
| 1:J:217:THR:HG22 | 1:J:361:PRO:HB3  | 1.94                     | 0.49              |
| 1:J:635:MET:HE1  | 1:J:640:PHE:HD1  | 1.77                     | 0.49              |
| 1:K:371:GLU:O    | 1:K:375:LYS:HG2  | 2.12                     | 0.49              |
| 1:K:378:PHE:HB2  | 1:K:392:PHE:CE1  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:PRO:HB3  | 1:A:337:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:923:ASP:HB2  | 1:A:954:SER:HB2  | 1.94                     | 0.49              |
| 1:B:930:CYS:HA   | 1:B:933:LEU:HB2  | 1.95                     | 0.49              |
| 1:C:239:TRP:CD1  | 1:C:252:LEU:HD13 | 2.48                     | 0.49              |
| 1:C:653:ILE:HD12 | 1:C:655:LEU:HD11 | 1.95                     | 0.49              |
| 1:C:902:THR:OG1  | 1:C:928:LEU:O    | 2.29                     | 0.49              |
| 1:D:371:GLU:HG3  | 1:D:402:PHE:CZ   | 2.47                     | 0.49              |
| 1:D:635:MET:HE1  | 1:D:640:PHE:HD1  | 1.77                     | 0.49              |
| 1:F:653:ILE:HD12 | 1:F:655:LEU:HD11 | 1.94                     | 0.49              |
| 1:H:930:CYS:HA   | 1:H:933:LEU:HB2  | 1.95                     | 0.49              |
| 1:I:137:ARG:HH21 | 1:I:239:TRP:NE1  | 2.10                     | 0.49              |
| 1:J:251:TYR:HB2  | 1:J:293:ILE:HG12 | 1.95                     | 0.49              |
| 1:L:304:GLN:HG2  | 1:L:307:PHE:CD2  | 2.48                     | 0.49              |
| 1:D:635:MET:HE1  | 1:D:640:PHE:CD1  | 2.48                     | 0.48              |
| 1:E:392:PHE:O    | 1:E:396:GLN:NE2  | 2.46                     | 0.48              |
| 1:E:635:MET:HE1  | 1:E:640:PHE:HD1  | 1.78                     | 0.48              |
| 1:E:861:GLU:N    | 1:E:889:VAL:O    | 2.36                     | 0.48              |
| 1:E:942:MET:SD   | 1:E:943:LEU:N    | 2.86                     | 0.48              |
| 1:G:635:MET:HE1  | 1:G:640:PHE:HD1  | 1.77                     | 0.48              |
| 1:H:304:GLN:HB2  | 1:H:567:GLU:OE1  | 2.12                     | 0.48              |
| 1:I:239:TRP:CD1  | 1:I:252:LEU:HD13 | 2.48                     | 0.48              |
| 1:I:746:SER:OG   | 1:I:747:ASP:OD1  | 2.26                     | 0.48              |
| 1:J:298:ASP:OD1  | 1:J:345:THR:OG1  | 2.29                     | 0.48              |
| 1:J:371:GLU:HG3  | 1:J:402:PHE:CZ   | 2.47                     | 0.48              |
| 1:J:635:MET:HE1  | 1:J:640:PHE:CD1  | 2.48                     | 0.48              |
| 1:K:350:ALA:HB3  | 1:K:568:LYS:HG3  | 1.93                     | 0.48              |
| 1:K:392:PHE:O    | 1:K:396:GLN:NE2  | 2.46                     | 0.48              |
| 1:K:635:MET:HE1  | 1:K:640:PHE:HD1  | 1.78                     | 0.48              |
| 1:K:861:GLU:N    | 1:K:889:VAL:O    | 2.36                     | 0.48              |
| 1:K:942:MET:SD   | 1:K:943:LEU:N    | 2.86                     | 0.48              |
| 1:C:137:ARG:HH21 | 1:C:239:TRP:NE1  | 2.11                     | 0.48              |
| 1:C:391:ALA:O    | 1:C:395:ILE:HG12 | 2.13                     | 0.48              |
| 1:D:358:LEU:HD13 | 1:D:361:PRO:HG3  | 1.94                     | 0.48              |
| 1:D:861:GLU:N    | 1:D:889:VAL:O    | 2.36                     | 0.48              |
| 1:E:251:TYR:HB2  | 1:E:293:ILE:HG12 | 1.94                     | 0.48              |
| 1:E:350:ALA:HB3  | 1:E:568:LYS:HG3  | 1.93                     | 0.48              |
| 1:E:930:CYS:HA   | 1:E:933:LEU:HB2  | 1.94                     | 0.48              |
| 1:I:391:ALA:O    | 1:I:395:ILE:HG12 | 2.13                     | 0.48              |
| 1:B:942:MET:SD   | 1:B:943:LEU:N    | 2.86                     | 0.48              |
| 1:A:140:VAL:HG23 | 1:A:240:ALA:HB2  | 1.95                     | 0.48              |
| 1:D:298:ASP:OD1  | 1:D:345:THR:OG1  | 2.30                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:917:ARG:HH22 | 1:K:1030:GLU:HG2 | 1.78                     | 0.48              |
| 1:G:746:SER:OG   | 1:G:747:ASP:OD1  | 2.25                     | 0.48              |
| 1:G:799:GLU:HB2  | 1:G:828:LYS:HB2  | 1.94                     | 0.48              |
| 1:H:581:LEU:HD22 | 1:H:590:LEU:HD22 | 1.94                     | 0.48              |
| 1:J:371:GLU:HG3  | 1:J:402:PHE:HZ   | 1.78                     | 0.48              |
| 1:B:300:PHE:CD1  | 1:B:303:LEU:HD12 | 2.49                     | 0.48              |
| 1:D:140:VAL:HG23 | 1:D:240:ALA:HB2  | 1.95                     | 0.48              |
| 1:D:291:SER:H    | 1:D:339:LYS:HZ2  | 1.61                     | 0.48              |
| 1:D:371:GLU:HG3  | 1:D:402:PHE:HZ   | 1.78                     | 0.48              |
| 1:D:398:ASN:ND2  | 1:D:432:SER:O    | 2.46                     | 0.48              |
| 1:E:653:ILE:HD12 | 1:E:655:LEU:HD11 | 1.96                     | 0.48              |
| 1:F:350:ALA:HB3  | 1:F:568:LYS:HG3  | 1.95                     | 0.48              |
| 1:G:140:VAL:HG23 | 1:G:240:ALA:HB2  | 1.95                     | 0.48              |
| 1:H:635:MET:HE1  | 1:H:640:PHE:HD1  | 1.78                     | 0.48              |
| 1:J:398:ASN:ND2  | 1:J:432:SER:O    | 2.46                     | 0.48              |
| 1:L:350:ALA:HB3  | 1:L:568:LYS:HG3  | 1.95                     | 0.48              |
| 1:L:653:ILE:HD12 | 1:L:655:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:358:LEU:HD13 | 1:A:361:PRO:HG3  | 1.94                     | 0.48              |
| 1:A:371:GLU:HG3  | 1:A:402:PHE:HZ   | 1.78                     | 0.48              |
| 1:A:580:GLY:O    | 1:A:586:ARG:NE   | 2.47                     | 0.48              |
| 1:A:940:LEU:HD21 | 1:A:943:LEU:HB2  | 1.94                     | 0.48              |
| 1:D:746:SER:OG   | 1:D:747:ASP:OD1  | 2.25                     | 0.48              |
| 1:F:239:TRP:CD1  | 1:F:252:LEU:HD13 | 2.48                     | 0.48              |
| 1:F:391:ALA:O    | 1:F:395:ILE:HG12 | 2.14                     | 0.48              |
| 1:F:619:LEU:HD22 | 1:F:622:GLN:NE2  | 2.29                     | 0.48              |
| 1:G:371:GLU:HG3  | 1:G:402:PHE:HZ   | 1.78                     | 0.48              |
| 1:G:580:GLY:O    | 1:G:586:ARG:NE   | 2.47                     | 0.48              |
| 1:I:304:GLN:HG2  | 1:I:307:PHE:CD2  | 2.48                     | 0.48              |
| 1:J:140:VAL:HG23 | 1:J:240:ALA:HB2  | 1.95                     | 0.48              |
| 1:J:167:LEU:HD22 | 1:J:368:GLY:HA2  | 1.95                     | 0.48              |
| 1:J:291:SER:H    | 1:J:339:LYS:HZ2  | 1.61                     | 0.48              |
| 1:J:358:LEU:HD13 | 1:J:361:PRO:HG3  | 1.95                     | 0.48              |
| 1:J:746:SER:OG   | 1:J:747:ASP:OD1  | 2.25                     | 0.48              |
| 1:K:653:ILE:HD12 | 1:K:655:LEU:HD11 | 1.96                     | 0.48              |
| 1:L:391:ALA:O    | 1:L:395:ILE:HG12 | 2.14                     | 0.48              |
| 1:A:900:ALA:O    | 1:A:904:VAL:HG23 | 2.14                     | 0.48              |
| 1:E:1030:GLU:HG2 | 1:J:917:ARG:HH22 | 1.79                     | 0.48              |
| 1:F:581:LEU:HD22 | 1:F:590:LEU:HD22 | 1.95                     | 0.48              |
| 1:F:809:ASP:OD1  | 1:F:810:PHE:N    | 2.47                     | 0.48              |
| 1:G:358:LEU:HD13 | 1:G:361:PRO:HG3  | 1.95                     | 0.48              |
| 1:K:239:TRP:CD1  | 1:K:252:LEU:HD13 | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:735:SER:HB2  | 1:K:764:HIS:HB3   | 1.95                     | 0.48              |
| 1:L:239:TRP:CD1  | 1:L:252:LEU:HD13  | 2.48                     | 0.48              |
| 1:L:619:LEU:HD22 | 1:L:622:GLN:NE2   | 2.29                     | 0.48              |
| 1:A:217:THR:HG22 | 1:A:361:PRO:HB3   | 1.94                     | 0.48              |
| 1:A:799:GLU:HB2  | 1:A:828:LYS:HB2   | 1.94                     | 0.48              |
| 1:B:239:TRP:CD1  | 1:B:252:LEU:HD13  | 2.49                     | 0.48              |
| 1:B:635:MET:HE1  | 1:B:640:PHE:HD1   | 1.78                     | 0.48              |
| 1:E:239:TRP:CD1  | 1:E:252:LEU:HD13  | 2.49                     | 0.48              |
| 1:F:563:TYR:CE1  | 1:F:572:ILE:HG12  | 2.48                     | 0.48              |
| 1:G:900:ALA:O    | 1:G:904:VAL:HG23  | 2.14                     | 0.48              |
| 1:G:940:LEU:HD21 | 1:G:943:LEU:HB2   | 1.94                     | 0.48              |
| 1:H:653:ILE:HD12 | 1:H:655:LEU:HD11  | 1.96                     | 0.48              |
| 1:L:809:ASP:OD1  | 1:L:810:PHE:N     | 2.47                     | 0.48              |
| 1:A:990:LEU:HD22 | 1:A:1025:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:579:PHE:HE1  | 1:B:606:LEU:HD22  | 1.78                     | 0.48              |
| 1:B:653:ILE:HD12 | 1:B:655:LEU:HD11  | 1.96                     | 0.48              |
| 1:C:371:GLU:HG3  | 1:C:402:PHE:CZ    | 2.48                     | 0.48              |
| 1:C:563:TYR:CE1  | 1:C:572:ILE:HG12  | 2.48                     | 0.48              |
| 1:C:746:SER:OG   | 1:C:747:ASP:OD1   | 2.26                     | 0.48              |
| 1:C:809:ASP:OD1  | 1:C:810:PHE:N     | 2.47                     | 0.48              |
| 1:C:1030:GLU:HG2 | 1:L:917:ARG:HH22  | 1.79                     | 0.48              |
| 1:D:304:GLN:HB2  | 1:D:567:GLU:OE1   | 2.13                     | 0.48              |
| 1:E:200:LYS:HB2  | 1:E:203:LEU:HG    | 1.96                     | 0.48              |
| 1:F:371:GLU:HG3  | 1:F:402:PHE:HZ    | 1.79                     | 0.48              |
| 1:H:224:ALA:HB2  | 1:H:347:ARG:HH21  | 1.79                     | 0.48              |
| 1:H:239:TRP:CD1  | 1:H:252:LEU:HD13  | 2.49                     | 0.48              |
| 1:H:330:SER:HA   | 1:H:335:LYS:NZ    | 2.29                     | 0.48              |
| 1:I:215:VAL:HG12 | 1:I:362:ARG:NH2   | 2.29                     | 0.48              |
| 1:K:809:ASP:OD1  | 1:K:810:PHE:N     | 2.47                     | 0.48              |
| 1:L:371:GLU:HG3  | 1:L:402:PHE:CZ    | 2.48                     | 0.48              |
| 1:L:902:THR:OG1  | 1:L:928:LEU:O     | 2.30                     | 0.48              |
| 1:C:215:VAL:HG12 | 1:C:362:ARG:NH2   | 2.29                     | 0.48              |
| 1:C:304:GLN:HG2  | 1:C:307:PHE:CD2   | 2.48                     | 0.48              |
| 1:C:923:ASP:HB2  | 1:C:954:SER:HB2   | 1.96                     | 0.48              |
| 1:E:809:ASP:OD1  | 1:E:810:PHE:N     | 2.47                     | 0.48              |
| 1:G:217:THR:HG22 | 1:G:361:PRO:HB3   | 1.94                     | 0.48              |
| 1:H:912:THR:OG1  | 1:H:913:HIS:ND1   | 2.33                     | 0.48              |
| 1:I:563:TYR:CE1  | 1:I:572:ILE:HG12  | 2.48                     | 0.48              |
| 1:I:809:ASP:OD1  | 1:I:810:PHE:N     | 2.47                     | 0.48              |
| 1:I:923:ASP:HB2  | 1:I:954:SER:HB2   | 1.96                     | 0.48              |
| 1:J:304:GLN:HB2  | 1:J:567:GLU:OE1   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:140:VAL:HG23 | 1:K:240:ALA:HB2   | 1.96                     | 0.48              |
| 1:L:581:LEU:HD22 | 1:L:590:LEU:HD22  | 1.95                     | 0.48              |
| 1:L:849:SER:OG   | 1:L:875:LYS:HD2   | 2.14                     | 0.48              |
| 1:A:637:GLU:O    | 1:A:641:VAL:HG23  | 2.14                     | 0.47              |
| 1:B:251:TYR:HB2  | 1:B:293:ILE:HG12  | 1.95                     | 0.47              |
| 1:C:619:LEU:HD22 | 1:C:622:GLN:NE2   | 2.29                     | 0.47              |
| 1:E:579:PHE:CE1  | 1:E:606:LEU:HD13  | 2.49                     | 0.47              |
| 1:F:797:LEU:HD21 | 1:F:800:LEU:HD12  | 1.95                     | 0.47              |
| 1:G:637:GLU:O    | 1:G:641:VAL:HG23  | 2.14                     | 0.47              |
| 1:G:990:LEU:HD22 | 1:G:1025:LEU:HD11 | 1.96                     | 0.47              |
| 1:H:579:PHE:CE1  | 1:H:606:LEU:HD13  | 2.49                     | 0.47              |
| 1:I:350:ALA:HB3  | 1:I:568:LYS:HG3   | 1.95                     | 0.47              |
| 1:I:619:LEU:HD22 | 1:I:622:GLN:NE2   | 2.29                     | 0.47              |
| 1:I:849:SER:OG   | 1:I:875:LYS:HD2   | 2.14                     | 0.47              |
| 1:K:251:TYR:HB2  | 1:K:293:ILE:HG12  | 1.95                     | 0.47              |
| 1:L:216:HIS:ND1  | 1:L:341:SER:OG    | 2.30                     | 0.47              |
| 1:A:251:TYR:HB2  | 1:A:293:ILE:HG12  | 1.95                     | 0.47              |
| 1:B:809:ASP:OD1  | 1:B:810:PHE:N     | 2.47                     | 0.47              |
| 1:C:797:LEU:HD21 | 1:C:800:LEU:HD12  | 1.95                     | 0.47              |
| 1:F:328:LEU:O    | 1:F:332:ILE:HG13  | 2.14                     | 0.47              |
| 1:G:304:GLN:HB2  | 1:G:567:GLU:OE1   | 2.13                     | 0.47              |
| 1:H:809:ASP:OD1  | 1:H:810:PHE:N     | 2.47                     | 0.47              |
| 1:I:371:GLU:HG3  | 1:I:402:PHE:CZ    | 2.49                     | 0.47              |
| 1:I:797:LEU:HD21 | 1:I:800:LEU:HD12  | 1.95                     | 0.47              |
| 1:K:200:LYS:HB2  | 1:K:203:LEU:HG    | 1.96                     | 0.47              |
| 1:K:224:ALA:HB2  | 1:K:347:ARG:HH21  | 1.79                     | 0.47              |
| 1:K:579:PHE:CE1  | 1:K:606:LEU:HD13  | 2.49                     | 0.47              |
| 1:L:215:VAL:HG12 | 1:L:362:ARG:NH2   | 2.29                     | 0.47              |
| 1:L:328:LEU:O    | 1:L:332:ILE:HG13  | 2.14                     | 0.47              |
| 1:A:304:GLN:HB2  | 1:A:567:GLU:OE1   | 2.13                     | 0.47              |
| 1:C:140:VAL:HG23 | 1:C:240:ALA:HB2   | 1.97                     | 0.47              |
| 1:C:849:SER:OG   | 1:C:875:LYS:HD2   | 2.14                     | 0.47              |
| 1:E:140:VAL:HG23 | 1:E:240:ALA:HB2   | 1.97                     | 0.47              |
| 1:E:735:SER:HB2  | 1:E:764:HIS:HB3   | 1.96                     | 0.47              |
| 1:F:136:TYR:OH   | 1:F:275:CYS:SG    | 2.55                     | 0.47              |
| 1:F:216:HIS:ND1  | 1:F:341:SER:OG    | 2.29                     | 0.47              |
| 1:G:167:LEU:HD22 | 1:G:368:GLY:HA2   | 1.95                     | 0.47              |
| 1:G:251:TYR:HB2  | 1:G:293:ILE:HG12  | 1.95                     | 0.47              |
| 1:H:251:TYR:HB2  | 1:H:293:ILE:HG12  | 1.95                     | 0.47              |
| 1:A:291:SER:H    | 1:A:339:LYS:HZ2   | 1.60                     | 0.47              |
| 1:B:224:ALA:HB2  | 1:B:347:ARG:HH21  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:300:PHE:CD1  | 1:E:303:LEU:HD12  | 2.50                     | 0.47              |
| 1:E:330:SER:HA   | 1:E:335:LYS:NZ    | 2.30                     | 0.47              |
| 1:F:215:VAL:HG12 | 1:F:362:ARG:NH2   | 2.29                     | 0.47              |
| 1:F:849:SER:OG   | 1:F:875:LYS:HD2   | 2.15                     | 0.47              |
| 1:G:291:SER:H    | 1:G:339:LYS:HZ2   | 1.60                     | 0.47              |
| 1:L:563:TYR:CE1  | 1:L:572:ILE:HG12  | 2.48                     | 0.47              |
| 1:C:251:TYR:HB2  | 1:C:293:ILE:HG12  | 1.96                     | 0.47              |
| 1:D:900:ALA:O    | 1:D:904:VAL:HG23  | 2.14                     | 0.47              |
| 1:E:224:ALA:HB2  | 1:E:347:ARG:HH21  | 1.79                     | 0.47              |
| 1:F:902:THR:OG1  | 1:F:928:LEU:O     | 2.29                     | 0.47              |
| 1:H:392:PHE:O    | 1:H:396:GLN:NE2   | 2.46                     | 0.47              |
| 1:K:300:PHE:CD1  | 1:K:303:LEU:HD12  | 2.50                     | 0.47              |
| 1:A:632:LEU:HD12 | 1:A:641:VAL:HG22  | 1.97                     | 0.47              |
| 1:B:392:PHE:O    | 1:B:396:GLN:NE2   | 2.46                     | 0.47              |
| 1:B:579:PHE:CE1  | 1:B:606:LEU:HD13  | 2.49                     | 0.47              |
| 1:B:637:GLU:O    | 1:B:641:VAL:HG23  | 2.15                     | 0.47              |
| 1:B:912:THR:OG1  | 1:B:913:HIS:ND1   | 2.34                     | 0.47              |
| 1:C:942:MET:SD   | 1:C:943:LEU:N     | 2.87                     | 0.47              |
| 1:F:917:ARG:HH22 | 1:I:1030:GLU:HG2  | 1.79                     | 0.47              |
| 1:F:942:MET:SD   | 1:F:943:LEU:N     | 2.87                     | 0.47              |
| 1:G:632:LEU:HD12 | 1:G:641:VAL:HG22  | 1.97                     | 0.47              |
| 1:H:735:SER:HB2  | 1:H:764:HIS:HB3   | 1.95                     | 0.47              |
| 1:I:140:VAL:HG23 | 1:I:240:ALA:HB2   | 1.97                     | 0.47              |
| 1:L:136:TYR:OH   | 1:L:275:CYS:SG    | 2.55                     | 0.47              |
| 1:L:797:LEU:HD21 | 1:L:800:LEU:HD12  | 1.95                     | 0.47              |
| 1:A:398:ASN:ND2  | 1:A:432:SER:O     | 2.46                     | 0.47              |
| 1:B:140:VAL:HG23 | 1:B:240:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:735:SER:HB2  | 1:B:764:HIS:HB3   | 1.95                     | 0.47              |
| 1:D:413:ILE:HD11 | 1:D:521:PHE:HZ    | 1.80                     | 0.47              |
| 1:D:637:GLU:O    | 1:D:641:VAL:HG23  | 2.14                     | 0.47              |
| 1:D:923:ASP:OD1  | 1:D:924:THR:N     | 2.48                     | 0.47              |
| 1:D:990:LEU:HD22 | 1:D:1025:LEU:HD11 | 1.96                     | 0.47              |
| 1:E:923:ASP:HB2  | 1:E:954:SER:HB2   | 1.97                     | 0.47              |
| 1:F:629:PHE:CE1  | 1:F:645:MET:HE3   | 2.50                     | 0.47              |
| 1:G:398:ASN:ND2  | 1:G:432:SER:O     | 2.46                     | 0.47              |
| 1:H:200:LYS:HB2  | 1:H:203:LEU:HG    | 1.96                     | 0.47              |
| 1:I:328:LEU:O    | 1:I:332:ILE:HG13  | 2.14                     | 0.47              |
| 1:I:355:GLN:HA   | 1:I:358:LEU:HD12  | 1.96                     | 0.47              |
| 1:I:942:MET:SD   | 1:I:943:LEU:N     | 2.87                     | 0.47              |
| 1:J:413:ILE:HD11 | 1:J:521:PHE:HZ    | 1.80                     | 0.47              |
| 1:J:637:GLU:O    | 1:J:641:VAL:HG23  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:900:ALA:O    | 1:J:904:VAL:HG23  | 2.14                     | 0.47              |
| 1:J:923:ASP:OD1  | 1:J:924:THR:N     | 2.48                     | 0.47              |
| 1:K:655:LEU:HG   | 1:K:660:ASP:HB3   | 1.97                     | 0.47              |
| 1:L:629:PHE:CE1  | 1:L:645:MET:HE3   | 2.50                     | 0.47              |
| 1:L:942:MET:SD   | 1:L:943:LEU:N     | 2.87                     | 0.47              |
| 1:E:355:GLN:HA   | 1:E:358:LEU:HD12  | 1.97                     | 0.47              |
| 1:E:655:LEU:HG   | 1:E:660:ASP:HB3   | 1.97                     | 0.47              |
| 1:H:582:VAL:HB   | 1:H:603:ARG:HG2   | 1.96                     | 0.47              |
| 1:H:637:GLU:O    | 1:H:641:VAL:HG23  | 2.15                     | 0.47              |
| 1:J:990:LEU:HD22 | 1:J:1025:LEU:HD11 | 1.96                     | 0.47              |
| 1:K:230:ILE:HG21 | 2:K:1501:ADP:C5   | 2.50                     | 0.47              |
| 1:K:355:GLN:HA   | 1:K:358:LEU:HD12  | 1.97                     | 0.47              |
| 1:L:519:MET:SD   | 1:L:519:MET:N     | 2.86                     | 0.47              |
| 1:A:809:ASP:OD1  | 1:A:810:PHE:N     | 2.48                     | 0.47              |
| 1:C:328:LEU:O    | 1:C:332:ILE:HG13  | 2.15                     | 0.47              |
| 1:D:167:LEU:HD22 | 1:D:368:GLY:HA2   | 1.97                     | 0.47              |
| 1:D:580:GLY:O    | 1:D:586:ARG:NE    | 2.47                     | 0.47              |
| 1:G:923:ASP:OD1  | 1:G:924:THR:N     | 2.48                     | 0.47              |
| 1:I:381:TYR:HE2  | 1:I:412:TRP:HD1   | 1.63                     | 0.47              |
| 1:J:580:GLY:O    | 1:J:586:ARG:NE    | 2.47                     | 0.47              |
| 1:A:132:TYR:HA   | 1:A:135:MET:HE2   | 1.98                     | 0.47              |
| 1:A:917:ARG:HH22 | 1:H:1030:GLU:HG2  | 1.79                     | 0.47              |
| 1:A:923:ASP:OD1  | 1:A:924:THR:N     | 2.48                     | 0.47              |
| 1:B:221:GLN:HB2  | 1:B:365:GLU:HG2   | 1.97                     | 0.47              |
| 1:C:580:GLY:O    | 1:C:586:ARG:NE    | 2.47                     | 0.47              |
| 1:D:417:GLY:O    | 1:D:421:GLN:HG2   | 2.15                     | 0.47              |
| 1:D:809:ASP:OD1  | 1:D:810:PHE:N     | 2.48                     | 0.47              |
| 1:E:230:ILE:HG21 | 2:E:1501:ADP:C5   | 2.50                     | 0.47              |
| 1:F:140:VAL:HG23 | 1:F:240:ALA:HB2   | 1.97                     | 0.47              |
| 1:G:132:TYR:HA   | 1:G:135:MET:HE2   | 1.97                     | 0.47              |
| 1:J:417:GLY:O    | 1:J:421:GLN:HG2   | 2.15                     | 0.47              |
| 1:J:809:ASP:OD1  | 1:J:810:PHE:N     | 2.48                     | 0.47              |
| 1:K:330:SER:HA   | 1:K:335:LYS:NZ    | 2.30                     | 0.47              |
| 1:L:417:GLY:O    | 1:L:421:GLN:HG2   | 2.15                     | 0.47              |
| 1:B:330:SER:HA   | 1:B:335:LYS:NZ    | 2.30                     | 0.46              |
| 1:B:655:LEU:HG   | 1:B:660:ASP:HB3   | 1.97                     | 0.46              |
| 1:B:677:LEU:HB2  | 1:B:740:LEU:HD11  | 1.97                     | 0.46              |
| 1:B:755:MET:HG2  | 1:B:779:LEU:HD13  | 1.97                     | 0.46              |
| 1:C:350:ALA:HB3  | 1:C:568:LYS:HG3   | 1.96                     | 0.46              |
| 1:E:637:GLU:O    | 1:E:641:VAL:HG23  | 2.15                     | 0.46              |
| 1:F:417:GLY:O    | 1:F:421:GLN:HG2   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:1030:GLU:HG2 | 1:I:917:ARG:HH22 | 1.79                     | 0.46              |
| 1:H:140:VAL:HG23 | 1:H:240:ALA:HB2  | 1.97                     | 0.46              |
| 1:H:328:LEU:O    | 1:H:332:ILE:HG13 | 2.15                     | 0.46              |
| 1:H:742:GLU:HG2  | 1:H:771:ARG:HD2  | 1.97                     | 0.46              |
| 1:I:304:GLN:HB2  | 1:I:567:GLU:OE1  | 2.14                     | 0.46              |
| 1:I:330:SER:HA   | 1:I:335:LYS:NZ   | 2.31                     | 0.46              |
| 1:L:140:VAL:HG23 | 1:L:240:ALA:HB2  | 1.97                     | 0.46              |
| 1:L:371:GLU:HG3  | 1:L:402:PHE:HZ   | 1.80                     | 0.46              |
| 1:L:559:LEU:HA   | 1:L:571:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:330:SER:HA   | 1:A:335:LYS:NZ   | 2.30                     | 0.46              |
| 1:B:742:GLU:HG2  | 1:B:771:ARG:HD2  | 1.97                     | 0.46              |
| 1:C:304:GLN:HB2  | 1:C:567:GLU:OE1  | 2.14                     | 0.46              |
| 1:C:330:SER:HA   | 1:C:335:LYS:NZ   | 2.31                     | 0.46              |
| 1:C:381:TYR:HE2  | 1:C:412:TRP:HD1  | 1.63                     | 0.46              |
| 1:C:917:ARG:HH22 | 1:L:1030:GLU:HG2 | 1.79                     | 0.46              |
| 1:C:930:CYS:O    | 1:C:934:LEU:HG   | 2.15                     | 0.46              |
| 1:E:831:LEU:HD12 | 1:E:859:ILE:HG22 | 1.97                     | 0.46              |
| 1:F:330:SER:HA   | 1:F:335:LYS:NZ   | 2.31                     | 0.46              |
| 1:F:519:MET:SD   | 1:F:519:MET:N    | 2.86                     | 0.46              |
| 1:G:330:SER:HA   | 1:G:335:LYS:NZ   | 2.30                     | 0.46              |
| 1:H:655:LEU:HG   | 1:H:660:ASP:HB3  | 1.97                     | 0.46              |
| 1:J:973:LEU:C    | 1:J:976:ASN:HD22 | 2.24                     | 0.46              |
| 1:K:637:GLU:O    | 1:K:641:VAL:HG23 | 2.15                     | 0.46              |
| 1:L:330:SER:HA   | 1:L:335:LYS:NZ   | 2.31                     | 0.46              |
| 1:L:923:ASP:OD1  | 1:L:924:THR:N    | 2.49                     | 0.46              |
| 1:B:200:LYS:HB2  | 1:B:203:LEU:HG   | 1.96                     | 0.46              |
| 1:D:330:SER:HA   | 1:D:335:LYS:NZ   | 2.30                     | 0.46              |
| 1:D:973:LEU:C    | 1:D:976:ASN:HD22 | 2.24                     | 0.46              |
| 1:F:923:ASP:OD1  | 1:F:924:THR:N    | 2.49                     | 0.46              |
| 1:G:413:ILE:HD11 | 1:G:521:PHE:HZ   | 1.80                     | 0.46              |
| 1:G:809:ASP:OD1  | 1:G:810:PHE:N    | 2.48                     | 0.46              |
| 1:H:355:GLN:HA   | 1:H:358:LEU:HD12 | 1.97                     | 0.46              |
| 1:H:755:MET:HG2  | 1:H:779:LEU:HD13 | 1.97                     | 0.46              |
| 1:I:930:CYS:O    | 1:I:934:LEU:HG   | 2.15                     | 0.46              |
| 1:J:902:THR:OG1  | 1:J:928:LEU:O    | 2.30                     | 0.46              |
| 1:B:1030:GLU:HG2 | 1:G:917:ARG:HH22 | 1.79                     | 0.46              |
| 1:D:895:SER:HA   | 1:D:898:CYS:SG   | 2.56                     | 0.46              |
| 1:F:300:PHE:CD1  | 1:F:303:LEU:HD12 | 2.50                     | 0.46              |
| 1:G:930:CYS:HA   | 1:G:933:LEU:HB2  | 1.96                     | 0.46              |
| 1:H:677:LEU:HB2  | 1:H:740:LEU:HD11 | 1.97                     | 0.46              |
| 1:J:330:SER:HA   | 1:J:335:LYS:NZ   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:895:SER:HA   | 1:J:898:CYS:SG   | 2.56                     | 0.46              |
| 1:K:831:LEU:HD12 | 1:K:859:ILE:HG22 | 1.98                     | 0.46              |
| 1:L:300:PHE:CD1  | 1:L:303:LEU:HD12 | 2.50                     | 0.46              |
| 1:A:413:ILE:HD11 | 1:A:521:PHE:HZ   | 1.80                     | 0.46              |
| 1:A:930:CYS:HA   | 1:A:933:LEU:HB2  | 1.96                     | 0.46              |
| 1:A:930:CYS:O    | 1:A:934:LEU:HG   | 2.16                     | 0.46              |
| 1:B:355:GLN:HA   | 1:B:358:LEU:HD12 | 1.97                     | 0.46              |
| 1:C:757:VAL:HA   | 1:C:760:GLU:CD   | 2.41                     | 0.46              |
| 1:E:742:GLU:HG2  | 1:E:771:ARG:HD2  | 1.97                     | 0.46              |
| 1:F:502:ASN:HB2  | 1:F:513:PHE:HB2  | 1.98                     | 0.46              |
| 1:F:559:LEU:HA   | 1:F:571:LEU:HD23 | 1.98                     | 0.46              |
| 1:G:930:CYS:O    | 1:G:934:LEU:HG   | 2.16                     | 0.46              |
| 1:I:613:LYS:HE3  | 1:I:622:GLN:HB2  | 1.97                     | 0.46              |
| 1:J:519:MET:SD   | 1:J:519:MET:N    | 2.88                     | 0.46              |
| 1:L:381:TYR:HE2  | 1:L:412:TRP:HD1  | 1.64                     | 0.46              |
| 1:C:613:LYS:HE3  | 1:C:622:GLN:HB2  | 1.97                     | 0.46              |
| 1:D:519:MET:SD   | 1:D:519:MET:N    | 2.88                     | 0.46              |
| 1:F:381:TYR:HE2  | 1:F:412:TRP:HD1  | 1.64                     | 0.46              |
| 1:I:757:VAL:HA   | 1:I:760:GLU:CD   | 2.41                     | 0.46              |
| 1:I:923:ASP:OD1  | 1:I:924:THR:N    | 2.49                     | 0.46              |
| 1:K:742:GLU:HG2  | 1:K:771:ARG:HD2  | 1.97                     | 0.46              |
| 1:L:873:CYS:O    | 1:L:877:LYS:HG3  | 2.16                     | 0.46              |
| 1:A:979:GLY:O    | 1:A:983:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:349:VAL:HB   | 1:C:568:LYS:HA   | 1.98                     | 0.46              |
| 1:D:930:CYS:O    | 1:D:934:LEU:HG   | 2.16                     | 0.46              |
| 1:F:304:GLN:HB2  | 1:F:567:GLU:OE1  | 2.15                     | 0.46              |
| 1:F:873:CYS:O    | 1:F:877:LYS:HG3  | 2.16                     | 0.46              |
| 1:G:979:GLY:O    | 1:G:983:VAL:HG23 | 2.16                     | 0.46              |
| 1:I:742:GLU:HG2  | 1:I:771:ARG:HD2  | 1.98                     | 0.46              |
| 1:I:861:GLU:N    | 1:I:889:VAL:O    | 2.37                     | 0.46              |
| 1:J:930:CYS:O    | 1:J:934:LEU:HG   | 2.16                     | 0.46              |
| 1:K:137:ARG:HH21 | 1:K:239:TRP:NE1  | 2.14                     | 0.46              |
| 1:K:923:ASP:OD1  | 1:K:924:THR:N    | 2.49                     | 0.46              |
| 1:K:974:GLY:O    | 1:K:976:ASN:ND2  | 2.48                     | 0.46              |
| 1:L:502:ASN:HB2  | 1:L:513:PHE:HB2  | 1.98                     | 0.46              |
| 1:A:502:ASN:HB2  | 1:A:513:PHE:HB2  | 1.98                     | 0.46              |
| 1:C:859:ILE:O    | 1:C:862:ASN:ND2  | 2.49                     | 0.46              |
| 1:C:923:ASP:OD1  | 1:C:924:THR:N    | 2.49                     | 0.46              |
| 1:F:923:ASP:HB2  | 1:F:954:SER:HB2  | 1.97                     | 0.46              |
| 1:F:930:CYS:O    | 1:F:934:LEU:HG   | 2.15                     | 0.46              |
| 1:I:300:PHE:CD1  | 1:I:303:LEU:HD12 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:757:VAL:HA   | 1:L:760:GLU:CD   | 2.41                     | 0.46              |
| 1:C:861:GLU:N    | 1:C:889:VAL:O    | 2.37                     | 0.46              |
| 1:C:873:CYS:O    | 1:C:877:LYS:HG3  | 2.16                     | 0.46              |
| 1:E:137:ARG:HH21 | 1:E:239:TRP:NE1  | 2.14                     | 0.46              |
| 1:F:757:VAL:HA   | 1:F:760:GLU:CD   | 2.41                     | 0.46              |
| 1:F:861:GLU:N    | 1:F:889:VAL:O    | 2.37                     | 0.46              |
| 1:G:502:ASN:HB2  | 1:G:513:PHE:HB2  | 1.98                     | 0.46              |
| 1:I:297:MET:HE2  | 1:I:342:LEU:HD22 | 1.98                     | 0.46              |
| 1:I:1010:GLU:HG3 | 1:I:1013:ARG:NH2 | 2.27                     | 0.46              |
| 1:L:861:GLU:N    | 1:L:889:VAL:O    | 2.37                     | 0.46              |
| 1:A:895:SER:HA   | 1:A:898:CYS:SG   | 2.56                     | 0.46              |
| 1:B:630:TYR:OH   | 1:B:660:ASP:OD1  | 2.23                     | 0.46              |
| 1:C:300:PHE:CD1  | 1:C:303:LEU:HD12 | 2.50                     | 0.46              |
| 1:C:371:GLU:HG3  | 1:C:402:PHE:HZ   | 1.81                     | 0.46              |
| 1:C:895:SER:HA   | 1:C:898:CYS:SG   | 2.56                     | 0.46              |
| 1:C:987:CYS:O    | 1:C:991:LYS:HG2  | 2.16                     | 0.46              |
| 1:E:930:CYS:O    | 1:E:934:LEU:HG   | 2.16                     | 0.46              |
| 1:G:417:GLY:O    | 1:G:421:GLN:HG2  | 2.15                     | 0.46              |
| 1:G:895:SER:HA   | 1:G:898:CYS:SG   | 2.56                     | 0.46              |
| 1:I:895:SER:HA   | 1:I:898:CYS:SG   | 2.56                     | 0.46              |
| 1:J:987:CYS:O    | 1:J:991:LYS:HG2  | 2.16                     | 0.46              |
| 1:L:304:GLN:HB2  | 1:L:567:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:167:LEU:HD22 | 1:A:368:GLY:HA2  | 1.97                     | 0.45              |
| 1:A:417:GLY:O    | 1:A:421:GLN:HG2  | 2.15                     | 0.45              |
| 1:A:563:TYR:CE1  | 1:A:572:ILE:HG12 | 2.51                     | 0.45              |
| 1:B:137:ARG:HH21 | 1:B:239:TRP:NE1  | 2.14                     | 0.45              |
| 1:B:328:LEU:O    | 1:B:332:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:328:LEU:O    | 1:D:332:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:987:CYS:O    | 1:D:991:LYS:HG2  | 2.17                     | 0.45              |
| 1:G:861:GLU:N    | 1:G:889:VAL:O    | 2.36                     | 0.45              |
| 1:I:320:LYS:HG3  | 1:I:322:VAL:HG23 | 1.98                     | 0.45              |
| 1:I:859:ILE:O    | 1:I:862:ASN:ND2  | 2.49                     | 0.45              |
| 1:I:873:CYS:O    | 1:I:877:LYS:HG3  | 2.16                     | 0.45              |
| 1:I:979:GLY:O    | 1:I:983:VAL:HG23 | 2.17                     | 0.45              |
| 1:J:328:LEU:O    | 1:J:332:ILE:HG13 | 2.16                     | 0.45              |
| 1:K:987:CYS:O    | 1:K:991:LYS:HG2  | 2.16                     | 0.45              |
| 1:A:861:GLU:N    | 1:A:889:VAL:O    | 2.36                     | 0.45              |
| 1:B:230:ILE:HG21 | 2:B:1501:ADP:C5  | 2.50                     | 0.45              |
| 1:C:320:LYS:HG3  | 1:C:322:VAL:HG23 | 1.98                     | 0.45              |
| 1:C:355:GLN:HA   | 1:C:358:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:979:GLY:O    | 1:C:983:VAL:HG23 | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:391:ALA:O    | 1:E:395:ILE:HG12 | 2.16                     | 0.45              |
| 1:F:895:SER:HA   | 1:F:898:CYS:SG   | 2.56                     | 0.45              |
| 1:G:563:TYR:CE1  | 1:G:572:ILE:HG12 | 2.51                     | 0.45              |
| 1:H:378:PHE:HB2  | 1:H:392:PHE:CE1  | 2.51                     | 0.45              |
| 1:H:417:GLY:O    | 1:H:421:GLN:HG2  | 2.16                     | 0.45              |
| 1:J:343:LEU:HD23 | 1:J:343:LEU:HA   | 1.86                     | 0.45              |
| 1:J:930:CYS:HA   | 1:J:933:LEU:HB2  | 1.97                     | 0.45              |
| 1:K:391:ALA:O    | 1:K:395:ILE:HG12 | 2.16                     | 0.45              |
| 1:L:370:SER:OG   | 1:L:373:LYS:HG2  | 2.16                     | 0.45              |
| 1:C:756:ARG:CZ   | 1:K:813:ARG:HH21 | 2.29                     | 0.45              |
| 1:C:1010:GLU:HG3 | 1:C:1013:ARG:NH2 | 2.27                     | 0.45              |
| 1:D:132:TYR:HA   | 1:D:135:MET:HE2  | 1.97                     | 0.45              |
| 1:D:930:CYS:HA   | 1:D:933:LEU:HB2  | 1.97                     | 0.45              |
| 1:E:417:GLY:O    | 1:E:421:GLN:HG2  | 2.17                     | 0.45              |
| 1:E:813:ARG:HH21 | 1:I:756:ARG:CZ   | 2.29                     | 0.45              |
| 1:E:987:CYS:O    | 1:E:991:LYS:HG2  | 2.16                     | 0.45              |
| 1:F:297:MET:HE2  | 1:F:342:LEU:HD22 | 1.97                     | 0.45              |
| 1:H:137:ARG:HH21 | 1:H:239:TRP:NE1  | 2.14                     | 0.45              |
| 1:I:987:CYS:O    | 1:I:991:LYS:HG2  | 2.16                     | 0.45              |
| 1:J:632:LEU:HD12 | 1:J:641:VAL:HG22 | 1.97                     | 0.45              |
| 1:A:328:LEU:O    | 1:A:332:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:343:LEU:HD23 | 1:D:343:LEU:HA   | 1.86                     | 0.45              |
| 1:D:632:LEU:HD12 | 1:D:641:VAL:HG22 | 1.97                     | 0.45              |
| 1:F:767:CYS:O    | 1:F:796:LYS:NZ   | 2.39                     | 0.45              |
| 1:G:902:THR:OG1  | 1:G:928:LEU:O    | 2.30                     | 0.45              |
| 1:H:930:CYS:O    | 1:H:934:LEU:HG   | 2.16                     | 0.45              |
| 1:J:132:TYR:HA   | 1:J:135:MET:HE2  | 1.98                     | 0.45              |
| 1:J:563:TYR:CE1  | 1:J:572:ILE:HG12 | 2.51                     | 0.45              |
| 1:K:417:GLY:O    | 1:K:421:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:519:MET:SD   | 1:A:519:MET:N    | 2.88                     | 0.45              |
| 1:A:902:THR:OG1  | 1:A:928:LEU:O    | 2.30                     | 0.45              |
| 1:B:930:CYS:O    | 1:B:934:LEU:HG   | 2.16                     | 0.45              |
| 1:C:735:SER:HB2  | 1:C:764:HIS:HB3  | 1.97                     | 0.45              |
| 1:D:224:ALA:HB2  | 1:D:347:ARG:HH21 | 1.82                     | 0.45              |
| 1:D:563:TYR:CE1  | 1:D:572:ILE:HG12 | 2.51                     | 0.45              |
| 1:E:358:LEU:HD13 | 1:E:361:PRO:HG3  | 1.97                     | 0.45              |
| 1:E:519:MET:SD   | 1:E:519:MET:N    | 2.88                     | 0.45              |
| 1:F:613:LYS:HE3  | 1:F:622:GLN:HB2  | 1.97                     | 0.45              |
| 1:F:979:GLY:O    | 1:F:983:VAL:HG23 | 2.17                     | 0.45              |
| 1:F:988:GLU:O    | 1:F:992:GLN:NE2  | 2.50                     | 0.45              |
| 1:G:137:ARG:HH21 | 1:G:239:TRP:NE1  | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:300:PHE:CD1  | 1:G:303:LEU:HD12 | 2.51                     | 0.45              |
| 1:G:328:LEU:O    | 1:G:332:ILE:HG13 | 2.16                     | 0.45              |
| 1:G:755:MET:HG2  | 1:G:779:LEU:HD13 | 1.99                     | 0.45              |
| 1:I:371:GLU:HG3  | 1:I:402:PHE:HZ   | 1.81                     | 0.45              |
| 1:I:912:THR:OG1  | 1:I:913:HIS:ND1  | 2.33                     | 0.45              |
| 1:J:216:HIS:ND1  | 1:J:341:SER:OG   | 2.32                     | 0.45              |
| 1:L:895:SER:HA   | 1:L:898:CYS:SG   | 2.57                     | 0.45              |
| 1:A:137:ARG:HH21 | 1:A:239:TRP:NE1  | 2.15                     | 0.45              |
| 1:A:300:PHE:CD1  | 1:A:303:LEU:HD12 | 2.51                     | 0.45              |
| 1:A:973:LEU:C    | 1:A:976:ASN:HD22 | 2.24                     | 0.45              |
| 1:B:979:GLY:O    | 1:B:983:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:291:SER:H    | 1:C:339:LYS:HZ2  | 1.63                     | 0.45              |
| 1:C:417:GLY:O    | 1:C:421:GLN:HG2  | 2.15                     | 0.45              |
| 1:C:607:LEU:HD12 | 1:C:640:PHE:CE1  | 2.52                     | 0.45              |
| 1:C:755:MET:HG2  | 1:C:779:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:912:THR:OG1  | 1:C:913:HIS:ND1  | 2.33                     | 0.45              |
| 1:D:137:ARG:HA   | 1:D:140:VAL:HG22 | 1.99                     | 0.45              |
| 1:D:625:GLN:HG2  | 1:D:629:PHE:CE2  | 2.52                     | 0.45              |
| 1:E:943:LEU:HG   | 1:E:945:LEU:CD2  | 2.47                     | 0.45              |
| 1:F:409:LEU:HD13 | 2:F:1501:ADP:H4' | 1.99                     | 0.45              |
| 1:G:973:LEU:C    | 1:G:976:ASN:HD22 | 2.24                     | 0.45              |
| 1:I:251:TYR:HB2  | 1:I:293:ILE:HG12 | 1.98                     | 0.45              |
| 1:I:349:VAL:HB   | 1:I:568:LYS:HA   | 1.99                     | 0.45              |
| 1:I:417:GLY:O    | 1:I:421:GLN:HG2  | 2.15                     | 0.45              |
| 1:I:735:SER:HB2  | 1:I:764:HIS:HB3  | 1.97                     | 0.45              |
| 1:I:755:MET:HG2  | 1:I:779:LEU:HD13 | 1.99                     | 0.45              |
| 1:J:300:PHE:CD1  | 1:J:303:LEU:HD12 | 2.51                     | 0.45              |
| 1:J:409:LEU:HD13 | 2:J:1501:ADP:H4' | 1.99                     | 0.45              |
| 1:L:251:TYR:HB2  | 1:L:293:ILE:HG12 | 1.97                     | 0.45              |
| 1:L:297:MET:HE2  | 1:L:342:LEU:HD22 | 1.97                     | 0.45              |
| 1:L:330:SER:HA   | 1:L:335:LYS:HZ1  | 1.81                     | 0.45              |
| 1:L:355:GLN:HA   | 1:L:358:LEU:HD12 | 1.98                     | 0.45              |
| 1:L:613:LYS:HE3  | 1:L:622:GLN:HB2  | 1.97                     | 0.45              |
| 1:L:742:GLU:HG2  | 1:L:771:ARG:HD2  | 1.98                     | 0.45              |
| 1:L:979:GLY:O    | 1:L:983:VAL:HG23 | 2.17                     | 0.45              |
| 1:L:988:GLU:O    | 1:L:992:GLN:NE2  | 2.50                     | 0.45              |
| 1:B:923:ASP:HB2  | 1:B:954:SER:HB2  | 1.98                     | 0.45              |
| 1:C:559:LEU:HA   | 1:C:571:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:742:GLU:HG2  | 1:C:771:ARG:HD2  | 1.99                     | 0.45              |
| 1:D:216:HIS:ND1  | 1:D:341:SER:OG   | 2.32                     | 0.45              |
| 1:D:409:LEU:HD13 | 2:D:1501:ADP:H4' | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:502:ASN:HB2  | 1:D:513:PHE:HB2   | 1.98                     | 0.45              |
| 1:F:742:GLU:HG2  | 1:F:771:ARG:HD2   | 1.98                     | 0.45              |
| 1:G:466:CYS:HB3  | 1:G:529:TYR:CB    | 2.46                     | 0.45              |
| 1:H:855:THR:OG1  | 1:H:856:ARG:N     | 2.50                     | 0.45              |
| 1:H:943:LEU:HG   | 1:H:945:LEU:CD2   | 2.47                     | 0.45              |
| 1:I:668:ILE:HA   | 1:I:671:CYS:SG    | 2.56                     | 0.45              |
| 1:J:137:ARG:HA   | 1:J:140:VAL:HG22  | 1.99                     | 0.45              |
| 1:J:625:GLN:HG2  | 1:J:629:PHE:CE2   | 2.52                     | 0.45              |
| 1:K:358:LEU:HD13 | 1:K:361:PRO:HG3   | 1.97                     | 0.45              |
| 1:L:349:VAL:HB   | 1:L:568:LYS:HA    | 1.99                     | 0.45              |
| 1:L:987:CYS:O    | 1:L:991:LYS:HG2   | 2.16                     | 0.45              |
| 1:A:466:CYS:HB3  | 1:A:529:TYR:CB    | 2.46                     | 0.45              |
| 1:A:646:ASP:HB3  | 1:A:673:ARG:NH1   | 2.32                     | 0.45              |
| 1:B:417:GLY:O    | 1:B:421:GLN:HG2   | 2.17                     | 0.45              |
| 1:B:831:LEU:HD12 | 1:B:859:ILE:HG22  | 1.97                     | 0.45              |
| 1:B:855:THR:OG1  | 1:B:856:ARG:N     | 2.50                     | 0.45              |
| 1:B:943:LEU:HG   | 1:B:945:LEU:CD2   | 2.47                     | 0.45              |
| 1:D:300:PHE:CD1  | 1:D:303:LEU:HD12  | 2.51                     | 0.45              |
| 1:F:990:LEU:HD22 | 1:F:1025:LEU:HD11 | 1.99                     | 0.45              |
| 1:G:409:LEU:HD13 | 2:G:1501:ADP:H4'  | 1.99                     | 0.45              |
| 1:G:519:MET:SD   | 1:G:519:MET:N     | 2.88                     | 0.45              |
| 1:G:646:ASP:HB3  | 1:G:673:ARG:NH1   | 2.32                     | 0.45              |
| 1:G:1002:LEU:C   | 1:G:1005:MET:HE3  | 2.42                     | 0.45              |
| 1:H:358:LEU:HD13 | 1:H:361:PRO:HG3   | 1.97                     | 0.45              |
| 1:H:831:LEU:HD12 | 1:H:859:ILE:HG22  | 1.97                     | 0.45              |
| 1:I:370:SER:OG   | 1:I:373:LYS:HG2   | 2.17                     | 0.45              |
| 1:J:207:PRO:HG3  | 1:J:215:VAL:HG11  | 1.99                     | 0.45              |
| 1:J:502:ASN:HB2  | 1:J:513:PHE:HB2   | 1.98                     | 0.45              |
| 1:J:979:GLY:O    | 1:J:983:VAL:HG23  | 2.16                     | 0.45              |
| 1:K:519:MET:SD   | 1:K:519:MET:N     | 2.88                     | 0.45              |
| 1:K:755:MET:HG2  | 1:K:779:LEU:HD13  | 1.97                     | 0.45              |
| 1:K:943:LEU:HG   | 1:K:945:LEU:CD2   | 2.47                     | 0.45              |
| 1:L:409:LEU:HD13 | 2:L:1501:ADP:H4'  | 1.99                     | 0.45              |
| 1:A:409:LEU:HD13 | 2:A:1501:ADP:H4'  | 1.99                     | 0.45              |
| 1:B:358:LEU:HD13 | 1:B:361:PRO:HG3   | 1.97                     | 0.45              |
| 1:B:580:GLY:O    | 1:B:586:ARG:NE    | 2.49                     | 0.45              |
| 1:C:370:SER:OG   | 1:C:373:LYS:HG2   | 2.17                     | 0.45              |
| 1:C:409:LEU:HD13 | 2:C:1501:ADP:H4'  | 1.99                     | 0.45              |
| 1:D:207:PRO:HG3  | 1:D:215:VAL:HG11  | 1.99                     | 0.45              |
| 1:D:355:GLN:HA   | 1:D:358:LEU:HD12  | 1.99                     | 0.45              |
| 1:D:979:GLY:O    | 1:D:983:VAL:HG23  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:755:MET:HG2  | 1:E:779:LEU:HD13  | 1.98                     | 0.45              |
| 1:F:355:GLN:HA   | 1:F:358:LEU:HD12  | 1.98                     | 0.45              |
| 1:F:859:ILE:O    | 1:F:862:ASN:ND2   | 2.49                     | 0.45              |
| 1:H:979:GLY:O    | 1:H:983:VAL:HG23  | 2.17                     | 0.45              |
| 1:J:224:ALA:HB2  | 1:J:347:ARG:HH21  | 1.82                     | 0.45              |
| 1:K:930:CYS:O    | 1:K:934:LEU:HG    | 2.17                     | 0.45              |
| 1:L:735:SER:HB2  | 1:L:764:HIS:HB3   | 1.97                     | 0.45              |
| 1:A:224:ALA:HB2  | 1:A:347:ARG:HH21  | 1.82                     | 0.45              |
| 1:A:1002:LEU:C   | 1:A:1005:MET:HE3  | 2.42                     | 0.45              |
| 1:C:990:LEU:HD22 | 1:C:1025:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:300:PHE:CE2  | 1:D:354:LEU:HD22  | 2.52                     | 0.45              |
| 1:F:370:SER:OG   | 1:F:373:LYS:HG2   | 2.17                     | 0.45              |
| 1:F:987:CYS:O    | 1:F:991:LYS:HG2   | 2.16                     | 0.45              |
| 1:I:409:LEU:HD13 | 2:I:1501:ADP:H4'  | 1.99                     | 0.45              |
| 1:J:646:ASP:HB3  | 1:J:673:ARG:NH1   | 2.32                     | 0.45              |
| 1:A:137:ARG:HA   | 1:A:140:VAL:HG22  | 1.99                     | 0.44              |
| 1:A:228:LYS:N    | 2:A:1501:ADP:O3B  | 2.51                     | 0.44              |
| 1:A:755:MET:HG2  | 1:A:779:LEU:HD13  | 1.99                     | 0.44              |
| 1:B:391:ALA:O    | 1:B:395:ILE:HG12  | 2.16                     | 0.44              |
| 1:C:988:GLU:O    | 1:C:992:GLN:NE2   | 2.50                     | 0.44              |
| 1:D:137:ARG:HH21 | 1:D:239:TRP:NE1   | 2.15                     | 0.44              |
| 1:D:230:ILE:HG21 | 2:D:1501:ADP:C5   | 2.52                     | 0.44              |
| 1:E:923:ASP:OD1  | 1:E:924:THR:N     | 2.50                     | 0.44              |
| 1:H:528:MET:HE3  | 1:H:532:LEU:HD21  | 1.98                     | 0.44              |
| 1:H:923:ASP:OD1  | 1:H:924:THR:N     | 2.50                     | 0.44              |
| 1:J:300:PHE:CE2  | 1:J:354:LEU:HD22  | 2.52                     | 0.44              |
| 1:K:855:THR:OG1  | 1:K:856:ARG:N     | 2.50                     | 0.44              |
| 1:L:859:ILE:O    | 1:L:862:ASN:ND2   | 2.50                     | 0.44              |
| 1:A:294:LEU:HD21 | 1:A:343:LEU:HD12  | 2.00                     | 0.44              |
| 1:A:300:PHE:CE2  | 1:A:354:LEU:HD22  | 2.52                     | 0.44              |
| 1:A:355:GLN:HA   | 1:A:358:LEU:HD12  | 1.99                     | 0.44              |
| 1:B:987:CYS:O    | 1:B:991:LYS:HG2   | 2.16                     | 0.44              |
| 1:D:646:ASP:HB3  | 1:D:673:ARG:NH1   | 2.32                     | 0.44              |
| 1:F:349:VAL:HB   | 1:F:568:LYS:HA    | 1.99                     | 0.44              |
| 1:G:137:ARG:HA   | 1:G:140:VAL:HG22  | 1.99                     | 0.44              |
| 1:G:228:LYS:N    | 2:G:1501:ADP:O2B  | 2.51                     | 0.44              |
| 1:G:294:LEU:HD21 | 1:G:343:LEU:HD12  | 2.00                     | 0.44              |
| 1:I:915:TYR:O    | 1:I:916:LEU:HD22  | 2.18                     | 0.44              |
| 1:J:137:ARG:HH21 | 1:J:239:TRP:NE1   | 2.15                     | 0.44              |
| 1:J:355:GLN:HA   | 1:J:358:LEU:HD12  | 1.99                     | 0.44              |
| 1:J:816:CYS:HB3  | 1:J:820:LYS:HE2   | 1.99                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:902:THR:OG1  | 1:K:928:LEU:O     | 2.31                     | 0.44              |
| 1:L:946:ASP:OD1  | 1:L:974:GLY:N     | 2.42                     | 0.44              |
| 1:L:990:LEU:HD22 | 1:L:1025:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:216:HIS:CE1  | 1:A:341:SER:HG    | 2.28                     | 0.44              |
| 1:A:370:SER:OG   | 1:A:373:LYS:HG2   | 2.17                     | 0.44              |
| 1:B:291:SER:H    | 1:B:339:LYS:HZ2   | 1.63                     | 0.44              |
| 1:B:923:ASP:OD1  | 1:B:924:THR:N     | 2.50                     | 0.44              |
| 1:C:531:LEU:O    | 1:C:598:ILE:HA    | 2.17                     | 0.44              |
| 1:D:294:LEU:HD21 | 1:D:343:LEU:HD12  | 2.00                     | 0.44              |
| 1:D:370:SER:OG   | 1:D:373:LYS:HG2   | 2.17                     | 0.44              |
| 1:D:816:CYS:HB3  | 1:D:820:LYS:HE2   | 1.99                     | 0.44              |
| 1:F:251:TYR:HB2  | 1:F:293:ILE:HG12  | 1.98                     | 0.44              |
| 1:G:297:MET:HE1  | 1:G:342:LEU:HD22  | 2.00                     | 0.44              |
| 1:G:298:ASP:OD1  | 1:G:345:THR:OG1   | 2.29                     | 0.44              |
| 1:G:300:PHE:CE2  | 1:G:354:LEU:HD22  | 2.52                     | 0.44              |
| 1:H:291:SER:H    | 1:H:339:LYS:HZ2   | 1.63                     | 0.44              |
| 1:H:391:ALA:O    | 1:H:395:ILE:HG12  | 2.16                     | 0.44              |
| 1:H:923:ASP:HB2  | 1:H:954:SER:HB2   | 1.99                     | 0.44              |
| 1:J:230:ILE:HG21 | 2:J:1501:ADP:C5   | 2.52                     | 0.44              |
| 1:J:294:LEU:HD21 | 1:J:343:LEU:HD12  | 2.00                     | 0.44              |
| 1:J:297:MET:HE1  | 1:J:342:LEU:HD22  | 2.00                     | 0.44              |
| 1:J:1002:LEU:C   | 1:J:1005:MET:HE3  | 2.42                     | 0.44              |
| 1:A:297:MET:HE1  | 1:A:342:LEU:HD22  | 2.00                     | 0.44              |
| 1:B:813:ARG:HH21 | 1:L:756:ARG:CZ    | 2.29                     | 0.44              |
| 1:C:625:GLN:HG2  | 1:C:629:PHE:CE2   | 2.52                     | 0.44              |
| 1:C:940:LEU:HD21 | 1:C:943:LEU:HD13  | 2.00                     | 0.44              |
| 1:D:1002:LEU:C   | 1:D:1005:MET:HE3  | 2.42                     | 0.44              |
| 1:E:328:LEU:O    | 1:E:332:ILE:HG13  | 2.16                     | 0.44              |
| 1:E:571:LEU:O    | 1:E:575:VAL:HG23  | 2.18                     | 0.44              |
| 1:E:974:GLY:O    | 1:E:976:ASN:ND2   | 2.50                     | 0.44              |
| 1:E:979:GLY:O    | 1:E:983:VAL:HG23  | 2.17                     | 0.44              |
| 1:F:300:PHE:CE2  | 1:F:354:LEU:HD22  | 2.52                     | 0.44              |
| 1:F:320:LYS:HG3  | 1:F:322:VAL:HG23  | 1.98                     | 0.44              |
| 1:F:930:CYS:HA   | 1:F:933:LEU:HB2   | 1.99                     | 0.44              |
| 1:G:224:ALA:HB2  | 1:G:347:ARG:HH21  | 1.82                     | 0.44              |
| 1:H:987:CYS:O    | 1:H:991:LYS:HG2   | 2.17                     | 0.44              |
| 1:K:221:GLN:HB2  | 1:K:365:GLU:HG2   | 1.99                     | 0.44              |
| 1:L:320:LYS:HG3  | 1:L:322:VAL:HG23  | 1.98                     | 0.44              |
| 1:A:298:ASP:OD1  | 1:A:345:THR:OG1   | 2.30                     | 0.44              |
| 1:A:987:CYS:O    | 1:A:991:LYS:HG2   | 2.16                     | 0.44              |
| 1:B:784:CYS:SG   | 1:B:807:LEU:HD22  | 2.57                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:297:MET:HE1   | 1:D:342:LEU:HD22  | 2.00                     | 0.44              |
| 1:E:207:PRO:HG3   | 1:E:215:VAL:HG11  | 1.99                     | 0.44              |
| 1:E:230:ILE:HG13  | 2:E:1501:ADP:C8   | 2.53                     | 0.44              |
| 1:F:755:MET:HG2   | 1:F:779:LEU:HD13  | 1.99                     | 0.44              |
| 1:G:230:ILE:HG21  | 2:G:1501:ADP:C5   | 2.52                     | 0.44              |
| 1:G:355:GLN:HA    | 1:G:358:LEU:HD12  | 1.99                     | 0.44              |
| 1:G:987:CYS:O     | 1:G:991:LYS:HG2   | 2.16                     | 0.44              |
| 1:H:221:GLN:HB2   | 1:H:365:GLU:HG2   | 2.00                     | 0.44              |
| 1:I:531:LEU:O     | 1:I:598:ILE:HA    | 2.17                     | 0.44              |
| 1:I:940:LEU:HD21  | 1:I:943:LEU:HD13  | 2.00                     | 0.44              |
| 1:K:230:ILE:HG13  | 2:K:1501:ADP:C8   | 2.53                     | 0.44              |
| 1:K:571:LEU:O     | 1:K:575:VAL:HG23  | 2.18                     | 0.44              |
| 1:K:979:GLY:O     | 1:K:983:VAL:HG23  | 2.17                     | 0.44              |
| 1:L:912:THR:OG1   | 1:L:913:HIS:ND1   | 2.33                     | 0.44              |
| 1:L:1018:LEU:HD11 | 1:L:1027:ILE:HG13 | 2.00                     | 0.44              |
| 1:A:230:ILE:HG21  | 2:A:1501:ADP:C5   | 2.52                     | 0.44              |
| 1:B:974:GLY:O     | 1:B:976:ASN:ND2   | 2.50                     | 0.44              |
| 1:C:617:LYS:HE2   | 1:L:956:TRP:CE3   | 2.51                     | 0.44              |
| 1:C:677:LEU:HB2   | 1:C:740:LEU:HD11  | 2.00                     | 0.44              |
| 1:C:915:TYR:O     | 1:C:916:LEU:HD22  | 2.18                     | 0.44              |
| 1:C:930:CYS:HA    | 1:C:933:LEU:HB2   | 1.99                     | 0.44              |
| 1:E:221:GLN:HB2   | 1:E:365:GLU:HG2   | 1.99                     | 0.44              |
| 1:F:756:ARG:CZ    | 1:H:813:ARG:HH21  | 2.30                     | 0.44              |
| 1:G:625:GLN:HG2   | 1:G:629:PHE:CE2   | 2.52                     | 0.44              |
| 1:H:300:PHE:CE2   | 1:H:354:LEU:HD22  | 2.53                     | 0.44              |
| 1:H:784:CYS:SG    | 1:H:807:LEU:HD22  | 2.57                     | 0.44              |
| 1:H:974:GLY:O     | 1:H:976:ASN:ND2   | 2.50                     | 0.44              |
| 1:I:677:LEU:HB2   | 1:I:740:LEU:HD11  | 2.00                     | 0.44              |
| 1:I:988:GLU:O     | 1:I:992:GLN:NE2   | 2.50                     | 0.44              |
| 1:I:990:LEU:HD22  | 1:I:1025:LEU:HD11 | 1.99                     | 0.44              |
| 1:K:580:GLY:O     | 1:K:586:ARG:NE    | 2.49                     | 0.44              |
| 1:L:668:ILE:HA    | 1:L:671:CYS:SG    | 2.56                     | 0.44              |
| 1:B:207:PRO:HG3   | 1:B:215:VAL:HG11  | 2.00                     | 0.44              |
| 1:B:571:LEU:O     | 1:B:575:VAL:HG23  | 2.18                     | 0.44              |
| 1:C:343:LEU:HD23  | 1:C:343:LEU:HA    | 1.86                     | 0.44              |
| 1:C:466:CYS:HB3   | 1:C:529:TYR:CB    | 2.46                     | 0.44              |
| 1:E:580:GLY:O     | 1:E:586:ARG:NE    | 2.49                     | 0.44              |
| 1:F:655:LEU:HG    | 1:F:660:ASP:HB3   | 2.00                     | 0.44              |
| 1:F:668:ILE:HA    | 1:F:671:CYS:SG    | 2.56                     | 0.44              |
| 1:G:216:HIS:ND1   | 1:G:341:SER:OG    | 2.32                     | 0.44              |
| 1:H:320:LYS:HA    | 1:H:320:LYS:HD2   | 1.84                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:291:SER:H     | 1:I:339:LYS:HZ2   | 1.64                     | 0.44              |
| 1:I:580:GLY:O     | 1:I:586:ARG:NE    | 2.50                     | 0.44              |
| 1:I:625:GLN:HG2   | 1:I:629:PHE:CE2   | 2.52                     | 0.44              |
| 1:I:655:LEU:HG    | 1:I:660:ASP:HB3   | 2.00                     | 0.44              |
| 1:J:228:LYS:N     | 2:J:1501:ADP:O2B  | 2.51                     | 0.44              |
| 1:L:300:PHE:CE2   | 1:L:354:LEU:HD22  | 2.53                     | 0.44              |
| 1:L:655:LEU:HG    | 1:L:660:ASP:HB3   | 2.00                     | 0.44              |
| 1:L:755:MET:HG2   | 1:L:779:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:625:GLN:HG2   | 1:A:629:PHE:CE2   | 2.52                     | 0.44              |
| 1:B:320:LYS:HA    | 1:B:320:LYS:HD2   | 1.84                     | 0.44              |
| 1:B:593:LYS:HA    | 1:B:593:LYS:HD3   | 1.82                     | 0.44              |
| 1:C:381:TYR:HE2   | 1:C:412:TRP:CD1   | 2.36                     | 0.44              |
| 1:C:668:ILE:HA    | 1:C:671:CYS:SG    | 2.57                     | 0.44              |
| 1:D:228:LYS:N     | 2:D:1501:ADP:O3B  | 2.51                     | 0.44              |
| 1:D:317:ASP:HB3   | 1:D:320:LYS:HB2   | 2.00                     | 0.44              |
| 1:F:531:LEU:O     | 1:F:598:ILE:HA    | 2.18                     | 0.44              |
| 1:F:912:THR:OG1   | 1:F:913:HIS:ND1   | 2.33                     | 0.44              |
| 1:I:930:CYS:HA    | 1:I:933:LEU:HB2   | 1.99                     | 0.44              |
| 1:K:328:LEU:O     | 1:K:332:ILE:HG13  | 2.16                     | 0.44              |
| 1:L:625:GLN:HG2   | 1:L:629:PHE:CE2   | 2.52                     | 0.44              |
| 1:C:137:ARG:HA    | 1:C:140:VAL:HG22  | 2.00                     | 0.44              |
| 1:C:954:SER:OG    | 1:C:957:ASN:OD1   | 2.28                     | 0.44              |
| 1:E:784:CYS:SG    | 1:E:807:LEU:HD22  | 2.57                     | 0.44              |
| 1:F:254:PHE:CZ    | 1:F:256:HIS:HB2   | 2.53                     | 0.44              |
| 1:F:1018:LEU:HD11 | 1:F:1027:ILE:HG13 | 2.00                     | 0.44              |
| 1:I:343:LEU:HD23  | 1:I:343:LEU:HA    | 1.87                     | 0.44              |
| 1:I:466:CYS:HB3   | 1:I:529:TYR:CB    | 2.46                     | 0.44              |
| 1:I:559:LEU:HA    | 1:I:571:LEU:HD23  | 1.99                     | 0.44              |
| 1:I:629:PHE:CE1   | 1:I:645:MET:HE3   | 2.50                     | 0.44              |
| 1:I:1018:LEU:HD11 | 1:I:1027:ILE:HG13 | 2.00                     | 0.44              |
| 1:J:466:CYS:HB3   | 1:J:529:TYR:CB    | 2.46                     | 0.44              |
| 1:K:784:CYS:SG    | 1:K:807:LEU:HD22  | 2.57                     | 0.44              |
| 1:L:254:PHE:CZ    | 1:L:256:HIS:HB2   | 2.53                     | 0.44              |
| 1:A:943:LEU:HG    | 1:A:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:C:655:LEU:HG    | 1:C:660:ASP:HB3   | 2.00                     | 0.43              |
| 1:D:466:CYS:HB3   | 1:D:529:TYR:CB    | 2.46                     | 0.43              |
| 1:F:580:GLY:O     | 1:F:586:ARG:NE    | 2.50                     | 0.43              |
| 1:F:625:GLN:HG2   | 1:F:629:PHE:CE2   | 2.52                     | 0.43              |
| 1:G:943:LEU:HG    | 1:G:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:H:254:PHE:CZ    | 1:H:256:HIS:HB2   | 2.53                     | 0.43              |
| 1:H:954:SER:O     | 1:H:957:ASN:HB2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:317:ASP:HB3  | 1:J:320:LYS:HB2   | 2.00                     | 0.43              |
| 1:K:973:LEU:C    | 1:K:976:ASN:HD22  | 2.26                     | 0.43              |
| 1:L:531:LEU:O    | 1:L:598:ILE:HA    | 2.18                     | 0.43              |
| 1:L:580:GLY:O    | 1:L:586:ARG:NE    | 2.50                     | 0.43              |
| 1:L:915:TYR:O    | 1:L:916:LEU:HD22  | 2.18                     | 0.43              |
| 1:D:755:MET:HG2  | 1:D:779:LEU:HD13  | 1.99                     | 0.43              |
| 1:D:915:TYR:O    | 1:D:916:LEU:HD22  | 2.19                     | 0.43              |
| 1:E:1007:LEU:HB3 | 1:E:1011:THR:HG21 | 2.01                     | 0.43              |
| 1:F:915:TYR:O    | 1:F:916:LEU:HD22  | 2.18                     | 0.43              |
| 1:I:381:TYR:HE2  | 1:I:412:TRP:CD1   | 2.36                     | 0.43              |
| 1:J:755:MET:HG2  | 1:J:779:LEU:HD13  | 1.99                     | 0.43              |
| 1:K:954:SER:OG   | 1:K:957:ASN:ND2   | 2.29                     | 0.43              |
| 1:K:1007:LEU:HB3 | 1:K:1011:THR:HG21 | 2.01                     | 0.43              |
| 1:K:1009:ARG:HA  | 1:K:1009:ARG:HD2  | 1.77                     | 0.43              |
| 1:L:381:TYR:HE2  | 1:L:412:TRP:CD1   | 2.36                     | 0.43              |
| 1:B:228:LYS:N    | 2:B:1501:ADP:O3B  | 2.51                     | 0.43              |
| 1:K:347:ARG:O    | 1:K:568:LYS:HE3   | 2.19                     | 0.43              |
| 1:K:466:CYS:HB3  | 1:K:529:TYR:CB    | 2.47                     | 0.43              |
| 1:A:816:CYS:HB3  | 1:A:820:LYS:HE2   | 1.99                     | 0.43              |
| 1:A:859:ILE:O    | 1:A:862:ASN:ND2   | 2.51                     | 0.43              |
| 1:B:230:ILE:HG13 | 2:B:1501:ADP:C8   | 2.53                     | 0.43              |
| 1:B:300:PHE:CE2  | 1:B:354:LEU:HD22  | 2.53                     | 0.43              |
| 1:B:940:LEU:HD21 | 1:B:943:LEU:HB2   | 1.99                     | 0.43              |
| 1:D:859:ILE:O    | 1:D:862:ASN:ND2   | 2.51                     | 0.43              |
| 1:E:300:PHE:CE2  | 1:E:354:LEU:HD22  | 2.54                     | 0.43              |
| 1:F:223:ALA:HB1  | 3:F:1502:7YN:N13  | 2.33                     | 0.43              |
| 1:F:943:LEU:HG   | 1:F:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:F:972:ASN:O    | 1:F:973:LEU:HD22  | 2.18                     | 0.43              |
| 1:G:207:PRO:HG3  | 1:G:215:VAL:HG11  | 1.99                     | 0.43              |
| 1:G:370:SER:OG   | 1:G:373:LYS:HG2   | 2.18                     | 0.43              |
| 1:G:859:ILE:O    | 1:G:862:ASN:ND2   | 2.51                     | 0.43              |
| 1:H:223:ALA:HB1  | 3:H:1502:7YN:N13  | 2.33                     | 0.43              |
| 1:J:370:SER:OG   | 1:J:373:LYS:HG2   | 2.18                     | 0.43              |
| 1:J:859:ILE:O    | 1:J:862:ASN:ND2   | 2.51                     | 0.43              |
| 1:K:223:ALA:HB1  | 3:K:1502:7YN:N13  | 2.33                     | 0.43              |
| 1:K:294:LEU:HD21 | 1:K:343:LEU:HD12  | 2.01                     | 0.43              |
| 1:K:300:PHE:CE2  | 1:K:354:LEU:HD22  | 2.54                     | 0.43              |
| 1:L:1016:GLU:O   | 1:L:1020:GLU:HG2  | 2.18                     | 0.43              |
| 1:A:207:PRO:HG3  | 1:A:215:VAL:HG11  | 1.99                     | 0.43              |
| 1:A:320:LYS:HA   | 1:A:320:LYS:HD2   | 1.83                     | 0.43              |
| 1:B:1016:GLU:O   | 1:B:1020:GLU:HG2  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:629:PHE:CE1   | 1:C:645:MET:HE3   | 2.51                     | 0.43              |
| 1:C:1018:LEU:HD11 | 1:C:1027:ILE:HG13 | 2.00                     | 0.43              |
| 1:E:228:LYS:N     | 2:E:1501:ADP:O3B  | 2.51                     | 0.43              |
| 1:E:466:CYS:HB3   | 1:E:529:TYR:CB    | 2.47                     | 0.43              |
| 1:E:786:ASP:O     | 1:E:789:SER:OG    | 2.32                     | 0.43              |
| 1:F:230:ILE:HG13  | 2:F:1501:ADP:C8   | 2.53                     | 0.43              |
| 1:F:381:TYR:HE2   | 1:F:412:TRP:CD1   | 2.37                     | 0.43              |
| 1:F:735:SER:HB2   | 1:F:764:HIS:HB3   | 1.99                     | 0.43              |
| 1:G:816:CYS:HB3   | 1:G:820:LYS:HE2   | 1.99                     | 0.43              |
| 1:I:137:ARG:HA    | 1:I:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:I:855:THR:OG1   | 1:I:856:ARG:N     | 2.52                     | 0.43              |
| 1:I:954:SER:OG    | 1:I:957:ASN:OD1   | 2.28                     | 0.43              |
| 1:K:254:PHE:CZ    | 1:K:256:HIS:HB2   | 2.53                     | 0.43              |
| 1:L:940:LEU:HD21  | 1:L:943:LEU:HD13  | 2.00                     | 0.43              |
| 1:L:972:ASN:O     | 1:L:973:LEU:HD22  | 2.18                     | 0.43              |
| 1:L:1007:LEU:HB3  | 1:L:1011:THR:HG21 | 2.00                     | 0.43              |
| 1:B:954:SER:O     | 1:B:957:ASN:HB2   | 2.18                     | 0.43              |
| 1:C:230:ILE:HG13  | 2:C:1501:ADP:C8   | 2.54                     | 0.43              |
| 1:C:855:THR:OG1   | 1:C:856:ARG:N     | 2.52                     | 0.43              |
| 1:E:223:ALA:HB1   | 3:E:1502:7YN:N13  | 2.33                     | 0.43              |
| 1:F:855:THR:OG1   | 1:F:856:ARG:N     | 2.52                     | 0.43              |
| 1:F:1016:GLU:O    | 1:F:1020:GLU:HG2  | 2.18                     | 0.43              |
| 1:I:740:LEU:HD12  | 1:I:740:LEU:HA    | 1.89                     | 0.43              |
| 1:I:767:CYS:O     | 1:I:796:LYS:NZ    | 2.39                     | 0.43              |
| 1:J:294:LEU:HA    | 1:J:341:SER:HB2   | 2.01                     | 0.43              |
| 1:J:799:GLU:CB    | 1:J:828:LYS:HB2   | 2.49                     | 0.43              |
| 1:J:915:TYR:O     | 1:J:916:LEU:HD22  | 2.19                     | 0.43              |
| 1:K:228:LYS:N     | 2:K:1501:ADP:O2B  | 2.51                     | 0.43              |
| 1:L:943:LEU:HG    | 1:L:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:B:137:ARG:HA    | 1:B:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:C:254:PHE:CZ    | 1:C:256:HIS:HB2   | 2.53                     | 0.43              |
| 1:C:943:LEU:HG    | 1:C:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:D:294:LEU:HA    | 1:D:341:SER:HB2   | 2.01                     | 0.43              |
| 1:D:799:GLU:CB    | 1:D:828:LYS:HB2   | 2.49                     | 0.43              |
| 1:E:347:ARG:O     | 1:E:568:LYS:HE3   | 2.19                     | 0.43              |
| 1:E:1009:ARG:HA   | 1:E:1009:ARG:HD2  | 1.76                     | 0.43              |
| 1:F:617:LYS:HE2   | 1:I:956:TRP:CE3   | 2.52                     | 0.43              |
| 1:F:940:LEU:HD21  | 1:F:943:LEU:HD13  | 2.00                     | 0.43              |
| 1:F:956:TRP:CE3   | 1:I:617:LYS:HE2   | 2.52                     | 0.43              |
| 1:F:1007:LEU:HB3  | 1:F:1011:THR:HG21 | 2.00                     | 0.43              |
| 1:H:294:LEU:HD21  | 1:H:343:LEU:HD12  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:1016:GLU:O    | 1:H:1020:GLU:HG2  | 2.19                     | 0.43              |
| 1:I:943:LEU:HG    | 1:I:945:LEU:CD2   | 2.48                     | 0.43              |
| 1:J:849:SER:OG    | 1:J:875:LYS:HE3   | 2.19                     | 0.43              |
| 1:J:1027:ILE:HG22 | 1:J:1029:PHE:N    | 2.34                     | 0.43              |
| 1:L:855:THR:OG1   | 1:L:856:ARG:N     | 2.52                     | 0.43              |
| 1:A:347:ARG:O     | 1:A:568:LYS:HE3   | 2.19                     | 0.43              |
| 1:A:954:SER:O     | 1:A:957:ASN:HB2   | 2.19                     | 0.43              |
| 1:C:167:LEU:HD22  | 1:C:368:GLY:HA2   | 2.01                     | 0.43              |
| 1:C:956:TRP:CE3   | 1:L:617:LYS:HE2   | 2.52                     | 0.43              |
| 1:C:972:ASN:O     | 1:C:973:LEU:HD22  | 2.18                     | 0.43              |
| 1:D:849:SER:OG    | 1:D:875:LYS:HE3   | 2.19                     | 0.43              |
| 1:E:254:PHE:CZ    | 1:E:256:HIS:HB2   | 2.54                     | 0.43              |
| 1:I:230:ILE:HG13  | 2:I:1501:ADP:C8   | 2.54                     | 0.43              |
| 1:J:230:ILE:HG13  | 2:J:1501:ADP:C8   | 2.54                     | 0.43              |
| 1:K:797:LEU:HD21  | 1:K:800:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:608:LYS:O     | 1:A:612:VAL:HG23  | 2.19                     | 0.43              |
| 1:B:294:LEU:HD21  | 1:B:343:LEU:HD12  | 2.01                     | 0.43              |
| 1:D:531:LEU:O     | 1:D:598:ILE:HA    | 2.19                     | 0.43              |
| 1:E:137:ARG:HA    | 1:E:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:E:940:LEU:HD21  | 1:E:943:LEU:HB2   | 2.00                     | 0.43              |
| 1:F:137:ARG:HA    | 1:F:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:G:900:ALA:O     | 1:G:903:SER:OG    | 2.28                     | 0.43              |
| 1:G:954:SER:O     | 1:G:957:ASN:HB2   | 2.19                     | 0.43              |
| 1:H:137:ARG:HA    | 1:H:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:H:230:ILE:HG13  | 2:H:1501:ADP:C8   | 2.53                     | 0.43              |
| 1:H:940:LEU:HD21  | 1:H:943:LEU:HB2   | 2.00                     | 0.43              |
| 1:I:380:LYS:HA    | 1:I:380:LYS:HD3   | 1.87                     | 0.43              |
| 1:J:531:LEU:O     | 1:J:598:ILE:HA    | 2.19                     | 0.43              |
| 1:J:943:LEU:HG    | 1:J:945:LEU:CD2   | 2.49                     | 0.43              |
| 1:K:137:ARG:HA    | 1:K:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:K:391:ALA:O     | 1:K:394:LEU:HG    | 2.19                     | 0.43              |
| 1:K:940:LEU:HD21  | 1:K:943:LEU:HB2   | 2.00                     | 0.43              |
| 1:L:137:ARG:HA    | 1:L:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:L:677:LEU:HB2   | 1:L:740:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:1018:LEU:HD11 | 1:A:1027:ILE:HD12 | 2.01                     | 0.43              |
| 1:B:254:PHE:CZ    | 1:B:256:HIS:HB2   | 2.54                     | 0.43              |
| 1:C:320:LYS:HA    | 1:C:320:LYS:HD2   | 1.84                     | 0.43              |
| 1:C:1016:GLU:O    | 1:C:1020:GLU:HG2  | 2.18                     | 0.43              |
| 1:D:391:ALA:O     | 1:D:395:ILE:HG12  | 2.19                     | 0.43              |
| 1:E:139:HIS:ND1   | 1:E:277:PRO:HB3   | 2.34                     | 0.43              |
| 1:E:391:ALA:O     | 1:E:394:LEU:HG    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:677:LEU:HB2   | 1:F:740:LEU:HD11  | 2.00                     | 0.43              |
| 1:G:320:LYS:HA    | 1:G:320:LYS:HD2   | 1.83                     | 0.43              |
| 1:G:347:ARG:O     | 1:G:568:LYS:HE3   | 2.19                     | 0.43              |
| 1:G:608:LYS:O     | 1:G:612:VAL:HG23  | 2.19                     | 0.43              |
| 1:G:915:TYR:O     | 1:G:916:LEU:HD22  | 2.19                     | 0.43              |
| 1:H:347:ARG:O     | 1:H:568:LYS:HE3   | 2.18                     | 0.43              |
| 1:H:519:MET:SD    | 1:H:519:MET:N     | 2.89                     | 0.43              |
| 1:H:1007:LEU:HB3  | 1:H:1011:THR:HG21 | 2.01                     | 0.43              |
| 1:I:223:ALA:HB1   | 3:I:1502:7YN:N13  | 2.34                     | 0.43              |
| 1:I:254:PHE:CZ    | 1:I:256:HIS:HB2   | 2.53                     | 0.43              |
| 1:J:391:ALA:O     | 1:J:395:ILE:HG12  | 2.19                     | 0.43              |
| 1:K:1016:GLU:O    | 1:K:1020:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:391:ALA:O     | 1:A:395:ILE:HG12  | 2.19                     | 0.42              |
| 1:A:915:TYR:O     | 1:A:916:LEU:HD22  | 2.19                     | 0.42              |
| 1:B:391:ALA:O     | 1:B:394:LEU:HG    | 2.19                     | 0.42              |
| 1:C:300:PHE:CE2   | 1:C:354:LEU:HD22  | 2.53                     | 0.42              |
| 1:C:354:LEU:O     | 1:C:358:LEU:HG    | 2.19                     | 0.42              |
| 1:C:380:LYS:HA    | 1:C:380:LYS:HD3   | 1.87                     | 0.42              |
| 1:C:767:CYS:O     | 1:C:796:LYS:NZ    | 2.39                     | 0.42              |
| 1:D:230:ILE:HG13  | 2:D:1501:ADP:C8   | 2.54                     | 0.42              |
| 1:D:320:LYS:HA    | 1:D:320:LYS:HD2   | 1.83                     | 0.42              |
| 1:E:1016:GLU:O    | 1:E:1020:GLU:HG2  | 2.19                     | 0.42              |
| 1:G:391:ALA:O     | 1:G:395:ILE:HG12  | 2.19                     | 0.42              |
| 1:H:307:PHE:CZ    | 1:H:329:SER:HB3   | 2.54                     | 0.42              |
| 1:H:902:THR:OG1   | 1:H:928:LEU:O     | 2.33                     | 0.42              |
| 1:H:940:LEU:HD21  | 1:H:943:LEU:HD13  | 2.02                     | 0.42              |
| 1:I:250:ASP:N     | 1:I:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:I:972:ASN:O     | 1:I:973:LEU:HD22  | 2.19                     | 0.42              |
| 1:A:307:PHE:CZ    | 1:A:329:SER:HB3   | 2.54                     | 0.42              |
| 1:A:900:ALA:O     | 1:A:903:SER:OG    | 2.28                     | 0.42              |
| 1:B:262:LEU:O     | 1:B:323:ARG:NE    | 2.37                     | 0.42              |
| 1:B:1007:LEU:HB3  | 1:B:1011:THR:HG21 | 2.01                     | 0.42              |
| 1:C:250:ASP:N     | 1:C:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:D:347:ARG:O     | 1:D:568:LYS:HE3   | 2.19                     | 0.42              |
| 1:D:943:LEU:HG    | 1:D:945:LEU:CD2   | 2.49                     | 0.42              |
| 1:E:307:PHE:CZ    | 1:E:329:SER:HB3   | 2.54                     | 0.42              |
| 1:E:677:LEU:HB2   | 1:E:740:LEU:HD11  | 2.00                     | 0.42              |
| 1:F:250:ASP:N     | 1:F:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:F:431:THR:O     | 1:F:434:THR:OG1   | 2.37                     | 0.42              |
| 1:G:230:ILE:HG13  | 2:G:1501:ADP:C8   | 2.54                     | 0.42              |
| 1:G:1018:LEU:HD11 | 1:G:1027:ILE:HD12 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:207:PRO:HG3   | 1:H:215:VAL:HG11  | 2.01                     | 0.42              |
| 1:H:250:ASP:N     | 1:H:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:I:320:LYS:HA    | 1:I:320:LYS:HD2   | 1.84                     | 0.42              |
| 1:J:320:LYS:HA    | 1:J:320:LYS:HD2   | 1.83                     | 0.42              |
| 1:J:608:LYS:O     | 1:J:612:VAL:HG23  | 2.19                     | 0.42              |
| 1:K:139:HIS:ND1   | 1:K:277:PRO:HB3   | 2.34                     | 0.42              |
| 1:K:207:PRO:HG3   | 1:K:215:VAL:HG11  | 2.01                     | 0.42              |
| 1:K:307:PHE:CZ    | 1:K:329:SER:HB3   | 2.54                     | 0.42              |
| 1:L:230:ILE:HG13  | 2:L:1501:ADP:C8   | 2.54                     | 0.42              |
| 1:L:431:THR:O     | 1:L:434:THR:OG1   | 2.37                     | 0.42              |
| 1:A:230:ILE:HG13  | 2:A:1501:ADP:C8   | 2.54                     | 0.42              |
| 1:B:307:PHE:CZ    | 1:B:329:SER:HB3   | 2.54                     | 0.42              |
| 1:B:608:LYS:O     | 1:B:612:VAL:HG23  | 2.19                     | 0.42              |
| 1:B:915:TYR:O     | 1:B:916:LEU:HD22  | 2.19                     | 0.42              |
| 1:C:637:GLU:O     | 1:C:641:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:608:LYS:O     | 1:D:612:VAL:HG23  | 2.19                     | 0.42              |
| 1:E:797:LEU:HD21  | 1:E:800:LEU:HD12  | 2.01                     | 0.42              |
| 1:G:307:PHE:CZ    | 1:G:329:SER:HB3   | 2.54                     | 0.42              |
| 1:H:370:SER:OG    | 1:H:373:LYS:HG2   | 2.19                     | 0.42              |
| 1:H:593:LYS:HA    | 1:H:593:LYS:HD3   | 1.83                     | 0.42              |
| 1:H:608:LYS:O     | 1:H:612:VAL:HG23  | 2.19                     | 0.42              |
| 1:H:915:TYR:O     | 1:H:916:LEU:HD22  | 2.19                     | 0.42              |
| 1:I:786:ASP:O     | 1:I:789:SER:OG    | 2.32                     | 0.42              |
| 1:J:307:PHE:CZ    | 1:J:329:SER:HB3   | 2.54                     | 0.42              |
| 1:K:531:LEU:O     | 1:K:598:ILE:HA    | 2.20                     | 0.42              |
| 1:B:223:ALA:HB1   | 3:B:1502:7YN:N13  | 2.34                     | 0.42              |
| 1:B:902:THR:OG1   | 1:B:928:LEU:O     | 2.33                     | 0.42              |
| 1:D:213:GLU:O     | 1:D:214:PRO:C     | 2.63                     | 0.42              |
| 1:D:307:PHE:CZ    | 1:D:329:SER:HB3   | 2.54                     | 0.42              |
| 1:E:531:LEU:O     | 1:E:598:ILE:HA    | 2.20                     | 0.42              |
| 1:E:915:TYR:O     | 1:E:916:LEU:HD22  | 2.19                     | 0.42              |
| 1:H:391:ALA:O     | 1:H:394:LEU:HG    | 2.20                     | 0.42              |
| 1:H:563:TYR:CE1   | 1:H:572:ILE:HG12  | 2.54                     | 0.42              |
| 1:H:571:LEU:O     | 1:H:575:VAL:HG23  | 2.19                     | 0.42              |
| 1:J:347:ARG:O     | 1:J:568:LYS:HE3   | 2.19                     | 0.42              |
| 1:K:873:CYS:O     | 1:K:877:LYS:HG3   | 2.19                     | 0.42              |
| 1:K:915:TYR:O     | 1:K:916:LEU:HD22  | 2.19                     | 0.42              |
| 1:B:1018:LEU:HD11 | 1:B:1027:ILE:HG13 | 2.00                     | 0.42              |
| 1:C:223:ALA:HB1   | 3:C:1502:7YN:N13  | 2.34                     | 0.42              |
| 1:D:216:HIS:CE1   | 1:D:341:SER:HG    | 2.29                     | 0.42              |
| 1:E:579:PHE:HA    | 1:E:582:VAL:HG22  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:940:LEU:HD21  | 1:E:943:LEU:HD13  | 2.01                     | 0.42              |
| 1:F:230:ILE:HG21  | 2:F:1501:ADP:C5   | 2.54                     | 0.42              |
| 1:F:946:ASP:OD1   | 1:F:972:ASN:HB3   | 2.19                     | 0.42              |
| 1:G:294:LEU:HA    | 1:G:341:SER:HB2   | 2.01                     | 0.42              |
| 1:G:849:SER:OG    | 1:G:875:LYS:HE3   | 2.19                     | 0.42              |
| 1:I:900:ALA:O     | 1:I:903:SER:OG    | 2.31                     | 0.42              |
| 1:J:213:GLU:O     | 1:J:214:PRO:C     | 2.62                     | 0.42              |
| 1:J:229:THR:HG22  | 1:J:298:ASP:OD2   | 2.19                     | 0.42              |
| 1:K:579:PHE:CE1   | 1:K:606:LEU:HD22  | 2.54                     | 0.42              |
| 1:L:946:ASP:OD1   | 1:L:972:ASN:HB3   | 2.20                     | 0.42              |
| 1:A:250:ASP:N     | 1:A:292:ARG:HB3   | 2.35                     | 0.42              |
| 1:A:294:LEU:HA    | 1:A:341:SER:HB2   | 2.01                     | 0.42              |
| 1:A:799:GLU:CB    | 1:A:828:LYS:HB2   | 2.49                     | 0.42              |
| 1:A:849:SER:OG    | 1:A:875:LYS:HE3   | 2.19                     | 0.42              |
| 1:A:967:SER:O     | 1:A:969:ARG:HG3   | 2.19                     | 0.42              |
| 1:B:563:TYR:CE1   | 1:B:572:ILE:HG12  | 2.55                     | 0.42              |
| 1:B:940:LEU:HD21  | 1:B:943:LEU:HD13  | 2.02                     | 0.42              |
| 1:B:973:LEU:C     | 1:B:976:ASN:HD22  | 2.28                     | 0.42              |
| 1:C:294:LEU:HD21  | 1:C:343:LEU:HD12  | 2.02                     | 0.42              |
| 1:D:250:ASP:N     | 1:D:292:ARG:HB3   | 2.35                     | 0.42              |
| 1:E:164:TYR:CZ    | 1:E:234:LYS:HE3   | 2.54                     | 0.42              |
| 1:E:250:ASP:N     | 1:E:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:E:294:LEU:HD21  | 1:E:343:LEU:HD12  | 2.01                     | 0.42              |
| 1:E:306:ALA:HB1   | 1:E:310:HIS:HD2   | 1.85                     | 0.42              |
| 1:E:579:PHE:HE1   | 1:E:606:LEU:HD13  | 1.85                     | 0.42              |
| 1:E:873:CYS:O     | 1:E:877:LYS:HG3   | 2.20                     | 0.42              |
| 1:G:856:ARG:HB2   | 1:G:885:LYS:HB2   | 2.02                     | 0.42              |
| 1:H:973:LEU:C     | 1:H:976:ASN:HD22  | 2.28                     | 0.42              |
| 1:I:1007:LEU:HB3  | 1:I:1011:THR:HG21 | 2.00                     | 0.42              |
| 1:I:1016:GLU:O    | 1:I:1020:GLU:HG2  | 2.18                     | 0.42              |
| 1:K:1018:LEU:HD11 | 1:K:1027:ILE:HG13 | 2.00                     | 0.42              |
| 1:L:167:LEU:HD22  | 1:L:368:GLY:HA2   | 2.00                     | 0.42              |
| 1:L:250:ASP:N     | 1:L:292:ARG:HB3   | 2.35                     | 0.42              |
| 1:A:317:ASP:HB3   | 1:A:320:LYS:HB2   | 2.00                     | 0.42              |
| 1:B:164:TYR:CZ    | 1:B:234:LYS:HE3   | 2.55                     | 0.42              |
| 1:B:213:GLU:O     | 1:B:214:PRO:C     | 2.63                     | 0.42              |
| 1:B:250:ASP:N     | 1:B:292:ARG:HB3   | 2.34                     | 0.42              |
| 1:B:579:PHE:HE1   | 1:B:606:LEU:HD13  | 1.85                     | 0.42              |
| 1:B:579:PHE:CE1   | 1:B:606:LEU:HD22  | 2.55                     | 0.42              |
| 1:C:786:ASP:O     | 1:C:789:SER:OG    | 2.32                     | 0.42              |
| 1:D:229:THR:HG22  | 1:D:298:ASP:OD2   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:967:SER:O     | 1:D:969:ARG:HG3  | 2.19                     | 0.42              |
| 1:E:579:PHE:CE1   | 1:E:606:LEU:HD22 | 2.54                     | 0.42              |
| 1:E:608:LYS:O     | 1:E:612:VAL:HG23 | 2.19                     | 0.42              |
| 1:E:973:LEU:C     | 1:E:976:ASN:HD22 | 2.28                     | 0.42              |
| 1:F:646:ASP:HB3   | 1:F:673:ARG:NH1  | 2.35                     | 0.42              |
| 1:F:1017:ALA:O    | 1:F:1020:GLU:N   | 2.52                     | 0.42              |
| 1:G:250:ASP:N     | 1:G:292:ARG:HB3  | 2.35                     | 0.42              |
| 1:G:799:GLU:CB    | 1:G:828:LYS:HB2  | 2.49                     | 0.42              |
| 1:G:967:SER:O     | 1:G:969:ARG:HG3  | 2.19                     | 0.42              |
| 1:H:139:HIS:ND1   | 1:H:277:PRO:HB3  | 2.34                     | 0.42              |
| 1:H:213:GLU:O     | 1:H:214:PRO:C    | 2.63                     | 0.42              |
| 1:I:645:MET:HE1   | 1:I:667:CYS:CB   | 2.39                     | 0.42              |
| 1:J:250:ASP:N     | 1:J:292:ARG:HB3  | 2.35                     | 0.42              |
| 1:K:164:TYR:CZ    | 1:K:234:LYS:HE3  | 2.54                     | 0.42              |
| 1:K:306:ALA:HB1   | 1:K:310:HIS:HD2  | 1.85                     | 0.42              |
| 1:K:579:PHE:HA    | 1:K:582:VAL:HG22 | 2.01                     | 0.42              |
| 1:K:608:LYS:O     | 1:K:612:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:856:ARG:HB2   | 1:A:885:LYS:HB2  | 2.02                     | 0.42              |
| 1:A:1027:ILE:HG22 | 1:A:1029:PHE:N   | 2.34                     | 0.42              |
| 1:B:139:HIS:ND1   | 1:B:277:PRO:HB3  | 2.34                     | 0.42              |
| 1:B:347:ARG:O     | 1:B:568:LYS:HE3  | 2.19                     | 0.42              |
| 1:B:579:PHE:HA    | 1:B:582:VAL:HG22 | 2.02                     | 0.42              |
| 1:B:679:LEU:HD12  | 1:B:745:LEU:HD21 | 2.02                     | 0.42              |
| 1:E:518:HIS:HD1   | 1:E:520:THR:HG23 | 1.84                     | 0.42              |
| 1:F:954:SER:O     | 1:F:957:ASN:HB2  | 2.20                     | 0.42              |
| 1:G:213:GLU:O     | 1:G:214:PRO:C    | 2.62                     | 0.42              |
| 1:G:317:ASP:HB3   | 1:G:320:LYS:HB2  | 2.00                     | 0.42              |
| 1:H:371:GLU:HG3   | 1:H:402:PHE:CZ   | 2.55                     | 0.42              |
| 1:H:861:GLU:N     | 1:H:889:VAL:O    | 2.36                     | 0.42              |
| 1:H:873:CYS:O     | 1:H:877:LYS:HG3  | 2.19                     | 0.42              |
| 1:J:216:HIS:CE1   | 1:J:341:SER:HG   | 2.29                     | 0.42              |
| 1:K:501:MET:HE1   | 1:K:514:TYR:CD2  | 2.54                     | 0.42              |
| 1:K:579:PHE:HE1   | 1:K:606:LEU:HD13 | 1.85                     | 0.42              |
| 1:K:677:LEU:HB2   | 1:K:740:LEU:HD11 | 2.01                     | 0.42              |
| 1:K:1002:LEU:O    | 1:K:1005:MET:HE3 | 2.20                     | 0.42              |
| 1:L:646:ASP:HB3   | 1:L:673:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:213:GLU:O     | 1:A:214:PRO:C    | 2.63                     | 0.42              |
| 1:A:593:LYS:HA    | 1:A:593:LYS:HD3  | 1.82                     | 0.42              |
| 1:C:645:MET:HE1   | 1:C:667:CYS:CB   | 2.39                     | 0.42              |
| 1:C:900:ALA:O     | 1:C:903:SER:OG   | 2.31                     | 0.42              |
| 1:D:518:HIS:HB3   | 1:D:521:PHE:CD2  | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1002:LEU:O    | 1:D:1005:MET:HE3  | 2.20                     | 0.42              |
| 1:F:228:LYS:N     | 2:F:1501:ADP:O3B  | 2.53                     | 0.42              |
| 1:G:1027:ILE:HG22 | 1:G:1029:PHE:N    | 2.34                     | 0.42              |
| 1:J:306:ALA:HB1   | 1:J:310:HIS:HD2   | 1.85                     | 0.42              |
| 1:J:518:HIS:HB3   | 1:J:521:PHE:CD2   | 2.55                     | 0.42              |
| 1:J:967:SER:O     | 1:J:969:ARG:HG3   | 2.19                     | 0.42              |
| 1:J:1002:LEU:O    | 1:J:1005:MET:HE3  | 2.20                     | 0.42              |
| 1:K:940:LEU:HD21  | 1:K:943:LEU:HD13  | 2.02                     | 0.42              |
| 1:L:466:CYS:HB3   | 1:L:529:TYR:CB    | 2.46                     | 0.42              |
| 1:L:786:ASP:O     | 1:L:789:SER:OG    | 2.32                     | 0.42              |
| 1:L:1017:ALA:O    | 1:L:1020:GLU:N    | 2.52                     | 0.42              |
| 1:B:873:CYS:O     | 1:B:877:LYS:HG3   | 2.20                     | 0.42              |
| 1:C:228:LYS:N     | 2:C:1501:ADP:O3B  | 2.53                     | 0.42              |
| 1:C:646:ASP:HB3   | 1:C:673:ARG:NH1   | 2.34                     | 0.42              |
| 1:C:742:GLU:HG2   | 1:C:771:ARG:HB3   | 2.02                     | 0.42              |
| 1:C:1007:LEU:HB3  | 1:C:1011:THR:HG21 | 2.00                     | 0.42              |
| 1:D:306:ALA:HB1   | 1:D:310:HIS:HD2   | 1.85                     | 0.42              |
| 1:D:677:LEU:HB2   | 1:D:740:LEU:HD11  | 2.02                     | 0.42              |
| 1:E:371:GLU:HG3   | 1:E:402:PHE:CZ    | 2.55                     | 0.42              |
| 1:E:1002:LEU:O    | 1:E:1005:MET:HE3  | 2.20                     | 0.42              |
| 1:H:580:GLY:O     | 1:H:586:ARG:NE    | 2.52                     | 0.42              |
| 1:H:1018:LEU:HD11 | 1:H:1027:ILE:HG13 | 2.01                     | 0.42              |
| 1:I:300:PHE:CE2   | 1:I:354:LEU:HD22  | 2.54                     | 0.42              |
| 1:K:317:ASP:HB3   | 1:K:320:LYS:HB2   | 2.02                     | 0.42              |
| 1:K:563:TYR:CE1   | 1:K:572:ILE:HG12  | 2.54                     | 0.42              |
| 1:L:230:ILE:HG21  | 2:L:1501:ADP:C5   | 2.55                     | 0.42              |
| 1:L:563:TYR:HD1   | 1:L:571:LEU:HB2   | 1.85                     | 0.42              |
| 1:A:677:LEU:HB2   | 1:A:740:LEU:HD11  | 2.02                     | 0.41              |
| 1:B:954:SER:OG    | 1:B:957:ASN:OD1   | 2.27                     | 0.41              |
| 1:D:1018:LEU:HD11 | 1:D:1027:ILE:HD12 | 2.01                     | 0.41              |
| 1:E:381:TYR:CE1   | 1:E:415:CYS:HB3   | 2.55                     | 0.41              |
| 1:F:294:LEU:HD21  | 1:F:343:LEU:HD12  | 2.01                     | 0.41              |
| 1:F:466:CYS:HB3   | 1:F:529:TYR:CB    | 2.46                     | 0.41              |
| 1:G:593:LYS:HA    | 1:G:593:LYS:HD3   | 1.82                     | 0.41              |
| 1:G:677:LEU:HB2   | 1:G:740:LEU:HD11  | 2.02                     | 0.41              |
| 1:H:679:LEU:HD12  | 1:H:745:LEU:HD21  | 2.02                     | 0.41              |
| 1:H:797:LEU:HD21  | 1:H:800:LEU:HD12  | 2.01                     | 0.41              |
| 1:L:320:LYS:HD2   | 1:L:320:LYS:HA    | 1.84                     | 0.41              |
| 1:L:816:CYS:HB3   | 1:L:820:LYS:HE2   | 2.02                     | 0.41              |
| 1:A:531:LEU:O     | 1:A:598:ILE:HA    | 2.19                     | 0.41              |
| 1:B:531:LEU:O     | 1:B:598:ILE:HA    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:740:LEU:HD12  | 1:B:740:LEU:HA    | 1.89                     | 0.41              |
| 1:C:230:ILE:HG21  | 2:C:1501:ADP:C5   | 2.55                     | 0.41              |
| 1:C:607:LEU:HD12  | 1:C:640:PHE:HE1   | 1.84                     | 0.41              |
| 1:D:1016:GLU:O    | 1:D:1020:GLU:HG2  | 2.20                     | 0.41              |
| 1:E:483:CYS:SG    | 1:E:487:LYS:NZ    | 2.80                     | 0.41              |
| 1:E:657:THR:O     | 1:E:661:HIS:ND1   | 2.53                     | 0.41              |
| 1:E:1018:LEU:HD11 | 1:E:1027:ILE:HG13 | 2.01                     | 0.41              |
| 1:F:306:ALA:HB1   | 1:F:310:HIS:HD2   | 1.85                     | 0.41              |
| 1:F:458:PHE:HA    | 1:F:461:TYR:HD2   | 1.86                     | 0.41              |
| 1:F:786:ASP:O     | 1:F:789:SER:OG    | 2.32                     | 0.41              |
| 1:F:816:CYS:HB3   | 1:F:820:LYS:HE2   | 2.02                     | 0.41              |
| 1:G:223:ALA:HB1   | 3:G:1502:7YN:N13  | 2.35                     | 0.41              |
| 1:G:518:HIS:HB3   | 1:G:521:PHE:CD2   | 2.55                     | 0.41              |
| 1:H:625:GLN:HG2   | 1:H:629:PHE:CE2   | 2.55                     | 0.41              |
| 1:I:230:ILE:HG21  | 2:I:1501:ADP:C5   | 2.55                     | 0.41              |
| 1:I:354:LEU:O     | 1:I:358:LEU:HG    | 2.20                     | 0.41              |
| 1:J:677:LEU:HB2   | 1:J:740:LEU:HD11  | 2.02                     | 0.41              |
| 1:J:1016:GLU:O    | 1:J:1020:GLU:HG2  | 2.20                     | 0.41              |
| 1:K:250:ASP:N     | 1:K:292:ARG:HB3   | 2.35                     | 0.41              |
| 1:K:371:GLU:HG3   | 1:K:402:PHE:CZ    | 2.55                     | 0.41              |
| 1:K:381:TYR:CE1   | 1:K:415:CYS:HB3   | 2.55                     | 0.41              |
| 1:L:228:LYS:N     | 2:L:1501:ADP:O2B  | 2.53                     | 0.41              |
| 1:A:518:HIS:HB3   | 1:A:521:PHE:CD2   | 2.55                     | 0.41              |
| 1:A:985:THR:O     | 1:A:988:GLU:HG3   | 2.21                     | 0.41              |
| 1:A:1010:GLU:HA   | 1:A:1013:ARG:HH12 | 1.86                     | 0.41              |
| 1:B:625:GLN:HG2   | 1:B:629:PHE:CE2   | 2.55                     | 0.41              |
| 1:B:797:LEU:HD21  | 1:B:800:LEU:HD12  | 2.01                     | 0.41              |
| 1:E:213:GLU:O     | 1:E:214:PRO:C     | 2.63                     | 0.41              |
| 1:E:954:SER:O     | 1:E:957:ASN:HB2   | 2.20                     | 0.41              |
| 1:G:531:LEU:O     | 1:G:598:ILE:HA    | 2.19                     | 0.41              |
| 1:G:985:THR:O     | 1:G:988:GLU:HG3   | 2.21                     | 0.41              |
| 1:I:213:GLU:O     | 1:I:214:PRO:C     | 2.64                     | 0.41              |
| 1:I:228:LYS:N     | 2:I:1501:ADP:O2B  | 2.53                     | 0.41              |
| 1:J:1018:LEU:HD11 | 1:J:1027:ILE:HD12 | 2.01                     | 0.41              |
| 1:K:213:GLU:O     | 1:K:214:PRO:C     | 2.63                     | 0.41              |
| 1:K:657:THR:O     | 1:K:661:HIS:ND1   | 2.53                     | 0.41              |
| 1:L:223:ALA:HB1   | 3:L:1502:7YN:N13  | 2.35                     | 0.41              |
| 1:L:294:LEU:HD21  | 1:L:343:LEU:HD12  | 2.02                     | 0.41              |
| 1:A:135:MET:HE3   | 1:A:135:MET:HB2   | 1.97                     | 0.41              |
| 1:B:371:GLU:HG3   | 1:B:402:PHE:CZ    | 2.55                     | 0.41              |
| 1:B:1002:LEU:O    | 1:B:1005:MET:HE3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:213:GLU:O    | 1:C:214:PRO:C     | 2.64                     | 0.41              |
| 1:C:946:ASP:OD1  | 1:C:974:GLY:N     | 2.42                     | 0.41              |
| 1:D:677:LEU:HD23 | 1:D:678:SER:N     | 2.35                     | 0.41              |
| 1:E:317:ASP:HB3  | 1:E:320:LYS:HB2   | 2.02                     | 0.41              |
| 1:E:625:GLN:HG2  | 1:E:629:PHE:CE2   | 2.55                     | 0.41              |
| 1:G:216:HIS:CE1  | 1:G:341:SER:HG    | 2.31                     | 0.41              |
| 1:G:1010:GLU:HA  | 1:G:1013:ARG:HH12 | 1.86                     | 0.41              |
| 1:H:201:LEU:O    | 1:H:204:LEU:HG    | 2.21                     | 0.41              |
| 1:H:371:GLU:HG3  | 1:H:402:PHE:HZ    | 1.85                     | 0.41              |
| 1:H:1002:LEU:O   | 1:H:1005:MET:HE3  | 2.20                     | 0.41              |
| 1:I:294:LEU:HD21 | 1:I:343:LEU:HD12  | 2.02                     | 0.41              |
| 1:I:317:ASP:HB3  | 1:I:320:LYS:HB2   | 2.02                     | 0.41              |
| 1:J:381:TYR:HE2  | 1:J:412:TRP:HD1   | 1.68                     | 0.41              |
| 1:J:900:ALA:O    | 1:J:903:SER:OG    | 2.28                     | 0.41              |
| 1:L:306:ALA:HB1  | 1:L:310:HIS:HD2   | 1.84                     | 0.41              |
| 1:L:632:LEU:HD12 | 1:L:641:VAL:HG22  | 2.02                     | 0.41              |
| 1:A:229:THR:HG22 | 1:A:298:ASP:OD2   | 2.19                     | 0.41              |
| 1:A:254:PHE:CZ   | 1:A:256:HIS:HB2   | 2.56                     | 0.41              |
| 1:B:164:TYR:CE2  | 1:B:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:B:519:MET:SD   | 1:B:519:MET:N     | 2.88                     | 0.41              |
| 1:C:306:ALA:HB1  | 1:C:310:HIS:HD2   | 1.85                     | 0.41              |
| 1:C:502:ASN:HB2  | 1:C:513:PHE:HB2   | 2.01                     | 0.41              |
| 1:E:320:LYS:HA   | 1:E:320:LYS:HD2   | 1.84                     | 0.41              |
| 1:E:563:TYR:CE1  | 1:E:572:ILE:HG12  | 2.55                     | 0.41              |
| 1:E:902:THR:OG1  | 1:E:928:LEU:O     | 2.33                     | 0.41              |
| 1:F:354:LEU:O    | 1:F:358:LEU:HG    | 2.19                     | 0.41              |
| 1:F:593:LYS:HA   | 1:F:593:LYS:HD3   | 1.82                     | 0.41              |
| 1:F:632:LEU:HD12 | 1:F:641:VAL:HG22  | 2.02                     | 0.41              |
| 1:F:742:GLU:HG2  | 1:F:771:ARG:HB3   | 2.02                     | 0.41              |
| 1:G:135:MET:HE3  | 1:G:135:MET:HB2   | 1.96                     | 0.41              |
| 1:G:431:THR:O    | 1:G:434:THR:OG1   | 2.38                     | 0.41              |
| 1:H:164:TYR:CZ   | 1:H:234:LYS:HE3   | 2.55                     | 0.41              |
| 1:H:306:ALA:HB1  | 1:H:310:HIS:HD2   | 1.85                     | 0.41              |
| 1:H:381:TYR:CD1  | 1:H:415:CYS:HB3   | 2.56                     | 0.41              |
| 1:H:971:LEU:HD12 | 1:H:971:LEU:HA    | 1.93                     | 0.41              |
| 1:I:502:ASN:HB2  | 1:I:513:PHE:HB2   | 2.01                     | 0.41              |
| 1:I:742:GLU:HG2  | 1:I:771:ARG:HB3   | 2.03                     | 0.41              |
| 1:K:646:ASP:HB3  | 1:K:673:ARG:NH1   | 2.36                     | 0.41              |
| 1:L:458:PHE:HA   | 1:L:461:TYR:HD2   | 1.86                     | 0.41              |
| 1:A:431:THR:O    | 1:A:434:THR:OG1   | 2.38                     | 0.41              |
| 1:B:300:PHE:HB3  | 1:B:346:THR:HG22  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:300:PHE:HB3  | 1:E:346:THR:HG22 | 2.01                     | 0.41              |
| 1:E:307:PHE:HE1  | 1:E:325:ASP:HB2  | 1.86                     | 0.41              |
| 1:E:646:ASP:HB3  | 1:E:673:ARG:NH1  | 2.36                     | 0.41              |
| 1:G:254:PHE:CZ   | 1:G:256:HIS:HB2  | 2.56                     | 0.41              |
| 1:H:409:LEU:HD13 | 2:H:1501:ADP:H4' | 2.02                     | 0.41              |
| 1:I:306:ALA:HB1  | 1:I:310:HIS:HD2  | 1.85                     | 0.41              |
| 1:I:632:LEU:HD12 | 1:I:641:VAL:HG22 | 2.02                     | 0.41              |
| 1:K:625:GLN:HG2  | 1:K:629:PHE:CE2  | 2.55                     | 0.41              |
| 1:L:213:GLU:O    | 1:L:214:PRO:C    | 2.64                     | 0.41              |
| 1:L:307:PHE:CZ   | 1:L:329:SER:HB3  | 2.56                     | 0.41              |
| 1:B:284:CYS:O    | 1:B:288:ARG:NE   | 2.53                     | 0.41              |
| 1:B:646:ASP:HB3  | 1:B:673:ARG:NH1  | 2.36                     | 0.41              |
| 1:B:971:LEU:HD12 | 1:B:971:LEU:HA   | 1.93                     | 0.41              |
| 1:C:381:TYR:CD1  | 1:C:415:CYS:HB3  | 2.56                     | 0.41              |
| 1:C:757:VAL:HA   | 1:C:760:GLU:OE2  | 2.21                     | 0.41              |
| 1:D:381:TYR:HE2  | 1:D:412:TRP:HD1  | 1.68                     | 0.41              |
| 1:D:436:THR:HG21 | 1:D:634:GLU:HA   | 2.03                     | 0.41              |
| 1:D:563:TYR:HD1  | 1:D:571:LEU:HB2  | 1.86                     | 0.41              |
| 1:E:284:CYS:O    | 1:E:288:ARG:NE   | 2.54                     | 0.41              |
| 1:E:343:LEU:HD23 | 1:E:343:LEU:HA   | 1.87                     | 0.41              |
| 1:F:307:PHE:CZ   | 1:F:329:SER:HB3  | 2.56                     | 0.41              |
| 1:F:946:ASP:OD1  | 1:F:974:GLY:N    | 2.42                     | 0.41              |
| 1:G:229:THR:HG22 | 1:G:298:ASP:OD2  | 2.19                     | 0.41              |
| 1:H:164:TYR:CE2  | 1:H:234:LYS:HE3  | 2.56                     | 0.41              |
| 1:H:646:ASP:HB3  | 1:H:673:ARG:NH1  | 2.36                     | 0.41              |
| 1:I:301:ASP:O    | 1:I:570:TYR:OH   | 2.22                     | 0.41              |
| 1:I:381:TYR:CD1  | 1:I:415:CYS:HB3  | 2.56                     | 0.41              |
| 1:I:646:ASP:HB3  | 1:I:673:ARG:NH1  | 2.35                     | 0.41              |
| 1:I:757:VAL:HA   | 1:I:760:GLU:OE2  | 2.21                     | 0.41              |
| 1:J:954:SER:O    | 1:J:957:ASN:HB2  | 2.21                     | 0.41              |
| 1:L:164:TYR:CZ   | 1:L:234:LYS:HE3  | 2.56                     | 0.41              |
| 1:L:354:LEU:O    | 1:L:358:LEU:HG   | 2.19                     | 0.41              |
| 1:L:381:TYR:CD1  | 1:L:415:CYS:HB3  | 2.56                     | 0.41              |
| 1:A:563:TYR:HD1  | 1:A:571:LEU:HB2  | 1.86                     | 0.41              |
| 1:B:373:LYS:HA   | 1:B:373:LYS:HD3  | 1.92                     | 0.41              |
| 1:C:317:ASP:HB3  | 1:C:320:LYS:HB2  | 2.03                     | 0.41              |
| 1:D:900:ALA:O    | 1:D:903:SER:OG   | 2.28                     | 0.41              |
| 1:D:954:SER:O    | 1:D:957:ASN:HB2  | 2.21                     | 0.41              |
| 1:E:988:GLU:O    | 1:E:992:GLN:NE2  | 2.54                     | 0.41              |
| 1:F:164:TYR:CZ   | 1:F:234:LYS:HE3  | 2.56                     | 0.41              |
| 1:F:213:GLU:O    | 1:F:214:PRO:C    | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1009:ARG:HA   | 1:G:1009:ARG:HD2  | 1.75                     | 0.41              |
| 1:H:483:CYS:SG    | 1:H:487:LYS:NZ    | 2.80                     | 0.41              |
| 1:H:1028:VAL:HG12 | 1:H:1028:VAL:O    | 2.21                     | 0.41              |
| 1:I:1028:VAL:O    | 1:I:1028:VAL:HG12 | 2.21                     | 0.41              |
| 1:J:436:THR:HG21  | 1:J:634:GLU:HA    | 2.03                     | 0.41              |
| 1:J:563:TYR:HD1   | 1:J:571:LEU:HB2   | 1.86                     | 0.41              |
| 1:J:856:ARG:HB2   | 1:J:885:LYS:HB2   | 2.02                     | 0.41              |
| 1:L:343:LEU:HD23  | 1:L:343:LEU:HA    | 1.87                     | 0.41              |
| 1:L:742:GLU:HG2   | 1:L:771:ARG:HB3   | 2.03                     | 0.41              |
| 1:A:826:LEU:HD12  | 1:A:826:LEU:HA    | 1.96                     | 0.41              |
| 1:A:1002:LEU:O    | 1:A:1005:MET:HE3  | 2.20                     | 0.41              |
| 1:B:306:ALA:HB1   | 1:B:310:HIS:HD2   | 1.85                     | 0.41              |
| 1:B:381:TYR:CE1   | 1:B:415:CYS:HB3   | 2.55                     | 0.41              |
| 1:B:466:CYS:HB3   | 1:B:529:TYR:CB    | 2.47                     | 0.41              |
| 1:B:657:THR:O     | 1:B:661:HIS:ND1   | 2.53                     | 0.41              |
| 1:B:1011:THR:O    | 1:B:1015:LEU:HG   | 2.21                     | 0.41              |
| 1:B:1028:VAL:HG12 | 1:B:1028:VAL:O    | 2.21                     | 0.41              |
| 1:C:816:CYS:HB3   | 1:C:820:LYS:HE2   | 2.02                     | 0.41              |
| 1:C:1028:VAL:O    | 1:C:1028:VAL:HG12 | 2.21                     | 0.41              |
| 1:D:139:HIS:CD2   | 1:D:277:PRO:HD3   | 2.56                     | 0.41              |
| 1:D:164:TYR:CZ    | 1:D:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:D:735:SER:HB2   | 1:D:764:HIS:HB3   | 2.03                     | 0.41              |
| 1:D:856:ARG:HB2   | 1:D:885:LYS:HB2   | 2.02                     | 0.41              |
| 1:D:942:MET:SD    | 1:D:943:LEU:N     | 2.94                     | 0.41              |
| 1:D:1010:GLU:HA   | 1:D:1013:ARG:HH12 | 1.86                     | 0.41              |
| 1:D:1018:LEU:HA   | 1:D:1021:GLU:OE2  | 2.21                     | 0.41              |
| 1:E:346:THR:OG1   | 1:E:351:LEU:HD21  | 2.21                     | 0.41              |
| 1:E:1011:THR:O    | 1:E:1015:LEU:HG   | 2.21                     | 0.41              |
| 1:E:1028:VAL:O    | 1:E:1028:VAL:HG12 | 2.21                     | 0.41              |
| 1:F:136:TYR:HE1   | 1:F:276:TRP:HA    | 1.86                     | 0.41              |
| 1:F:317:ASP:HB3   | 1:F:320:LYS:HB2   | 2.02                     | 0.41              |
| 1:F:320:LYS:HD2   | 1:F:320:LYS:HA    | 1.85                     | 0.41              |
| 1:F:757:VAL:HA    | 1:F:760:GLU:OE2   | 2.21                     | 0.41              |
| 1:G:330:SER:HA    | 1:G:335:LYS:HZ1   | 1.86                     | 0.41              |
| 1:G:563:TYR:HD1   | 1:G:571:LEU:HB2   | 1.86                     | 0.41              |
| 1:H:320:LYS:HG3   | 1:H:322:VAL:HG23  | 2.03                     | 0.41              |
| 1:H:378:PHE:HE2   | 1:H:411:CYS:HB3   | 1.85                     | 0.41              |
| 1:H:381:TYR:CE1   | 1:H:415:CYS:HB3   | 2.56                     | 0.41              |
| 1:H:740:LEU:HD12  | 1:H:740:LEU:HA    | 1.89                     | 0.41              |
| 1:H:988:GLU:O     | 1:H:992:GLN:NE2   | 2.54                     | 0.41              |
| 1:H:1011:THR:O    | 1:H:1015:LEU:HG   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:458:PHE:HA   | 1:I:461:TYR:HD2   | 1.86                     | 0.41              |
| 1:I:946:ASP:OD1  | 1:I:974:GLY:N     | 2.42                     | 0.41              |
| 1:J:139:HIS:CD2  | 1:J:277:PRO:HD3   | 2.56                     | 0.41              |
| 1:J:164:TYR:CZ   | 1:J:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:J:677:LEU:HD23 | 1:J:678:SER:N     | 2.36                     | 0.41              |
| 1:J:735:SER:HB2  | 1:J:764:HIS:HB3   | 2.03                     | 0.41              |
| 1:J:942:MET:SD   | 1:J:943:LEU:N     | 2.94                     | 0.41              |
| 1:J:1018:LEU:HA  | 1:J:1021:GLU:OE2  | 2.21                     | 0.41              |
| 1:K:167:LEU:HD22 | 1:K:368:GLY:HA2   | 2.02                     | 0.41              |
| 1:K:307:PHE:HE1  | 1:K:325:ASP:HB2   | 1.86                     | 0.41              |
| 1:K:320:LYS:HA   | 1:K:320:LYS:HD2   | 1.84                     | 0.41              |
| 1:K:343:LEU:HD23 | 1:K:343:LEU:HA    | 1.88                     | 0.41              |
| 1:K:458:PHE:HA   | 1:K:461:TYR:HD2   | 1.86                     | 0.41              |
| 1:K:1011:THR:O   | 1:K:1015:LEU:HG   | 2.21                     | 0.41              |
| 1:K:1028:VAL:O   | 1:K:1028:VAL:HG12 | 2.21                     | 0.41              |
| 1:L:657:THR:O    | 1:L:661:HIS:ND1   | 2.54                     | 0.41              |
| 1:A:223:ALA:HB1  | 3:A:1502:7YN:N13  | 2.36                     | 0.41              |
| 1:C:164:TYR:CZ   | 1:C:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:C:632:LEU:HD12 | 1:C:641:VAL:HG13  | 2.02                     | 0.41              |
| 1:C:1017:ALA:O   | 1:C:1020:GLU:N    | 2.52                     | 0.41              |
| 1:G:826:LEU:HD12 | 1:G:826:LEU:HA    | 1.96                     | 0.41              |
| 1:G:1002:LEU:O   | 1:G:1005:MET:HE3  | 2.20                     | 0.41              |
| 1:H:657:THR:O    | 1:H:661:HIS:ND1   | 2.53                     | 0.41              |
| 1:I:164:TYR:CZ   | 1:I:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:I:637:GLU:O    | 1:I:641:VAL:HG23  | 2.21                     | 0.41              |
| 1:J:223:ALA:HB1  | 3:J:1502:7YN:N13  | 2.35                     | 0.41              |
| 1:K:164:TYR:CE2  | 1:K:234:LYS:HE3   | 2.56                     | 0.41              |
| 1:K:201:LEU:O    | 1:K:204:LEU:HG    | 2.21                     | 0.41              |
| 1:K:346:THR:OG1  | 1:K:351:LEU:HD21  | 2.21                     | 0.41              |
| 1:K:518:HIS:HD1  | 1:K:520:THR:HG23  | 1.86                     | 0.41              |
| 1:K:954:SER:O    | 1:K:957:ASN:HB2   | 2.20                     | 0.41              |
| 1:K:988:GLU:O    | 1:K:992:GLN:NE2   | 2.54                     | 0.41              |
| 1:A:436:THR:HG21 | 1:A:634:GLU:HA    | 2.03                     | 0.40              |
| 1:A:767:CYS:O    | 1:A:796:LYS:NZ    | 2.41                     | 0.40              |
| 1:A:1018:LEU:HA  | 1:A:1021:GLU:OE2  | 2.21                     | 0.40              |
| 1:B:375:LYS:HA   | 1:B:375:LYS:HD3   | 1.93                     | 0.40              |
| 1:B:581:LEU:HD22 | 1:B:590:LEU:HD22  | 2.02                     | 0.40              |
| 1:B:988:GLU:O    | 1:B:992:GLN:NE2   | 2.54                     | 0.40              |
| 1:F:343:LEU:HD23 | 1:F:343:LEU:HA    | 1.87                     | 0.40              |
| 1:F:639:ASP:OD1  | 1:F:640:PHE:N     | 2.54                     | 0.40              |
| 1:F:657:THR:O    | 1:F:661:HIS:ND1   | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1028:VAL:HG12 | 1:F:1028:VAL:O    | 2.21                     | 0.40              |
| 1:G:436:THR:HG21  | 1:G:634:GLU:HA    | 2.03                     | 0.40              |
| 1:G:1016:GLU:O    | 1:G:1020:GLU:HG2  | 2.20                     | 0.40              |
| 1:I:639:ASP:OD1   | 1:I:640:PHE:N     | 2.55                     | 0.40              |
| 1:I:816:CYS:HB3   | 1:I:820:LYS:HE2   | 2.02                     | 0.40              |
| 1:J:1010:GLU:HA   | 1:J:1013:ARG:HH12 | 1.86                     | 0.40              |
| 1:L:593:LYS:HA    | 1:L:593:LYS:HD3   | 1.82                     | 0.40              |
| 1:L:639:ASP:OD1   | 1:L:640:PHE:N     | 2.54                     | 0.40              |
| 1:L:757:VAL:HA    | 1:L:760:GLU:OE2   | 2.21                     | 0.40              |
| 1:A:201:LEU:O     | 1:A:204:LEU:HG    | 2.22                     | 0.40              |
| 1:A:677:LEU:HD23  | 1:A:678:SER:N     | 2.36                     | 0.40              |
| 1:B:320:LYS:HG3   | 1:B:322:VAL:HG23  | 2.04                     | 0.40              |
| 1:B:370:SER:OG    | 1:B:373:LYS:HG2   | 2.21                     | 0.40              |
| 1:B:371:GLU:HG3   | 1:B:402:PHE:HZ    | 1.86                     | 0.40              |
| 1:C:563:TYR:HD1   | 1:C:571:LEU:HB2   | 1.86                     | 0.40              |
| 1:C:958:LEU:O     | 1:C:962:LEU:HG    | 2.21                     | 0.40              |
| 1:D:1028:VAL:O    | 1:D:1028:VAL:HG12 | 2.22                     | 0.40              |
| 1:E:164:TYR:CE2   | 1:E:234:LYS:HE3   | 2.56                     | 0.40              |
| 1:E:167:LEU:HD22  | 1:E:368:GLY:HA2   | 2.02                     | 0.40              |
| 1:E:371:GLU:HG3   | 1:E:402:PHE:HZ    | 1.86                     | 0.40              |
| 1:E:458:PHE:HA    | 1:E:461:TYR:HD2   | 1.87                     | 0.40              |
| 1:E:679:LEU:HD12  | 1:E:745:LEU:HD21  | 2.02                     | 0.40              |
| 1:F:563:TYR:HD1   | 1:F:571:LEU:HB2   | 1.86                     | 0.40              |
| 1:F:967:SER:O     | 1:F:969:ARG:HG3   | 2.21                     | 0.40              |
| 1:G:164:TYR:CZ    | 1:G:234:LYS:HE3   | 2.56                     | 0.40              |
| 1:G:306:ALA:HB1   | 1:G:310:HIS:HD2   | 1.85                     | 0.40              |
| 1:G:1018:LEU:HA   | 1:G:1021:GLU:OE2  | 2.21                     | 0.40              |
| 1:H:230:ILE:HG21  | 2:H:1501:ADP:C5   | 2.56                     | 0.40              |
| 1:H:373:LYS:HA    | 1:H:373:LYS:HD3   | 1.92                     | 0.40              |
| 1:H:480:PHE:HB2   | 1:H:514:TYR:HB2   | 2.03                     | 0.40              |
| 1:H:958:LEU:O     | 1:H:962:LEU:HG    | 2.21                     | 0.40              |
| 1:I:229:THR:HG22  | 1:I:298:ASP:OD2   | 2.21                     | 0.40              |
| 1:I:307:PHE:CZ    | 1:I:329:SER:HB3   | 2.56                     | 0.40              |
| 1:J:380:LYS:HA    | 1:J:380:LYS:HD3   | 1.88                     | 0.40              |
| 1:J:1028:VAL:O    | 1:J:1028:VAL:HG12 | 2.22                     | 0.40              |
| 1:K:284:CYS:O     | 1:K:288:ARG:NE    | 2.54                     | 0.40              |
| 1:K:370:SER:OG    | 1:K:373:LYS:HG2   | 2.21                     | 0.40              |
| 1:L:1028:VAL:O    | 1:L:1028:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:164:TYR:CZ    | 1:A:234:LYS:HE3   | 2.56                     | 0.40              |
| 1:A:306:ALA:HB1   | 1:A:310:HIS:HD2   | 1.85                     | 0.40              |
| 1:A:1016:GLU:O    | 1:A:1020:GLU:HG2  | 2.20                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:876:MET:HE1   | 1:C:886:LEU:HD13 | 2.04                     | 0.40              |
| 1:D:300:PHE:HB3   | 1:D:346:THR:HG22 | 2.03                     | 0.40              |
| 1:E:958:LEU:O     | 1:E:962:LEU:HG   | 2.21                     | 0.40              |
| 1:F:139:HIS:ND1   | 1:F:277:PRO:HB3  | 2.37                     | 0.40              |
| 1:F:740:LEU:HD12  | 1:F:740:LEU:HA   | 1.89                     | 0.40              |
| 1:G:139:HIS:CD2   | 1:G:277:PRO:HD3  | 2.56                     | 0.40              |
| 1:G:677:LEU:HD23  | 1:G:678:SER:N    | 2.36                     | 0.40              |
| 1:I:431:THR:O     | 1:I:434:THR:OG1  | 2.37                     | 0.40              |
| 1:I:876:MET:HE1   | 1:I:886:LEU:HD13 | 2.04                     | 0.40              |
| 1:I:985:THR:O     | 1:I:988:GLU:HG3  | 2.21                     | 0.40              |
| 1:J:300:PHE:HB3   | 1:J:346:THR:HG22 | 2.03                     | 0.40              |
| 1:K:371:GLU:HG3   | 1:K:402:PHE:HZ   | 1.86                     | 0.40              |
| 1:K:679:LEU:HD12  | 1:K:745:LEU:HD21 | 2.02                     | 0.40              |
| 1:L:139:HIS:ND1   | 1:L:277:PRO:HB3  | 2.37                     | 0.40              |
| 1:L:934:LEU:HD21  | 1:L:960:THR:HG22 | 2.02                     | 0.40              |
| 1:L:967:SER:O     | 1:L:969:ARG:HG3  | 2.21                     | 0.40              |
| 1:L:985:THR:O     | 1:L:988:GLU:HG3  | 2.21                     | 0.40              |
| 1:A:139:HIS:CD2   | 1:A:277:PRO:HD3  | 2.56                     | 0.40              |
| 1:A:1009:ARG:HA   | 1:A:1009:ARG:HD2 | 1.75                     | 0.40              |
| 1:B:215:VAL:HB    | 1:B:362:ARG:HH22 | 1.86                     | 0.40              |
| 1:C:307:PHE:CZ    | 1:C:329:SER:HB3  | 2.56                     | 0.40              |
| 1:D:254:PHE:CZ    | 1:D:256:HIS:HB2  | 2.56                     | 0.40              |
| 1:D:307:PHE:HE1   | 1:D:325:ASP:HB2  | 1.87                     | 0.40              |
| 1:D:985:THR:O     | 1:D:988:GLU:HG3  | 2.21                     | 0.40              |
| 1:E:370:SER:OG    | 1:E:373:LYS:HG2  | 2.21                     | 0.40              |
| 1:F:207:PRO:HG3   | 1:F:215:VAL:HG11 | 2.03                     | 0.40              |
| 1:F:381:TYR:CD1   | 1:F:415:CYS:HB3  | 2.56                     | 0.40              |
| 1:F:985:THR:O     | 1:F:988:GLU:HG3  | 2.21                     | 0.40              |
| 1:G:201:LEU:O     | 1:G:204:LEU:HG   | 2.22                     | 0.40              |
| 1:G:381:TYR:HE2   | 1:G:412:TRP:HD1  | 1.68                     | 0.40              |
| 1:H:954:SER:OG    | 1:H:957:ASN:OD1  | 2.28                     | 0.40              |
| 1:I:167:LEU:HD22  | 1:I:368:GLY:HA2  | 2.04                     | 0.40              |
| 1:I:265:PRO:HG3   | 1:I:323:ARG:HD2  | 2.04                     | 0.40              |
| 1:I:958:LEU:O     | 1:I:962:LEU:HG   | 2.21                     | 0.40              |
| 1:J:254:PHE:CZ    | 1:J:256:HIS:HB2  | 2.56                     | 0.40              |
| 1:A:942:MET:SD    | 1:A:943:LEU:N    | 2.94                     | 0.40              |
| 1:B:381:TYR:CD1   | 1:B:415:CYS:HB3  | 2.57                     | 0.40              |
| 1:B:518:HIS:HD1   | 1:B:520:THR:HG23 | 1.85                     | 0.40              |
| 1:B:958:LEU:O     | 1:B:962:LEU:HG   | 2.21                     | 0.40              |
| 1:B:1000:LEU:HD12 | 1:B:1001:GLN:H   | 1.86                     | 0.40              |
| 1:C:431:THR:O     | 1:C:434:THR:OG1  | 2.37                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:946:ASP:OD1 | 1:C:972:ASN:HB3  | 2.20                     | 0.40              |
| 1:C:985:THR:O   | 1:C:988:GLU:HG3  | 2.21                     | 0.40              |
| 1:D:215:VAL:HB  | 1:D:362:ARG:HH22 | 1.87                     | 0.40              |
| 1:E:376:GLU:O   | 1:E:380:LYS:HG2  | 2.21                     | 0.40              |
| 1:E:378:PHE:HE1 | 1:E:411:CYS:HB3  | 1.87                     | 0.40              |
| 1:E:381:TYR:CD1 | 1:E:415:CYS:HB3  | 2.57                     | 0.40              |
| 1:E:593:LYS:HA  | 1:E:593:LYS:HD3  | 1.82                     | 0.40              |
| 1:F:330:SER:HA  | 1:F:335:LYS:HZ1  | 1.86                     | 0.40              |
| 1:F:391:ALA:O   | 1:F:394:LEU:HG   | 2.22                     | 0.40              |
| 1:G:139:HIS:CE1 | 1:G:143:ARG:HD2  | 2.57                     | 0.40              |
| 1:G:300:PHE:HB3 | 1:G:346:THR:HG22 | 2.03                     | 0.40              |
| 1:G:942:MET:SD  | 1:G:943:LEU:N    | 2.94                     | 0.40              |
| 1:H:284:CYS:O   | 1:H:288:ARG:NE   | 2.54                     | 0.40              |
| 1:I:946:ASP:OD1 | 1:I:972:ASN:HB3  | 2.20                     | 0.40              |
| 1:I:967:SER:O   | 1:I:969:ARG:HG3  | 2.21                     | 0.40              |
| 1:I:1017:ALA:O  | 1:I:1020:GLU:N   | 2.52                     | 0.40              |
| 1:J:307:PHE:HE1 | 1:J:325:ASP:HB2  | 1.87                     | 0.40              |
| 1:J:988:GLU:HA  | 1:J:991:LYS:HG3  | 2.03                     | 0.40              |
| 1:K:215:VAL:HB  | 1:K:362:ARG:HH22 | 1.86                     | 0.40              |
| 1:L:207:PRO:HG3 | 1:L:215:VAL:HG11 | 2.03                     | 0.40              |
| 1:L:317:ASP:HB3 | 1:L:320:LYS:HB2  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 775/1057 (73%) | 732 (94%) | 43 (6%) | 0        | 100         | 100 |
| 1   | B     | 775/1057 (73%) | 731 (94%) | 44 (6%) | 0        | 100         | 100 |
| 1   | C     | 775/1057 (73%) | 732 (94%) | 43 (6%) | 0        | 100         | 100 |
| 1   | D     | 775/1057 (73%) | 732 (94%) | 43 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | E     | 775/1057 (73%)   | 730 (94%)  | 45 (6%)  | 0        | 100         | 100 |
| 1   | F     | 775/1057 (73%)   | 732 (94%)  | 43 (6%)  | 0        | 100         | 100 |
| 1   | G     | 775/1057 (73%)   | 732 (94%)  | 43 (6%)  | 0        | 100         | 100 |
| 1   | H     | 775/1057 (73%)   | 731 (94%)  | 44 (6%)  | 0        | 100         | 100 |
| 1   | I     | 775/1057 (73%)   | 732 (94%)  | 43 (6%)  | 0        | 100         | 100 |
| 1   | J     | 775/1057 (73%)   | 732 (94%)  | 43 (6%)  | 0        | 100         | 100 |
| 1   | K     | 775/1057 (73%)   | 732 (94%)  | 43 (6%)  | 0        | 100         | 100 |
| 1   | L     | 775/1057 (73%)   | 731 (94%)  | 44 (6%)  | 0        | 100         | 100 |
| All | All   | 9300/12684 (73%) | 8779 (94%) | 521 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | A     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | B     | 718/958 (75%)    | 717 (100%)  | 1 (0%)   | 88          | 87  |
| 1   | C     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | D     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | E     | 718/958 (75%)    | 717 (100%)  | 1 (0%)   | 88          | 87  |
| 1   | F     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | G     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | H     | 718/958 (75%)    | 717 (100%)  | 1 (0%)   | 88          | 87  |
| 1   | I     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | J     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| 1   | K     | 718/958 (75%)    | 717 (100%)  | 1 (0%)   | 88          | 87  |
| 1   | L     | 718/958 (75%)    | 718 (100%)  | 0        | 100         | 100 |
| All | All   | 8616/11496 (75%) | 8612 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 396 | GLN  |
| 1   | E     | 396 | GLN  |
| 1   | H     | 396 | GLN  |
| 1   | K     | 396 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 221 | GLN  |
| 1   | A     | 502 | ASN  |
| 1   | A     | 584 | GLN  |
| 1   | A     | 821 | HIS  |
| 1   | A     | 842 | GLN  |
| 1   | A     | 957 | ASN  |
| 1   | A     | 966 | HIS  |
| 1   | B     | 502 | ASN  |
| 1   | B     | 584 | GLN  |
| 1   | B     | 683 | HIS  |
| 1   | B     | 821 | HIS  |
| 1   | B     | 966 | HIS  |
| 1   | C     | 502 | ASN  |
| 1   | C     | 584 | GLN  |
| 1   | C     | 622 | GLN  |
| 1   | C     | 683 | HIS  |
| 1   | C     | 821 | HIS  |
| 1   | C     | 966 | HIS  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 502 | ASN  |
| 1   | D     | 584 | GLN  |
| 1   | D     | 821 | HIS  |
| 1   | D     | 842 | GLN  |
| 1   | E     | 221 | GLN  |
| 1   | E     | 502 | ASN  |
| 1   | E     | 584 | GLN  |
| 1   | E     | 683 | HIS  |
| 1   | E     | 821 | HIS  |
| 1   | E     | 966 | HIS  |
| 1   | F     | 502 | ASN  |
| 1   | F     | 584 | GLN  |
| 1   | F     | 600 | GLN  |
| 1   | F     | 622 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 683 | HIS  |
| 1   | F     | 821 | HIS  |
| 1   | F     | 842 | GLN  |
| 1   | F     | 966 | HIS  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 502 | ASN  |
| 1   | G     | 584 | GLN  |
| 1   | G     | 821 | HIS  |
| 1   | G     | 842 | GLN  |
| 1   | G     | 957 | ASN  |
| 1   | G     | 966 | HIS  |
| 1   | H     | 502 | ASN  |
| 1   | H     | 584 | GLN  |
| 1   | H     | 683 | HIS  |
| 1   | H     | 821 | HIS  |
| 1   | H     | 966 | HIS  |
| 1   | I     | 502 | ASN  |
| 1   | I     | 584 | GLN  |
| 1   | I     | 600 | GLN  |
| 1   | I     | 622 | GLN  |
| 1   | I     | 683 | HIS  |
| 1   | I     | 821 | HIS  |
| 1   | I     | 966 | HIS  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 502 | ASN  |
| 1   | J     | 584 | GLN  |
| 1   | J     | 821 | HIS  |
| 1   | J     | 842 | GLN  |
| 1   | K     | 221 | GLN  |
| 1   | K     | 502 | ASN  |
| 1   | K     | 584 | GLN  |
| 1   | K     | 683 | HIS  |
| 1   | K     | 821 | HIS  |
| 1   | K     | 966 | HIS  |
| 1   | L     | 502 | ASN  |
| 1   | L     | 584 | GLN  |
| 1   | L     | 600 | GLN  |
| 1   | L     | 622 | GLN  |
| 1   | L     | 683 | HIS  |
| 1   | L     | 821 | HIS  |
| 1   | L     | 842 | GLN  |
| 1   | L     | 966 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 976 | 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 ⓘ

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ADP  | I     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 2   | ADP  | K     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 3   | 7YN  | I     | 1502 | -    | 28,31,31     | 2.00 | 5 (17%)  | 33,48,48    | 2.06 | 10 (30%) |
| 3   | 7YN  | K     | 1502 | -    | 28,31,31     | 1.99 | 5 (17%)  | 33,48,48    | 2.05 | 10 (30%) |
| 3   | 7YN  | D     | 1502 | -    | 28,31,31     | 1.99 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 2   | ADP  | B     | 1501 | -    | 28,29,29     | 1.39 | 4 (14%)  | 43,45,45    | 1.87 | 8 (18%)  |
| 2   | ADP  | A     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.87 | 8 (18%)  |
| 2   | ADP  | C     | 1501 | -    | 28,29,29     | 1.41 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 3   | 7YN  | H     | 1502 | -    | 28,31,31     | 1.98 | 5 (17%)  | 33,48,48    | 2.05 | 10 (30%) |
| 2   | ADP  | H     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.87 | 8 (18%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | 7YN  | C     | 1502 | -    | 28,31,31     | 2.00 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 3   | 7YN  | A     | 1502 | -    | 28,31,31     | 1.99 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 2   | ADP  | J     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 3   | 7YN  | J     | 1502 | -    | 28,31,31     | 1.98 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 2   | ADP  | F     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 3   | 7YN  | F     | 1502 | -    | 28,31,31     | 2.01 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 2   | ADP  | G     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 3   | 7YN  | G     | 1502 | -    | 28,31,31     | 1.98 | 5 (17%)  | 33,48,48    | 2.05 | 11 (33%) |
| 3   | 7YN  | L     | 1502 | -    | 28,31,31     | 2.00 | 5 (17%)  | 33,48,48    | 2.06 | 11 (33%) |
| 3   | 7YN  | B     | 1502 | -    | 28,31,31     | 1.98 | 5 (17%)  | 33,48,48    | 2.05 | 10 (30%) |
| 2   | ADP  | E     | 1501 | -    | 28,29,29     | 1.41 | 4 (14%)  | 43,45,45    | 1.87 | 8 (18%)  |
| 2   | ADP  | L     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.88 | 8 (18%)  |
| 2   | ADP  | D     | 1501 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.87 | 8 (18%)  |
| 3   | 7YN  | E     | 1502 | -    | 28,31,31     | 1.98 | 5 (17%)  | 33,48,48    | 2.05 | 10 (30%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ADP  | I     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 2   | ADP  | K     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | I     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |
| 3   | 7YN  | K     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |
| 3   | 7YN  | D     | 1502 | -    | -       | 4/19/33/33 | 0/4/4/4 |
| 2   | ADP  | B     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 2   | ADP  | A     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 2   | ADP  | C     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | H     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |
| 2   | ADP  | H     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | C     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |
| 3   | 7YN  | A     | 1502 | -    | -       | 4/19/33/33 | 0/4/4/4 |
| 2   | ADP  | J     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | J     | 1502 | -    | -       | 4/19/33/33 | 0/4/4/4 |
| 2   | ADP  | F     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | F     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ADP  | G     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | G     | 1502 | -    | -       | 4/19/33/33 | 0/4/4/4 |
| 3   | 7YN  | L     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |
| 3   | 7YN  | B     | 1502 | -    | -       | 5/19/33/33 | 0/4/4/4 |
| 2   | ADP  | E     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 2   | ADP  | L     | 1501 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 2   | ADP  | D     | 1501 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 3   | 7YN  | E     | 1502 | -    | -       | 6/19/33/33 | 0/4/4/4 |

All (108) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | L     | 1502 | 7YN  | S17-N15 | 6.87 | 1.70        | 1.64     |
| 3   | F     | 1502 | 7YN  | S17-N15 | 6.85 | 1.70        | 1.64     |
| 3   | I     | 1502 | 7YN  | S17-N15 | 6.82 | 1.70        | 1.64     |
| 3   | G     | 1502 | 7YN  | S17-N15 | 6.81 | 1.70        | 1.64     |
| 3   | J     | 1502 | 7YN  | S17-N15 | 6.81 | 1.70        | 1.64     |
| 3   | A     | 1502 | 7YN  | S17-N15 | 6.79 | 1.70        | 1.64     |
| 3   | D     | 1502 | 7YN  | S17-N15 | 6.79 | 1.70        | 1.64     |
| 3   | H     | 1502 | 7YN  | S17-N15 | 6.78 | 1.70        | 1.64     |
| 3   | K     | 1502 | 7YN  | S17-N15 | 6.75 | 1.70        | 1.64     |
| 3   | C     | 1502 | 7YN  | S17-N15 | 6.75 | 1.70        | 1.64     |
| 3   | E     | 1502 | 7YN  | S17-N15 | 6.70 | 1.70        | 1.64     |
| 3   | B     | 1502 | 7YN  | S17-N15 | 6.66 | 1.70        | 1.64     |
| 2   | E     | 1501 | ADP  | C5-C4   | 4.75 | 1.47        | 1.39     |
| 2   | G     | 1501 | ADP  | C5-C4   | 4.75 | 1.47        | 1.39     |
| 2   | J     | 1501 | ADP  | C5-C4   | 4.75 | 1.47        | 1.39     |
| 2   | F     | 1501 | ADP  | C5-C4   | 4.74 | 1.47        | 1.39     |
| 2   | L     | 1501 | ADP  | C5-C4   | 4.74 | 1.47        | 1.39     |
| 2   | I     | 1501 | ADP  | C5-C4   | 4.74 | 1.47        | 1.39     |
| 2   | H     | 1501 | ADP  | C5-C4   | 4.74 | 1.47        | 1.39     |
| 2   | K     | 1501 | ADP  | C5-C4   | 4.73 | 1.47        | 1.39     |
| 2   | A     | 1501 | ADP  | C5-C4   | 4.72 | 1.47        | 1.39     |
| 2   | C     | 1501 | ADP  | C5-C4   | 4.72 | 1.47        | 1.39     |
| 2   | D     | 1501 | ADP  | C5-C4   | 4.72 | 1.47        | 1.39     |
| 2   | B     | 1501 | ADP  | C5-C4   | 4.69 | 1.47        | 1.39     |
| 3   | C     | 1502 | 7YN  | C14-N15 | 3.41 | 1.47        | 1.39     |
| 3   | F     | 1502 | 7YN  | C14-N15 | 3.38 | 1.46        | 1.39     |
| 3   | E     | 1502 | 7YN  | C14-N15 | 3.38 | 1.46        | 1.39     |
| 3   | I     | 1502 | 7YN  | C14-N15 | 3.37 | 1.46        | 1.39     |
| 3   | K     | 1502 | 7YN  | C14-N15 | 3.36 | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 1502 | 7YN  | C14-N15 | 3.35  | 1.46        | 1.39     |
| 3   | L     | 1502 | 7YN  | C14-N15 | 3.34  | 1.46        | 1.39     |
| 3   | H     | 1502 | 7YN  | C14-N15 | 3.32  | 1.46        | 1.39     |
| 3   | A     | 1502 | 7YN  | C14-N15 | 3.32  | 1.46        | 1.39     |
| 3   | D     | 1502 | 7YN  | C14-N15 | 3.32  | 1.46        | 1.39     |
| 3   | G     | 1502 | 7YN  | C14-N15 | 3.32  | 1.46        | 1.39     |
| 3   | J     | 1502 | 7YN  | C14-N15 | 3.32  | 1.46        | 1.39     |
| 3   | E     | 1502 | 7YN  | C24-C22 | -3.15 | 1.50        | 1.52     |
| 3   | G     | 1502 | 7YN  | C09-C08 | 3.14  | 1.53        | 1.36     |
| 3   | J     | 1502 | 7YN  | C09-C08 | 3.14  | 1.53        | 1.36     |
| 3   | B     | 1502 | 7YN  | C09-C08 | 3.14  | 1.53        | 1.36     |
| 3   | C     | 1502 | 7YN  | C24-C22 | -3.14 | 1.50        | 1.52     |
| 3   | I     | 1502 | 7YN  | C24-C22 | -3.14 | 1.50        | 1.52     |
| 3   | C     | 1502 | 7YN  | C09-C08 | 3.13  | 1.53        | 1.36     |
| 3   | H     | 1502 | 7YN  | C09-C08 | 3.13  | 1.53        | 1.36     |
| 3   | A     | 1502 | 7YN  | C09-C08 | 3.13  | 1.53        | 1.36     |
| 3   | D     | 1502 | 7YN  | C09-C08 | 3.13  | 1.53        | 1.36     |
| 3   | K     | 1502 | 7YN  | C09-C08 | 3.13  | 1.53        | 1.36     |
| 3   | E     | 1502 | 7YN  | C09-C08 | 3.12  | 1.53        | 1.36     |
| 3   | B     | 1502 | 7YN  | C24-C22 | -3.12 | 1.50        | 1.52     |
| 3   | B     | 1502 | 7YN  | O26-C24 | -3.12 | 1.40        | 1.43     |
| 3   | I     | 1502 | 7YN  | C09-C08 | 3.12  | 1.53        | 1.36     |
| 3   | F     | 1502 | 7YN  | C09-C08 | 3.12  | 1.53        | 1.36     |
| 3   | L     | 1502 | 7YN  | C09-C08 | 3.12  | 1.53        | 1.36     |
| 3   | C     | 1502 | 7YN  | O26-C24 | -3.11 | 1.40        | 1.43     |
| 3   | K     | 1502 | 7YN  | C24-C22 | -3.10 | 1.50        | 1.52     |
| 3   | F     | 1502 | 7YN  | C24-C22 | -3.10 | 1.50        | 1.52     |
| 3   | L     | 1502 | 7YN  | C24-C22 | -3.10 | 1.50        | 1.52     |
| 3   | H     | 1502 | 7YN  | O26-C24 | -3.09 | 1.40        | 1.43     |
| 3   | E     | 1502 | 7YN  | O26-C24 | -3.07 | 1.40        | 1.43     |
| 3   | K     | 1502 | 7YN  | O26-C24 | -3.07 | 1.40        | 1.43     |
| 3   | H     | 1502 | 7YN  | C24-C22 | -3.06 | 1.50        | 1.52     |
| 3   | F     | 1502 | 7YN  | O26-C24 | -3.05 | 1.40        | 1.43     |
| 3   | I     | 1502 | 7YN  | O26-C24 | -3.04 | 1.40        | 1.43     |
| 3   | G     | 1502 | 7YN  | O26-C24 | -3.04 | 1.40        | 1.43     |
| 3   | J     | 1502 | 7YN  | O26-C24 | -3.04 | 1.40        | 1.43     |
| 3   | A     | 1502 | 7YN  | C24-C22 | -3.03 | 1.50        | 1.52     |
| 3   | D     | 1502 | 7YN  | C24-C22 | -3.03 | 1.50        | 1.52     |
| 3   | L     | 1502 | 7YN  | O26-C24 | -3.02 | 1.40        | 1.43     |
| 3   | A     | 1502 | 7YN  | O26-C24 | -3.00 | 1.40        | 1.43     |
| 3   | D     | 1502 | 7YN  | O26-C24 | -3.00 | 1.40        | 1.43     |
| 3   | G     | 1502 | 7YN  | C24-C22 | -2.89 | 1.50        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | J     | 1502 | 7YN  | C24-C22 | -2.89 | 1.50        | 1.52     |
| 2   | A     | 1501 | ADP  | C5-C6   | 2.69  | 1.48        | 1.41     |
| 2   | D     | 1501 | ADP  | C5-C6   | 2.69  | 1.48        | 1.41     |
| 2   | E     | 1501 | ADP  | C5-C6   | 2.69  | 1.48        | 1.41     |
| 2   | H     | 1501 | ADP  | C5-C6   | 2.69  | 1.48        | 1.41     |
| 2   | B     | 1501 | ADP  | C5-C6   | 2.68  | 1.48        | 1.41     |
| 2   | K     | 1501 | ADP  | C5-C6   | 2.68  | 1.48        | 1.41     |
| 2   | C     | 1501 | ADP  | C5-C6   | 2.68  | 1.48        | 1.41     |
| 2   | I     | 1501 | ADP  | C5-C6   | 2.68  | 1.48        | 1.41     |
| 2   | L     | 1501 | ADP  | C5-C6   | 2.66  | 1.48        | 1.41     |
| 2   | G     | 1501 | ADP  | C5-C6   | 2.66  | 1.48        | 1.41     |
| 2   | J     | 1501 | ADP  | C5-C6   | 2.66  | 1.48        | 1.41     |
| 2   | F     | 1501 | ADP  | C5-C6   | 2.66  | 1.48        | 1.41     |
| 2   | E     | 1501 | ADP  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 2   | H     | 1501 | ADP  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 2   | C     | 1501 | ADP  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 2   | F     | 1501 | ADP  | C5-N7   | -2.35 | 1.34        | 1.39     |
| 2   | L     | 1501 | ADP  | C5-N7   | -2.34 | 1.34        | 1.39     |
| 2   | K     | 1501 | ADP  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 2   | I     | 1501 | ADP  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 2   | A     | 1501 | ADP  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 2   | D     | 1501 | ADP  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 2   | G     | 1501 | ADP  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 2   | J     | 1501 | ADP  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 2   | B     | 1501 | ADP  | C5-N7   | -2.29 | 1.34        | 1.39     |
| 2   | E     | 1501 | ADP  | C8-N7   | 2.25  | 1.36        | 1.31     |
| 2   | A     | 1501 | ADP  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 2   | D     | 1501 | ADP  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 2   | G     | 1501 | ADP  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 2   | J     | 1501 | ADP  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 2   | K     | 1501 | ADP  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 2   | H     | 1501 | ADP  | C8-N7   | 2.22  | 1.36        | 1.31     |
| 2   | L     | 1501 | ADP  | C8-N7   | 2.22  | 1.35        | 1.31     |
| 2   | C     | 1501 | ADP  | C8-N7   | 2.22  | 1.35        | 1.31     |
| 2   | F     | 1501 | ADP  | C8-N7   | 2.22  | 1.35        | 1.31     |
| 2   | I     | 1501 | ADP  | C8-N7   | 2.22  | 1.35        | 1.31     |
| 2   | B     | 1501 | ADP  | C8-N7   | 2.22  | 1.35        | 1.31     |

All (223) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 1501 | ADP  | C5-C4-N3 | -6.14 | 118.26      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | K     | 1501 | ADP  | C5-C4-N3    | -6.14 | 118.27      | 126.72   |
| 2   | H     | 1501 | ADP  | C5-C4-N3    | -6.12 | 118.29      | 126.72   |
| 2   | I     | 1501 | ADP  | C5-C4-N3    | -6.11 | 118.30      | 126.72   |
| 2   | E     | 1501 | ADP  | C5-C4-N3    | -6.11 | 118.30      | 126.72   |
| 2   | G     | 1501 | ADP  | C5-C4-N3    | -6.09 | 118.34      | 126.72   |
| 2   | J     | 1501 | ADP  | C5-C4-N3    | -6.09 | 118.34      | 126.72   |
| 2   | F     | 1501 | ADP  | C5-C4-N3    | -6.08 | 118.35      | 126.72   |
| 2   | L     | 1501 | ADP  | C5-C4-N3    | -6.07 | 118.35      | 126.72   |
| 2   | D     | 1501 | ADP  | C5-C4-N3    | -6.07 | 118.36      | 126.72   |
| 2   | C     | 1501 | ADP  | C5-C4-N3    | -6.07 | 118.36      | 126.72   |
| 2   | A     | 1501 | ADP  | C5-C4-N3    | -6.06 | 118.37      | 126.72   |
| 2   | K     | 1501 | ADP  | N3-C4-N9    | 4.97  | 135.62      | 127.17   |
| 2   | H     | 1501 | ADP  | N3-C4-N9    | 4.97  | 135.61      | 127.17   |
| 2   | I     | 1501 | ADP  | N3-C4-N9    | 4.96  | 135.61      | 127.17   |
| 2   | L     | 1501 | ADP  | N3-C4-N9    | 4.96  | 135.60      | 127.17   |
| 2   | E     | 1501 | ADP  | N3-C4-N9    | 4.96  | 135.60      | 127.17   |
| 2   | G     | 1501 | ADP  | N3-C4-N9    | 4.93  | 135.56      | 127.17   |
| 2   | J     | 1501 | ADP  | N3-C4-N9    | 4.93  | 135.56      | 127.17   |
| 2   | B     | 1501 | ADP  | N3-C4-N9    | 4.93  | 135.55      | 127.17   |
| 2   | C     | 1501 | ADP  | N3-C4-N9    | 4.93  | 135.55      | 127.17   |
| 2   | F     | 1501 | ADP  | N3-C4-N9    | 4.92  | 135.54      | 127.17   |
| 2   | D     | 1501 | ADP  | N3-C4-N9    | 4.92  | 135.53      | 127.17   |
| 2   | A     | 1501 | ADP  | N3-C4-N9    | 4.91  | 135.51      | 127.17   |
| 3   | L     | 1502 | 7YN  | C04-C02-C01 | -4.34 | 116.03      | 122.56   |
| 3   | I     | 1502 | 7YN  | C04-C02-C01 | -4.34 | 116.04      | 122.56   |
| 3   | F     | 1502 | 7YN  | C04-C02-C01 | -4.34 | 116.04      | 122.56   |
| 3   | B     | 1502 | 7YN  | C04-C02-C01 | -4.33 | 116.04      | 122.56   |
| 3   | K     | 1502 | 7YN  | C04-C02-C01 | -4.33 | 116.05      | 122.56   |
| 3   | C     | 1502 | 7YN  | C04-C02-C01 | -4.31 | 116.08      | 122.56   |
| 3   | G     | 1502 | 7YN  | C04-C02-C01 | -4.31 | 116.08      | 122.56   |
| 3   | J     | 1502 | 7YN  | C04-C02-C01 | -4.31 | 116.08      | 122.56   |
| 3   | E     | 1502 | 7YN  | C04-C02-C01 | -4.31 | 116.08      | 122.56   |
| 3   | H     | 1502 | 7YN  | C04-C02-C01 | -4.31 | 116.08      | 122.56   |
| 3   | A     | 1502 | 7YN  | C04-C02-C01 | -4.30 | 116.09      | 122.56   |
| 3   | D     | 1502 | 7YN  | C04-C02-C01 | -4.30 | 116.09      | 122.56   |
| 3   | E     | 1502 | 7YN  | C06-C05-C03 | -4.20 | 116.21      | 122.25   |
| 3   | K     | 1502 | 7YN  | C06-C05-C03 | -4.20 | 116.21      | 122.25   |
| 3   | H     | 1502 | 7YN  | C06-C05-C03 | -4.19 | 116.22      | 122.25   |
| 3   | I     | 1502 | 7YN  | C06-C05-C03 | -4.19 | 116.22      | 122.25   |
| 3   | L     | 1502 | 7YN  | C06-C05-C03 | -4.18 | 116.24      | 122.25   |
| 3   | F     | 1502 | 7YN  | C06-C05-C03 | -4.17 | 116.25      | 122.25   |
| 3   | B     | 1502 | 7YN  | C06-C05-C03 | -4.17 | 116.25      | 122.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | C     | 1502 | 7YN  | C06-C05-C03 | -4.17 | 116.25      | 122.25   |
| 3   | A     | 1502 | 7YN  | C06-C05-C03 | -4.16 | 116.26      | 122.25   |
| 3   | D     | 1502 | 7YN  | C06-C05-C03 | -4.16 | 116.26      | 122.25   |
| 3   | G     | 1502 | 7YN  | C06-C05-C03 | -4.16 | 116.27      | 122.25   |
| 3   | J     | 1502 | 7YN  | C06-C05-C03 | -4.16 | 116.27      | 122.25   |
| 3   | F     | 1502 | 7YN  | C27-C24-C25 | -3.72 | 107.43      | 111.06   |
| 2   | G     | 1501 | ADP  | C2-N3-C4    | 3.72  | 120.91      | 111.83   |
| 2   | J     | 1501 | ADP  | C2-N3-C4    | 3.72  | 120.91      | 111.83   |
| 3   | I     | 1502 | 7YN  | C27-C24-C25 | -3.72 | 107.43      | 111.06   |
| 2   | C     | 1501 | ADP  | C2-N3-C4    | 3.71  | 120.90      | 111.83   |
| 2   | I     | 1501 | ADP  | C2-N3-C4    | 3.71  | 120.89      | 111.83   |
| 3   | B     | 1502 | 7YN  | C27-C24-C25 | -3.71 | 107.44      | 111.06   |
| 3   | C     | 1502 | 7YN  | C27-C24-C25 | -3.71 | 107.44      | 111.06   |
| 2   | K     | 1501 | ADP  | C2-N3-C4    | 3.71  | 120.88      | 111.83   |
| 3   | G     | 1502 | 7YN  | C27-C24-C25 | -3.70 | 107.45      | 111.06   |
| 3   | J     | 1502 | 7YN  | C27-C24-C25 | -3.70 | 107.45      | 111.06   |
| 2   | L     | 1501 | ADP  | C2-N3-C4    | 3.70  | 120.87      | 111.83   |
| 2   | A     | 1501 | ADP  | C2-N3-C4    | 3.70  | 120.86      | 111.83   |
| 2   | F     | 1501 | ADP  | C2-N3-C4    | 3.70  | 120.86      | 111.83   |
| 2   | H     | 1501 | ADP  | C2-N3-C4    | 3.70  | 120.86      | 111.83   |
| 3   | A     | 1502 | 7YN  | C27-C24-C25 | -3.70 | 107.45      | 111.06   |
| 3   | D     | 1502 | 7YN  | C27-C24-C25 | -3.70 | 107.45      | 111.06   |
| 2   | D     | 1501 | ADP  | C2-N3-C4    | 3.69  | 120.85      | 111.83   |
| 2   | E     | 1501 | ADP  | C2-N3-C4    | 3.69  | 120.84      | 111.83   |
| 3   | L     | 1502 | 7YN  | C27-C24-C25 | -3.69 | 107.46      | 111.06   |
| 2   | B     | 1501 | ADP  | C2-N3-C4    | 3.68  | 120.83      | 111.83   |
| 3   | K     | 1502 | 7YN  | C27-C24-C25 | -3.68 | 107.47      | 111.06   |
| 3   | H     | 1502 | 7YN  | C27-C24-C25 | -3.66 | 107.49      | 111.06   |
| 3   | E     | 1502 | 7YN  | C27-C24-C25 | -3.65 | 107.49      | 111.06   |
| 3   | H     | 1502 | 7YN  | C02-N13-C14 | 3.49  | 127.47      | 121.95   |
| 3   | E     | 1502 | 7YN  | C02-N13-C14 | 3.49  | 127.46      | 121.95   |
| 3   | B     | 1502 | 7YN  | C02-N13-C14 | 3.47  | 127.43      | 121.95   |
| 3   | K     | 1502 | 7YN  | C02-N13-C14 | 3.46  | 127.41      | 121.95   |
| 3   | I     | 1502 | 7YN  | C02-N13-C14 | 3.45  | 127.40      | 121.95   |
| 2   | G     | 1501 | ADP  | C4-C5-N7    | -3.41 | 106.69      | 110.58   |
| 2   | J     | 1501 | ADP  | C4-C5-N7    | -3.41 | 106.69      | 110.58   |
| 3   | F     | 1502 | 7YN  | C02-N13-C14 | 3.40  | 127.33      | 121.95   |
| 2   | A     | 1501 | ADP  | C4-C5-N7    | -3.40 | 106.69      | 110.58   |
| 2   | D     | 1501 | ADP  | C4-C5-N7    | -3.40 | 106.69      | 110.58   |
| 2   | F     | 1501 | ADP  | C4-C5-N7    | -3.40 | 106.70      | 110.58   |
| 2   | B     | 1501 | ADP  | C4-C5-N7    | -3.40 | 106.70      | 110.58   |
| 2   | I     | 1501 | ADP  | C4-C5-N7    | -3.39 | 106.71      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L     | 1502 | 7YN  | C02-N13-C14 | 3.39  | 127.30      | 121.95   |
| 3   | K     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.67      | 133.20   |
| 3   | E     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.68      | 133.20   |
| 2   | C     | 1501 | ADP  | C4-C5-N7    | -3.37 | 106.73      | 110.58   |
| 3   | C     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.69      | 133.20   |
| 2   | K     | 1501 | ADP  | C4-C5-N7    | -3.37 | 106.73      | 110.58   |
| 3   | A     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.69      | 133.20   |
| 3   | D     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.69      | 133.20   |
| 3   | I     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.70      | 133.20   |
| 3   | L     | 1502 | 7YN  | C05-C06-C09 | -3.37 | 123.70      | 133.20   |
| 2   | L     | 1501 | ADP  | C4-C5-N7    | -3.36 | 106.73      | 110.58   |
| 2   | H     | 1501 | ADP  | C4-C5-N7    | -3.36 | 106.74      | 110.58   |
| 3   | C     | 1502 | 7YN  | C02-N13-C14 | 3.36  | 127.26      | 121.95   |
| 3   | F     | 1502 | 7YN  | C05-C06-C09 | -3.36 | 123.72      | 133.20   |
| 3   | B     | 1502 | 7YN  | C05-C06-C09 | -3.36 | 123.73      | 133.20   |
| 2   | E     | 1501 | ADP  | C4-C5-N7    | -3.35 | 106.75      | 110.58   |
| 3   | H     | 1502 | 7YN  | C05-C06-C09 | -3.35 | 123.73      | 133.20   |
| 3   | G     | 1502 | 7YN  | C05-C06-C09 | -3.35 | 123.75      | 133.20   |
| 3   | J     | 1502 | 7YN  | C05-C06-C09 | -3.35 | 123.75      | 133.20   |
| 3   | A     | 1502 | 7YN  | C02-N13-C14 | 3.31  | 127.19      | 121.95   |
| 3   | D     | 1502 | 7YN  | C02-N13-C14 | 3.31  | 127.19      | 121.95   |
| 3   | G     | 1502 | 7YN  | C02-N13-C14 | 3.29  | 127.16      | 121.95   |
| 3   | J     | 1502 | 7YN  | C02-N13-C14 | 3.29  | 127.16      | 121.95   |
| 3   | G     | 1502 | 7YN  | C12-C03-C01 | 3.11  | 112.88      | 110.27   |
| 3   | J     | 1502 | 7YN  | C12-C03-C01 | 3.11  | 112.88      | 110.27   |
| 2   | C     | 1501 | ADP  | N3-C2-N1    | -3.11 | 123.88      | 128.58   |
| 2   | F     | 1501 | ADP  | N3-C2-N1    | -3.10 | 123.89      | 128.58   |
| 3   | C     | 1502 | 7YN  | C12-C03-C01 | 3.09  | 112.87      | 110.27   |
| 2   | G     | 1501 | ADP  | N3-C2-N1    | -3.09 | 123.90      | 128.58   |
| 2   | J     | 1501 | ADP  | N3-C2-N1    | -3.09 | 123.90      | 128.58   |
| 3   | L     | 1502 | 7YN  | C12-C03-C01 | 3.09  | 112.86      | 110.27   |
| 2   | L     | 1501 | ADP  | N3-C2-N1    | -3.08 | 123.91      | 128.58   |
| 2   | A     | 1501 | ADP  | N3-C2-N1    | -3.08 | 123.92      | 128.58   |
| 2   | I     | 1501 | ADP  | N3-C2-N1    | -3.08 | 123.92      | 128.58   |
| 3   | F     | 1502 | 7YN  | C12-C03-C01 | 3.07  | 112.85      | 110.27   |
| 3   | I     | 1502 | 7YN  | C12-C03-C01 | 3.07  | 112.85      | 110.27   |
| 3   | H     | 1502 | 7YN  | C12-C03-C01 | 3.07  | 112.84      | 110.27   |
| 2   | D     | 1501 | ADP  | N3-C2-N1    | -3.06 | 123.94      | 128.58   |
| 3   | E     | 1502 | 7YN  | C12-C03-C01 | 3.06  | 112.83      | 110.27   |
| 2   | K     | 1501 | ADP  | N3-C2-N1    | -3.06 | 123.96      | 128.58   |
| 3   | K     | 1502 | 7YN  | C12-C03-C01 | 3.04  | 112.82      | 110.27   |
| 3   | B     | 1502 | 7YN  | C12-C03-C01 | 3.04  | 112.82      | 110.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 1501 | ADP  | N3-C2-N1    | -3.04 | 123.98      | 128.58   |
| 2   | H     | 1501 | ADP  | N3-C2-N1    | -3.03 | 124.00      | 128.58   |
| 3   | A     | 1502 | 7YN  | C12-C03-C01 | 3.02  | 112.81      | 110.27   |
| 3   | D     | 1502 | 7YN  | C12-C03-C01 | 3.02  | 112.81      | 110.27   |
| 2   | E     | 1501 | ADP  | N3-C2-N1    | -3.02 | 124.01      | 128.58   |
| 3   | I     | 1502 | 7YN  | C05-C03-C01 | 2.79  | 122.52      | 120.52   |
| 3   | F     | 1502 | 7YN  | C05-C03-C01 | 2.78  | 122.51      | 120.52   |
| 3   | B     | 1502 | 7YN  | C05-C03-C01 | 2.77  | 122.50      | 120.52   |
| 3   | H     | 1502 | 7YN  | C05-C03-C01 | 2.77  | 122.50      | 120.52   |
| 3   | K     | 1502 | 7YN  | C05-C03-C01 | 2.77  | 122.50      | 120.52   |
| 3   | E     | 1502 | 7YN  | C05-C03-C01 | 2.77  | 122.50      | 120.52   |
| 3   | A     | 1502 | 7YN  | C05-C03-C01 | 2.73  | 122.47      | 120.52   |
| 3   | D     | 1502 | 7YN  | C05-C03-C01 | 2.73  | 122.47      | 120.52   |
| 3   | L     | 1502 | 7YN  | C05-C03-C01 | 2.73  | 122.47      | 120.52   |
| 3   | C     | 1502 | 7YN  | C05-C03-C01 | 2.72  | 122.47      | 120.52   |
| 3   | G     | 1502 | 7YN  | C05-C03-C01 | 2.71  | 122.46      | 120.52   |
| 3   | J     | 1502 | 7YN  | C05-C03-C01 | 2.71  | 122.46      | 120.52   |
| 2   | H     | 1501 | ADP  | C3'-C2'-C1' | 2.68  | 106.53      | 101.46   |
| 2   | G     | 1501 | ADP  | C4-N9-C8    | 2.67  | 108.54      | 105.74   |
| 2   | J     | 1501 | ADP  | C4-N9-C8    | 2.67  | 108.54      | 105.74   |
| 2   | F     | 1501 | ADP  | C3'-C2'-C1' | 2.67  | 106.51      | 101.46   |
| 2   | L     | 1501 | ADP  | C4-N9-C8    | 2.66  | 108.53      | 105.74   |
| 2   | C     | 1501 | ADP  | C3'-C2'-C1' | 2.66  | 106.49      | 101.46   |
| 2   | A     | 1501 | ADP  | C4-N9-C8    | 2.65  | 108.52      | 105.74   |
| 2   | D     | 1501 | ADP  | C4-N9-C8    | 2.65  | 108.52      | 105.74   |
| 2   | L     | 1501 | ADP  | C3'-C2'-C1' | 2.65  | 106.48      | 101.46   |
| 2   | I     | 1501 | ADP  | C3'-C2'-C1' | 2.65  | 106.47      | 101.46   |
| 2   | I     | 1501 | ADP  | C4-N9-C8    | 2.64  | 108.52      | 105.74   |
| 2   | G     | 1501 | ADP  | C3'-C2'-C1' | 2.64  | 106.45      | 101.46   |
| 2   | J     | 1501 | ADP  | C3'-C2'-C1' | 2.64  | 106.45      | 101.46   |
| 2   | F     | 1501 | ADP  | C4-N9-C8    | 2.63  | 108.50      | 105.74   |
| 2   | D     | 1501 | ADP  | C3'-C2'-C1' | 2.62  | 106.43      | 101.46   |
| 2   | B     | 1501 | ADP  | C3'-C2'-C1' | 2.62  | 106.42      | 101.46   |
| 2   | C     | 1501 | ADP  | C4-N9-C8    | 2.62  | 108.49      | 105.74   |
| 2   | A     | 1501 | ADP  | C3'-C2'-C1' | 2.62  | 106.41      | 101.46   |
| 2   | E     | 1501 | ADP  | C3'-C2'-C1' | 2.61  | 106.41      | 101.46   |
| 2   | K     | 1501 | ADP  | C3'-C2'-C1' | 2.61  | 106.41      | 101.46   |
| 2   | E     | 1501 | ADP  | C4-N9-C8    | 2.61  | 108.48      | 105.74   |
| 3   | I     | 1502 | 7YN  | C12-C03-C05 | -2.61 | 124.64      | 129.31   |
| 3   | F     | 1502 | 7YN  | C12-C03-C05 | -2.60 | 124.64      | 129.31   |
| 3   | H     | 1502 | 7YN  | C12-C03-C05 | -2.60 | 124.65      | 129.31   |
| 3   | G     | 1502 | 7YN  | C12-C03-C05 | -2.60 | 124.66      | 129.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | J     | 1502 | 7YN  | C12-C03-C05 | -2.60 | 124.66      | 129.31   |
| 2   | K     | 1501 | ADP  | C4-N9-C8    | 2.59  | 108.46      | 105.74   |
| 3   | L     | 1502 | 7YN  | C12-C03-C05 | -2.59 | 124.66      | 129.31   |
| 3   | C     | 1502 | 7YN  | C12-C03-C05 | -2.59 | 124.67      | 129.31   |
| 3   | E     | 1502 | 7YN  | C12-C03-C05 | -2.59 | 124.67      | 129.31   |
| 3   | B     | 1502 | 7YN  | C12-C03-C05 | -2.59 | 124.67      | 129.31   |
| 3   | K     | 1502 | 7YN  | C12-C03-C05 | -2.58 | 124.68      | 129.31   |
| 2   | H     | 1501 | ADP  | C4-N9-C8    | 2.57  | 108.44      | 105.74   |
| 2   | F     | 1501 | ADP  | C5-N7-C8    | 2.57  | 107.48      | 103.45   |
| 3   | A     | 1502 | 7YN  | C12-C03-C05 | -2.56 | 124.72      | 129.31   |
| 3   | D     | 1502 | 7YN  | C12-C03-C05 | -2.56 | 124.72      | 129.31   |
| 2   | B     | 1501 | ADP  | C4-N9-C8    | 2.55  | 108.42      | 105.74   |
| 2   | A     | 1501 | ADP  | C5-N7-C8    | 2.54  | 107.44      | 103.45   |
| 2   | D     | 1501 | ADP  | C5-N7-C8    | 2.54  | 107.44      | 103.45   |
| 2   | G     | 1501 | ADP  | C5-N7-C8    | 2.54  | 107.44      | 103.45   |
| 2   | J     | 1501 | ADP  | C5-N7-C8    | 2.54  | 107.44      | 103.45   |
| 2   | H     | 1501 | ADP  | C5-N7-C8    | 2.54  | 107.44      | 103.45   |
| 2   | C     | 1501 | ADP  | C5-N7-C8    | 2.53  | 107.43      | 103.45   |
| 2   | E     | 1501 | ADP  | C5-N7-C8    | 2.53  | 107.42      | 103.45   |
| 2   | L     | 1501 | ADP  | C5-N7-C8    | 2.53  | 107.42      | 103.45   |
| 2   | I     | 1501 | ADP  | C5-N7-C8    | 2.52  | 107.42      | 103.45   |
| 2   | K     | 1501 | ADP  | C5-N7-C8    | 2.52  | 107.41      | 103.45   |
| 2   | B     | 1501 | ADP  | C5-N7-C8    | 2.52  | 107.40      | 103.45   |
| 3   | A     | 1502 | 7YN  | N15-C14-N13 | 2.38  | 118.66      | 114.87   |
| 3   | D     | 1502 | 7YN  | N15-C14-N13 | 2.38  | 118.66      | 114.87   |
| 3   | G     | 1502 | 7YN  | N15-C14-N13 | 2.36  | 118.62      | 114.87   |
| 3   | J     | 1502 | 7YN  | N15-C14-N13 | 2.36  | 118.62      | 114.87   |
| 3   | L     | 1502 | 7YN  | N15-C14-N13 | 2.36  | 118.62      | 114.87   |
| 3   | C     | 1502 | 7YN  | N15-C14-N13 | 2.33  | 118.57      | 114.87   |
| 3   | A     | 1502 | 7YN  | C24-C22-C20 | 2.32  | 129.81      | 125.27   |
| 3   | D     | 1502 | 7YN  | C24-C22-C20 | 2.32  | 129.81      | 125.27   |
| 3   | I     | 1502 | 7YN  | C24-C22-C20 | 2.31  | 129.80      | 125.27   |
| 3   | G     | 1502 | 7YN  | C24-C22-C20 | 2.31  | 129.79      | 125.27   |
| 3   | J     | 1502 | 7YN  | C24-C22-C20 | 2.31  | 129.79      | 125.27   |
| 3   | F     | 1502 | 7YN  | N15-C14-N13 | 2.31  | 118.54      | 114.87   |
| 3   | I     | 1502 | 7YN  | N15-C14-N13 | 2.30  | 118.53      | 114.87   |
| 3   | H     | 1502 | 7YN  | C24-C22-C20 | 2.30  | 129.78      | 125.27   |
| 3   | E     | 1502 | 7YN  | C24-C22-C20 | 2.30  | 129.77      | 125.27   |
| 3   | K     | 1502 | 7YN  | C24-C22-C20 | 2.29  | 129.76      | 125.27   |
| 3   | L     | 1502 | 7YN  | C24-C22-C20 | 2.29  | 129.76      | 125.27   |
| 3   | B     | 1502 | 7YN  | C24-C22-C20 | 2.28  | 129.74      | 125.27   |
| 3   | C     | 1502 | 7YN  | C24-C22-C20 | 2.27  | 129.71      | 125.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | F     | 1502 | 7YN  | C24-C22-C20 | 2.27 | 129.71      | 125.27   |
| 3   | B     | 1502 | 7YN  | N15-C14-N13 | 2.25 | 118.44      | 114.87   |
| 3   | H     | 1502 | 7YN  | N15-C14-N13 | 2.24 | 118.43      | 114.87   |
| 3   | K     | 1502 | 7YN  | N15-C14-N13 | 2.23 | 118.42      | 114.87   |
| 3   | E     | 1502 | 7YN  | N15-C14-N13 | 2.22 | 118.40      | 114.87   |
| 3   | G     | 1502 | 7YN  | C11-C10-C01 | 2.03 | 106.12      | 103.57   |
| 3   | J     | 1502 | 7YN  | C11-C10-C01 | 2.03 | 106.12      | 103.57   |
| 3   | L     | 1502 | 7YN  | C11-C10-C01 | 2.02 | 106.11      | 103.57   |
| 3   | C     | 1502 | 7YN  | C11-C10-C01 | 2.02 | 106.11      | 103.57   |
| 3   | F     | 1502 | 7YN  | C11-C10-C01 | 2.02 | 106.11      | 103.57   |
| 3   | A     | 1502 | 7YN  | C11-C10-C01 | 2.01 | 106.10      | 103.57   |
| 3   | D     | 1502 | 7YN  | C11-C10-C01 | 2.01 | 106.10      | 103.57   |

There are no chirality outliers.

All (69) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | B     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | C     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | D     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | E     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | F     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | G     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | H     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | I     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | J     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | K     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | L     | 1502 | 7YN  | C20-C19-S17-N15 |
| 3   | A     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | B     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | C     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | D     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | E     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | F     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | G     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | H     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | I     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | J     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | K     | 1502 | 7YN  | C23-C22-C24-C25 |
| 3   | L     | 1502 | 7YN  | C23-C22-C24-C25 |
| 2   | A     | 1501 | ADP  | C5'-O5'-PA-O1A  |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 1501 | ADP  | C5'-O5'-PA-O1A  |
| 2   | C     | 1501 | ADP  | C5'-O5'-PA-O1A  |
| 2   | D     | 1501 | ADP  | C5'-O5'-PA-O1A  |
| 2   | E     | 1501 | ADP  | C5'-O5'-PA-O1A  |
| 2   | F     | 1501 | ADP  | C5'-O5'-PA-O1A  |
| 3   | A     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | B     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | C     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | D     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | E     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | F     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | G     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | H     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | I     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | J     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | K     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | L     | 1502 | 7YN  | C20-C19-S17-O28 |
| 3   | B     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | E     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | H     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | I     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | K     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | B     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | C     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | E     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | F     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | H     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | K     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | L     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | C     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | E     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | F     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | H     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | I     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | K     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | L     | 1502 | 7YN  | C20-C19-S17-O18 |
| 3   | A     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | C     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | D     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | F     | 1502 | 7YN  | C20-C22-C24-C25 |
| 3   | G     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | I     | 1502 | 7YN  | C20-C22-C24-C25 |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | J     | 1502 | 7YN  | C20-C22-C24-C27 |
| 3   | L     | 1502 | 7YN  | C20-C22-C24-C25 |

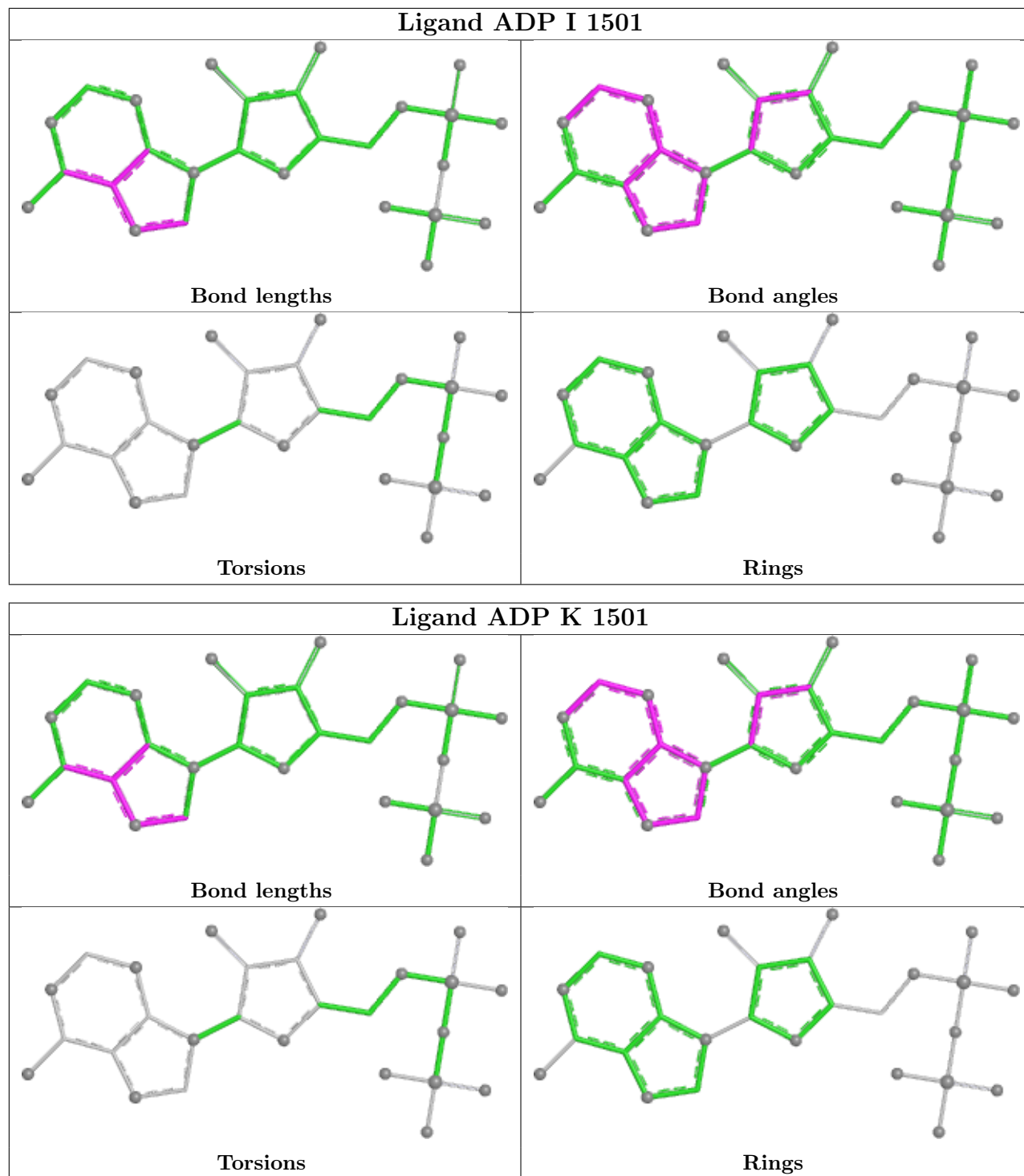
There are no ring outliers.

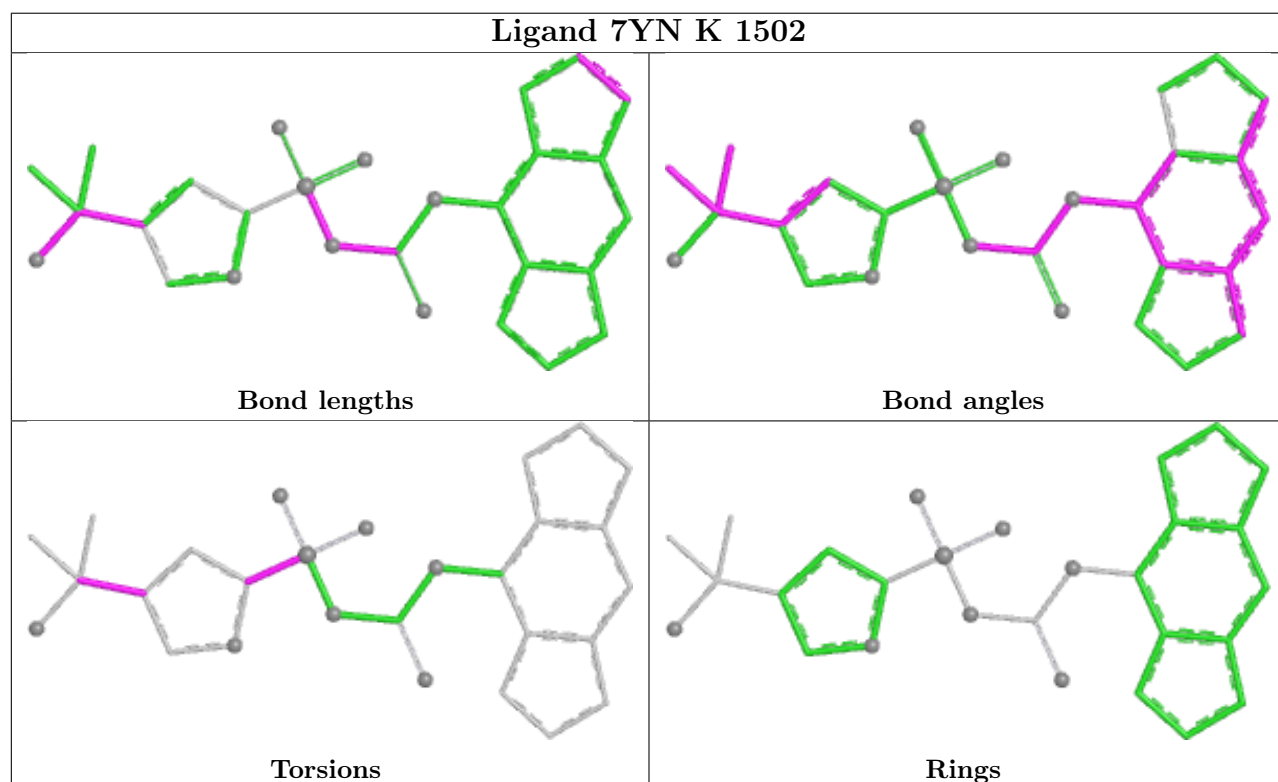
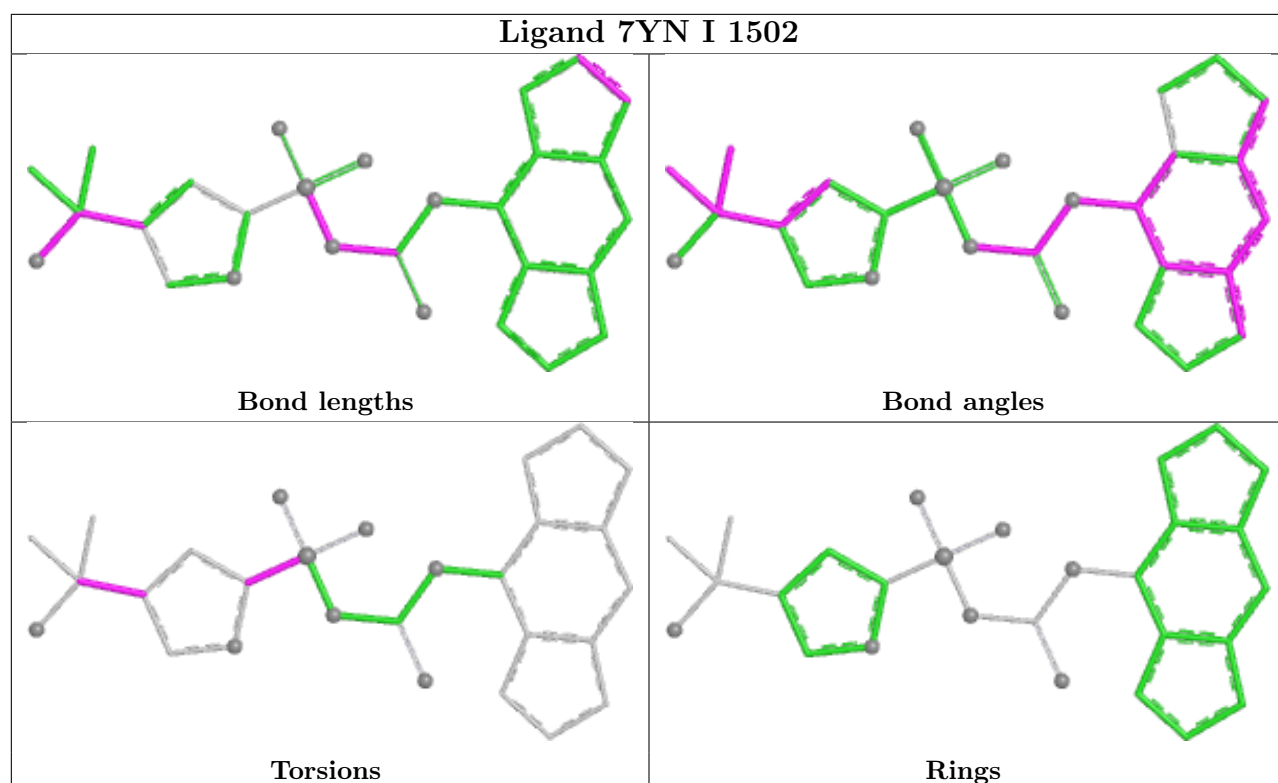
23 monomers are involved in 55 short contacts:

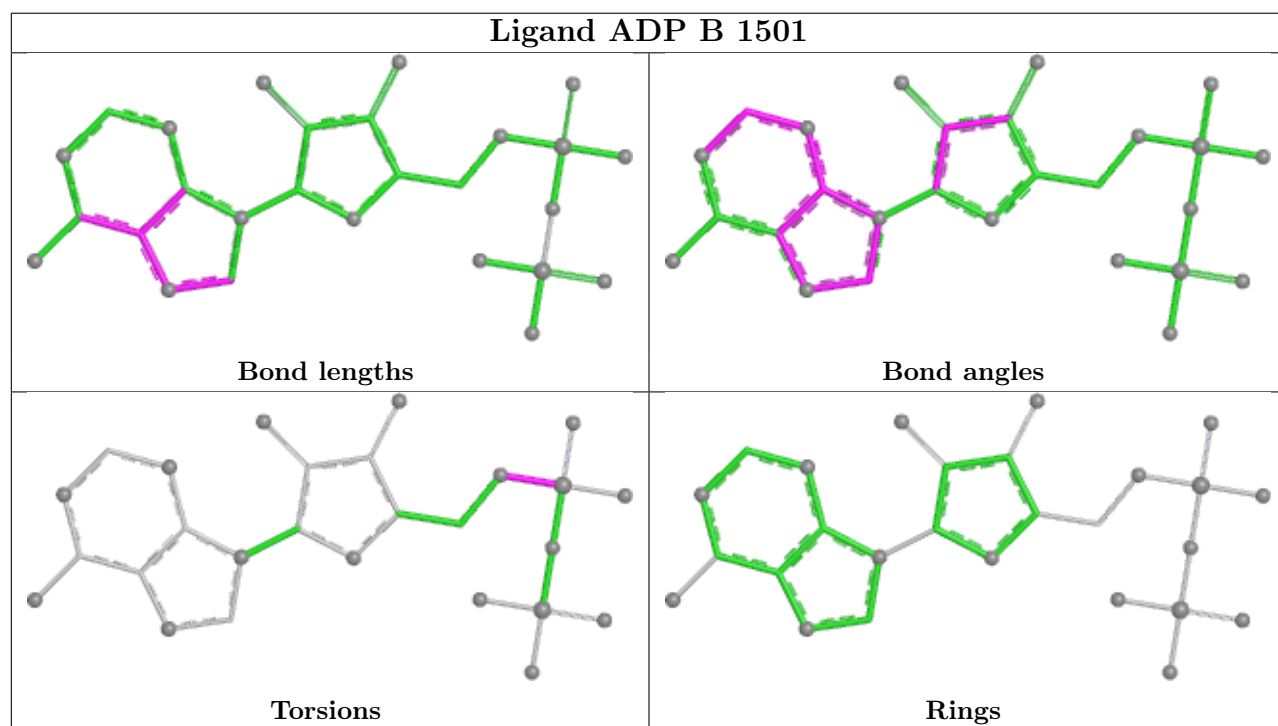
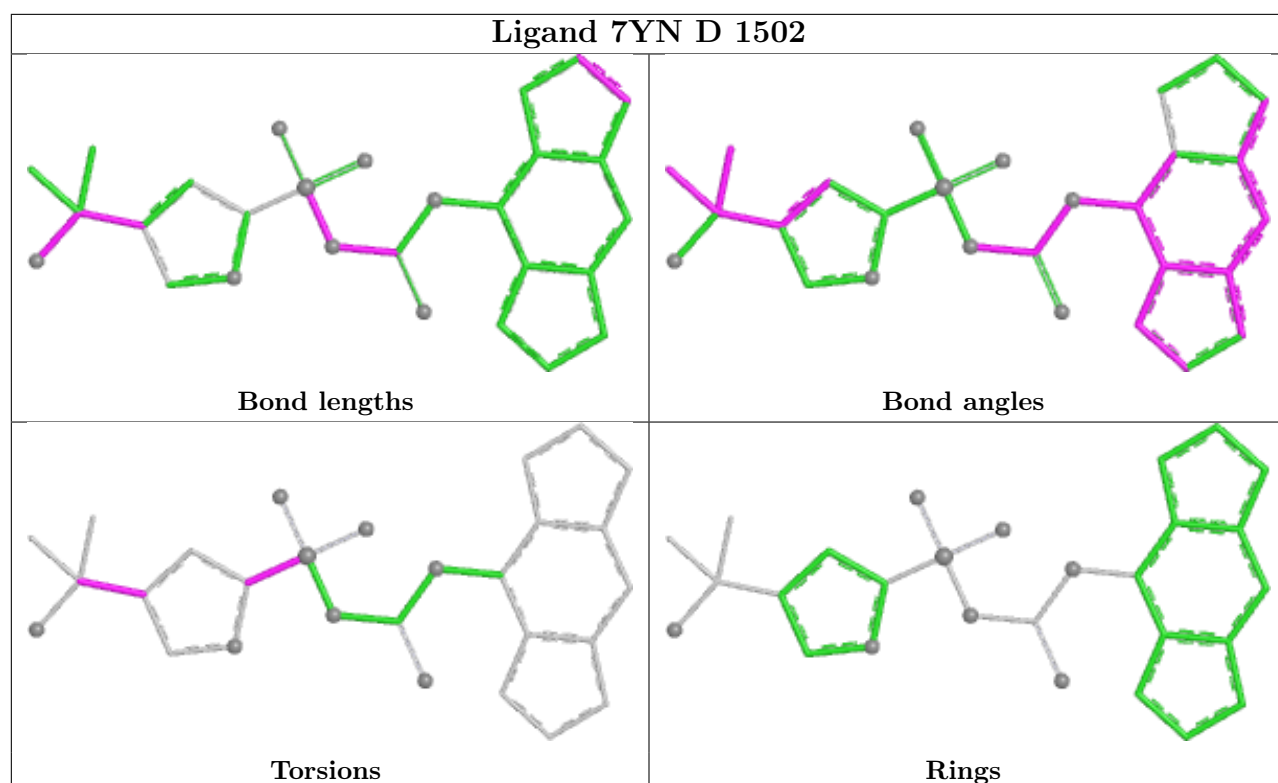
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | I     | 1501 | ADP  | 4       | 0            |
| 2   | K     | 1501 | ADP  | 3       | 0            |
| 3   | I     | 1502 | 7YN  | 1       | 0            |
| 3   | K     | 1502 | 7YN  | 1       | 0            |
| 2   | B     | 1501 | ADP  | 3       | 0            |
| 2   | A     | 1501 | ADP  | 4       | 0            |
| 2   | C     | 1501 | ADP  | 4       | 0            |
| 3   | H     | 1502 | 7YN  | 1       | 0            |
| 2   | H     | 1501 | ADP  | 3       | 0            |
| 3   | C     | 1502 | 7YN  | 1       | 0            |
| 3   | A     | 1502 | 7YN  | 1       | 0            |
| 2   | J     | 1501 | ADP  | 4       | 0            |
| 3   | J     | 1502 | 7YN  | 1       | 0            |
| 2   | F     | 1501 | ADP  | 4       | 0            |
| 3   | F     | 1502 | 7YN  | 1       | 0            |
| 2   | G     | 1501 | ADP  | 4       | 0            |
| 3   | G     | 1502 | 7YN  | 1       | 0            |
| 3   | L     | 1502 | 7YN  | 1       | 0            |
| 3   | B     | 1502 | 7YN  | 1       | 0            |
| 2   | E     | 1501 | ADP  | 3       | 0            |
| 2   | L     | 1501 | ADP  | 4       | 0            |
| 2   | D     | 1501 | ADP  | 4       | 0            |
| 3   | E     | 1502 | 7YN  | 1       | 0            |

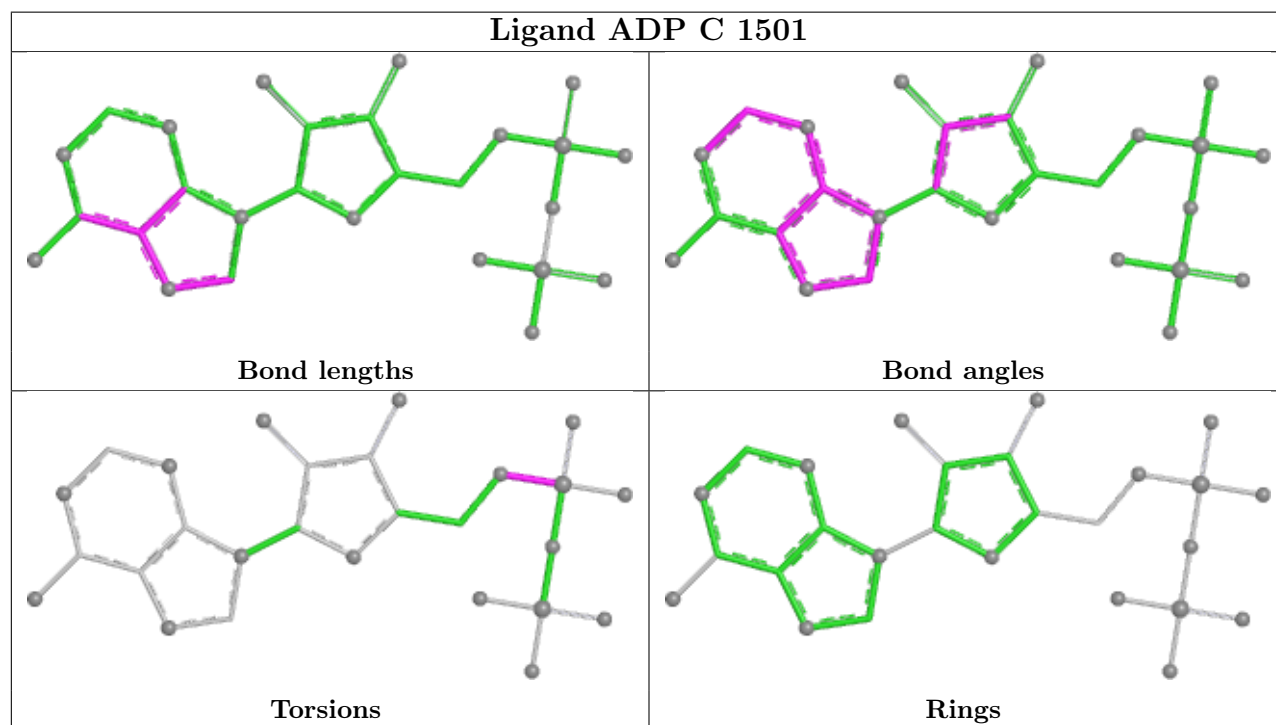
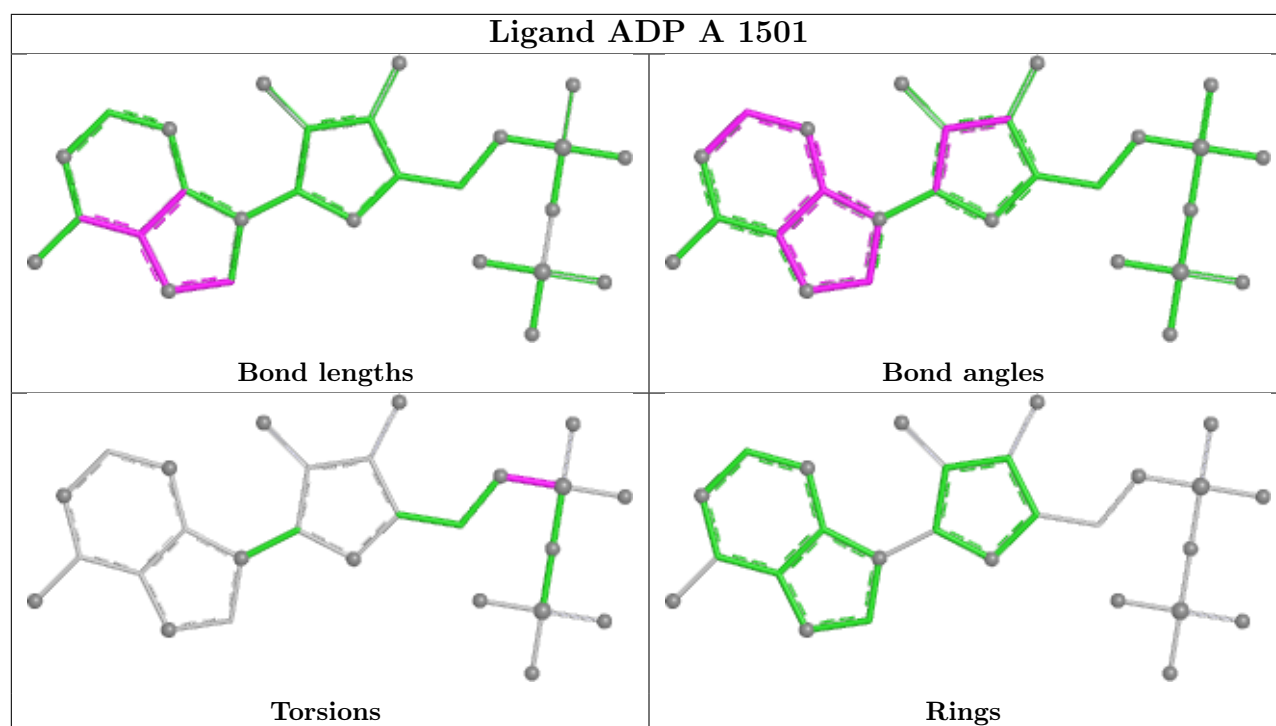
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

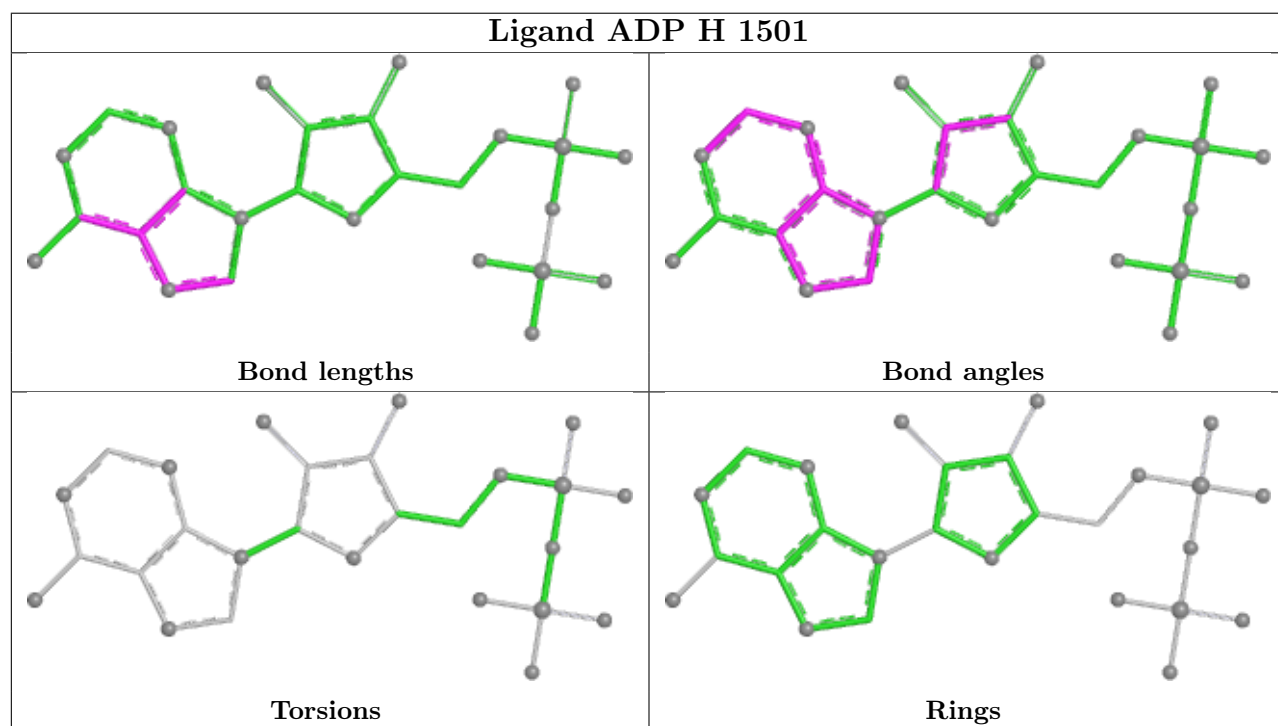
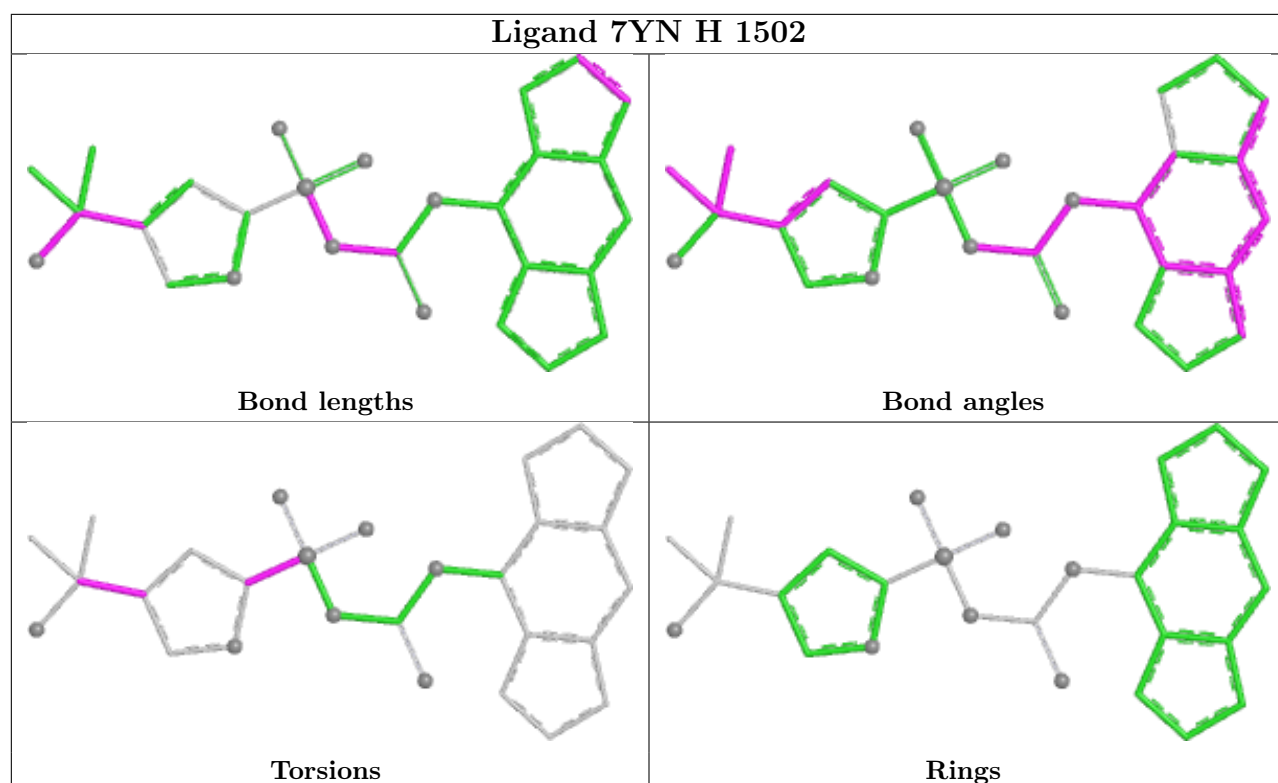
equivalents in the CSD to analyse the geometry.

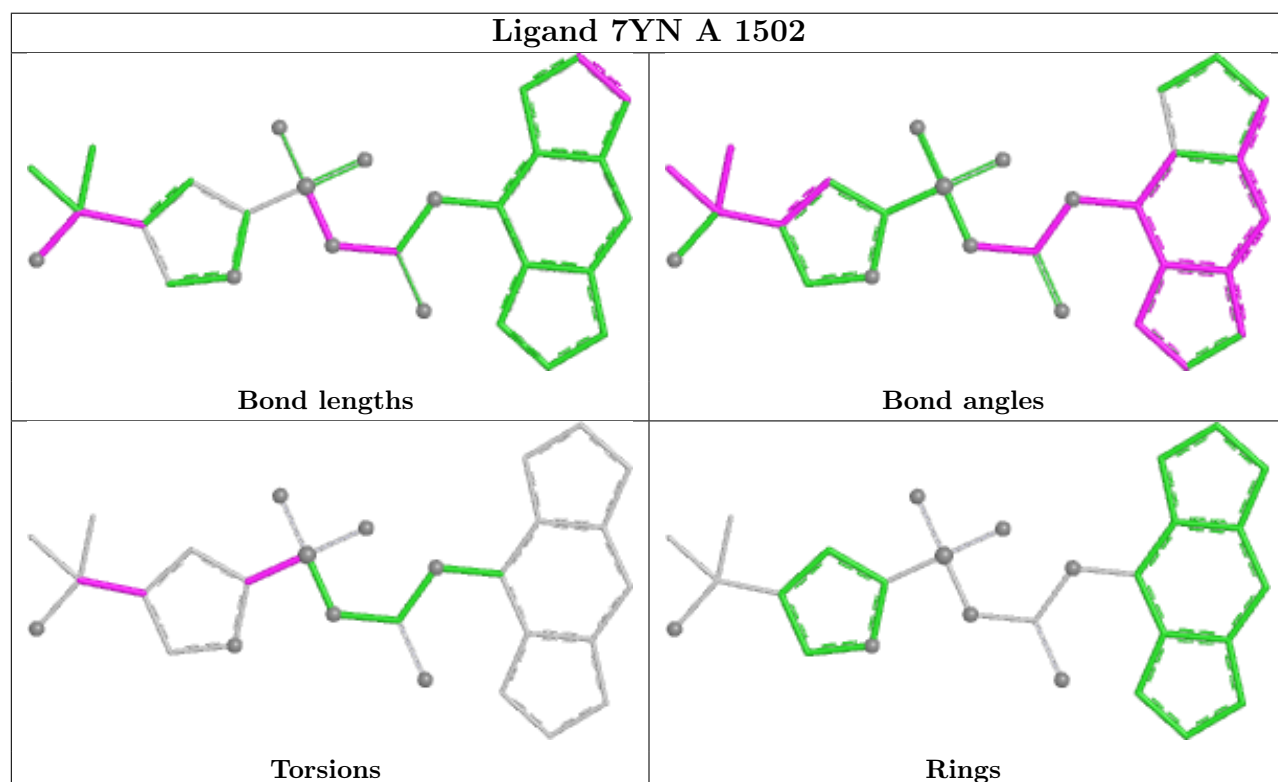
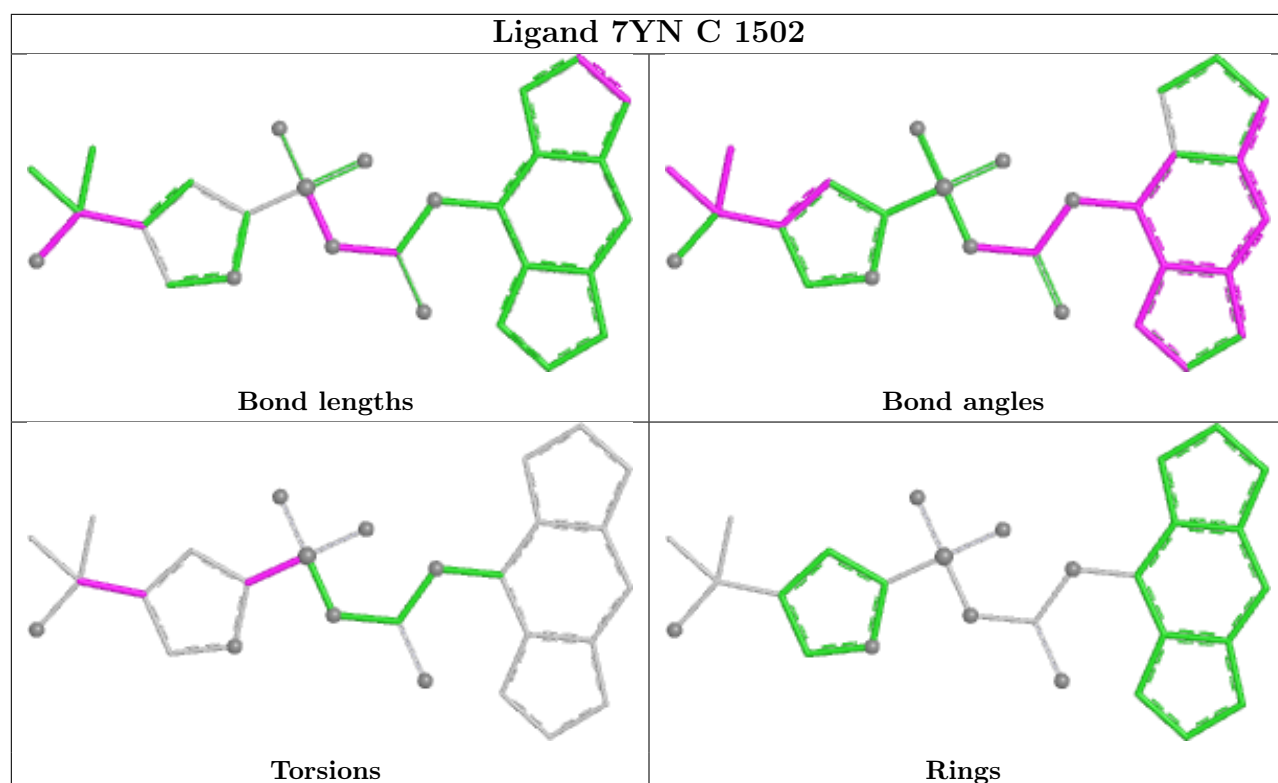


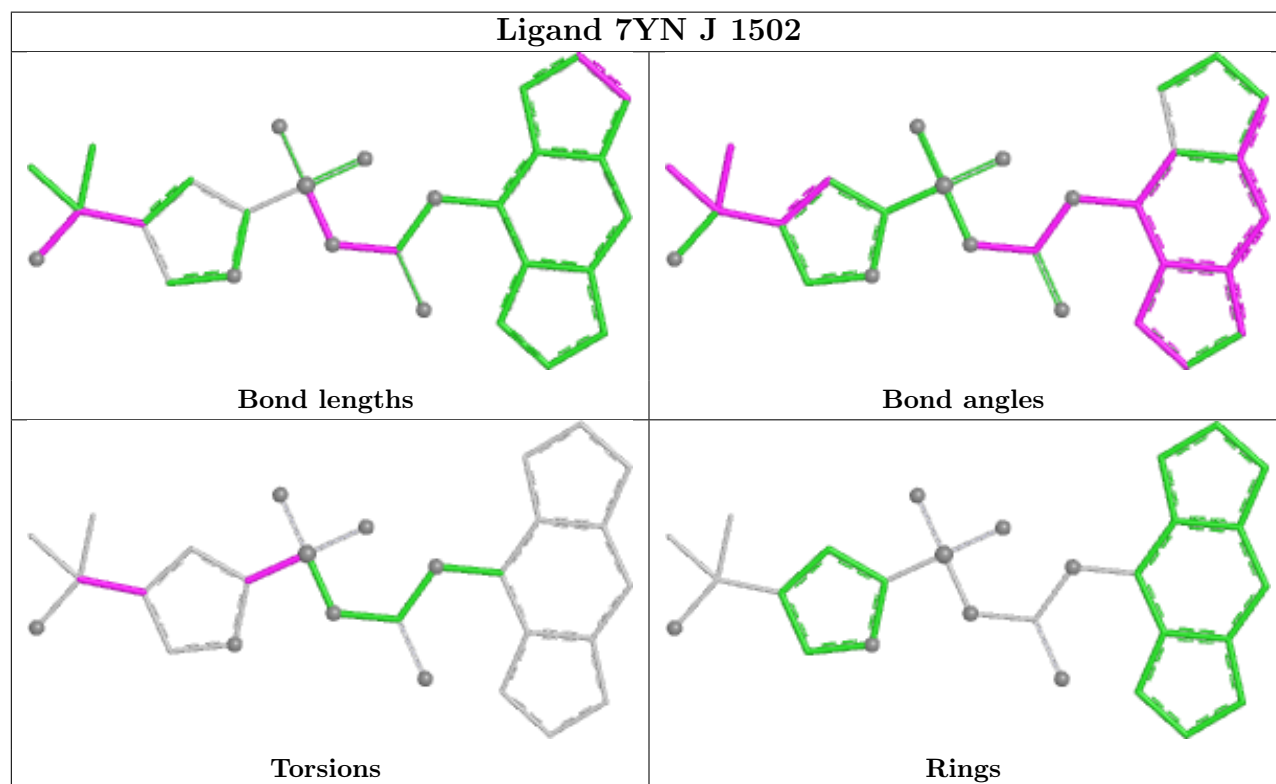
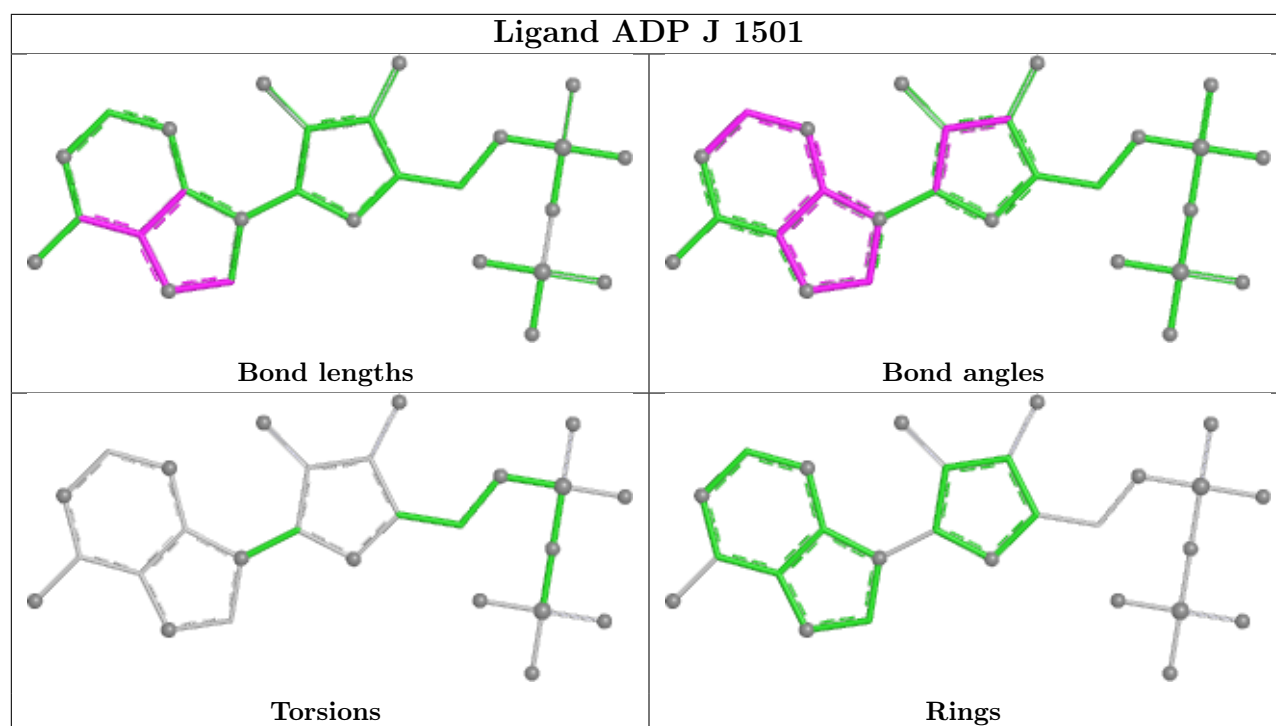


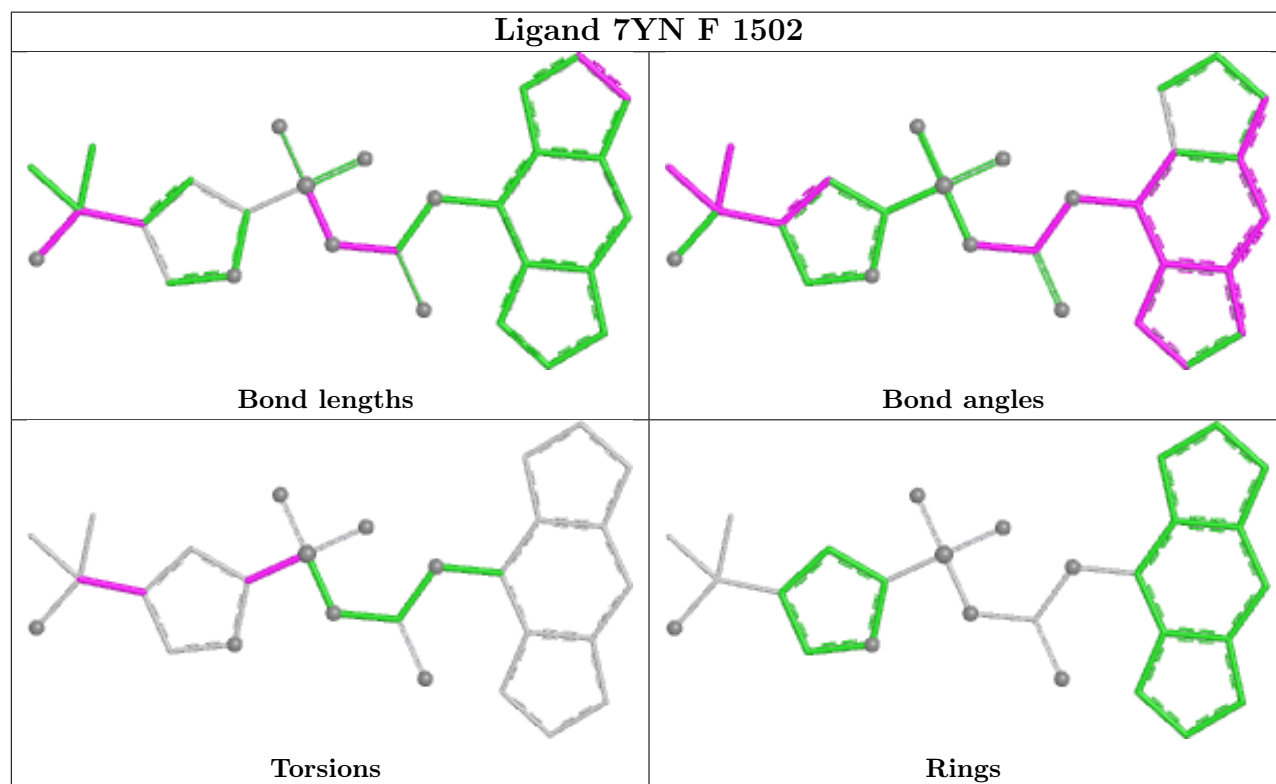
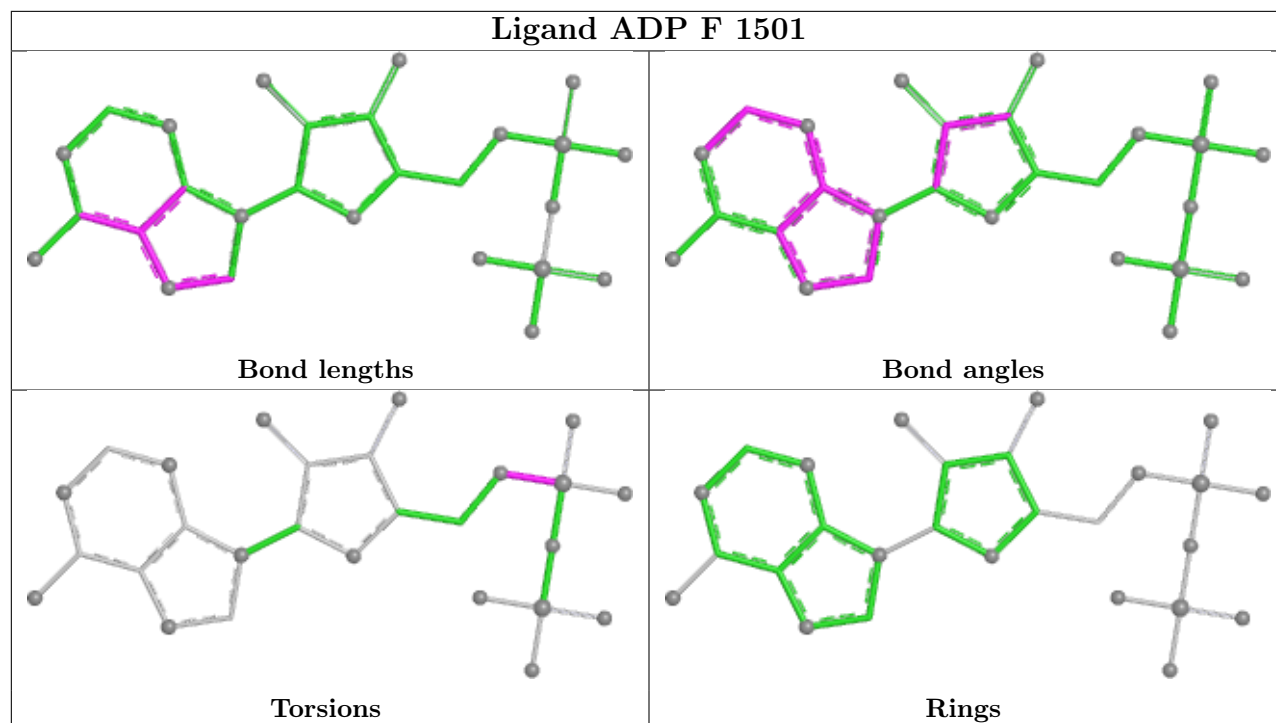


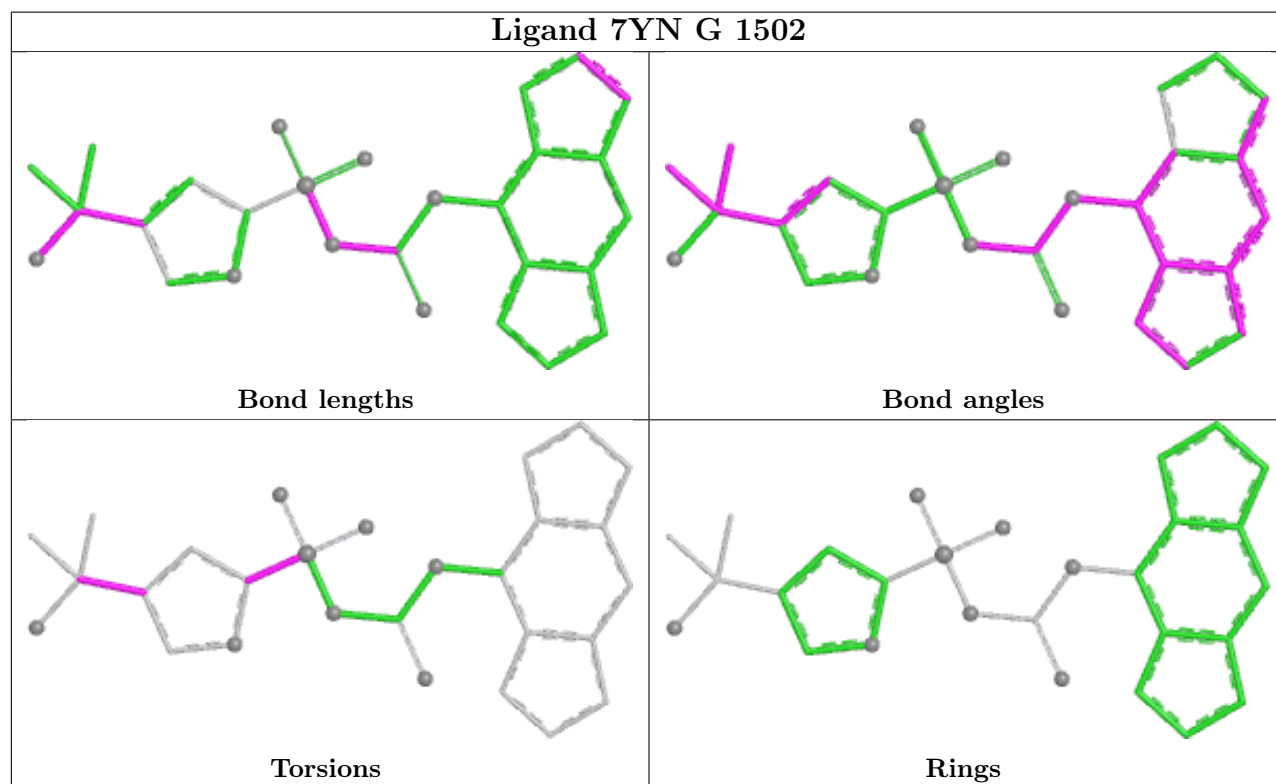
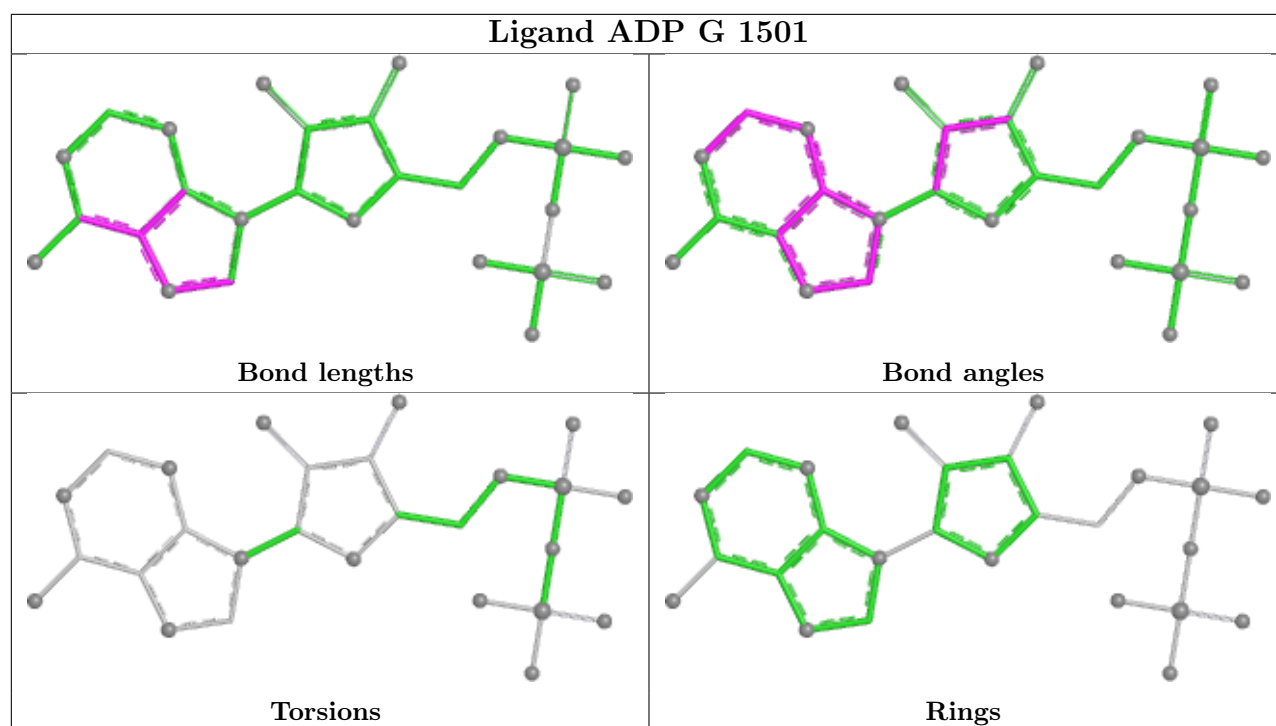


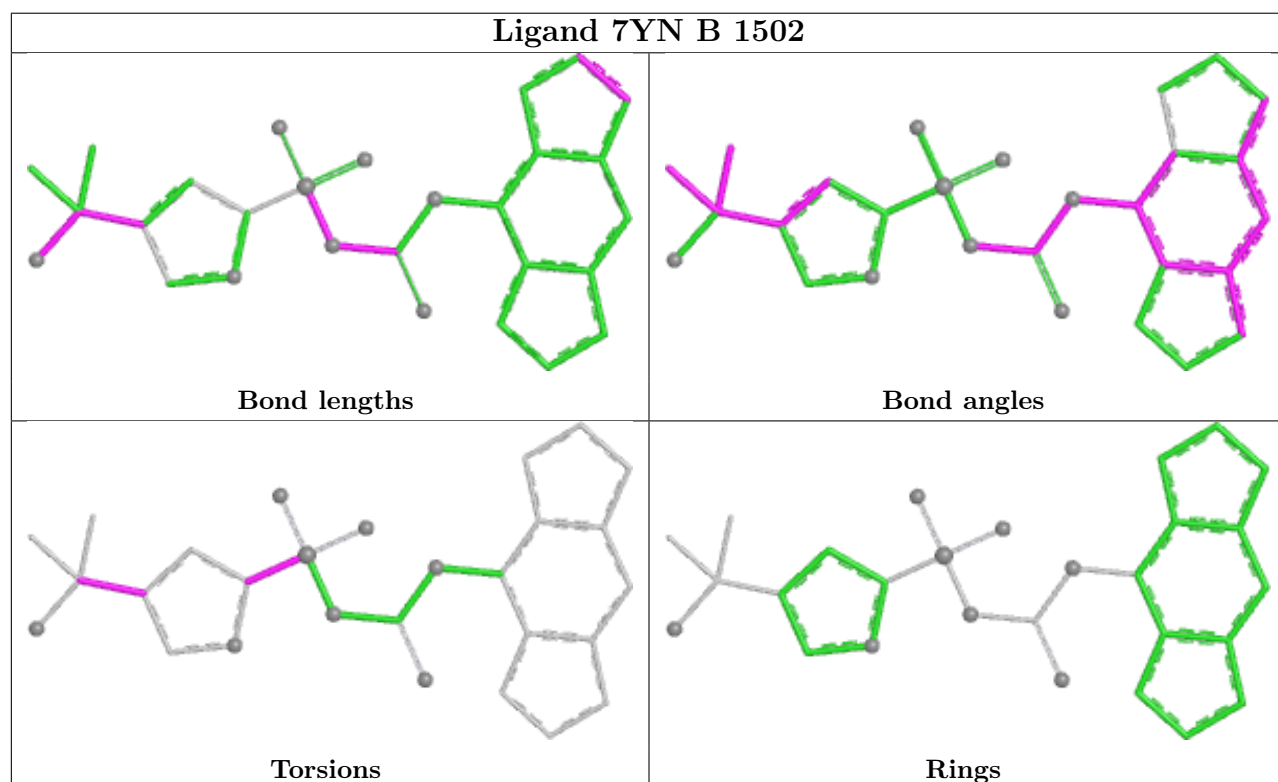
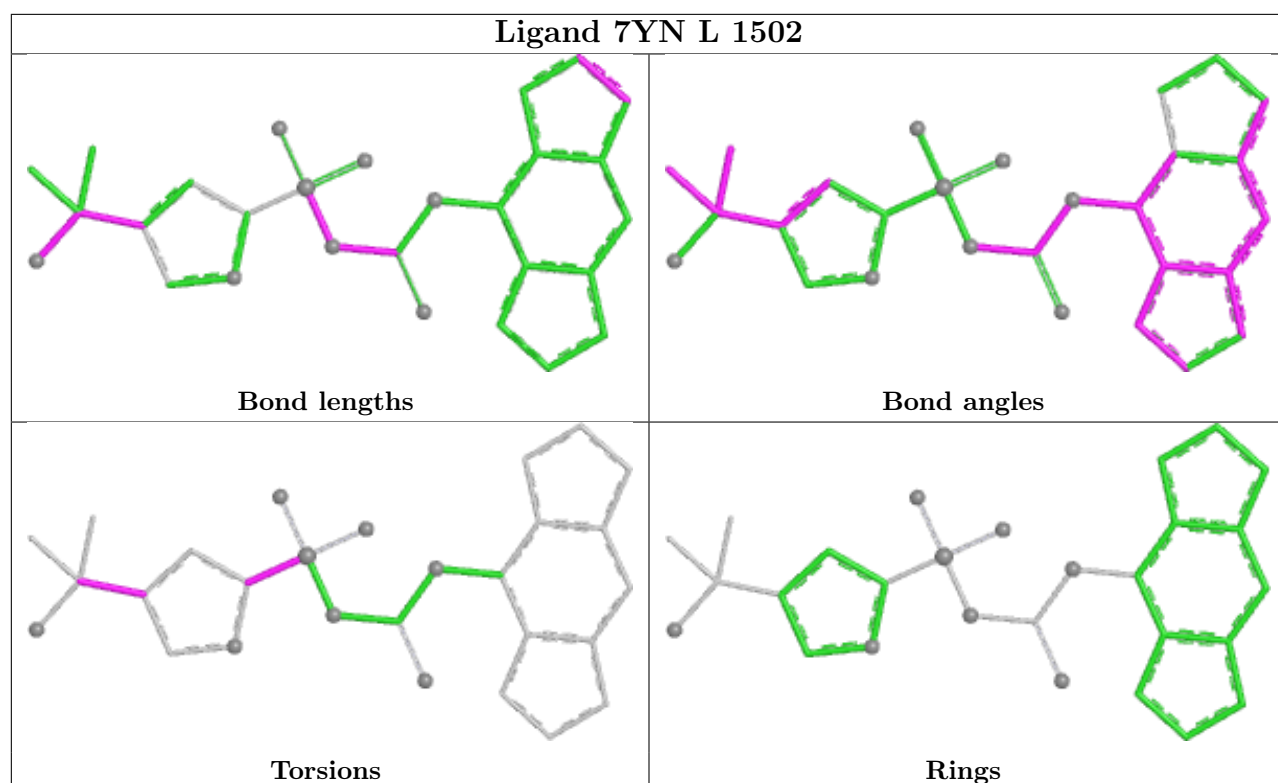


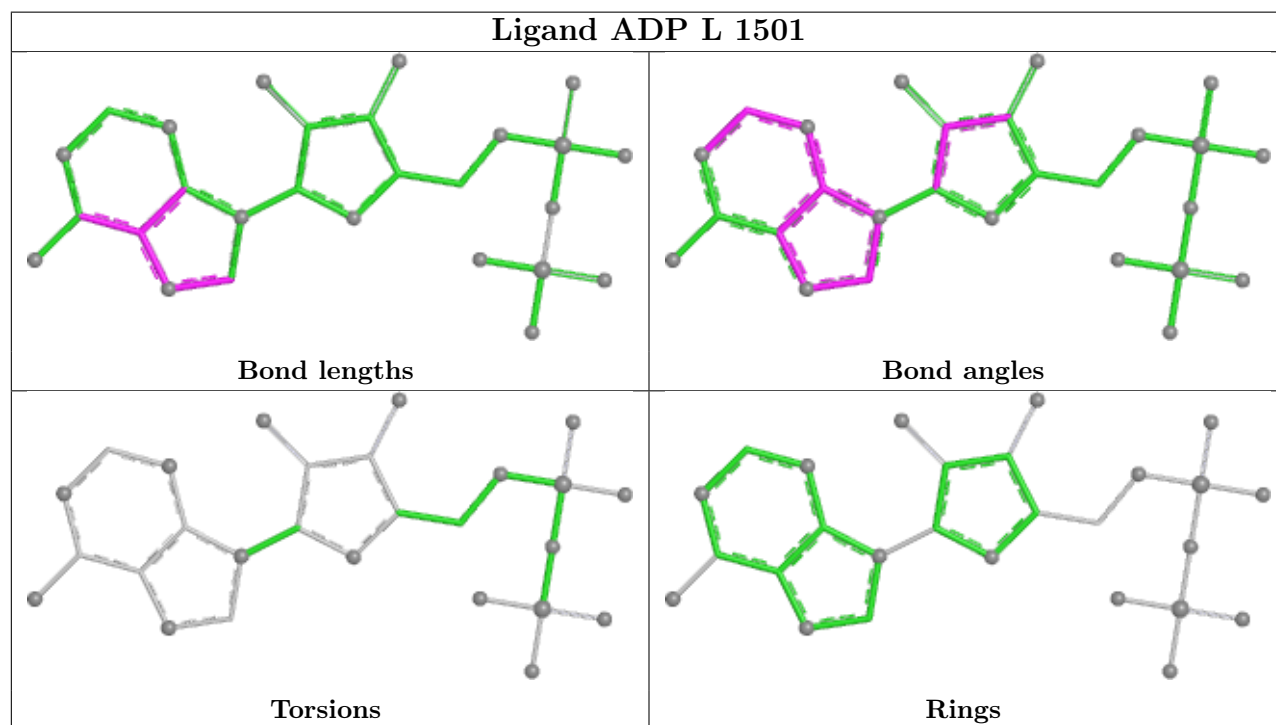
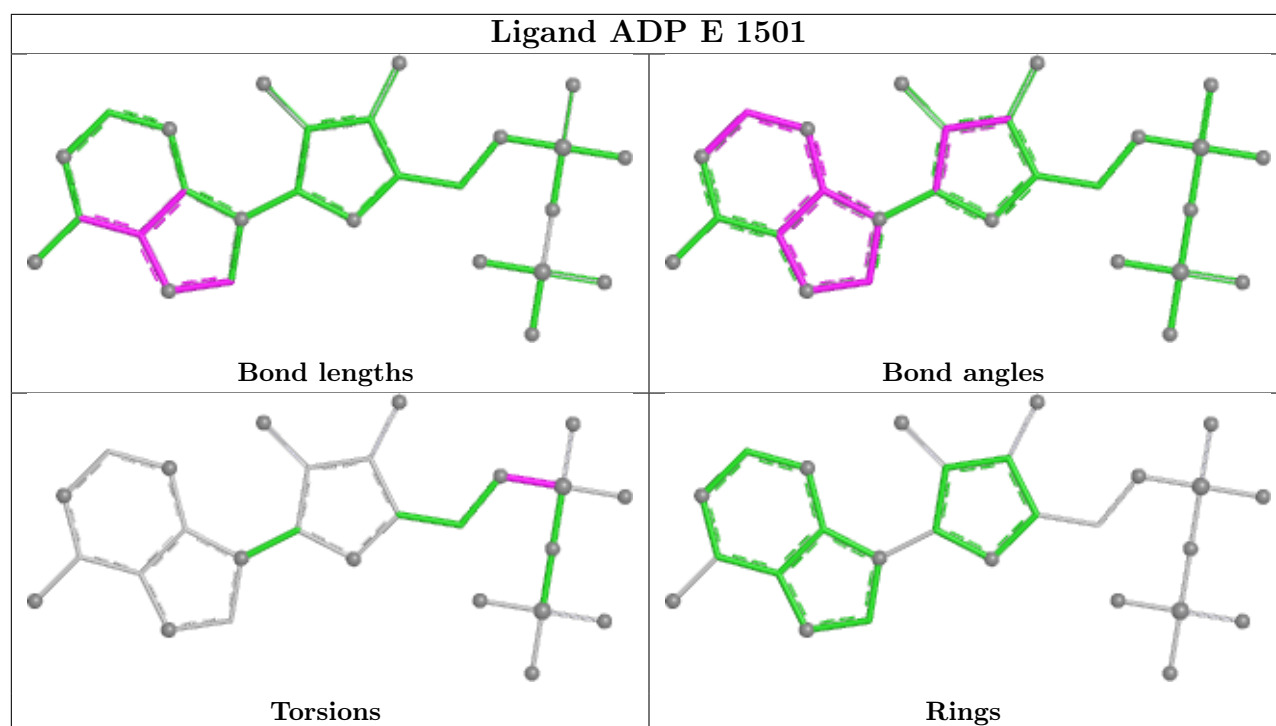


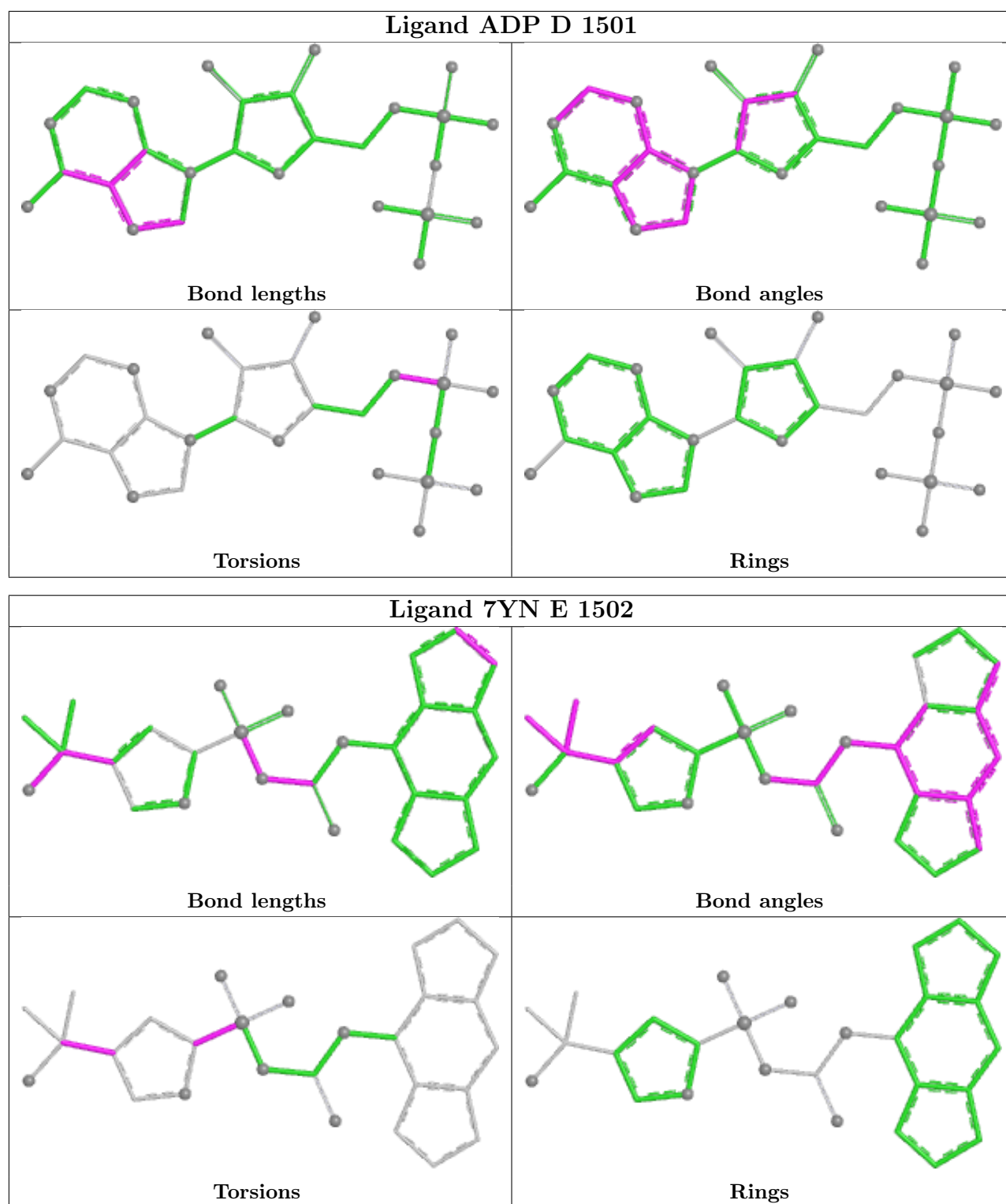












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

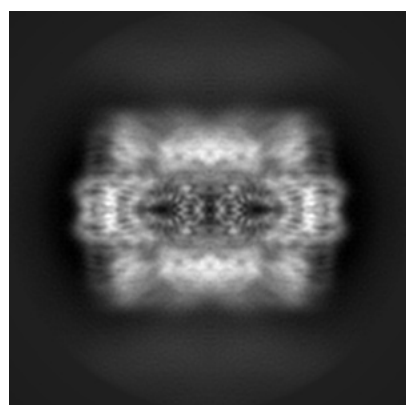
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32120. These allow visual inspection of the internal detail of the map and identification of artifacts.

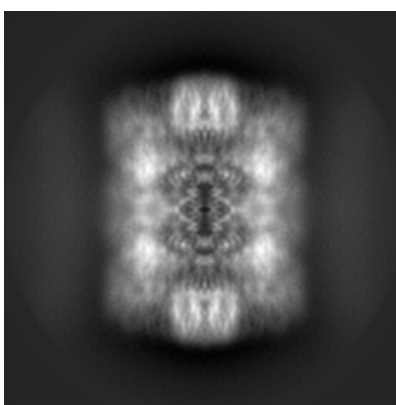
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

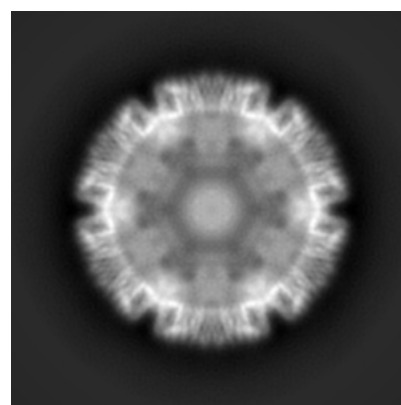
#### 6.1.1 Primary map



X



Y

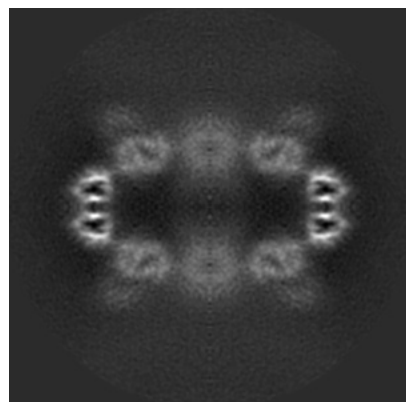


Z

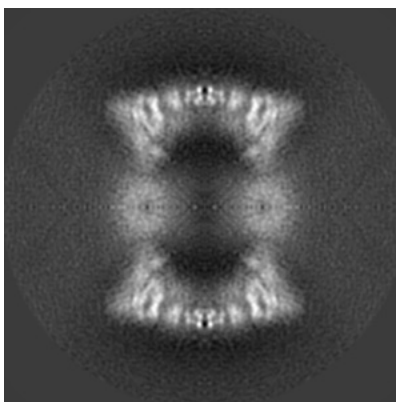
The images above show the map projected in three orthogonal directions.

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

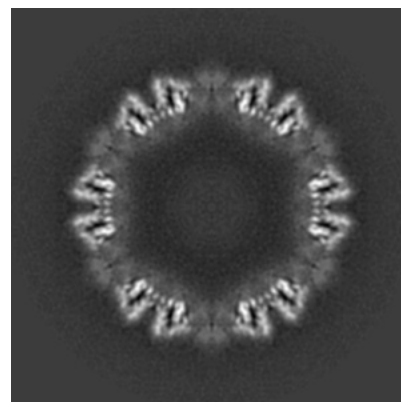
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

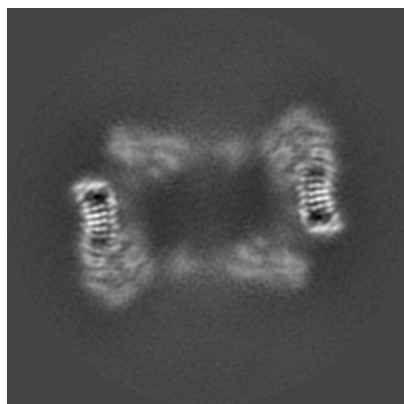


Z Index: 120

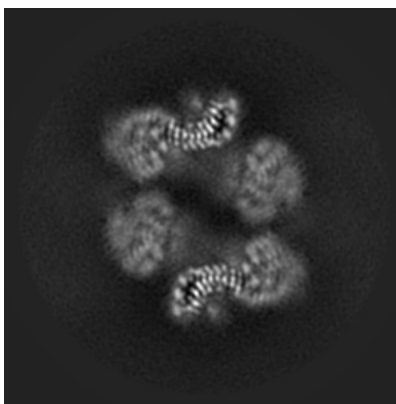
The images above show central slices of the map in three orthogonal directions.

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

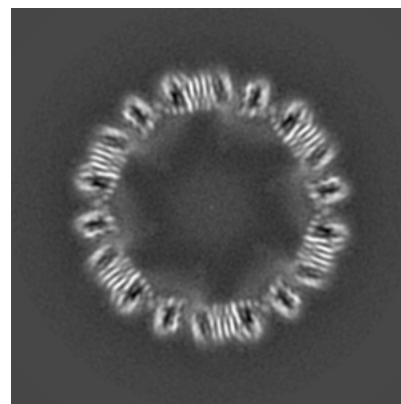
### 6.3.1 Primary map



X Index: 98



Y Index: 72

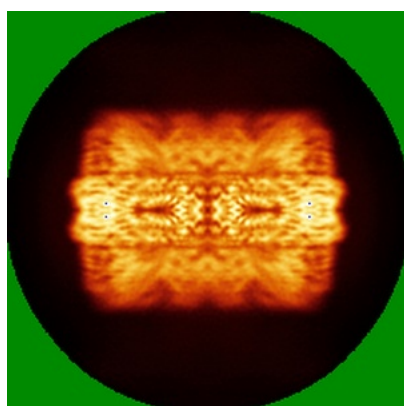


Z Index: 114

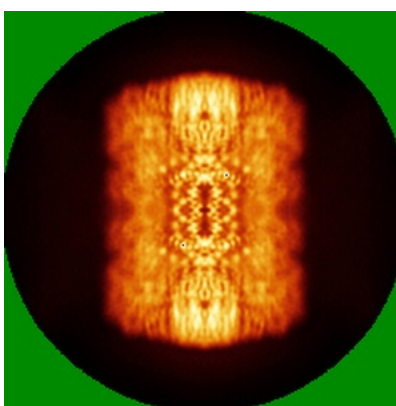
The images above show the largest variance slices of the map in three orthogonal directions.

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

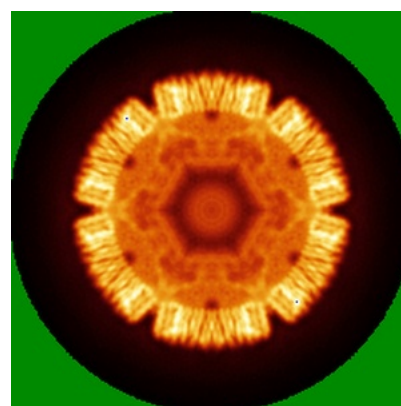
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

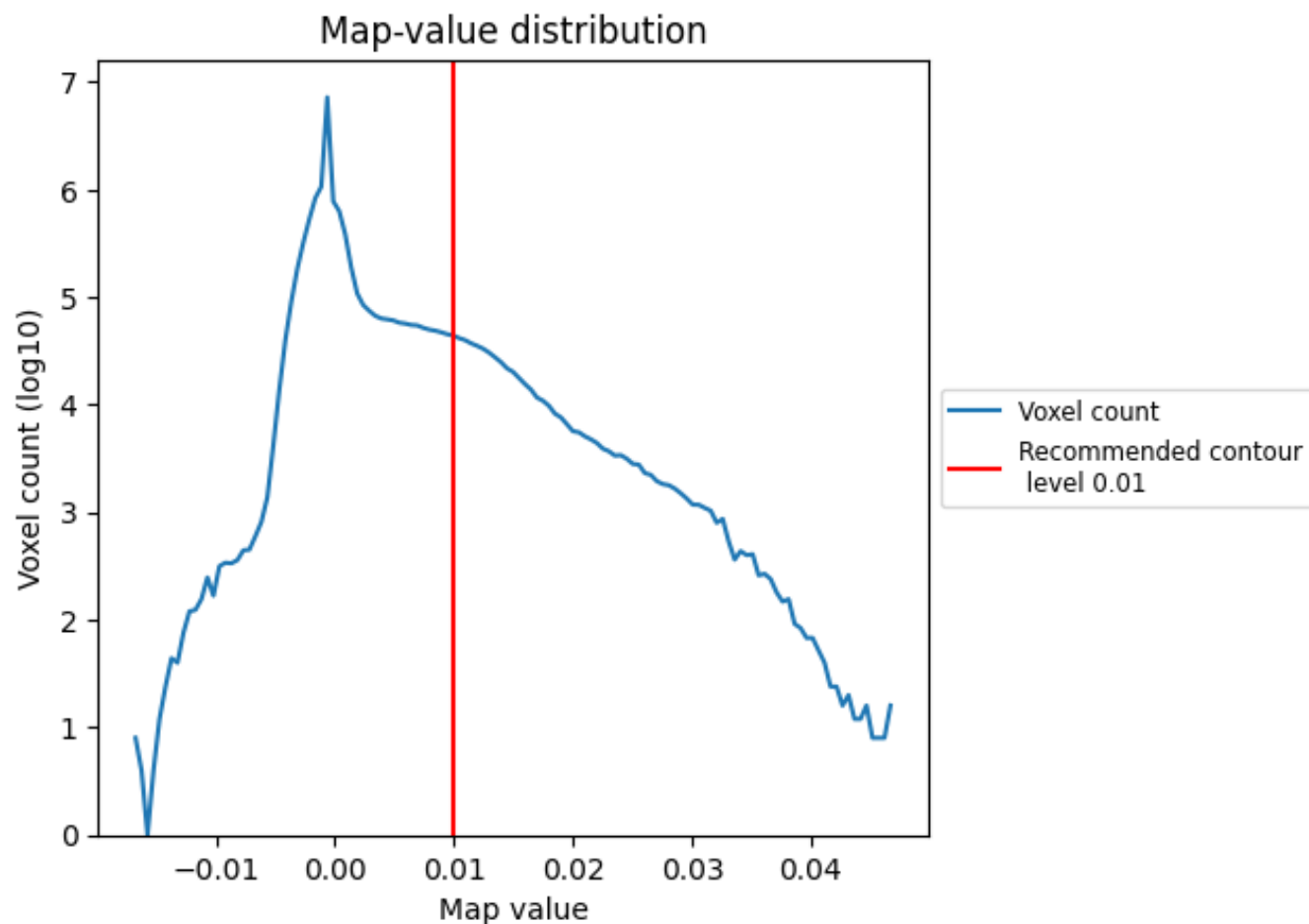
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

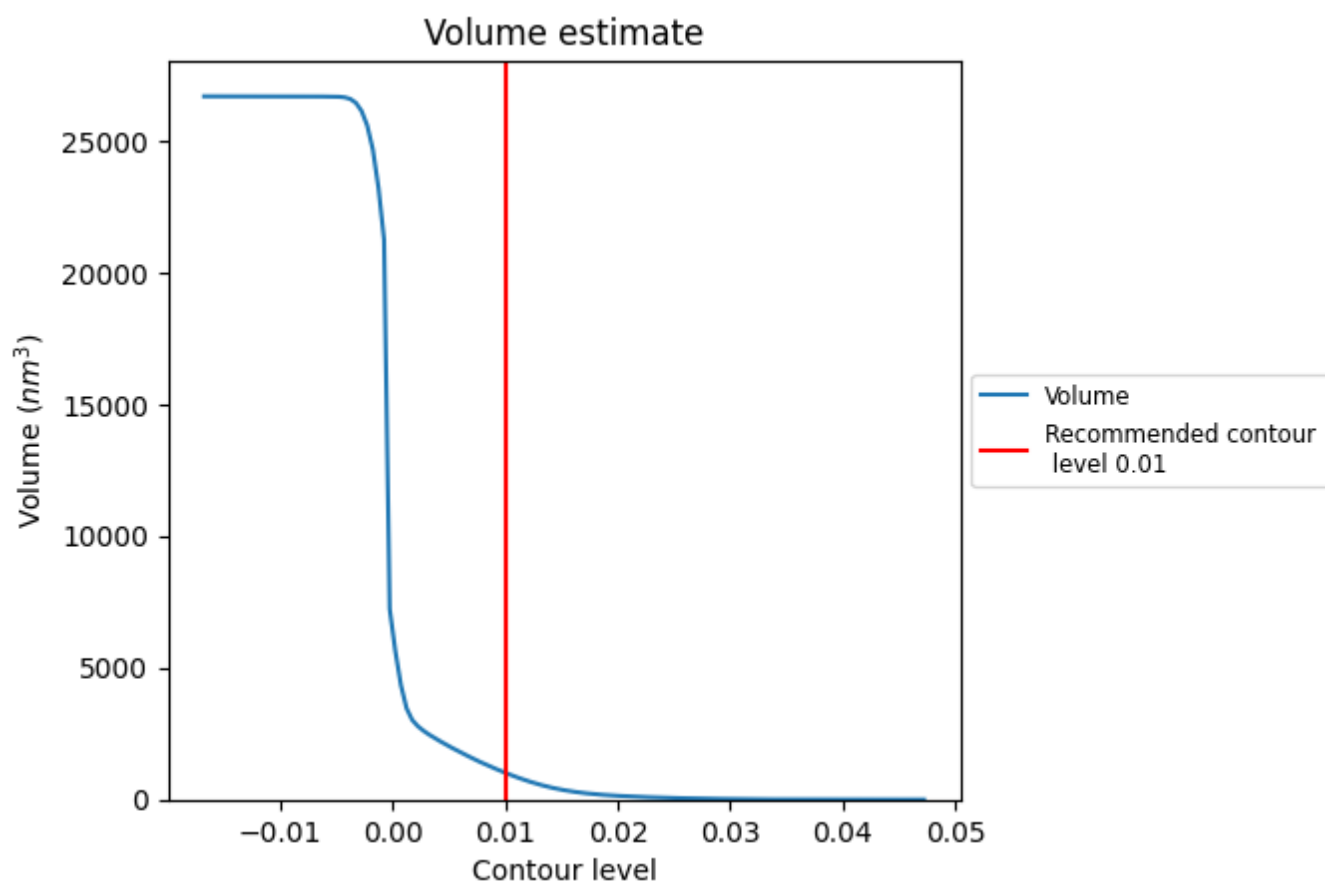
This section contains the results of statistical analysis of the map.

### 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.

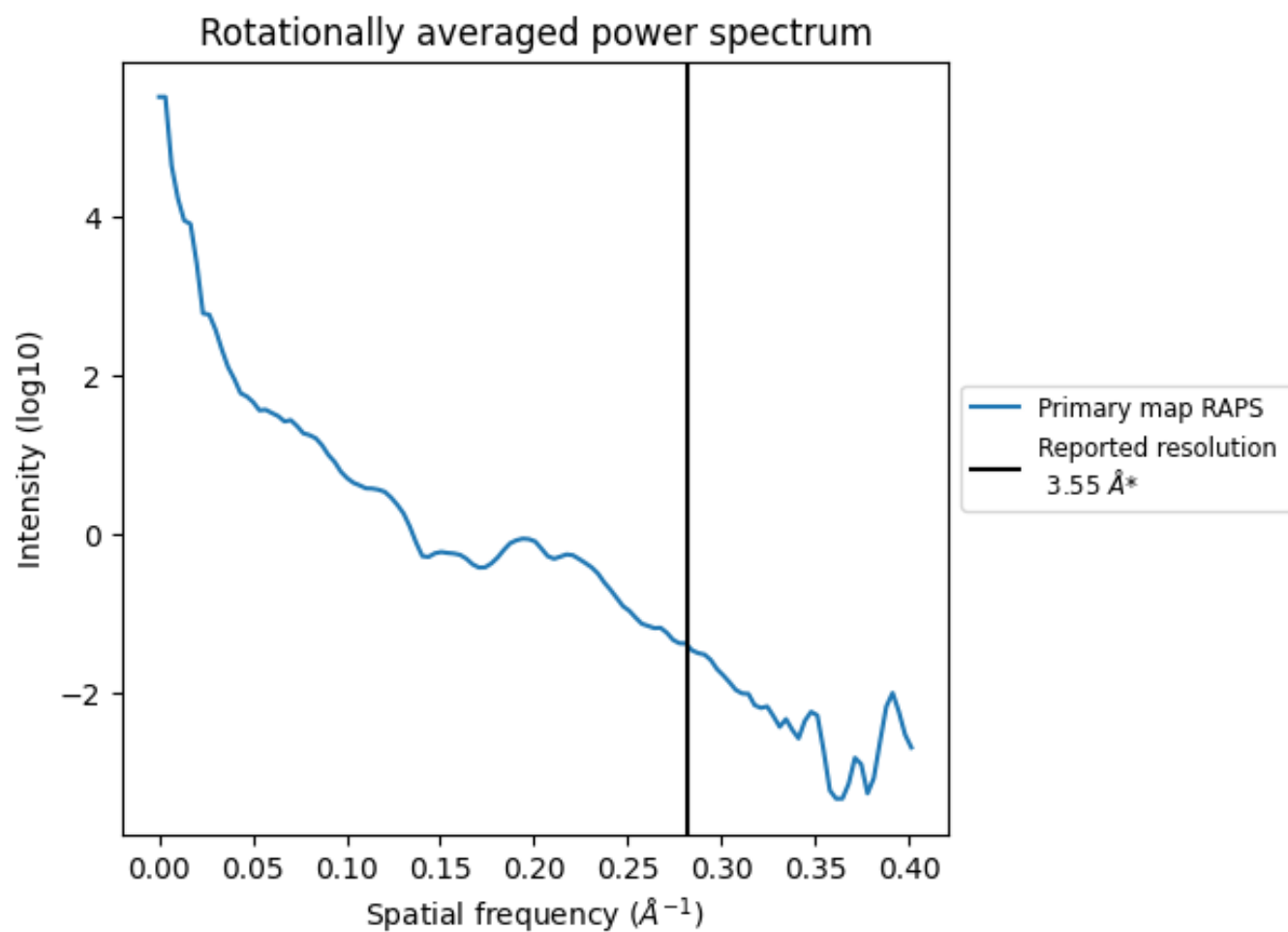
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1016 nm<sup>3</sup>; this corresponds to an approximate mass of 918 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 0.282 Å<sup>-1</sup>

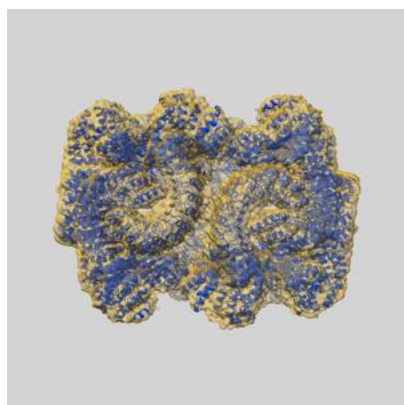
## 8 Fourier-Shell correlation

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

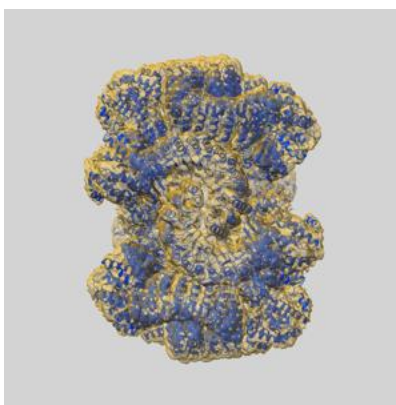
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32120 and PDB model 7VTQ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

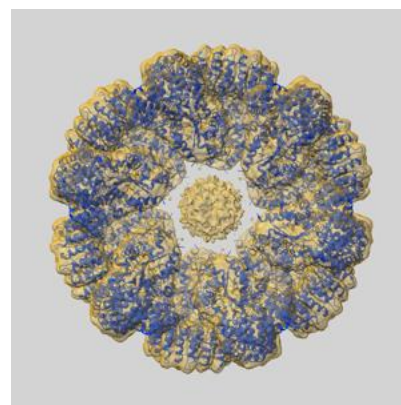
### 9.1 Map-model overlay [i](#)



X



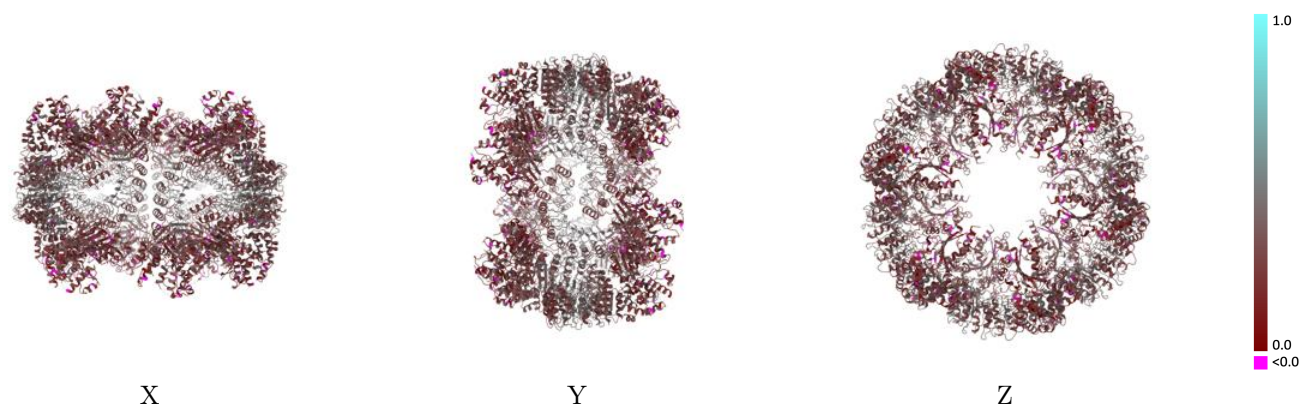
Y



Z

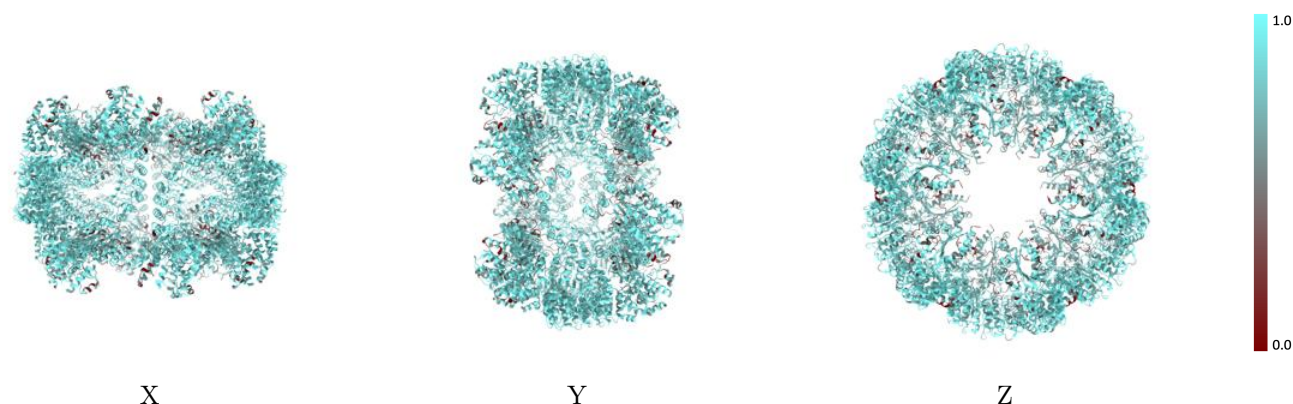
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



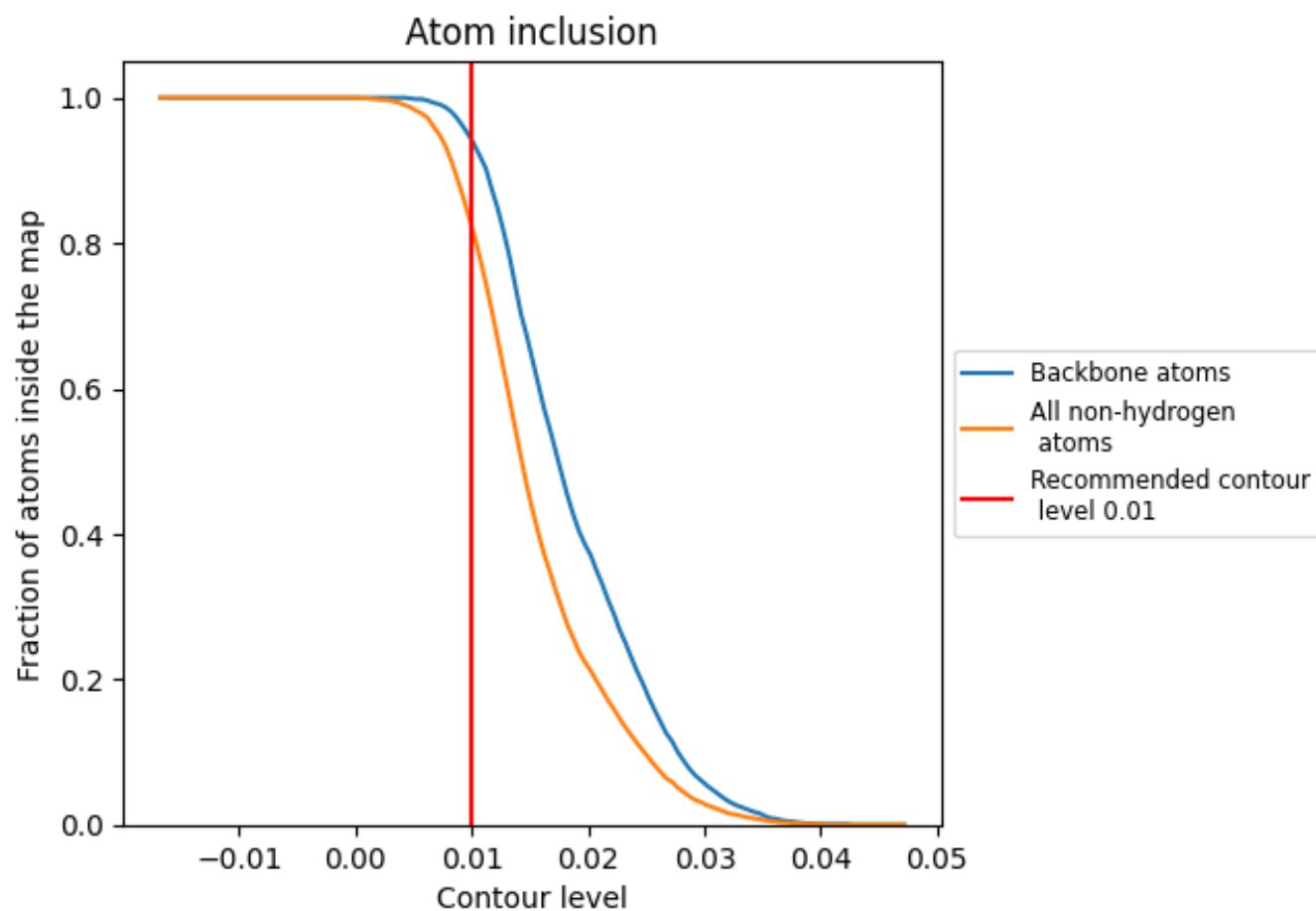
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8230 | <div><div></div></div> 0.2940 |
| A     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2930 |
| B     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2930 |
| C     | <div><div></div></div> 0.8250 | <div><div></div></div> 0.2930 |
| D     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2920 |
| E     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2940 |
| F     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.2940 |
| G     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2940 |
| H     | <div><div></div></div> 0.8210 | <div><div></div></div> 0.2950 |
| I     | <div><div></div></div> 0.8250 | <div><div></div></div> 0.2940 |
| J     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2930 |
| K     | <div><div></div></div> 0.8220 | <div><div></div></div> 0.2940 |
| L     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.2950 |

