



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:33 AM UTC

PDB ID : 8AKX / pdb\_00008akx  
EMDB ID : EMD-15496  
Title : 305 A SynPspA rod after incubation with ATP  
Authors : Junglas, B.; Hudina, E.; Schoennenbeck, P.; Ritter, I.; Santiago-Schuebel, B.;  
Huesgen, P.; Sachse, C.  
Deposited on : 2022-07-31  
Resolution : 6.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

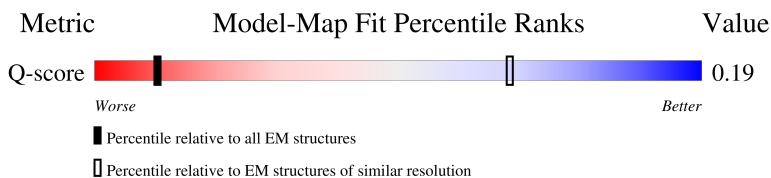
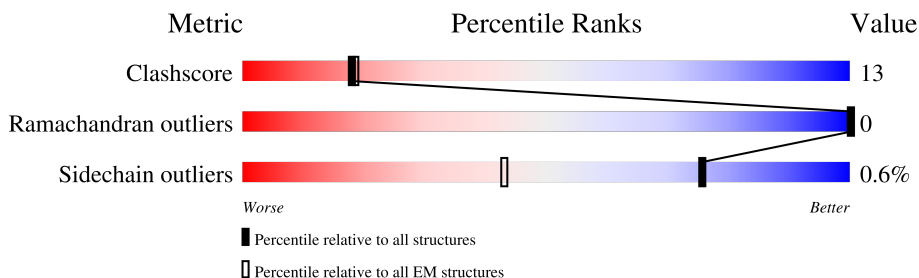
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 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                       | 531 ( 6.10 - 7.10 )                                      |

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   | 0     | 246    | <div> <div>16%</div> <div>56%</div> <div>24%</div> <div>20%</div> </div> |
| 1   | 1     | 246    | <div> <div>13%</div> <div>55%</div> <div>24%</div> <div>20%</div> </div> |
| 1   | 2     | 246    | <div> <div>11%</div> <div>56%</div> <div>24%</div> <div>20%</div> </div> |
| 1   | 3     | 246    | <div> <div>11%</div> <div>56%</div> <div>24%</div> <div>20%</div> </div> |

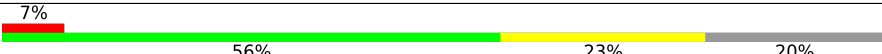
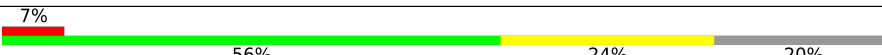
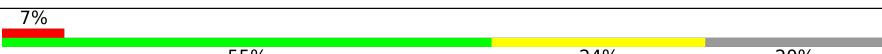
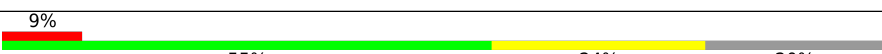
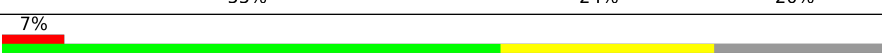
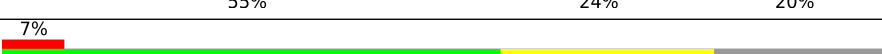
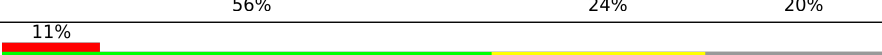
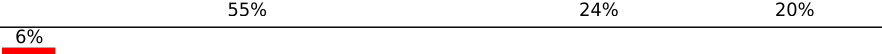
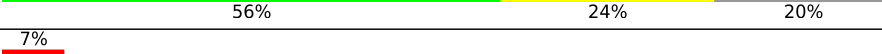
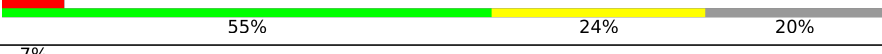
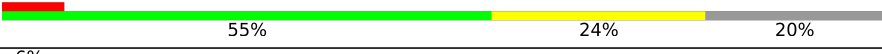
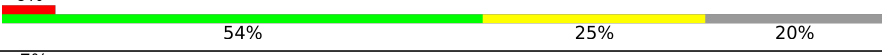
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 4     | 246    |                  |
| 1   | 5     | 246    |                  |
| 1   | 6     | 246    |                  |
| 1   | 7     | 246    |                  |
| 1   | A     | 246    |                  |
| 1   | B     | 246    |                  |
| 1   | C     | 246    |                  |
| 1   | D     | 246    |                  |
| 1   | E     | 246    |                  |
| 1   | F     | 246    |                  |
| 1   | G     | 246    |                  |
| 1   | H     | 246    |                  |
| 1   | I     | 246    |                  |
| 1   | J     | 246    |                  |
| 1   | K     | 246    |                  |
| 1   | L     | 246    |                  |
| 1   | M     | 246    |                  |
| 1   | N     | 246    |                  |
| 1   | O     | 246    |                  |
| 1   | P     | 246    |                  |
| 1   | Q     | 246    |                  |
| 1   | R     | 246    |                  |
| 1   | S     | 246    |                  |
| 1   | T     | 246    |                  |
| 1   | U     | 246    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | V     | 246    |    |
| 1   | W     | 246    |    |
| 1   | X     | 246    |    |
| 1   | Y     | 246    |    |
| 1   | Z     | 246    |    |
| 1   | a     | 246    |    |
| 1   | b     | 246    |    |
| 1   | c     | 246    |    |
| 1   | d     | 246    |    |
| 1   | e     | 246    |    |
| 1   | f     | 246    |    |
| 1   | g     | 246    |    |
| 1   | h     | 246    |   |
| 1   | i     | 246    |  |
| 1   | j     | 246    |  |
| 1   | k     | 246    |  |
| 1   | l     | 246    |  |
| 1   | m     | 246    |  |
| 1   | n     | 246    |  |
| 1   | o     | 246    |  |
| 1   | p     | 246    |  |
| 1   | q     | 246    |  |
| 1   | r     | 246    |  |
| 1   | s     | 246    |  |
| 1   | t     | 246    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | u     | 246    |                  |
| 1   | v     | 246    |                  |
| 1   | w     | 246    |                  |
| 1   | x     | 246    |                  |
| 1   | y     | 246    |                  |
| 1   | z     | 246    |                  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 190860 atoms, of which 96240 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 Chloroplast membrane-associated 30 kD protein.

| Mol | Chain | Residues | Atoms         |          |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|-----------|----------|----------|--------|---------|-------|
| 1   | 0     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 1     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 2     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 3     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 4     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 5     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 6     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | 7     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | A     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | B     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | C     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | D     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | E     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | F     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | G     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | H     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | I     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |          |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|-----------|----------|----------|--------|---------|-------|
| 1   | J     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | K     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | L     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | M     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | N     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | O     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | P     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | Q     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | R     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | S     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | T     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | U     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | V     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | W     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | X     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | Y     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | Z     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | a     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | b     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | c     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | d     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |          |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|-----------|----------|----------|--------|---------|-------|
| 1   | e     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | f     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | g     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | h     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | i     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | j     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | k     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | l     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | m     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | n     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | o     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | p     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | q     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | r     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | s     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | t     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | u     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | v     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | w     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | x     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |
| 1   | y     | 196      | Total<br>3181 | C<br>978 | H<br>1604 | N<br>289 | O<br>308 | S<br>2 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | z     | 196      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3181  | 978 | 1604 | 289 | 308 | 2 |         |       |

There are 1380 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 0     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| 0     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| 0     | -20     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -12     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -11     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -10     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| 0     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| 0     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| 0     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| 0     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| 0     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| 0     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| 0     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| 0     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| 0     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| 1     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| 1     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| 1     | -20     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -12     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -11     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -10     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 1     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| 1     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| 1     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| 1     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| 1     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| 1     | -4      | LEU      | -      | expression tag        | UNP P74717 |
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| 2     | -2      | GLN      | -      | expression tag        | UNP P74717 |
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| 2     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| 3     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 3     | -14     | HIS      | -      | expression tag        | UNP P74717 |

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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 5     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 5     | -18     | HIS      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 5     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| 5     | -16     | HIS      | -      | expression tag        | UNP P74717 |
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| 6     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| 7     | -22     | MET      | -      | initiating methionine | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| A     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| A     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| A     | -3      | PHE      | -      | expression tag        | UNP P74717 |

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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| A     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| B     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| B     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| C     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| C     | -7      | LEU      | -      | expression tag        | UNP P74717 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| C     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| C     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| C     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| C     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| D     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| D     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| D     | -20     | SER      | -      | expression tag        | UNP P74717 |
| D     | -19     | SER      | -      | expression tag        | UNP P74717 |
| D     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| D     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| D     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| E     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| E     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| E     | -20     | SER      | -      | expression tag        | UNP P74717 |
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| E     | -12     | SER      | -      | expression tag        | UNP P74717 |
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*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| E     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| E     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| F     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| F     | -20     | SER      | -      | expression tag        | UNP P74717 |
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| F     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| F     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| G     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| G     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| G     | -19     | SER      | -      | expression tag        | UNP P74717 |
| G     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| G     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| G     | -15     | HIS      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| I     | -20     | SER      | -      | expression tag        | UNP P74717 |
| I     | -19     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| I     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| T     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| T     | -20     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| e     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| r     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| r     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| r     | -15     | HIS      | -      | expression tag        | UNP P74717 |
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| r     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| s     | -20     | SER      | -      | expression tag        | UNP P74717 |
| s     | -19     | SER      | -      | expression tag        | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| t     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| t     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| u     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| u     | -20     | SER      | -      | expression tag        | UNP P74717 |
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| u     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| u     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| u     | -12     | SER      | -      | expression tag        | UNP P74717 |
| u     | -11     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| u     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| u     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| u     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| u     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| u     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| v     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| w     | -16     | HIS      | -      | expression tag        | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| w     | -11     | SER      | -      | expression tag        | UNP P74717 |
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| w     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| w     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| w     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| w     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| w     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| w     | -2      | GLN      | -      | expression tag        | UNP P74717 |
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| x     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| x     | -20     | SER      | -      | expression tag        | UNP P74717 |
| x     | -19     | SER      | -      | expression tag        | UNP P74717 |
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| x     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -15     | HIS      | -      | expression tag        | UNP P74717 |
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| x     | -13     | HIS      | -      | expression tag        | UNP P74717 |
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| x     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| x     | -3      | PHE      | -      | expression tag        | UNP P74717 |
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| x     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| y     | -20     | SER      | -      | expression tag        | UNP P74717 |
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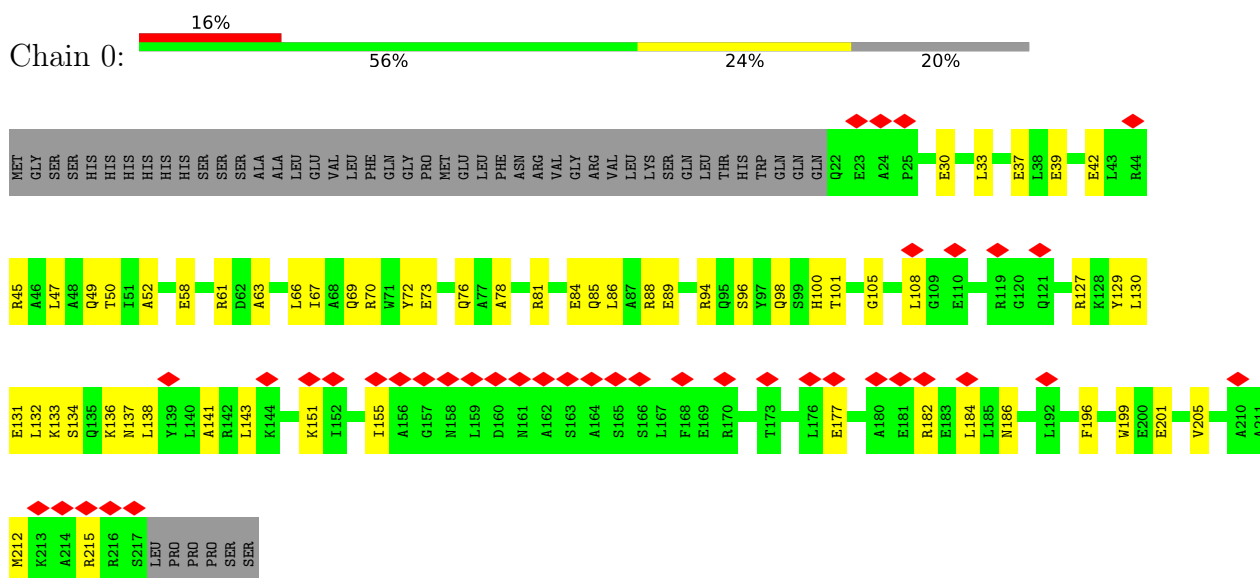
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| y     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| y     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| y     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| y     | -13     | HIS      | -      | expression tag        | UNP P74717 |
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| y     | -5      | VAL      | -      | expression tag        | UNP P74717 |
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| y     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| y     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| y     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| y     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| z     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| z     | -20     | SER      | -      | expression tag        | UNP P74717 |
| z     | -19     | SER      | -      | expression tag        | UNP P74717 |
| z     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| z     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| z     | -11     | SER      | -      | expression tag        | UNP P74717 |
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| z     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| z     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| z     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| z     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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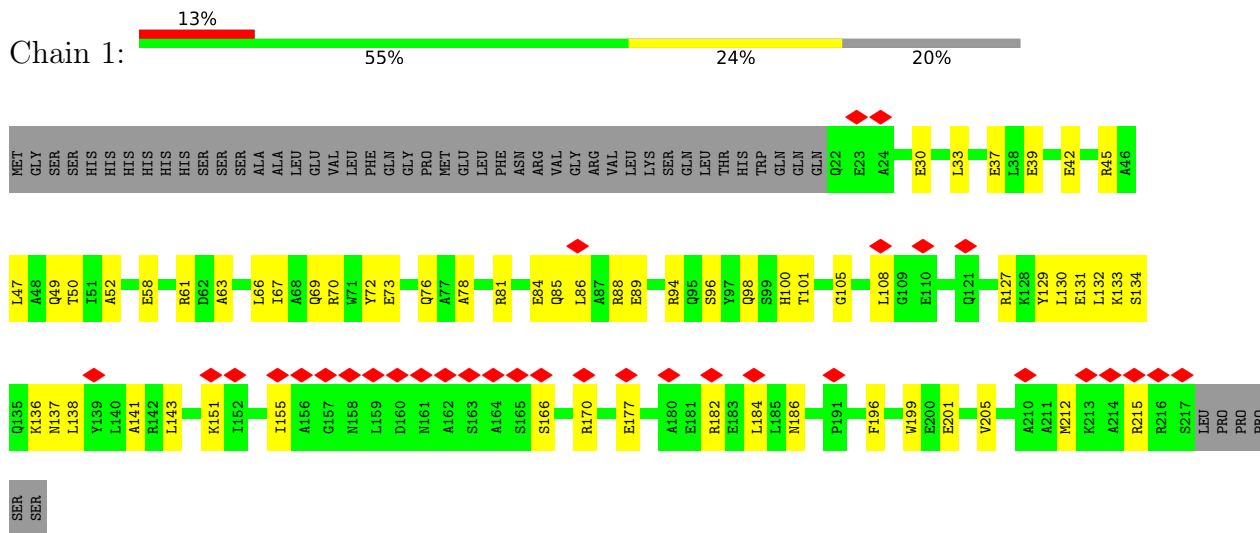
### 3 Residue-property plots

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

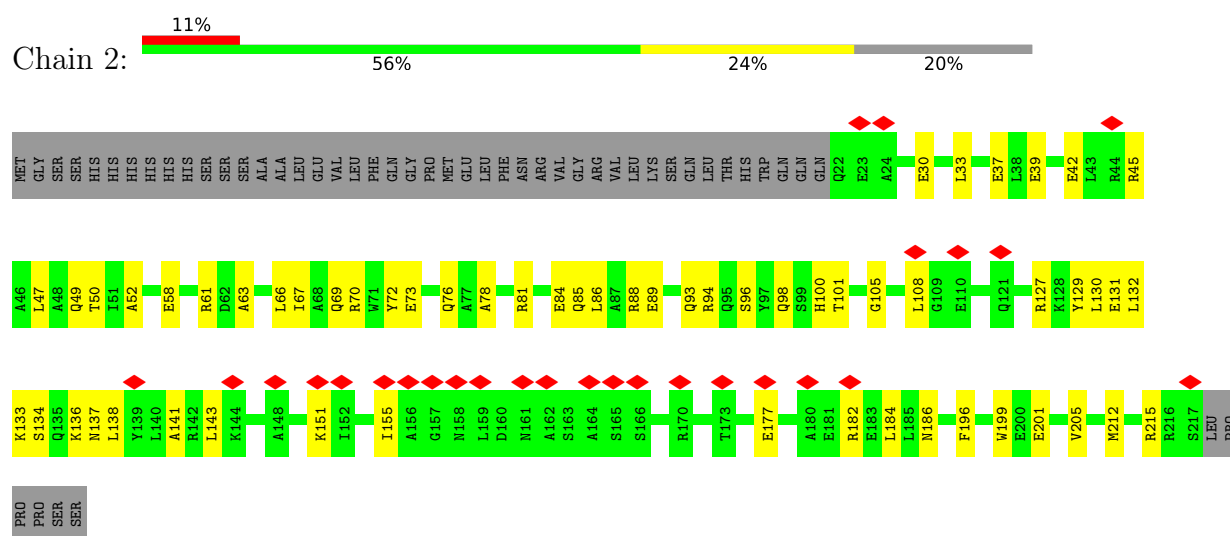
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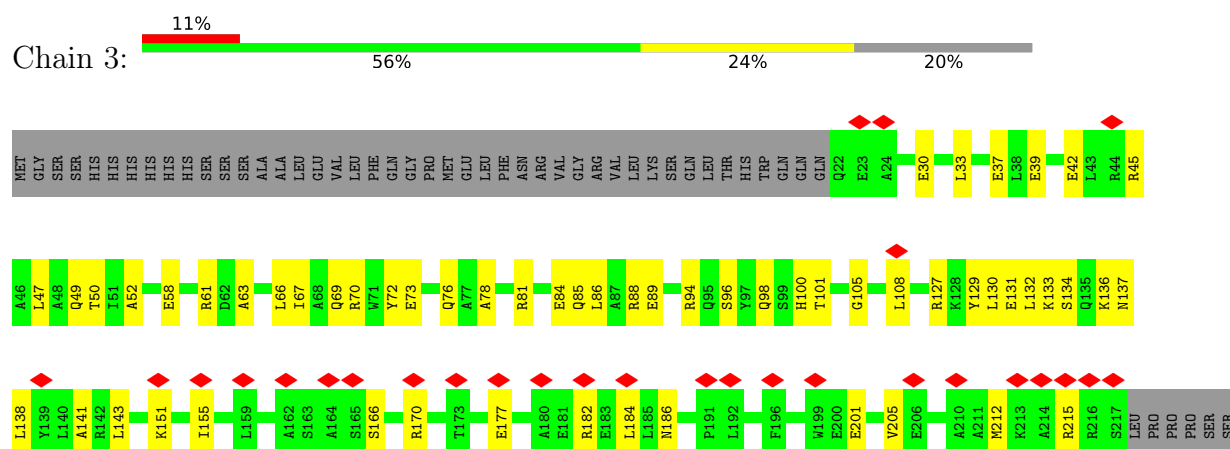
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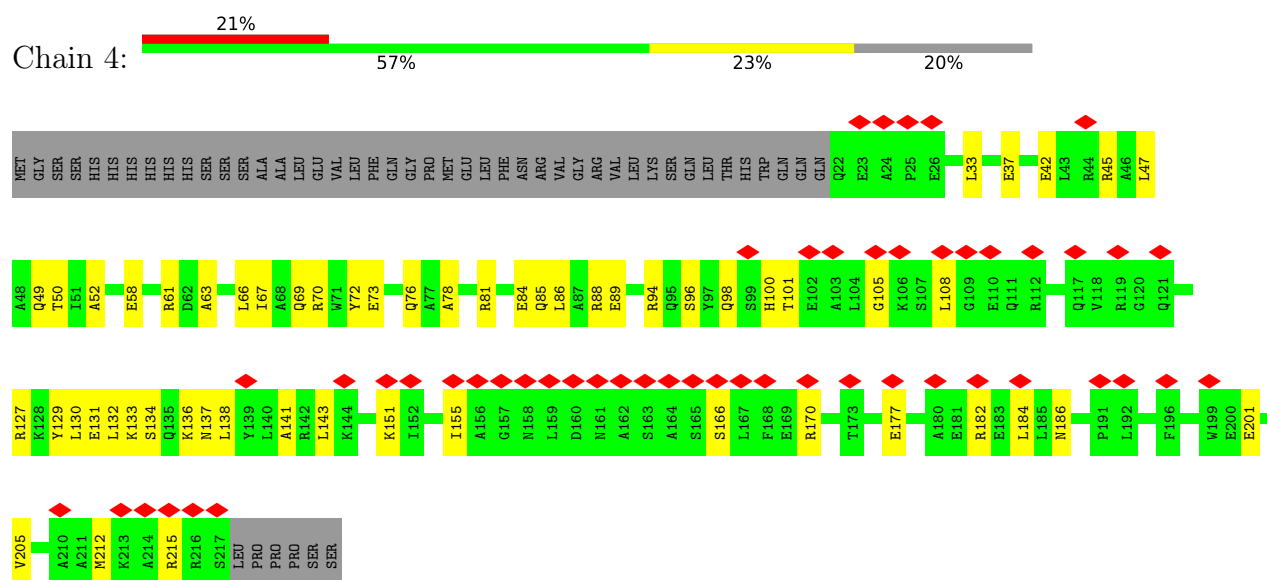
- Molecule 1: Chloroplast membrane-associated 30 kD protein



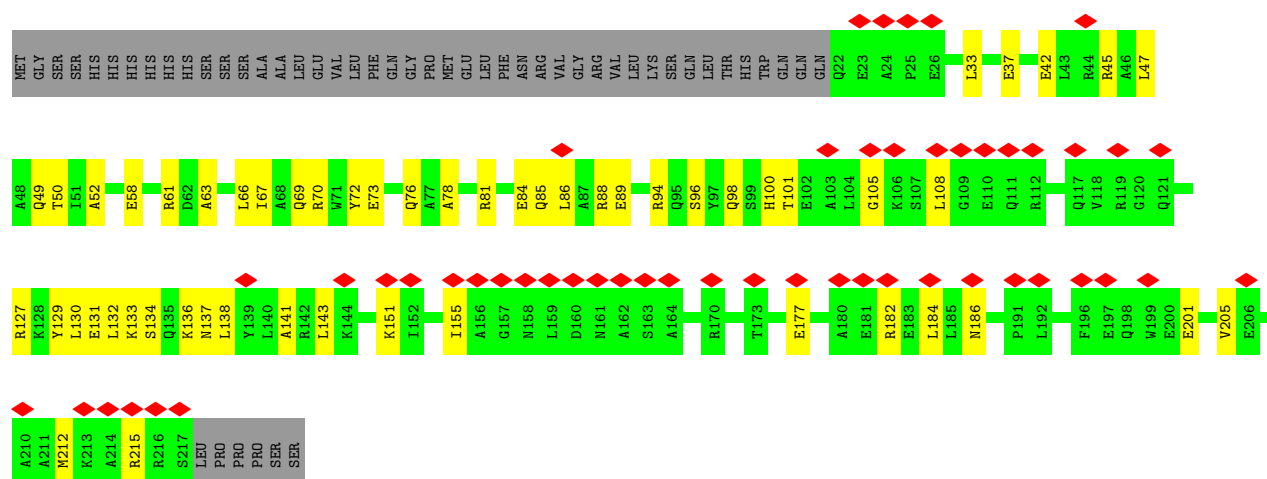
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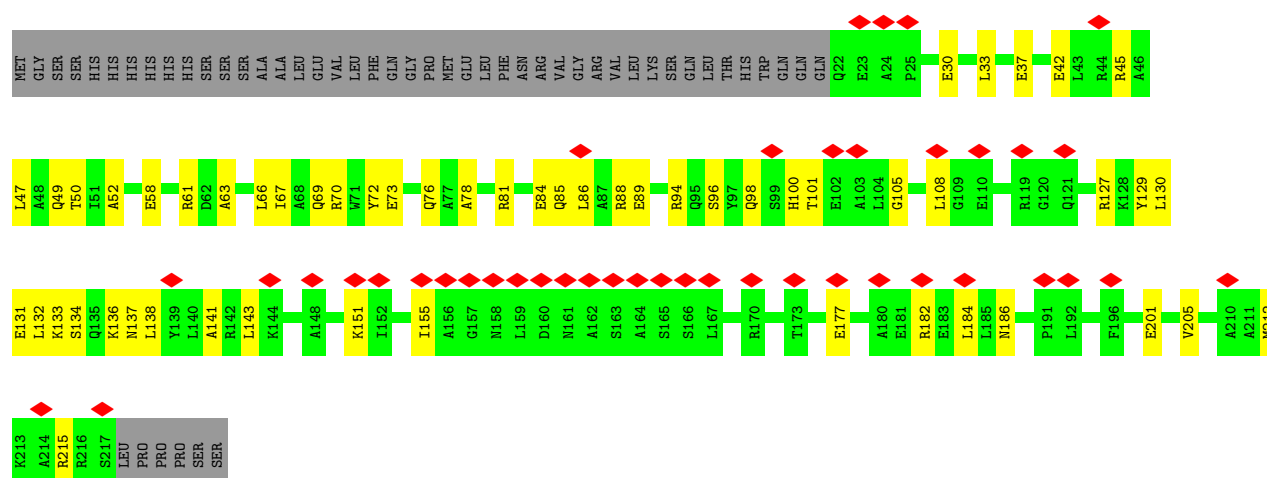
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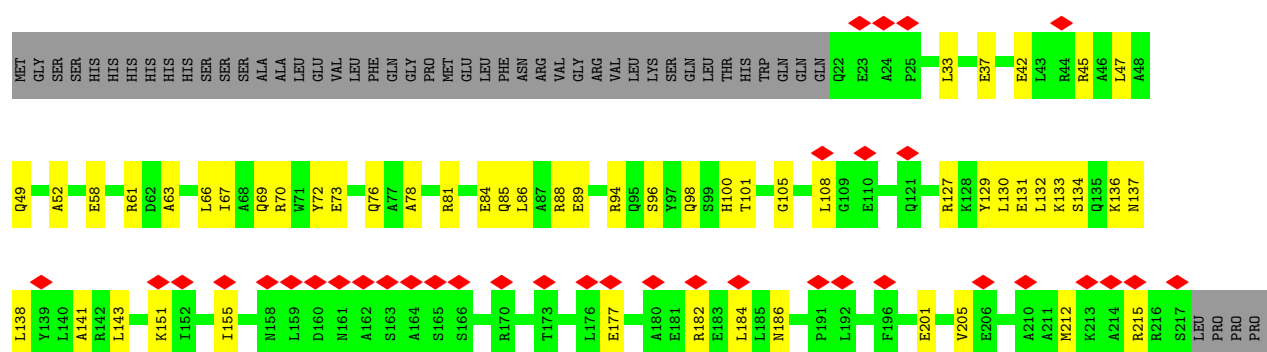
- Molecule 1: Chloroplast membrane-associated 30 kD protein.



- Molecule 1: Chloroplast membrane-associated 30 kD protein

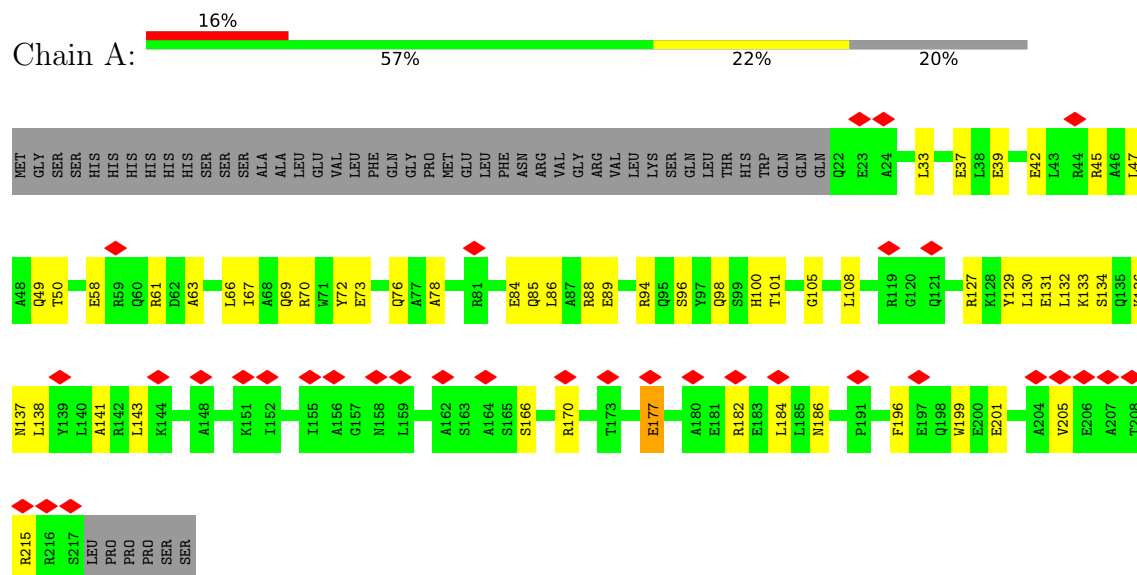


- Molecule 1: Chloroplast membrane-associated 30 kD protein

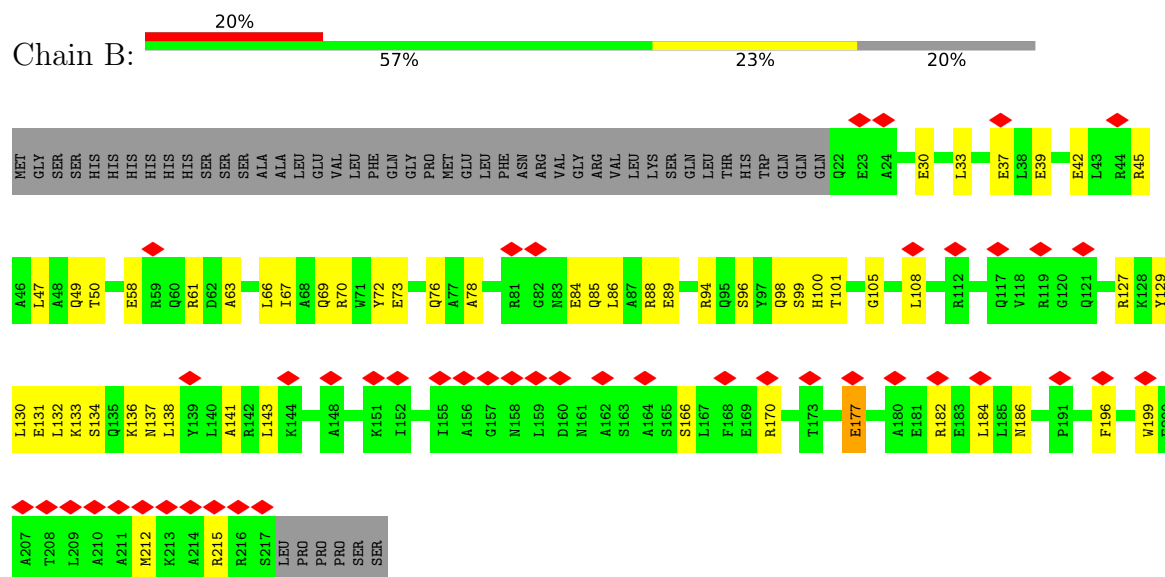


SER

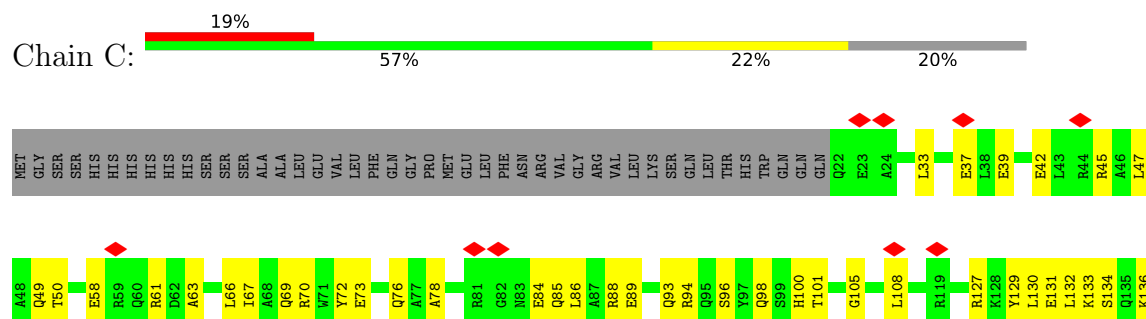
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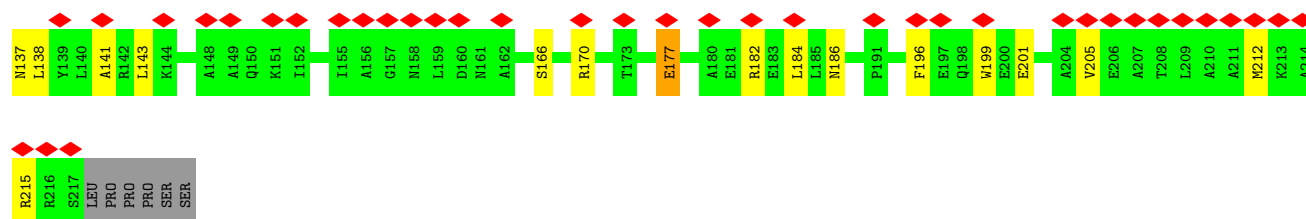


- Molecule 1: Chloroplast membrane-associated 30 kD protein

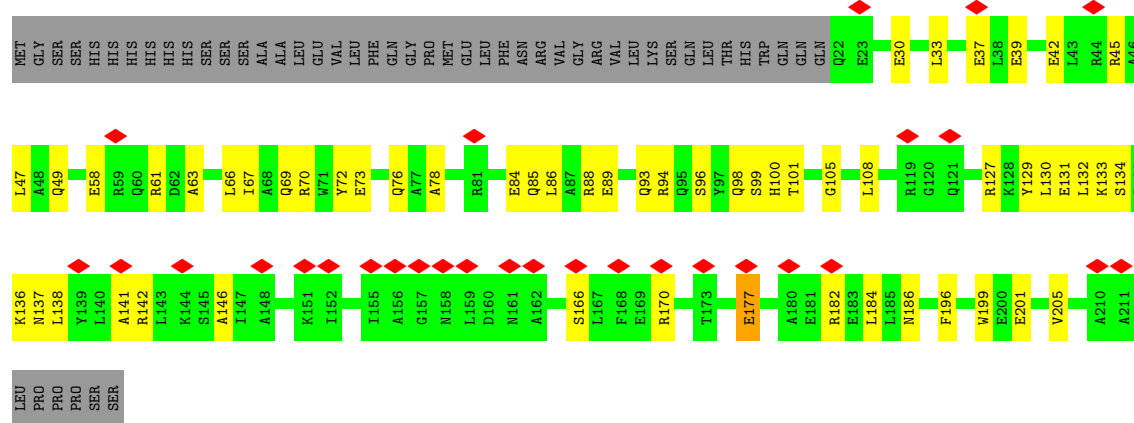


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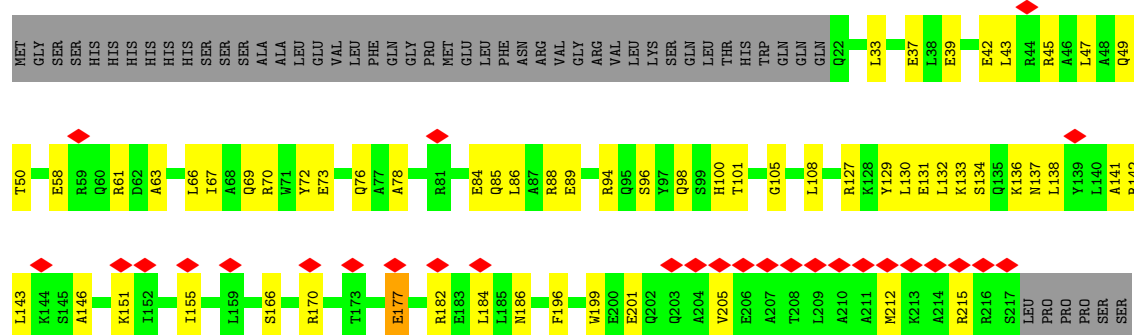




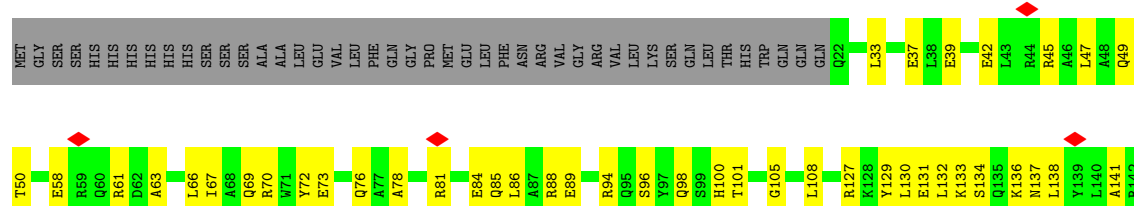
- Molecule 1: Chloroplast membrane-associated 30 kD protein

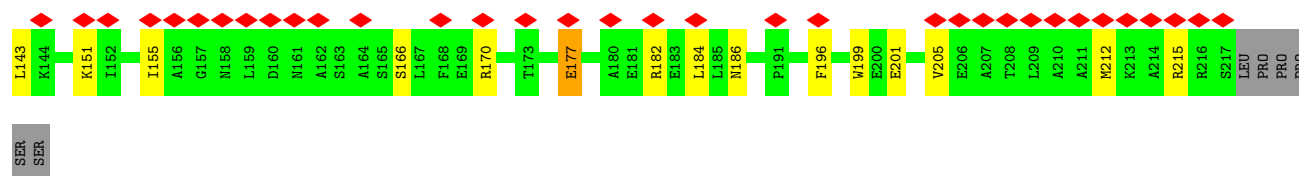


- Molecule 1: Chloroplast membrane-associated 30 kD protein

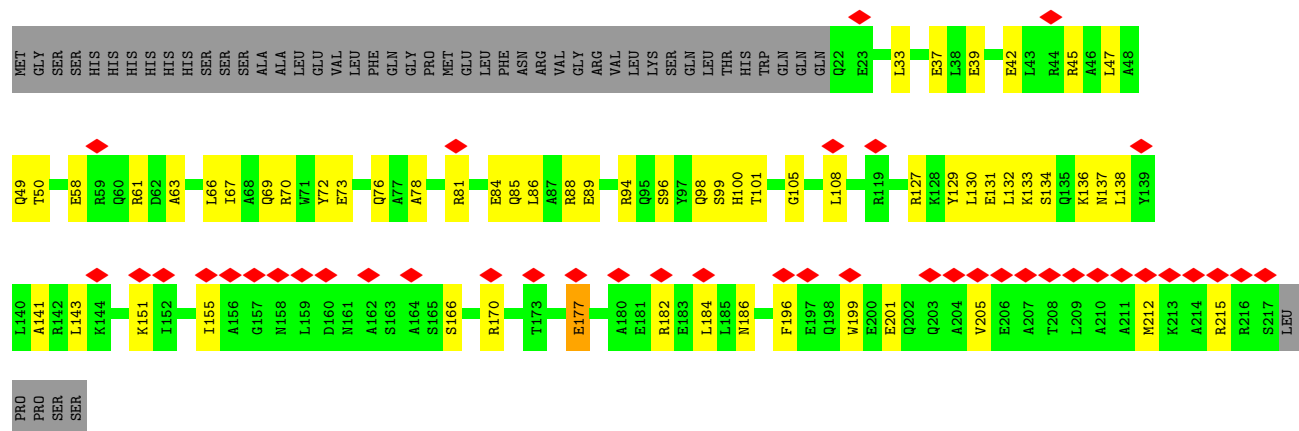


- Molecule 1: Chloroplast membrane-associated 30 kD protein

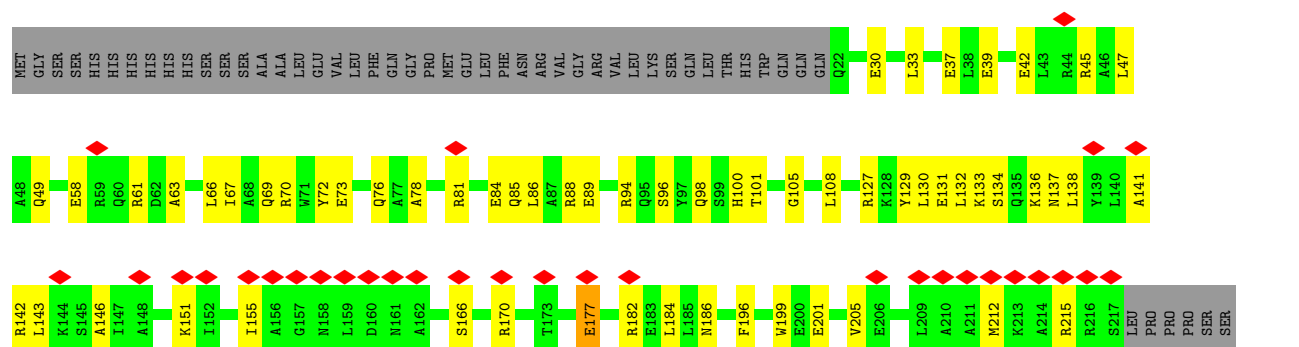




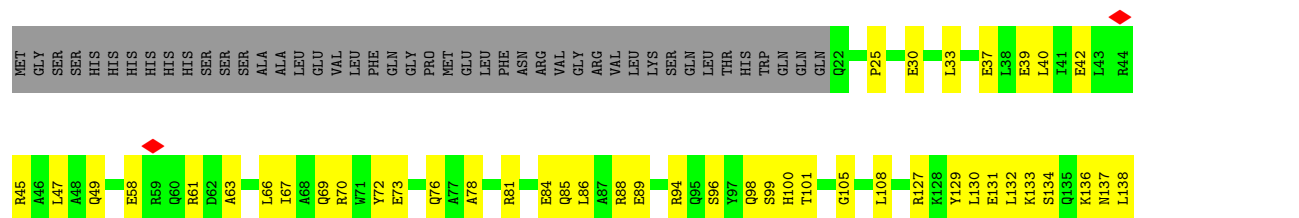
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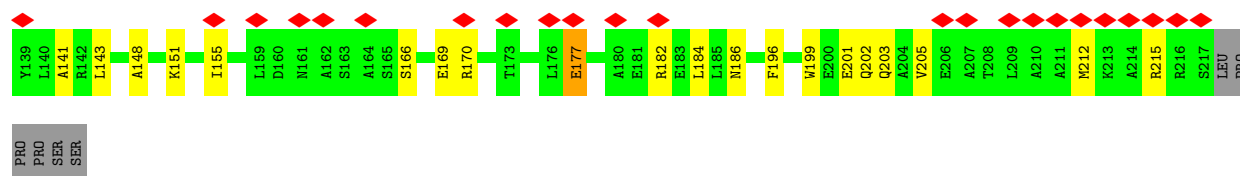


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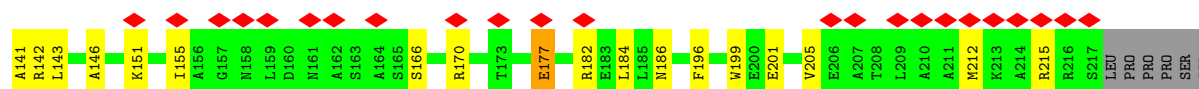
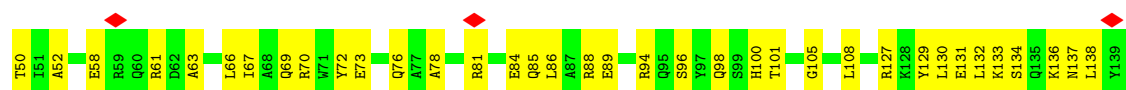
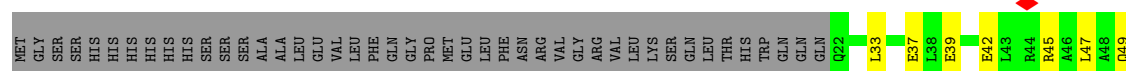


- Molecule 1: Chloroplast membrane-associated 30 kD protein

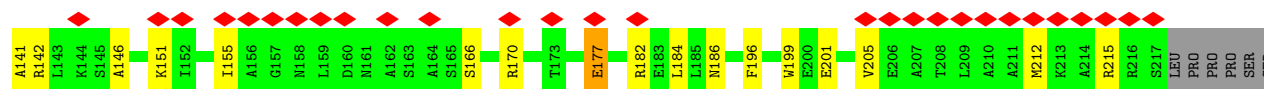
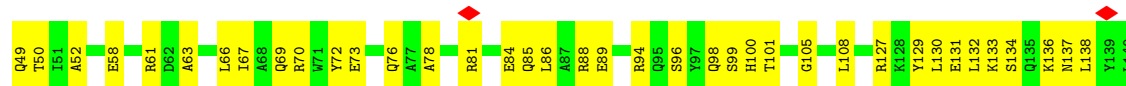
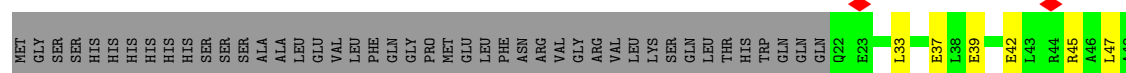




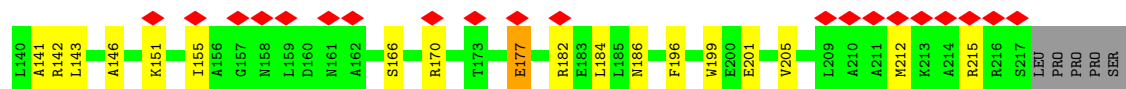
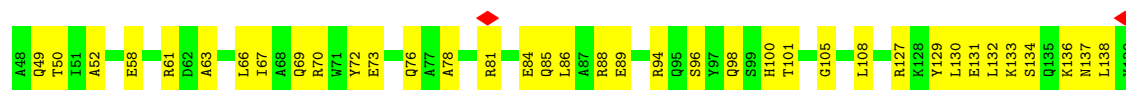
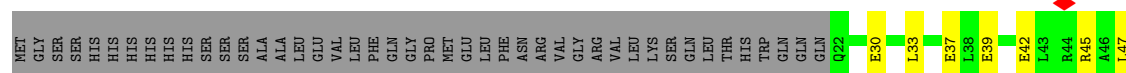
- Molecule 1: Chloroplast membrane-associated 30 kD protein



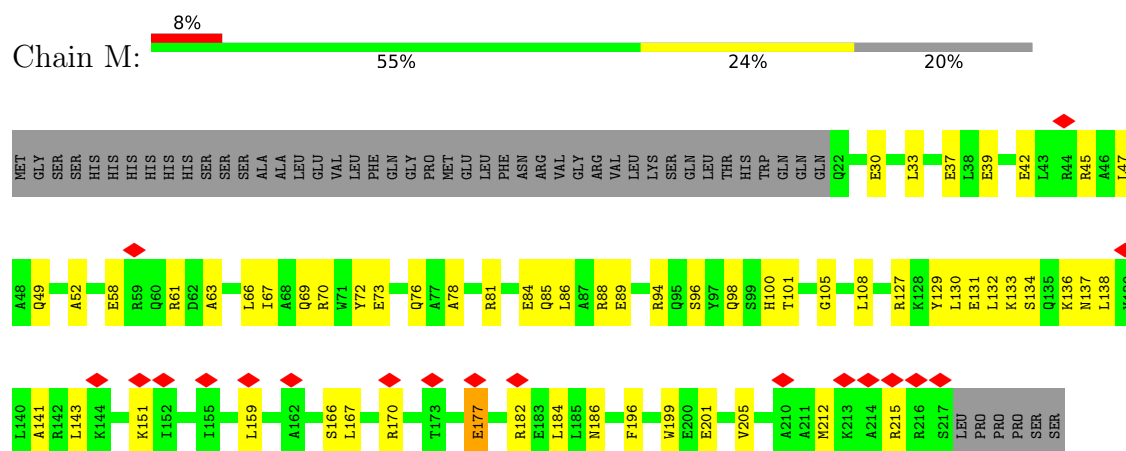
- Molecule 1: Chloroplast membrane-associated 30 kD protein



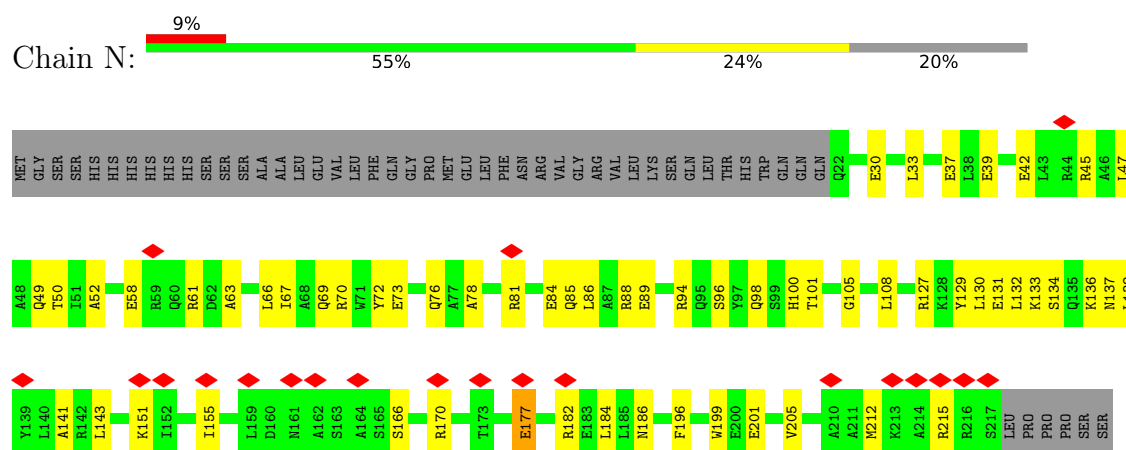
- Molecule 1: Chloroplast membrane-associated 30 kD protein



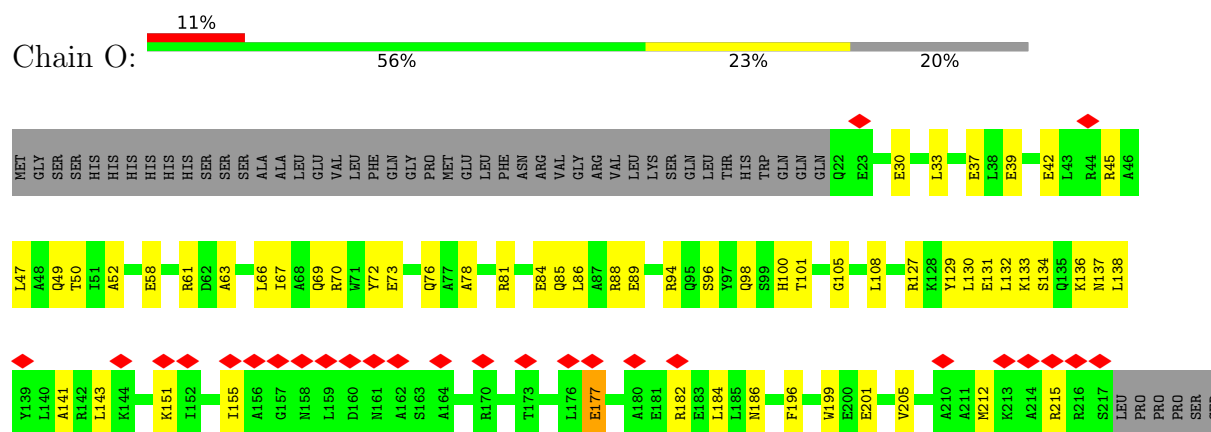
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

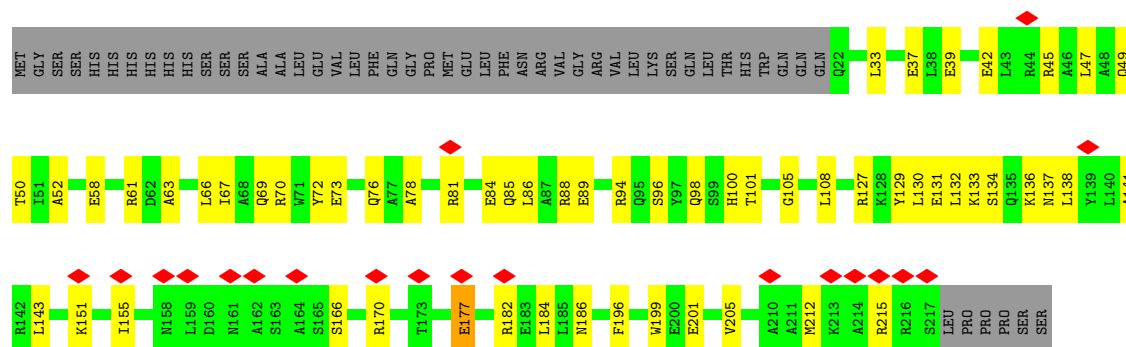


- Molecule 1: Chloroplast membrane-associated 30 kD protein

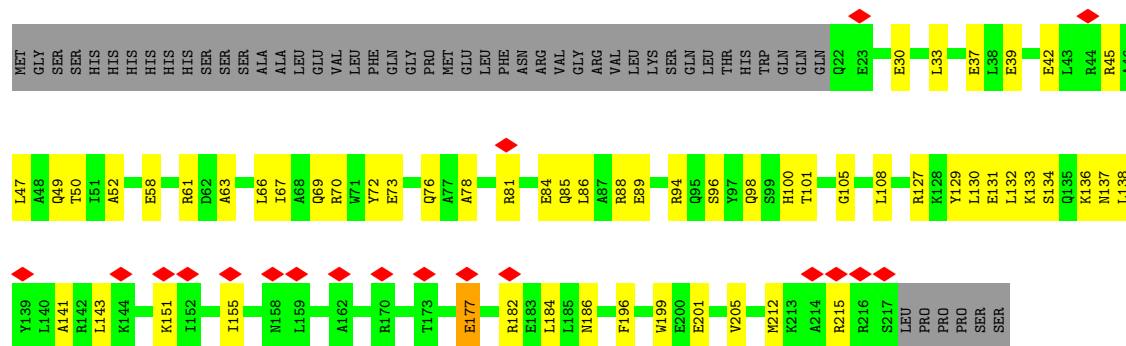


- Molecule 1: Chloroplast membrane-associated 30 kD protein

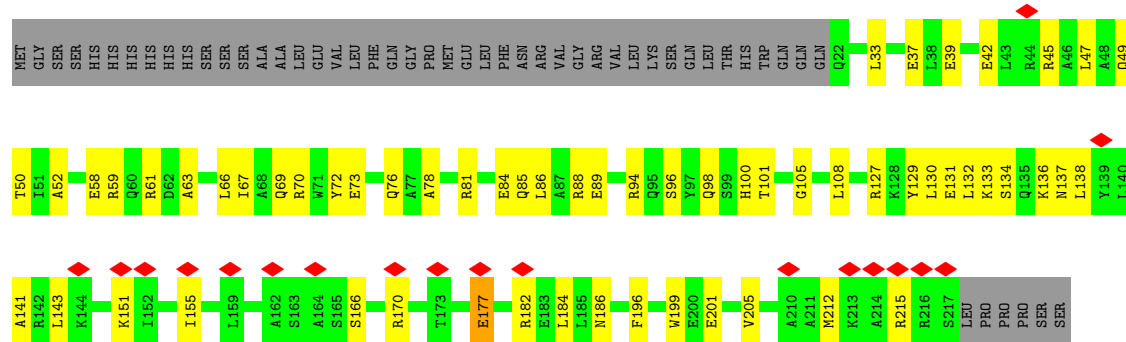




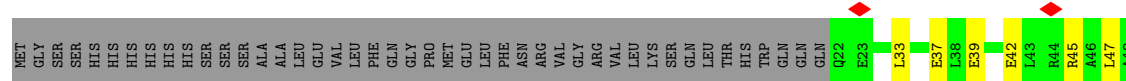
- Molecule 1: Chloroplast membrane-associated 30 kD protein

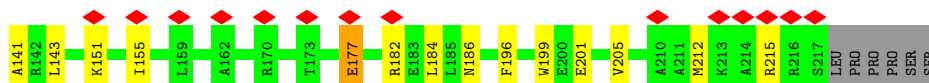


- Molecule 1: Chloroplast membrane-associated 30 kD protein

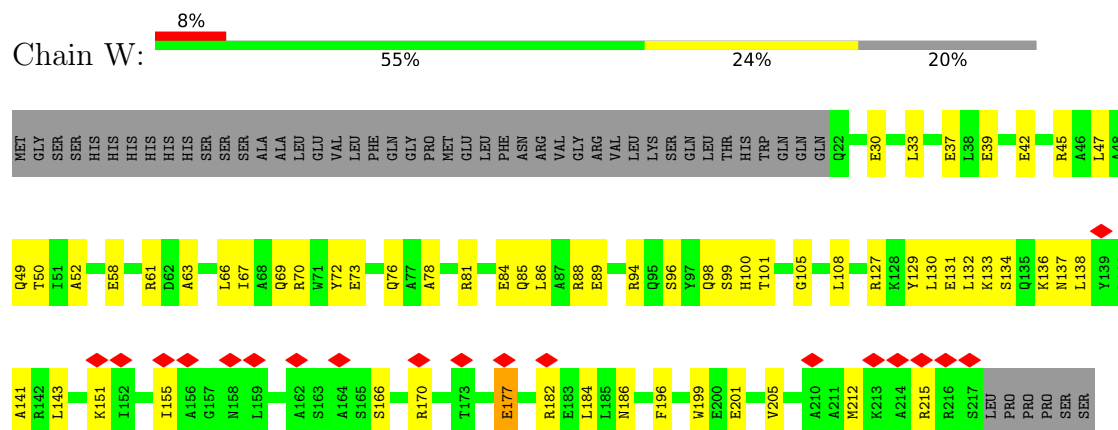


- Molecule 1: Chloroplast membrane-associated 30 kD protein

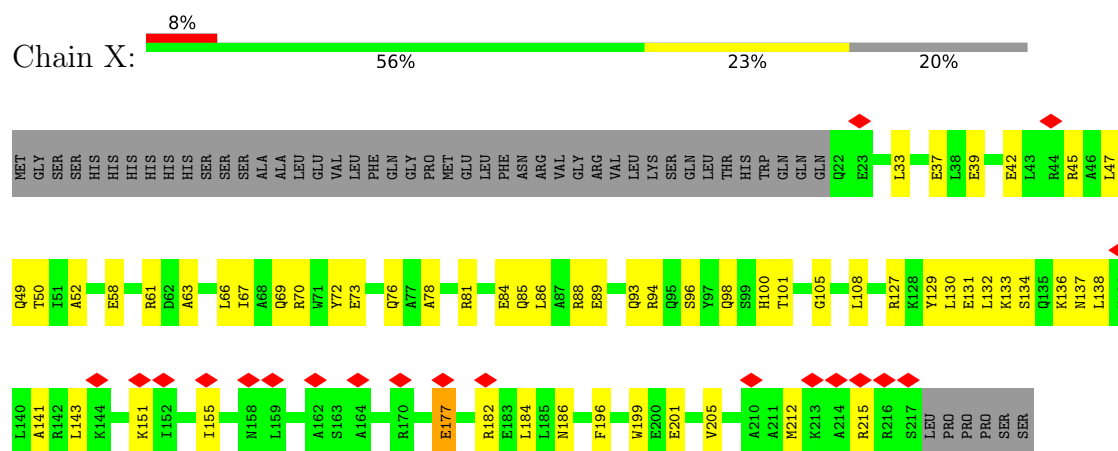




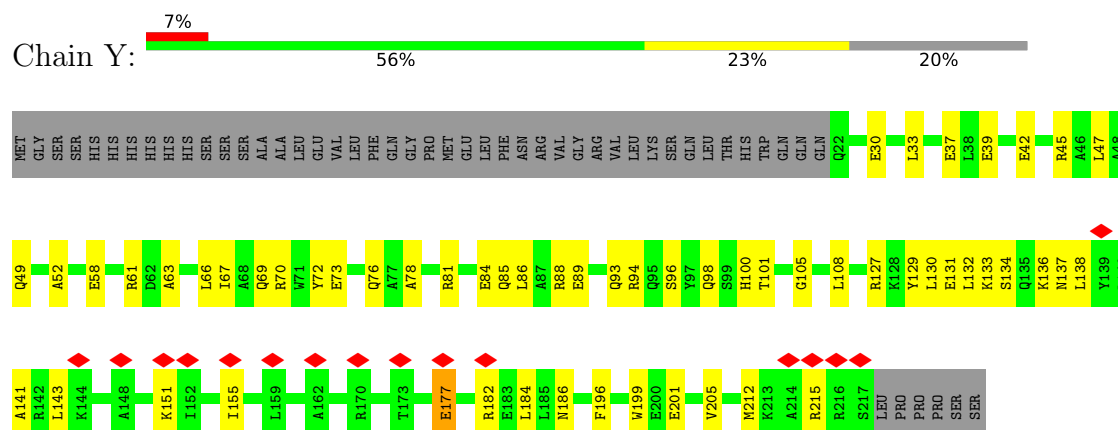
- Molecule 1: Chloroplast membrane-associated 30 kD protein



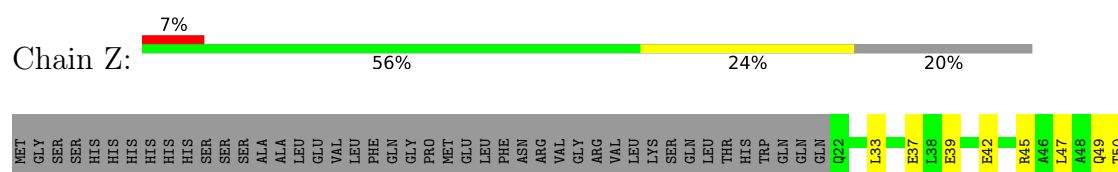
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

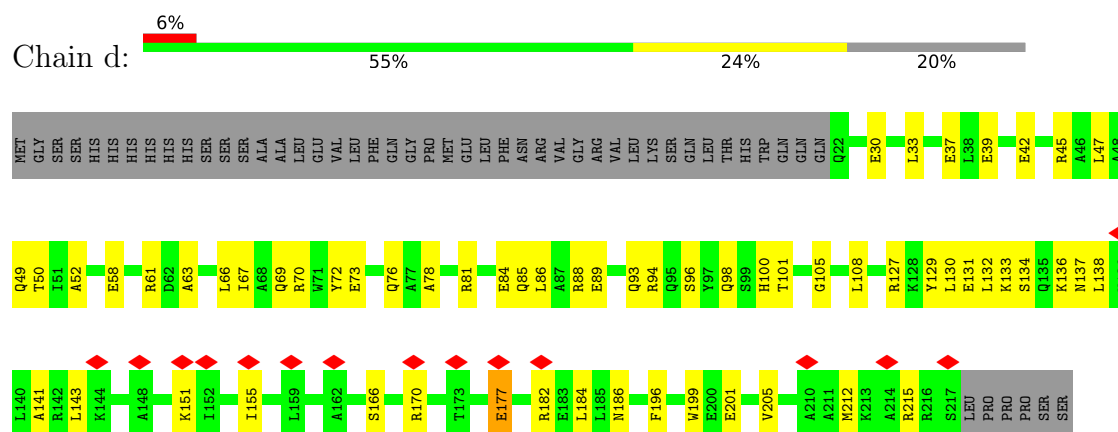


- Molecule 1: Chloroplast membrane-associated 30 kD protein

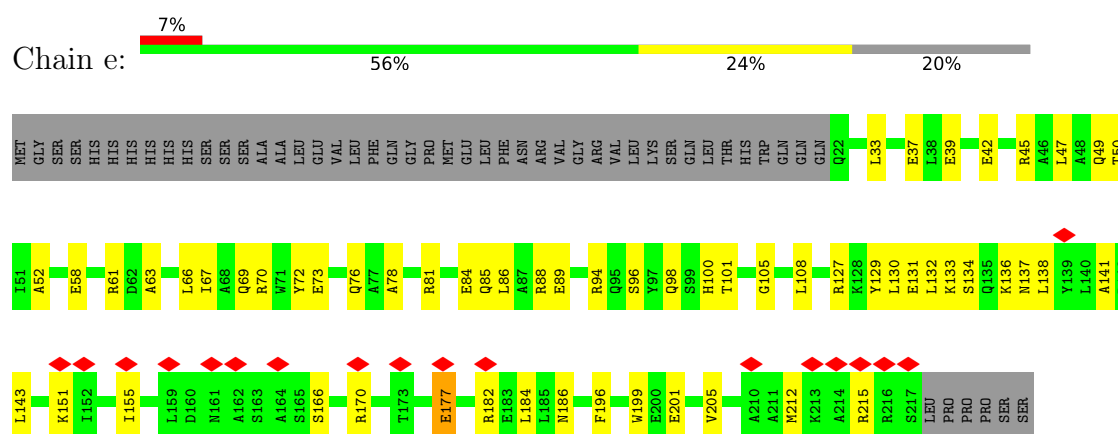




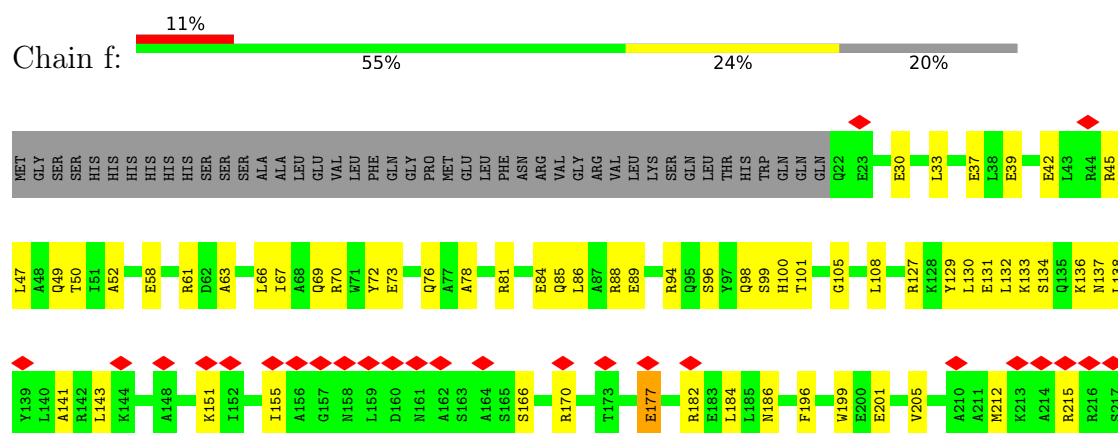
- Molecule 1: Chloroplast membrane-associated 30 kD protein



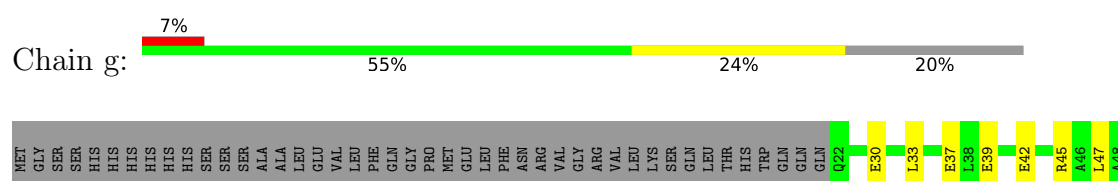
- Molecule 1: Chloroplast membrane-associated 30 kD protein

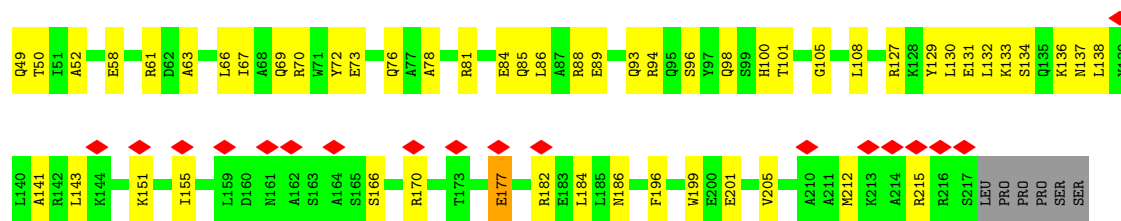


- Molecule 1: Chloroplast membrane-associated 30 kD protein

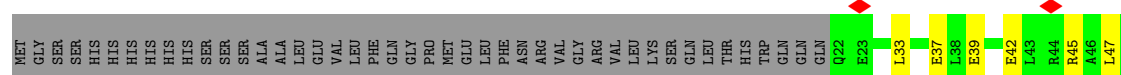


- Molecule 1: Chloroplast membrane-associated 30 kD protein

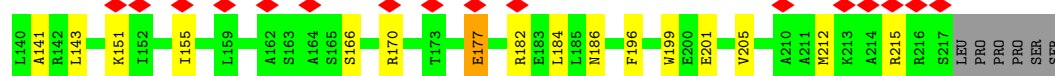
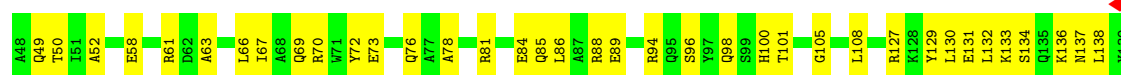
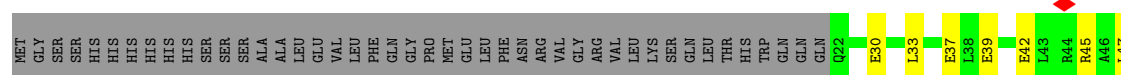




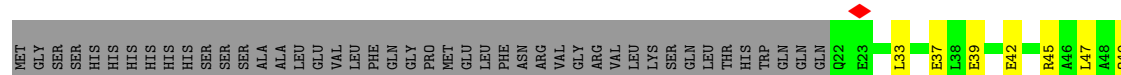
- Molecule 1: Chloroplast membrane-associated 30 kD protein

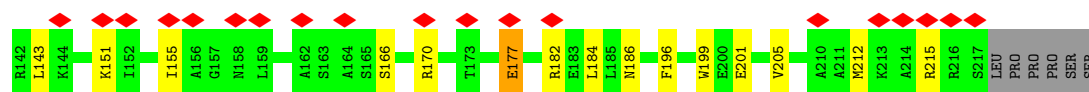


- Molecule 1: Chloroplast membrane-associated 30 kD protein

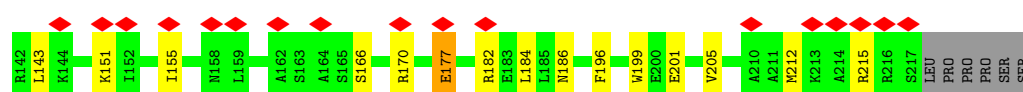
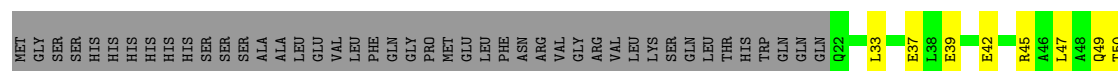


- Molecule 1: Chloroplast membrane-associated 30 kD protein

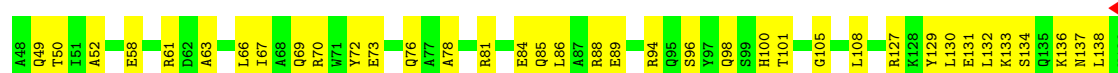
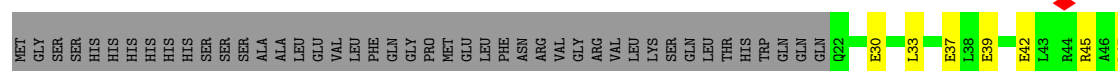




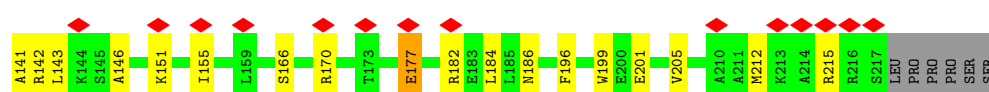
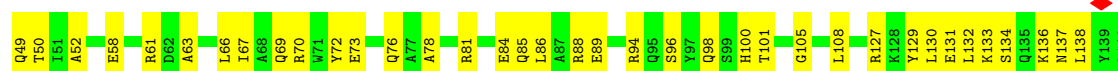
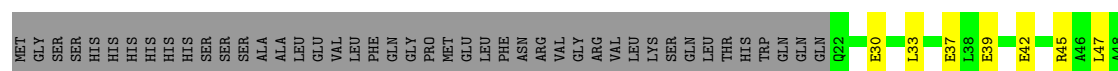
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

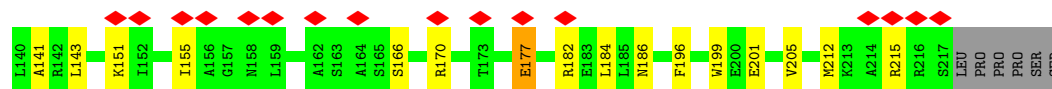


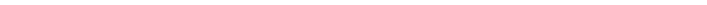
- Molecule 1: Chloroplast membrane-associated 30 kD protein

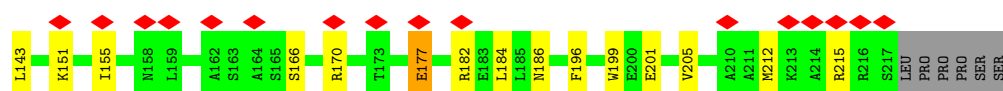


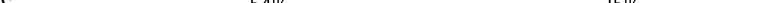
- Molecule 1: Chloroplast membrane-associated 30 kD protein



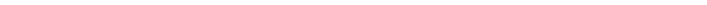


- Chain o:  7% 55% 24% 20%

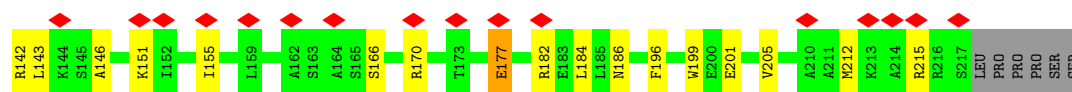


- Chain p: 

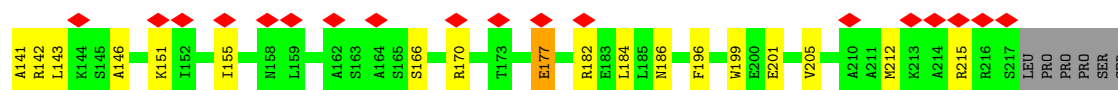
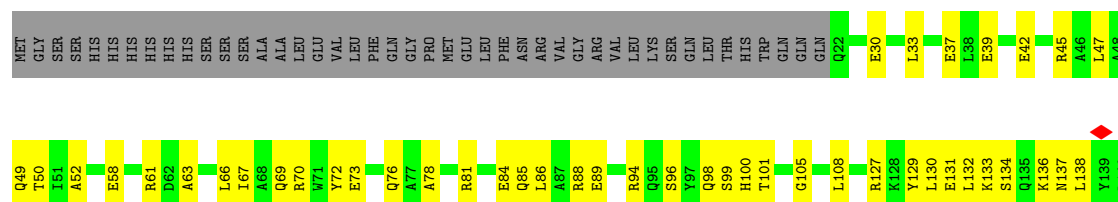


- Chain g:  7% 55% 24% 20%

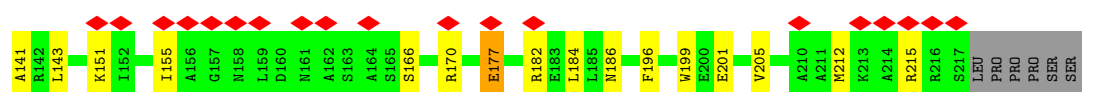
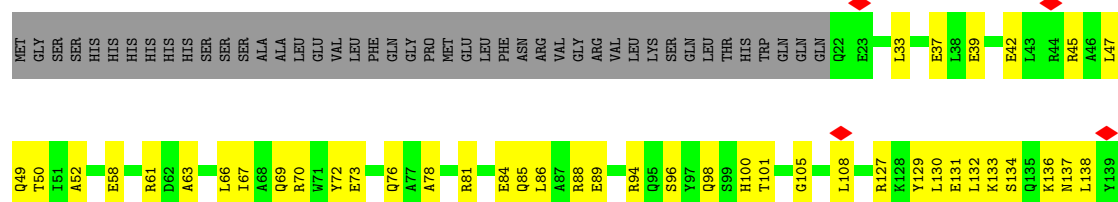




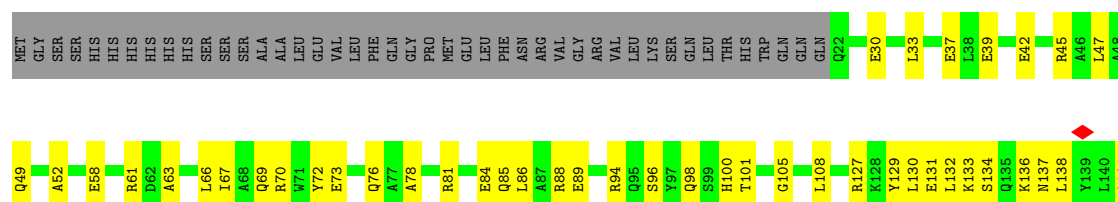
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

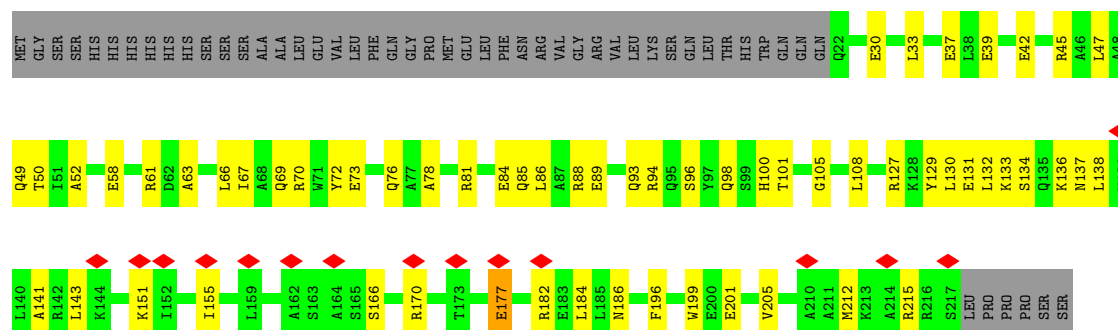


- Molecule 1: Chloroplast membrane-associated 30 kD protein

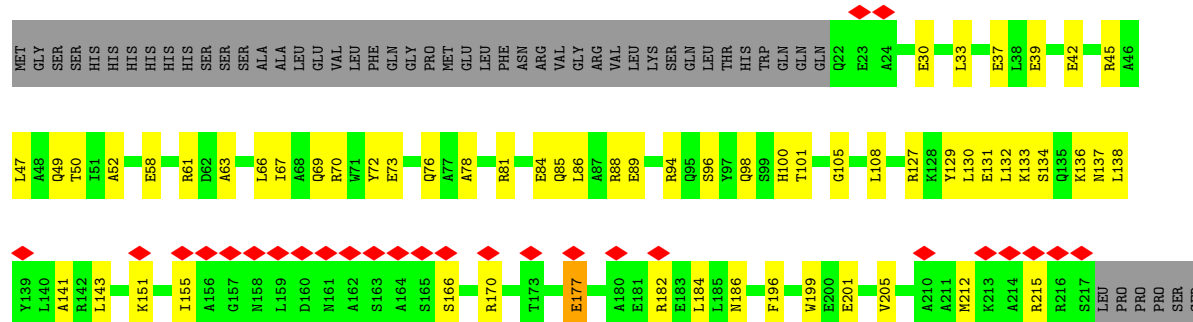


- Molecule 1: Chloroplast membrane-associated 30 kD protein

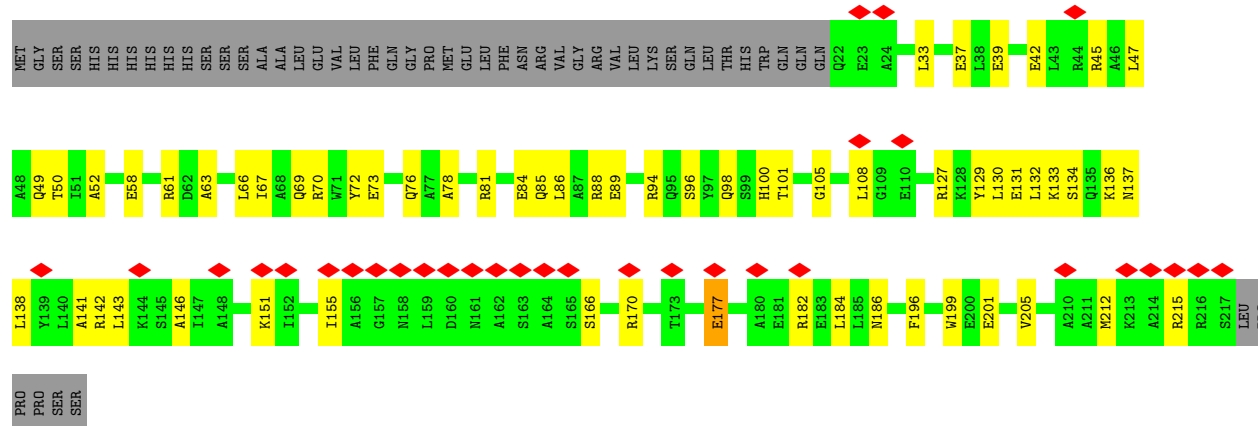




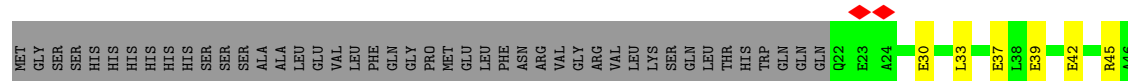
• Molecule 1: Chloroplast membrane-associated 30 kD protein

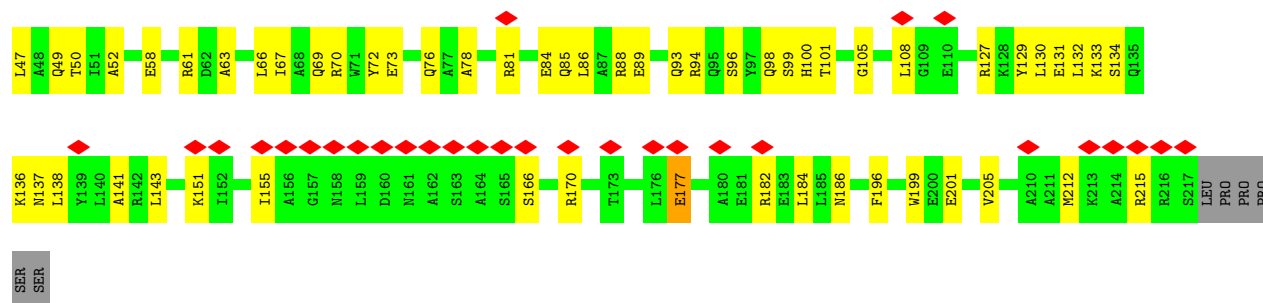


• Molecule 1: Chloroplast membrane-associated 30 kD protein

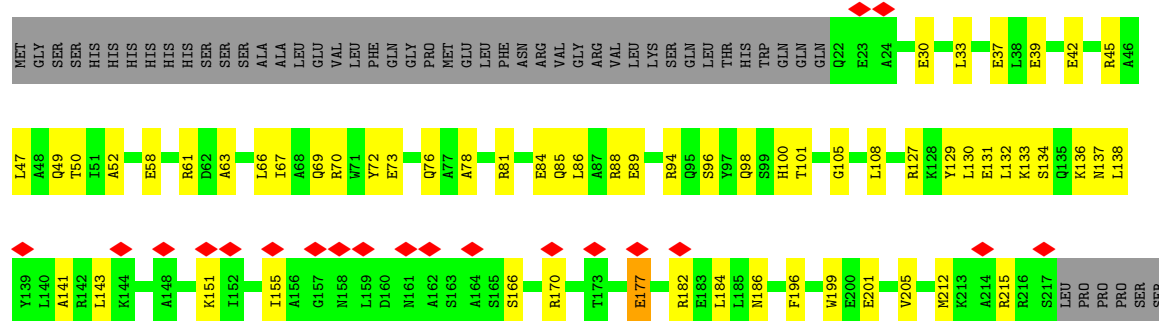


• Molecule 1: Chloroplast membrane-associated 30 kD protein

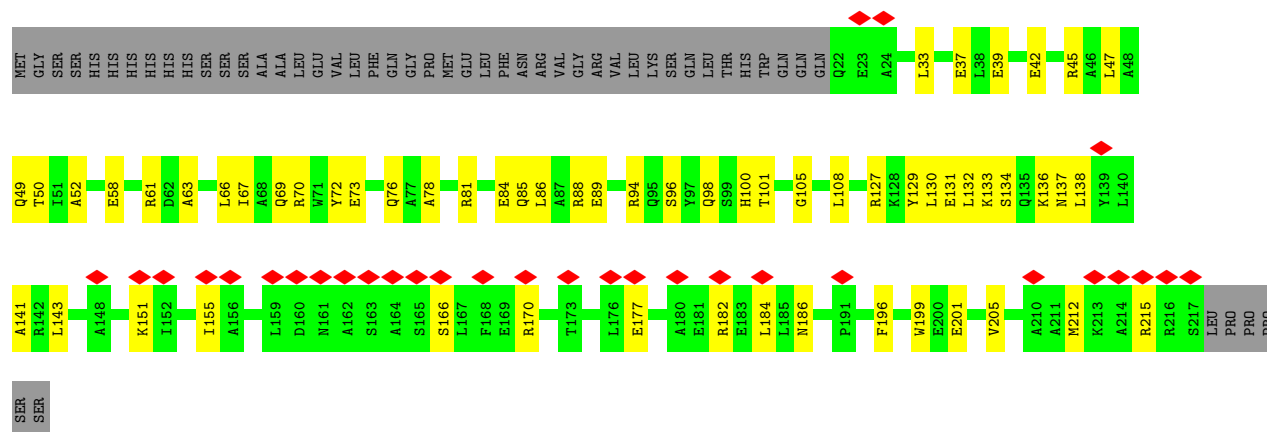




- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=-85.0°, rise=1.64 Å, axial sym=C1 | Depositor |
| Number of segments used            | 25901                                            | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION          | Depositor |
| Microscope                         | FEI TALOS ARCTICA                                | Depositor |
| Voltage (kV)                       | 200                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 58                                               | Depositor |
| Minimum defocus (nm)               | 1000                                             | Depositor |
| Maximum defocus (nm)               | 4000                                             | Depositor |
| Magnification                      | Not provided                                     |           |
| Image detector                     | GATAN K3 BIOQUANTUM (6k x 4k)                    | Depositor |
| Maximum map value                  | 0.427                                            | Depositor |
| Minimum map value                  | -0.178                                           | Depositor |
| Average map value                  | 0.002                                            | Depositor |
| Map value standard deviation       | 0.014                                            | Depositor |
| Recommended contour level          | 0.1                                              | Depositor |
| Map size (Å)                       | 544.8, 544.8, 544.8                              | wwPDB     |
| Map dimensions                     | 400, 400, 400                                    | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                  | 1.362, 1.362, 1.362                              | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$ |
| 1   | 0     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 1     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 2     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 3     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 4     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 5     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 6     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | 7     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | A     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | B     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | C     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | D     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | E     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | F     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | G     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | H     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | I     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | J     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | K     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | L     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | M     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | N     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | O     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | P     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | Q     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | R     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | S     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | T     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | U     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | V     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | W     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | X     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | Y     | 0.10         | 0/1593      | 0.22        | 0/2138      |
| 1   | Z     | 0.10         | 0/1593      | 0.22        | 0/2138      |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | a     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | b     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | c     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | d     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | e     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | f     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | g     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | h     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | i     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | j     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | k     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | l     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | m     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | n     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | o     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | p     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | q     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | r     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | s     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | t     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | u     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | v     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | w     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | x     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | y     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| 1   | z     | 0.10         | 0/1593  | 0.22        | 0/2138   |
| All | All   | 0.10         | 0/95580 | 0.22        | 0/128280 |

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   | 0     | 1577  | 1604     | 1603     | 45      | 0            |
| 1   | 1     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | 2     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | 3     | 1577  | 1604     | 1603     | 44      | 0            |
| 1   | 4     | 1577  | 1604     | 1603     | 42      | 0            |
| 1   | 5     | 1577  | 1604     | 1603     | 40      | 0            |
| 1   | 6     | 1577  | 1604     | 1603     | 42      | 0            |
| 1   | 7     | 1577  | 1604     | 1603     | 40      | 0            |
| 1   | A     | 1577  | 1604     | 1603     | 42      | 0            |
| 1   | B     | 1577  | 1604     | 1603     | 43      | 0            |
| 1   | C     | 1577  | 1604     | 1603     | 43      | 0            |
| 1   | D     | 1577  | 1604     | 1603     | 43      | 0            |
| 1   | E     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | F     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | G     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | H     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | I     | 1577  | 1604     | 1603     | 62      | 0            |
| 1   | J     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | K     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | L     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | M     | 1577  | 1604     | 1603     | 51      | 0            |
| 1   | N     | 1577  | 1604     | 1603     | 52      | 0            |
| 1   | O     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | P     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | Q     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | R     | 1577  | 1604     | 1603     | 50      | 0            |
| 1   | S     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | T     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | U     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | V     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | W     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | X     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | Y     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | Z     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | a     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | b     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | c     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | d     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | e     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | f     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | g     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | h     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | i     | 1577  | 1604     | 1603     | 47      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | j     | 1577  | 1604     | 1603     | 46      | 0            |
| 1   | k     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | l     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | m     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | n     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | o     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | p     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | q     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | r     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | s     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | t     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | u     | 1577  | 1604     | 1603     | 49      | 0            |
| 1   | v     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | w     | 1577  | 1604     | 1603     | 47      | 0            |
| 1   | x     | 1577  | 1604     | 1603     | 50      | 0            |
| 1   | y     | 1577  | 1604     | 1603     | 48      | 0            |
| 1   | z     | 1577  | 1604     | 1603     | 46      | 0            |
| All | All   | 94620 | 96240    | 96180    | 2530    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2530) 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:196:PHE:CZ  | 1:N:86:LEU:HD21 | 2.08                     | 0.87              |
| 1:I:39:GLU:O    | 1:M:151:LYS:NZ  | 2.15                     | 0.78              |
| 1:a:127:ARG:NH2 | 1:a:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:A:127:ARG:NH2 | 1:A:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:T:127:ARG:NH2 | 1:T:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:h:127:ARG:NH2 | 1:h:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:l:127:ARG:NH2 | 1:l:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:5:127:ARG:NH2 | 1:5:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:E:127:ARG:NH2 | 1:E:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:K:127:ARG:NH2 | 1:K:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:N:127:ARG:NH2 | 1:N:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:d:127:ARG:NH2 | 1:d:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:g:127:ARG:NH2 | 1:g:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:m:127:ARG:NH2 | 1:m:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:q:127:ARG:NH2 | 1:q:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:z:127:ARG:NH2 | 1:z:131:GLU:OE1 | 2.19                     | 0.76              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:127:ARG:NH2 | 1:B:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:c:127:ARG:NH2 | 1:c:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:j:127:ARG:NH2 | 1:j:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:l:127:ARG:NH2 | 1:l:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:p:127:ARG:NH2 | 1:p:131:GLU:OE1 | 2.19                     | 0.76              |
| 1:H:127:ARG:NH2 | 1:H:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:i:127:ARG:NH2 | 1:i:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:s:127:ARG:NH2 | 1:s:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:w:127:ARG:NH2 | 1:w:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:I:127:ARG:NH2 | 1:I:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:R:127:ARG:NH2 | 1:R:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:W:127:ARG:NH2 | 1:W:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:X:127:ARG:NH2 | 1:X:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:Y:127:ARG:NH2 | 1:Y:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:n:127:ARG:NH2 | 1:n:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:2:127:ARG:NH2 | 1:2:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:6:127:ARG:NH2 | 1:6:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:D:127:ARG:NH2 | 1:D:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:G:127:ARG:NH2 | 1:G:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:P:127:ARG:NH2 | 1:P:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:v:127:ARG:NH2 | 1:v:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:F:127:ARG:NH2 | 1:F:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:O:127:ARG:NH2 | 1:O:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:Q:127:ARG:NH2 | 1:Q:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:e:127:ARG:NH2 | 1:e:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:Z:127:ARG:NH2 | 1:Z:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:f:127:ARG:NH2 | 1:f:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:t:127:ARG:NH2 | 1:t:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:U:127:ARG:NH2 | 1:U:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:o:127:ARG:NH2 | 1:o:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:u:127:ARG:NH2 | 1:u:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:y:127:ARG:NH2 | 1:y:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:3:127:ARG:NH2 | 1:3:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:J:127:ARG:NH2 | 1:J:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:4:127:ARG:NH2 | 1:4:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:I:199:TRP:O   | 1:N:81:ARG:NH2  | 2.19                     | 0.75              |
| 1:r:127:ARG:NH2 | 1:r:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:0:127:ARG:NH2 | 1:0:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:7:127:ARG:NH2 | 1:7:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:M:127:ARG:NH2 | 1:M:131:GLU:OE1 | 2.19                     | 0.75              |
| 1:k:127:ARG:NH2 | 1:k:131:GLU:OE1 | 2.19                     | 0.75              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:127:ARG:NH2 | 1:L:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:x:127:ARG:NH2 | 1:x:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:C:127:ARG:NH2 | 1:C:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:V:127:ARG:NH2 | 1:V:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:b:127:ARG:NH2 | 1:b:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:S:127:ARG:NH2 | 1:S:131:GLU:OE1 | 2.19                     | 0.74              |
| 1:k:37:GLU:OE2  | 1:k:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:s:37:GLU:OE2  | 1:s:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:C:37:GLU:OE2  | 1:C:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:G:37:GLU:OE2  | 1:G:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:K:37:GLU:OE2  | 1:K:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:L:37:GLU:OE2  | 1:L:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:o:37:GLU:OE2  | 1:o:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:t:37:GLU:OE2  | 1:t:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:x:37:GLU:OE2  | 1:x:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:H:37:GLU:OE2  | 1:H:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:P:37:GLU:OE2  | 1:P:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:g:37:GLU:OE2  | 1:g:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:l:37:GLU:OE2  | 1:l:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:c:37:GLU:OE2  | 1:c:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:p:37:GLU:OE2  | 1:p:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:w:37:GLU:OE2  | 1:w:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:O:37:GLU:OE2  | 1:O:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:T:37:GLU:OE2  | 1:T:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:D:37:GLU:OE2  | 1:D:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:0:37:GLU:OE2  | 1:0:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:5:37:GLU:OE2  | 1:5:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:Y:37:GLU:OE2  | 1:Y:133:LYS:NZ  | 2.22                     | 0.73              |
| 1:j:37:GLU:OE2  | 1:j:133:LYS:NZ  | 2.21                     | 0.73              |
| 1:3:37:GLU:OE2  | 1:3:133:LYS:NZ  | 2.22                     | 0.72              |
| 1:B:37:GLU:OE2  | 1:B:133:LYS:NZ  | 2.22                     | 0.72              |
| 1:R:37:GLU:OE2  | 1:R:133:LYS:NZ  | 2.21                     | 0.72              |
| 1:U:37:GLU:OE2  | 1:U:133:LYS:NZ  | 2.22                     | 0.72              |
| 1:l:37:GLU:OE2  | 1:l:133:LYS:NZ  | 2.21                     | 0.72              |
| 1:n:37:GLU:OE2  | 1:n:133:LYS:NZ  | 2.21                     | 0.72              |
| 1:2:37:GLU:OE2  | 1:2:133:LYS:NZ  | 2.22                     | 0.72              |
| 1:6:37:GLU:OE2  | 1:6:133:LYS:NZ  | 2.22                     | 0.72              |
| 1:7:37:GLU:OE2  | 1:7:133:LYS:NZ  | 2.21                     | 0.72              |
| 1:F:37:GLU:OE2  | 1:F:133:LYS:NZ  | 2.21                     | 0.72              |
| 1:I:203:GLN:HB2 | 1:N:81:ARG:HH21 | 1.53                     | 0.72              |
| 1:Q:37:GLU:OE2  | 1:Q:133:LYS:NZ  | 2.22                     | 0.72              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:S:37:GLU:OE2  | 1:S:133:LYS:NZ | 2.21                     | 0.72              |
| 1:V:37:GLU:OE2  | 1:V:133:LYS:NZ | 2.21                     | 0.72              |
| 1:X:37:GLU:OE2  | 1:X:133:LYS:NZ | 2.21                     | 0.72              |
| 1:y:37:GLU:OE2  | 1:y:133:LYS:NZ | 2.21                     | 0.72              |
| 1:z:37:GLU:OE2  | 1:z:133:LYS:NZ | 2.22                     | 0.72              |
| 1:I:169:GLU:OE2 | 1:R:59:ARG:NH2 | 2.22                     | 0.72              |
| 1:N:37:GLU:OE2  | 1:N:133:LYS:NZ | 2.22                     | 0.72              |
| 1:f:37:GLU:OE2  | 1:f:133:LYS:NZ | 2.22                     | 0.72              |
| 1:A:37:GLU:OE2  | 1:A:133:LYS:NZ | 2.22                     | 0.72              |
| 1:Z:37:GLU:OE2  | 1:Z:133:LYS:NZ | 2.22                     | 0.72              |
| 1:i:37:GLU:OE2  | 1:i:133:LYS:NZ | 2.21                     | 0.72              |
| 1:r:37:GLU:OE2  | 1:r:133:LYS:NZ | 2.22                     | 0.72              |
| 1:v:37:GLU:OE2  | 1:v:133:LYS:NZ | 2.22                     | 0.72              |
| 1:E:37:GLU:OE2  | 1:E:133:LYS:NZ | 2.21                     | 0.72              |
| 1:J:37:GLU:OE2  | 1:J:133:LYS:NZ | 2.21                     | 0.72              |
| 1:M:37:GLU:OE2  | 1:M:133:LYS:NZ | 2.22                     | 0.72              |
| 1:m:37:GLU:OE2  | 1:m:133:LYS:NZ | 2.22                     | 0.72              |
| 1:u:37:GLU:OE2  | 1:u:133:LYS:NZ | 2.21                     | 0.72              |
| 1:4:37:GLU:OE2  | 1:4:133:LYS:NZ | 2.22                     | 0.72              |
| 1:q:37:GLU:OE2  | 1:q:133:LYS:NZ | 2.22                     | 0.72              |
| 1:I:37:GLU:OE2  | 1:I:133:LYS:NZ | 2.22                     | 0.72              |
| 1:b:37:GLU:OE2  | 1:b:133:LYS:NZ | 2.22                     | 0.72              |
| 1:b:85:GLN:NE2  | 1:b:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:B:85:GLN:NE2  | 1:B:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:X:85:GLN:NE2  | 1:X:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:d:37:GLU:OE2  | 1:d:133:LYS:NZ | 2.22                     | 0.72              |
| 1:e:37:GLU:OE2  | 1:e:133:LYS:NZ | 2.22                     | 0.72              |
| 1:f:85:GLN:NE2  | 1:f:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:j:85:GLN:NE2  | 1:j:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:5:85:GLN:NE2  | 1:5:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:F:85:GLN:NE2  | 1:F:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:n:85:GLN:NE2  | 1:n:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:T:85:GLN:NE2  | 1:T:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:h:37:GLU:OE2  | 1:h:133:LYS:NZ | 2.22                     | 0.72              |
| 1:r:85:GLN:NE2  | 1:r:89:GLU:OE2 | 2.23                     | 0.72              |
| 1:l:85:GLN:NE2  | 1:l:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:G:85:GLN:NE2  | 1:G:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:J:85:GLN:NE2  | 1:J:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:K:85:GLN:NE2  | 1:K:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:W:37:GLU:OE2  | 1:W:133:LYS:NZ | 2.22                     | 0.71              |
| 1:s:85:GLN:NE2  | 1:s:89:GLU:OE2 | 2.23                     | 0.71              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:w:85:GLN:NE2 | 1:w:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:y:85:GLN:NE2 | 1:y:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:3:137:ASN:O  | 1:3:141:ALA:N  | 2.24                     | 0.71              |
| 1:M:85:GLN:NE2 | 1:M:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:P:85:GLN:NE2 | 1:P:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:Q:85:GLN:NE2 | 1:Q:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:a:37:GLU:OE2 | 1:a:133:LYS:NZ | 2.22                     | 0.71              |
| 1:o:85:GLN:NE2 | 1:o:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:p:137:ASN:O  | 1:p:141:ALA:N  | 2.24                     | 0.71              |
| 1:2:85:GLN:NE2 | 1:2:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:D:45:ARG:NH1 | 1:D:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:D:137:ASN:O  | 1:D:141:ALA:N  | 2.24                     | 0.71              |
| 1:M:137:ASN:O  | 1:M:141:ALA:N  | 2.24                     | 0.71              |
| 1:R:137:ASN:O  | 1:R:141:ALA:N  | 2.24                     | 0.71              |
| 1:V:137:ASN:O  | 1:V:141:ALA:N  | 2.24                     | 0.71              |
| 1:u:85:GLN:NE2 | 1:u:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:u:137:ASN:O  | 1:u:141:ALA:N  | 2.24                     | 0.71              |
| 1:v:85:GLN:NE2 | 1:v:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:y:137:ASN:O  | 1:y:141:ALA:N  | 2.24                     | 0.71              |
| 1:2:45:ARG:NH1 | 1:2:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:7:137:ASN:O  | 1:7:141:ALA:N  | 2.24                     | 0.71              |
| 1:H:137:ASN:O  | 1:H:141:ALA:N  | 2.24                     | 0.71              |
| 1:N:85:GLN:NE2 | 1:N:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:O:85:GLN:NE2 | 1:O:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:Q:137:ASN:O  | 1:Q:141:ALA:N  | 2.24                     | 0.71              |
| 1:e:137:ASN:O  | 1:e:141:ALA:N  | 2.24                     | 0.71              |
| 1:l:45:ARG:NH1 | 1:l:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:p:45:ARG:NH1 | 1:p:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:x:85:GLN:NE2 | 1:x:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:y:45:ARG:NH1 | 1:y:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:6:45:ARG:NH1 | 1:6:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:C:85:GLN:NE2 | 1:C:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:H:45:ARG:NH1 | 1:H:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:I:137:ASN:O  | 1:I:141:ALA:N  | 2.24                     | 0.71              |
| 1:L:45:ARG:NH1 | 1:L:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:M:45:ARG:NH1 | 1:M:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:Q:45:ARG:NH1 | 1:Q:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:U:45:ARG:NH1 | 1:U:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:U:85:GLN:NE2 | 1:U:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:V:85:GLN:NE2 | 1:V:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:l:137:ASN:O  | 1:l:141:ALA:N  | 2.24                     | 0.71              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:t:45:ARG:NH1 | 1:t:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:u:45:ARG:NH1 | 1:u:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:z:137:ASN:O  | 1:z:141:ALA:N  | 2.24                     | 0.71              |
| 1:1:45:ARG:NH1 | 1:1:49:GLN:OE1 | 2.23                     | 0.71              |
| 1:7:85:GLN:NE2 | 1:7:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:I:85:GLN:NE2 | 1:I:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:P:45:ARG:NH1 | 1:P:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:Y:45:ARG:NH1 | 1:Y:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:Z:137:ASN:O  | 1:Z:141:ALA:N  | 2.24                     | 0.71              |
| 1:a:137:ASN:O  | 1:a:141:ALA:N  | 2.24                     | 0.71              |
| 1:t:137:ASN:O  | 1:t:141:ALA:N  | 2.24                     | 0.71              |
| 1:x:45:ARG:NH1 | 1:x:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:0:85:GLN:NE2 | 1:0:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:2:137:ASN:O  | 1:2:141:ALA:N  | 2.24                     | 0.71              |
| 1:3:85:GLN:NE2 | 1:3:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:L:85:GLN:NE2 | 1:L:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:Z:85:GLN:NE2 | 1:Z:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:c:45:ARG:NH1 | 1:c:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:g:45:ARG:NH1 | 1:g:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:h:45:ARG:NH1 | 1:h:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:q:45:ARG:NH1 | 1:q:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:z:85:GLN:NE2 | 1:z:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:0:45:ARG:NH1 | 1:0:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:6:85:GLN:NE2 | 1:6:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:I:45:ARG:NH1 | 1:I:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:J:45:ARG:NH1 | 1:J:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:R:85:GLN:NE2 | 1:R:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:T:45:ARG:NH1 | 1:T:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:g:137:ASN:O  | 1:g:141:ALA:N  | 2.24                     | 0.71              |
| 1:k:137:ASN:O  | 1:k:141:ALA:N  | 2.24                     | 0.71              |
| 1:q:85:GLN:NE2 | 1:q:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:q:137:ASN:O  | 1:q:141:ALA:N  | 2.24                     | 0.71              |
| 1:4:45:ARG:NH1 | 1:4:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:D:85:GLN:NE2 | 1:D:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:E:45:ARG:NH1 | 1:E:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:H:85:GLN:NE2 | 1:H:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:L:137:ASN:O  | 1:L:141:ALA:N  | 2.24                     | 0.71              |
| 1:N:137:ASN:O  | 1:N:141:ALA:N  | 2.24                     | 0.71              |
| 1:S:45:ARG:NH1 | 1:S:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:a:85:GLN:NE2 | 1:a:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:c:137:ASN:O  | 1:c:141:ALA:N  | 2.24                     | 0.71              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:d:45:ARG:NH1 | 1:d:49:GLN:OE1 | 2.24                     | 0.71              |
| 1:i:137:ASN:O  | 1:i:141:ALA:N  | 2.24                     | 0.71              |
| 1:k:85:GLN:NE2 | 1:k:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:p:85:GLN:NE2 | 1:p:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:r:45:ARG:NH1 | 1:r:49:GLN:OE1 | 2.23                     | 0.71              |
| 1:t:85:GLN:NE2 | 1:t:89:GLU:OE2 | 2.23                     | 0.71              |
| 1:5:45:ARG:NH1 | 1:5:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:N:45:ARG:NH1 | 1:N:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:O:45:ARG:NH1 | 1:O:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:U:137:ASN:O  | 1:U:141:ALA:N  | 2.24                     | 0.70              |
| 1:W:137:ASN:O  | 1:W:141:ALA:N  | 2.24                     | 0.70              |
| 1:Y:85:GLN:NE2 | 1:Y:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:e:85:GLN:NE2 | 1:e:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:k:45:ARG:NH1 | 1:k:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:v:45:ARG:NH1 | 1:v:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:w:45:ARG:NH1 | 1:w:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:4:85:GLN:NE2 | 1:4:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:C:137:ASN:O  | 1:C:141:ALA:N  | 2.24                     | 0.70              |
| 1:E:85:GLN:NE2 | 1:E:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:F:45:ARG:NH1 | 1:F:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:S:85:GLN:NE2 | 1:S:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:W:45:ARG:NH1 | 1:W:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:d:85:GLN:NE2 | 1:d:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:h:137:ASN:O  | 1:h:141:ALA:N  | 2.24                     | 0.70              |
| 1:l:85:GLN:NE2 | 1:l:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:m:45:ARG:NH1 | 1:m:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:C:45:ARG:NH1 | 1:C:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:W:85:GLN:NE2 | 1:W:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:X:45:ARG:NH1 | 1:X:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:Z:45:ARG:NH1 | 1:Z:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:j:137:ASN:O  | 1:j:141:ALA:N  | 2.24                     | 0.70              |
| 1:n:45:ARG:NH1 | 1:n:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:x:137:ASN:O  | 1:x:141:ALA:N  | 2.24                     | 0.70              |
| 1:4:137:ASN:O  | 1:4:141:ALA:N  | 2.24                     | 0.70              |
| 1:7:45:ARG:NH1 | 1:7:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:B:45:ARG:NH1 | 1:B:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:B:137:ASN:O  | 1:B:141:ALA:N  | 2.24                     | 0.70              |
| 1:E:137:ASN:O  | 1:E:141:ALA:N  | 2.24                     | 0.70              |
| 1:K:45:ARG:NH1 | 1:K:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:f:137:ASN:O  | 1:f:141:ALA:N  | 2.24                     | 0.70              |
| 1:n:137:ASN:O  | 1:n:141:ALA:N  | 2.24                     | 0.70              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:o:137:ASN:O  | 1:o:141:ALA:N  | 2.24                     | 0.70              |
| 1:v:137:ASN:O  | 1:v:141:ALA:N  | 2.24                     | 0.70              |
| 1:z:45:ARG:NH1 | 1:z:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:A:45:ARG:NH1 | 1:A:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:A:137:ASN:O  | 1:A:141:ALA:N  | 2.24                     | 0.70              |
| 1:b:137:ASN:O  | 1:b:141:ALA:N  | 2.24                     | 0.70              |
| 1:h:85:GLN:NE2 | 1:h:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:i:85:GLN:NE2 | 1:i:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:j:45:ARG:NH1 | 1:j:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:o:45:ARG:NH1 | 1:o:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:6:137:ASN:O  | 1:6:141:ALA:N  | 2.24                     | 0.70              |
| 1:F:137:ASN:O  | 1:F:141:ALA:N  | 2.24                     | 0.70              |
| 1:V:45:ARG:NH1 | 1:V:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:m:85:GLN:NE2 | 1:m:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:G:45:ARG:NH1 | 1:G:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:G:137:ASN:O  | 1:G:141:ALA:N  | 2.24                     | 0.70              |
| 1:R:45:ARG:NH1 | 1:R:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:Y:137:ASN:O  | 1:Y:141:ALA:N  | 2.24                     | 0.70              |
| 1:a:45:ARG:NH1 | 1:a:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:s:45:ARG:NH1 | 1:s:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:3:45:ARG:NH1 | 1:3:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:P:137:ASN:O  | 1:P:141:ALA:N  | 2.24                     | 0.70              |
| 1:S:137:ASN:O  | 1:S:141:ALA:N  | 2.24                     | 0.70              |
| 1:X:137:ASN:O  | 1:X:141:ALA:N  | 2.24                     | 0.70              |
| 1:b:45:ARG:NH1 | 1:b:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:f:45:ARG:NH1 | 1:f:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:i:45:ARG:NH1 | 1:i:49:GLN:OE1 | 2.24                     | 0.70              |
| 1:m:137:ASN:O  | 1:m:141:ALA:N  | 2.24                     | 0.70              |
| 1:A:85:GLN:NE2 | 1:A:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:r:137:ASN:O  | 1:r:141:ALA:N  | 2.24                     | 0.70              |
| 1:5:137:ASN:O  | 1:5:141:ALA:N  | 2.24                     | 0.70              |
| 1:J:137:ASN:O  | 1:J:141:ALA:N  | 2.24                     | 0.70              |
| 1:c:85:GLN:NE2 | 1:c:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:g:85:GLN:NE2 | 1:g:89:GLU:OE2 | 2.23                     | 0.70              |
| 1:s:137:ASN:O  | 1:s:141:ALA:N  | 2.24                     | 0.70              |
| 1:0:137:ASN:O  | 1:0:141:ALA:N  | 2.24                     | 0.69              |
| 1:T:137:ASN:O  | 1:T:141:ALA:N  | 2.24                     | 0.69              |
| 1:K:137:ASN:O  | 1:K:141:ALA:N  | 2.24                     | 0.69              |
| 1:e:45:ARG:NH1 | 1:e:49:GLN:OE1 | 2.24                     | 0.69              |
| 1:1:137:ASN:O  | 1:1:141:ALA:N  | 2.24                     | 0.69              |
| 1:d:137:ASN:O  | 1:d:141:ALA:N  | 2.24                     | 0.69              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:w:137:ASN:O   | 1:w:141:ALA:N   | 2.24                     | 0.69              |
| 1:O:137:ASN:O   | 1:O:141:ALA:N   | 2.24                     | 0.69              |
| 1:I:196:PHE:CE1 | 1:N:86:LEU:HD21 | 2.27                     | 0.68              |
| 1:M:130:LEU:O   | 1:M:134:SER:N   | 2.28                     | 0.67              |
| 1:u:130:LEU:O   | 1:u:134:SER:N   | 2.28                     | 0.67              |
| 1:y:130:LEU:O   | 1:y:134:SER:N   | 2.28                     | 0.67              |
| 1:I:130:LEU:O   | 1:I:134:SER:N   | 2.28                     | 0.67              |
| 1:Q:130:LEU:O   | 1:Q:134:SER:N   | 2.28                     | 0.67              |
| 1:2:130:LEU:O   | 1:2:134:SER:N   | 2.28                     | 0.67              |
| 1:H:130:LEU:O   | 1:H:134:SER:N   | 2.28                     | 0.67              |
| 1:p:130:LEU:O   | 1:p:134:SER:N   | 2.28                     | 0.67              |
| 1:t:130:LEU:O   | 1:t:134:SER:N   | 2.28                     | 0.67              |
| 1:3:130:LEU:O   | 1:3:134:SER:N   | 2.28                     | 0.67              |
| 1:D:130:LEU:O   | 1:D:134:SER:N   | 2.28                     | 0.67              |
| 1:R:130:LEU:O   | 1:R:134:SER:N   | 2.28                     | 0.67              |
| 1:U:130:LEU:O   | 1:U:134:SER:N   | 2.28                     | 0.67              |
| 1:q:130:LEU:O   | 1:q:134:SER:N   | 2.28                     | 0.67              |
| 1:E:130:LEU:O   | 1:E:134:SER:N   | 2.28                     | 0.67              |
| 1:L:130:LEU:O   | 1:L:134:SER:N   | 2.28                     | 0.67              |
| 1:V:130:LEU:O   | 1:V:134:SER:N   | 2.28                     | 0.67              |
| 1:z:130:LEU:O   | 1:z:134:SER:N   | 2.28                     | 0.67              |
| 1:7:130:LEU:O   | 1:7:134:SER:N   | 2.28                     | 0.67              |
| 1:N:130:LEU:O   | 1:N:134:SER:N   | 2.28                     | 0.67              |
| 1:x:130:LEU:O   | 1:x:134:SER:N   | 2.28                     | 0.67              |
| 1:6:130:LEU:O   | 1:6:134:SER:N   | 2.28                     | 0.67              |
| 1:l:130:LEU:O   | 1:l:134:SER:N   | 2.28                     | 0.67              |
| 1:P:130:LEU:O   | 1:P:134:SER:N   | 2.28                     | 0.66              |
| 1:Z:130:LEU:O   | 1:Z:134:SER:N   | 2.28                     | 0.66              |
| 1:m:130:LEU:O   | 1:m:134:SER:N   | 2.28                     | 0.66              |
| 1:v:130:LEU:O   | 1:v:134:SER:N   | 2.28                     | 0.66              |
| 1:Y:130:LEU:O   | 1:Y:134:SER:N   | 2.28                     | 0.66              |
| 1:1:130:LEU:O   | 1:1:134:SER:N   | 2.28                     | 0.66              |
| 1:J:130:LEU:O   | 1:J:134:SER:N   | 2.28                     | 0.66              |
| 1:A:130:LEU:O   | 1:A:134:SER:N   | 2.28                     | 0.66              |
| 1:h:130:LEU:O   | 1:h:134:SER:N   | 2.28                     | 0.66              |
| 1:r:130:LEU:O   | 1:r:134:SER:N   | 2.28                     | 0.66              |
| 1:T:130:LEU:O   | 1:T:134:SER:N   | 2.28                     | 0.66              |
| 1:d:130:LEU:O   | 1:d:134:SER:N   | 2.28                     | 0.66              |
| 1:C:130:LEU:O   | 1:C:134:SER:N   | 2.28                     | 0.66              |
| 1:F:130:LEU:O   | 1:F:134:SER:N   | 2.28                     | 0.66              |
| 1:G:130:LEU:O   | 1:G:134:SER:N   | 2.28                     | 0.66              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:N:39:GLU:O   | 1:R:151:LYS:NZ | 2.29                     | 0.66              |
| 1:i:130:LEU:O  | 1:i:134:SER:N  | 2.28                     | 0.66              |
| 1:o:130:LEU:O  | 1:o:134:SER:N  | 2.28                     | 0.66              |
| 1:4:130:LEU:O  | 1:4:134:SER:N  | 2.28                     | 0.66              |
| 1:B:39:GLU:O   | 1:F:151:LYS:NZ | 2.29                     | 0.66              |
| 1:W:130:LEU:O  | 1:W:134:SER:N  | 2.28                     | 0.66              |
| 1:a:130:LEU:O  | 1:a:134:SER:N  | 2.28                     | 0.66              |
| 1:j:39:GLU:O   | 1:n:151:LYS:NZ | 2.29                     | 0.66              |
| 1:k:130:LEU:O  | 1:k:134:SER:N  | 2.28                     | 0.66              |
| 1:v:39:GLU:O   | 1:z:151:LYS:NZ | 2.29                     | 0.66              |
| 1:0:130:LEU:O  | 1:0:134:SER:N  | 2.28                     | 0.66              |
| 1:0:151:LYS:NZ | 1:w:39:GLU:O   | 2.29                     | 0.66              |
| 1:5:130:LEU:O  | 1:5:134:SER:N  | 2.28                     | 0.66              |
| 1:A:39:GLU:O   | 1:E:151:LYS:NZ | 2.29                     | 0.66              |
| 1:K:130:LEU:O  | 1:K:134:SER:N  | 2.28                     | 0.66              |
| 1:O:130:LEU:O  | 1:O:134:SER:N  | 2.28                     | 0.66              |
| 1:S:130:LEU:O  | 1:S:134:SER:N  | 2.28                     | 0.66              |
| 1:W:39:GLU:O   | 1:a:151:LYS:NZ | 2.29                     | 0.66              |
| 1:a:39:GLU:O   | 1:e:151:LYS:NZ | 2.29                     | 0.66              |
| 1:g:130:LEU:O  | 1:g:134:SER:N  | 2.28                     | 0.66              |
| 1:s:130:LEU:O  | 1:s:134:SER:N  | 2.28                     | 0.66              |
| 1:w:130:LEU:O  | 1:w:134:SER:N  | 2.28                     | 0.66              |
| 1:3:151:LYS:NZ | 1:z:39:GLU:O   | 2.29                     | 0.65              |
| 1:K:39:GLU:O   | 1:O:151:LYS:NZ | 2.29                     | 0.65              |
| 1:O:39:GLU:O   | 1:S:151:LYS:NZ | 2.29                     | 0.65              |
| 1:c:130:LEU:O  | 1:c:134:SER:N  | 2.28                     | 0.65              |
| 1:e:130:LEU:O  | 1:e:134:SER:N  | 2.28                     | 0.65              |
| 1:n:39:GLU:O   | 1:r:151:LYS:NZ | 2.29                     | 0.65              |
| 1:n:130:LEU:O  | 1:n:134:SER:N  | 2.28                     | 0.65              |
| 1:i:39:GLU:O   | 1:m:151:LYS:NZ | 2.29                     | 0.65              |
| 1:m:39:GLU:O   | 1:q:151:LYS:NZ | 2.29                     | 0.65              |
| 1:J:39:GLU:O   | 1:N:151:LYS:NZ | 2.29                     | 0.65              |
| 1:X:39:GLU:O   | 1:b:151:LYS:NZ | 2.29                     | 0.65              |
| 1:B:130:LEU:O  | 1:B:134:SER:N  | 2.28                     | 0.65              |
| 1:X:130:LEU:O  | 1:X:134:SER:N  | 2.28                     | 0.65              |
| 1:s:39:GLU:O   | 1:w:151:LYS:NZ | 2.29                     | 0.65              |
| 1:0:39:GLU:O   | 1:4:151:LYS:NZ | 2.29                     | 0.65              |
| 1:R:39:GLU:O   | 1:V:151:LYS:NZ | 2.29                     | 0.65              |
| 1:b:39:GLU:O   | 1:f:151:LYS:NZ | 2.29                     | 0.65              |
| 1:f:39:GLU:O   | 1:j:151:LYS:NZ | 2.29                     | 0.65              |
| 1:j:130:LEU:O  | 1:j:134:SER:N  | 2.28                     | 0.65              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:39:GLU:O    | 1:J:151:LYS:NZ  | 2.29                     | 0.65              |
| 1:r:39:GLU:O    | 1:v:151:LYS:NZ  | 2.29                     | 0.65              |
| 1:V:39:GLU:O    | 1:Z:151:LYS:NZ  | 2.29                     | 0.65              |
| 1:k:39:GLU:O    | 1:o:151:LYS:NZ  | 2.29                     | 0.65              |
| 1:G:39:GLU:O    | 1:K:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:H:39:GLU:O    | 1:L:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:U:39:GLU:O    | 1:Y:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:b:130:LEU:O   | 1:b:134:SER:N   | 2.28                     | 0.64              |
| 1:d:39:GLU:O    | 1:h:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:e:39:GLU:O    | 1:i:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:g:39:GLU:O    | 1:k:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:p:39:GLU:O    | 1:t:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:q:39:GLU:O    | 1:u:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:2:151:LYS:NZ  | 1:y:39:GLU:O    | 2.29                     | 0.64              |
| 1:M:39:GLU:O    | 1:Q:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:S:39:GLU:O    | 1:W:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:c:39:GLU:O    | 1:g:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:3:39:GLU:O    | 1:7:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:f:130:LEU:O   | 1:f:134:SER:N   | 2.28                     | 0.64              |
| 1:h:39:GLU:O    | 1:l:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:2:39:GLU:O    | 1:6:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:u:39:GLU:O    | 1:y:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:1:39:GLU:O    | 1:5:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:1:151:LYS:NZ  | 1:x:39:GLU:O    | 2.29                     | 0.64              |
| 1:P:39:GLU:O    | 1:T:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:o:39:GLU:O    | 1:s:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:t:39:GLU:O    | 1:x:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:D:39:GLU:O    | 1:H:151:LYS:NZ  | 2.29                     | 0.64              |
| 1:l:39:GLU:O    | 1:p:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:C:39:GLU:O    | 1:G:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:Z:39:GLU:O    | 1:d:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:L:39:GLU:O    | 1:P:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:Q:39:GLU:O    | 1:U:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:Y:39:GLU:O    | 1:c:151:LYS:NZ  | 2.29                     | 0.63              |
| 1:T:39:GLU:O    | 1:X:151:LYS:NZ  | 2.29                     | 0.62              |
| 1:2:86:LEU:HD21 | 1:x:196:PHE:CZ  | 2.36                     | 0.61              |
| 1:0:96:SER:O    | 1:0:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:C:196:PHE:CZ  | 1:H:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:X:96:SER:O    | 1:X:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:Y:196:PHE:CZ  | 1:d:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:0:86:LEU:HD21 | 1:v:196:PHE:CZ  | 2.36                     | 0.61              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:5:96:SER:O   | 1:5:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:P:196:PHE:CZ | 1:U:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:i:196:PHE:CZ | 1:n:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:l:196:PHE:CZ | 1:q:86:LEU:HD21 | 2.35                     | 0.61              |
| 1:o:196:PHE:CZ | 1:t:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:L:196:PHE:CZ | 1:Q:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:N:96:SER:O   | 1:N:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:N:196:PHE:CZ | 1:S:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:O:96:SER:O   | 1:O:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:P:37:GLU:N   | 1:P:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:R:96:SER:O   | 1:R:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:a:196:PHE:CZ | 1:f:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:c:37:GLU:N   | 1:c:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:k:196:PHE:CZ | 1:p:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:o:37:GLU:OE1 | 1:o:37:GLU:N    | 2.34                     | 0.61              |
| 1:z:96:SER:O   | 1:z:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:0:37:GLU:N   | 1:0:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:1:37:GLU:OE1 | 1:1:37:GLU:N    | 2.34                     | 0.61              |
| 1:3:96:SER:O   | 1:3:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:A:196:PHE:CZ | 1:F:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:B:196:PHE:CZ | 1:G:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:G:37:GLU:OE1 | 1:G:37:GLU:N    | 2.34                     | 0.61              |
| 1:S:37:GLU:N   | 1:S:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:T:96:SER:O   | 1:T:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:V:196:PHE:CZ | 1:a:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:b:37:GLU:OE1 | 1:b:37:GLU:N    | 2.34                     | 0.61              |
| 1:b:196:PHE:CZ | 1:g:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:c:196:PHE:CZ | 1:h:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:1:196:PHE:CZ | 1:6:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:4:37:GLU:OE1 | 1:4:37:GLU:N    | 2.34                     | 0.61              |
| 1:D:37:GLU:OE1 | 1:D:37:GLU:N    | 2.34                     | 0.61              |
| 1:F:37:GLU:OE1 | 1:F:37:GLU:N    | 2.34                     | 0.61              |
| 1:V:96:SER:O   | 1:V:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:f:37:GLU:OE1 | 1:f:37:GLU:N    | 2.34                     | 0.61              |
| 1:n:196:PHE:CZ | 1:s:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:v:96:SER:O   | 1:v:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:w:96:SER:O   | 1:w:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:7:96:SER:O   | 1:7:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:C:37:GLU:OE1 | 1:C:37:GLU:N    | 2.34                     | 0.61              |
| 1:J:196:PHE:CZ | 1:O:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:O:196:PHE:CZ | 1:T:86:LEU:HD21 | 2.35                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:37:GLU:OE1  | 1:T:37:GLU:N    | 2.34                     | 0.61              |
| 1:W:196:PHE:CZ  | 1:b:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:n:37:GLU:OE1  | 1:n:37:GLU:N    | 2.34                     | 0.61              |
| 1:p:37:GLU:N    | 1:p:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:r:37:GLU:OE1  | 1:r:37:GLU:N    | 2.34                     | 0.61              |
| 1:x:37:GLU:OE1  | 1:x:37:GLU:N    | 2.34                     | 0.61              |
| 1:0:196:PHE:CZ  | 1:5:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:1:96:SER:O    | 1:1:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:G:196:PHE:CZ  | 1:L:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:J:96:SER:O    | 1:J:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:O:37:GLU:OE1  | 1:O:37:GLU:N    | 2.34                     | 0.61              |
| 1:l:37:GLU:OE1  | 1:l:37:GLU:N    | 2.34                     | 0.61              |
| 1:q:196:PHE:CZ  | 1:v:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:J:37:GLU:OE1  | 1:J:37:GLU:N    | 2.34                     | 0.61              |
| 1:K:96:SER:O    | 1:K:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:Y:37:GLU:OE1  | 1:Y:37:GLU:N    | 2.34                     | 0.61              |
| 1:Z:96:SER:O    | 1:Z:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:e:37:GLU:OE1  | 1:e:37:GLU:N    | 2.34                     | 0.61              |
| 1:h:196:PHE:CZ  | 1:m:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:j:196:PHE:CZ  | 1:o:86:LEU:HD21 | 2.35                     | 0.61              |
| 1:q:37:GLU:OE1  | 1:q:37:GLU:N    | 2.34                     | 0.61              |
| 1:s:37:GLU:N    | 1:s:37:GLU:OE1  | 2.34                     | 0.61              |
| 1:u:196:PHE:CZ  | 1:z:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:3:86:LEU:HD21 | 1:y:196:PHE:CZ  | 2.36                     | 0.61              |
| 1:4:86:LEU:HD21 | 1:z:196:PHE:CZ  | 2.36                     | 0.61              |
| 1:M:196:PHE:CZ  | 1:R:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:X:196:PHE:CZ  | 1:c:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:g:37:GLU:OE1  | 1:g:37:GLU:N    | 2.34                     | 0.61              |
| 1:g:96:SER:O    | 1:g:100:HIS:ND1 | 2.33                     | 0.61              |
| 1:m:196:PHE:CZ  | 1:r:86:LEU:HD21 | 2.36                     | 0.61              |
| 1:F:196:PHE:CZ  | 1:K:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:H:37:GLU:N    | 1:H:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:I:37:GLU:OE1  | 1:I:37:GLU:N    | 2.34                     | 0.60              |
| 1:M:37:GLU:N    | 1:M:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:P:96:SER:O    | 1:P:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:W:37:GLU:OE1  | 1:W:37:GLU:N    | 2.34                     | 0.60              |
| 1:p:196:PHE:CZ  | 1:u:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:r:96:SER:O    | 1:r:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:t:196:PHE:CZ  | 1:y:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:y:37:GLU:OE1  | 1:y:37:GLU:N    | 2.34                     | 0.60              |
| 1:1:86:LEU:HD21 | 1:w:196:PHE:CZ  | 2.35                     | 0.60              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:5:37:GLU:N   | 1:5:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:7:182:ARG:O  | 1:7:186:ASN:N   | 2.34                     | 0.60              |
| 1:Q:37:GLU:OE1 | 1:Q:37:GLU:N    | 2.34                     | 0.60              |
| 1:R:37:GLU:OE1 | 1:R:37:GLU:N    | 2.34                     | 0.60              |
| 1:U:196:PHE:CZ | 1:Z:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:c:96:SER:O   | 1:c:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:c:182:ARG:O  | 1:c:186:ASN:N   | 2.34                     | 0.60              |
| 1:d:196:PHE:CZ | 1:i:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:h:37:GLU:N   | 1:h:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:i:37:GLU:OE1 | 1:i:37:GLU:N    | 2.34                     | 0.60              |
| 1:k:37:GLU:N   | 1:k:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:s:96:SER:O   | 1:s:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:z:37:GLU:OE1 | 1:z:37:GLU:N    | 2.34                     | 0.60              |
| 1:B:37:GLU:OE1 | 1:B:37:GLU:N    | 2.34                     | 0.60              |
| 1:S:196:PHE:CZ | 1:X:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:T:196:PHE:CZ | 1:Y:86:LEU:HD21 | 2.35                     | 0.60              |
| 1:V:37:GLU:OE1 | 1:V:37:GLU:N    | 2.34                     | 0.60              |
| 1:Z:182:ARG:O  | 1:Z:186:ASN:N   | 2.34                     | 0.60              |
| 1:Z:196:PHE:CZ | 1:e:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:f:196:PHE:CZ | 1:k:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:v:37:GLU:N   | 1:v:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:2:37:GLU:OE1 | 1:2:37:GLU:N    | 2.34                     | 0.60              |
| 1:2:196:PHE:CZ | 1:7:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:3:37:GLU:OE1 | 1:3:37:GLU:N    | 2.34                     | 0.60              |
| 1:7:37:GLU:OE1 | 1:7:37:GLU:N    | 2.34                     | 0.60              |
| 1:F:96:SER:O   | 1:F:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:L:37:GLU:OE1 | 1:L:37:GLU:N    | 2.34                     | 0.60              |
| 1:Q:196:PHE:CZ | 1:V:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:Z:37:GLU:OE1 | 1:Z:37:GLU:N    | 2.34                     | 0.60              |
| 1:e:182:ARG:O  | 1:e:186:ASN:N   | 2.34                     | 0.60              |
| 1:e:196:PHE:CZ | 1:j:86:LEU:HD21 | 2.35                     | 0.60              |
| 1:g:182:ARG:O  | 1:g:186:ASN:N   | 2.34                     | 0.60              |
| 1:j:37:GLU:OE1 | 1:j:37:GLU:N    | 2.34                     | 0.60              |
| 1:p:47:LEU:O   | 1:p:50:THR:OG1  | 2.20                     | 0.60              |
| 1:u:37:GLU:OE1 | 1:u:37:GLU:N    | 2.34                     | 0.60              |
| 1:w:37:GLU:OE1 | 1:w:37:GLU:N    | 2.34                     | 0.60              |
| 1:y:47:LEU:O   | 1:y:50:THR:OG1  | 2.20                     | 0.60              |
| 1:K:37:GLU:OE1 | 1:K:37:GLU:N    | 2.34                     | 0.60              |
| 1:R:196:PHE:CZ | 1:W:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:U:47:LEU:O   | 1:U:50:THR:OG1  | 2.20                     | 0.60              |
| 1:Y:96:SER:O   | 1:Y:100:HIS:ND1 | 2.33                     | 0.60              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:a:37:GLU:OE1 | 1:a:37:GLU:N    | 2.34                     | 0.60              |
| 1:d:96:SER:O   | 1:d:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:d:182:ARG:O  | 1:d:186:ASN:N   | 2.34                     | 0.60              |
| 1:r:196:PHE:CZ | 1:w:86:LEU:HD21 | 2.35                     | 0.60              |
| 1:6:37:GLU:OE1 | 1:6:37:GLU:N    | 2.34                     | 0.60              |
| 1:6:96:SER:O   | 1:6:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:A:37:GLU:OE1 | 1:A:37:GLU:N    | 2.34                     | 0.60              |
| 1:E:196:PHE:CZ | 1:J:86:LEU:HD21 | 2.35                     | 0.60              |
| 1:H:196:PHE:CZ | 1:M:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:l:47:LEU:O   | 1:l:50:THR:OG1  | 2.20                     | 0.60              |
| 1:t:37:GLU:OE1 | 1:t:37:GLU:N    | 2.34                     | 0.60              |
| 1:x:96:SER:O   | 1:x:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:2:96:SER:O   | 1:2:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:D:199:TRP:O  | 1:I:81:ARG:NH2  | 2.35                     | 0.60              |
| 1:G:96:SER:O   | 1:G:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:U:37:GLU:OE1 | 1:U:37:GLU:N    | 2.34                     | 0.60              |
| 1:U:96:SER:O   | 1:U:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:X:37:GLU:N   | 1:X:37:GLU:OE1  | 2.34                     | 0.60              |
| 1:s:196:PHE:CZ | 1:x:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:1:47:LEU:O   | 1:1:50:THR:OG1  | 2.20                     | 0.60              |
| 1:L:96:SER:O   | 1:L:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:Q:96:SER:O   | 1:Q:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:g:196:PHE:CZ | 1:l:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:i:47:LEU:O   | 1:i:50:THR:OG1  | 2.20                     | 0.60              |
| 1:n:96:SER:O   | 1:n:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:y:96:SER:O   | 1:y:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:I:96:SER:O   | 1:I:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:M:96:SER:O   | 1:M:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:N:37:GLU:OE1 | 1:N:37:GLU:N    | 2.34                     | 0.60              |
| 1:h:182:ARG:O  | 1:h:186:ASN:N   | 2.34                     | 0.60              |
| 1:i:182:ARG:O  | 1:i:186:ASN:N   | 2.34                     | 0.60              |
| 1:k:182:ARG:O  | 1:k:186:ASN:N   | 2.34                     | 0.60              |
| 1:m:37:GLU:OE1 | 1:m:37:GLU:N    | 2.34                     | 0.60              |
| 1:u:96:SER:O   | 1:u:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:K:196:PHE:CZ | 1:P:86:LEU:HD21 | 2.36                     | 0.60              |
| 1:h:96:SER:O   | 1:h:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:q:96:SER:O   | 1:q:100:HIS:ND1 | 2.33                     | 0.60              |
| 1:A:182:ARG:O  | 1:A:186:ASN:N   | 2.34                     | 0.59              |
| 1:B:96:SER:O   | 1:B:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:E:96:SER:O   | 1:E:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:N:47:LEU:O   | 1:N:50:THR:OG1  | 2.20                     | 0.59              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:R:47:LEU:O   | 1:R:50:THR:OG1  | 2.20                     | 0.59              |
| 1:d:37:GLU:OE1 | 1:d:37:GLU:N    | 2.34                     | 0.59              |
| 1:j:182:ARG:O  | 1:j:186:ASN:N   | 2.34                     | 0.59              |
| 1:o:96:SER:O   | 1:o:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:l:182:ARG:O  | 1:l:186:ASN:N   | 2.34                     | 0.59              |
| 1:B:182:ARG:O  | 1:B:186:ASN:N   | 2.34                     | 0.59              |
| 1:C:182:ARG:O  | 1:C:186:ASN:N   | 2.34                     | 0.59              |
| 1:l:96:SER:O   | 1:l:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:m:96:SER:O   | 1:m:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:t:96:SER:O   | 1:t:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:A:96:SER:O   | 1:A:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:D:182:ARG:O  | 1:D:186:ASN:N   | 2.34                     | 0.59              |
| 1:E:37:GLU:N   | 1:E:37:GLU:OE1  | 2.34                     | 0.59              |
| 1:T:47:LEU:O   | 1:T:50:THR:OG1  | 2.20                     | 0.59              |
| 1:m:182:ARG:O  | 1:m:186:ASN:N   | 2.34                     | 0.59              |
| 1:r:47:LEU:O   | 1:r:50:THR:OG1  | 2.20                     | 0.59              |
| 1:D:96:SER:O   | 1:D:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:j:96:SER:O   | 1:j:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:n:182:ARG:O  | 1:n:186:ASN:N   | 2.34                     | 0.59              |
| 1:C:96:SER:O   | 1:C:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:H:96:SER:O   | 1:H:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:o:182:ARG:O  | 1:o:186:ASN:N   | 2.34                     | 0.59              |
| 1:p:182:ARG:O  | 1:p:186:ASN:N   | 2.34                     | 0.59              |
| 1:p:96:SER:O   | 1:p:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:E:182:ARG:O  | 1:E:186:ASN:N   | 2.34                     | 0.59              |
| 1:F:182:ARG:O  | 1:F:186:ASN:N   | 2.34                     | 0.59              |
| 1:H:182:ARG:O  | 1:H:186:ASN:N   | 2.34                     | 0.59              |
| 1:J:47:LEU:O   | 1:J:50:THR:OG1  | 2.20                     | 0.59              |
| 1:i:96:SER:O   | 1:i:100:HIS:ND1 | 2.33                     | 0.59              |
| 1:v:47:LEU:O   | 1:v:50:THR:OG1  | 2.20                     | 0.59              |
| 1:q:47:LEU:O   | 1:q:50:THR:OG1  | 2.20                     | 0.59              |
| 1:G:182:ARG:O  | 1:G:186:ASN:N   | 2.34                     | 0.58              |
| 1:B:47:LEU:O   | 1:B:50:THR:OG1  | 2.20                     | 0.58              |
| 1:O:47:LEU:O   | 1:O:50:THR:OG1  | 2.20                     | 0.58              |
| 1:V:47:LEU:O   | 1:V:50:THR:OG1  | 2.20                     | 0.58              |
| 1:c:78:ALA:HB1 | 1:c:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:k:96:SER:O   | 1:k:100:HIS:ND1 | 2.33                     | 0.58              |
| 1:l:78:ALA:HB1 | 1:l:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:q:182:ARG:O  | 1:q:186:ASN:N   | 2.34                     | 0.58              |
| 1:x:78:ALA:HB1 | 1:x:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:6:78:ALA:HB1 | 1:6:86:LEU:HD22 | 1.86                     | 0.58              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:C:78:ALA:HB1 | 1:C:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:D:78:ALA:HB1 | 1:D:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:H:78:ALA:HB1 | 1:H:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:T:78:ALA:HB1 | 1:T:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:r:182:ARG:O  | 1:r:186:ASN:N   | 2.34                     | 0.58              |
| 1:1:78:ALA:HB1 | 1:1:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:L:78:ALA:HB1 | 1:L:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:Q:78:ALA:HB1 | 1:Q:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:X:78:ALA:HB1 | 1:X:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:p:78:ALA:HB1 | 1:p:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:s:78:ALA:HB1 | 1:s:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:t:182:ARG:O  | 1:t:186:ASN:N   | 2.34                     | 0.58              |
| 1:2:78:ALA:HB1 | 1:2:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:P:78:ALA:HB1 | 1:P:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:Y:78:ALA:HB1 | 1:Y:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:g:78:ALA:HB1 | 1:g:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:o:78:ALA:HB1 | 1:o:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:t:78:ALA:HB1 | 1:t:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:5:78:ALA:HB1 | 1:5:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:I:182:ARG:O  | 1:I:186:ASN:N   | 2.34                     | 0.58              |
| 1:M:78:ALA:HB1 | 1:M:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:U:78:ALA:HB1 | 1:U:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:h:78:ALA:HB1 | 1:h:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:s:182:ARG:O  | 1:s:186:ASN:N   | 2.34                     | 0.58              |
| 1:A:199:TRP:O  | 1:F:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:G:78:ALA:HB1 | 1:G:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:J:182:ARG:O  | 1:J:186:ASN:N   | 2.34                     | 0.58              |
| 1:b:78:ALA:HB1 | 1:b:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:e:96:SER:O   | 1:e:100:HIS:ND1 | 2.33                     | 0.58              |
| 1:f:96:SER:O   | 1:f:100:HIS:ND1 | 2.33                     | 0.58              |
| 1:j:47:LEU:O   | 1:j:50:THR:OG1  | 2.20                     | 0.58              |
| 1:k:78:ALA:HB1 | 1:k:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:u:78:ALA:HB1 | 1:u:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:E:199:TRP:O  | 1:J:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:K:78:ALA:HB1 | 1:K:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:L:182:ARG:O  | 1:L:186:ASN:N   | 2.34                     | 0.58              |
| 1:m:199:TRP:O  | 1:r:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:w:78:ALA:HB1 | 1:w:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:I:177:GLU:CD | 1:R:52:ALA:HB3  | 2.28                     | 0.58              |
| 1:O:78:ALA:HB1 | 1:O:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:i:199:TRP:O  | 1:n:81:ARG:NH2  | 2.37                     | 0.58              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:q:78:ALA:HB1 | 1:q:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:y:78:ALA:HB1 | 1:y:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:0:81:ARG:NH2 | 1:v:199:TRP:O   | 2.37                     | 0.58              |
| 1:F:199:TRP:O  | 1:K:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:J:199:TRP:O  | 1:O:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:Z:78:ALA:HB1 | 1:Z:86:LEU:HD22 | 1.86                     | 0.58              |
| 1:e:199:TRP:O  | 1:j:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:q:199:TRP:O  | 1:v:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:r:199:TRP:O  | 1:w:81:ARG:NH2  | 2.37                     | 0.58              |
| 1:u:182:ARG:O  | 1:u:186:ASN:N   | 2.34                     | 0.58              |
| 1:4:47:LEU:O   | 1:4:50:THR:OG1  | 2.20                     | 0.57              |
| 1:D:196:PHE:CZ | 1:I:86:LEU:HD21 | 2.38                     | 0.57              |
| 1:I:78:ALA:HB1 | 1:I:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:K:182:ARG:O  | 1:K:186:ASN:N   | 2.34                     | 0.57              |
| 1:V:78:ALA:HB1 | 1:V:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:v:182:ARG:O  | 1:v:186:ASN:N   | 2.34                     | 0.57              |
| 1:7:78:ALA:HB1 | 1:7:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:B:199:TRP:O  | 1:G:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:N:199:TRP:O  | 1:S:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:S:78:ALA:HB1 | 1:S:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:d:78:ALA:HB1 | 1:d:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:f:78:ALA:HB1 | 1:f:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:j:78:ALA:HB1 | 1:j:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:n:199:TRP:O  | 1:s:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:o:47:LEU:O   | 1:o:50:THR:OG1  | 2.20                     | 0.57              |
| 1:E:78:ALA:HB1 | 1:E:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:h:199:TRP:O  | 1:m:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:m:78:ALA:HB1 | 1:m:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:u:199:TRP:O  | 1:z:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:x:182:ARG:O  | 1:x:186:ASN:N   | 2.34                     | 0.57              |
| 1:z:33:LEU:O   | 1:z:129:TYR:OH  | 2.21                     | 0.57              |
| 1:4:78:ALA:HB1 | 1:4:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:4:81:ARG:NH2 | 1:z:199:TRP:O   | 2.37                     | 0.57              |
| 1:B:78:ALA:HB1 | 1:B:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:R:78:ALA:HB1 | 1:R:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:d:199:TRP:O  | 1:i:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:j:199:TRP:O  | 1:o:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:n:78:ALA:HB1 | 1:n:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:2:81:ARG:NH2 | 1:x:199:TRP:O   | 2.37                     | 0.57              |
| 1:M:182:ARG:O  | 1:M:186:ASN:N   | 2.34                     | 0.57              |
| 1:M:199:TRP:O  | 1:R:81:ARG:NH2  | 2.37                     | 0.57              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:P:199:TRP:O  | 1:U:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:Z:199:TRP:O  | 1:e:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:w:182:ARG:O  | 1:w:186:ASN:N   | 2.34                     | 0.57              |
| 1:O:78:ALA:HB1 | 1:O:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:O:182:ARG:O  | 1:O:186:ASN:N   | 2.34                     | 0.57              |
| 1:1:199:TRP:O  | 1:6:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:3:78:ALA:HB1 | 1:3:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:A:78:ALA:HB1 | 1:A:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:L:199:TRP:O  | 1:Q:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:N:78:ALA:HB1 | 1:N:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:N:182:ARG:O  | 1:N:186:ASN:N   | 2.34                     | 0.57              |
| 1:O:182:ARG:O  | 1:O:186:ASN:N   | 2.34                     | 0.57              |
| 1:W:78:ALA:HB1 | 1:W:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:X:182:ARG:O  | 1:X:186:ASN:N   | 2.34                     | 0.57              |
| 1:a:199:TRP:O  | 1:f:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:b:182:ARG:O  | 1:b:186:ASN:N   | 2.34                     | 0.57              |
| 1:r:78:ALA:HB1 | 1:r:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:v:78:ALA:HB1 | 1:v:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:G:199:TRP:O  | 1:L:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:R:199:TRP:O  | 1:W:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:T:199:TRP:O  | 1:Y:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:i:78:ALA:HB1 | 1:i:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:l:199:TRP:O  | 1:q:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:5:182:ARG:O  | 1:5:186:ASN:N   | 2.34                     | 0.57              |
| 1:C:199:TRP:O  | 1:H:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:P:182:ARG:O  | 1:P:186:ASN:N   | 2.34                     | 0.57              |
| 1:S:182:ARG:O  | 1:S:186:ASN:N   | 2.34                     | 0.57              |
| 1:a:78:ALA:HB1 | 1:a:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:a:96:SER:O   | 1:a:100:HIS:ND1 | 2.33                     | 0.57              |
| 1:e:47:LEU:O   | 1:e:50:THR:OG1  | 2.20                     | 0.57              |
| 1:o:199:TRP:O  | 1:t:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:s:199:TRP:O  | 1:x:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:z:78:ALA:HB1 | 1:z:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:F:78:ALA:HB1 | 1:F:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:J:78:ALA:HB1 | 1:J:86:LEU:HD22 | 1.86                     | 0.57              |
| 1:Z:33:LEU:O   | 1:Z:129:TYR:OH  | 2.21                     | 0.57              |
| 1:b:96:SER:O   | 1:b:100:HIS:ND1 | 2.33                     | 0.57              |
| 1:f:182:ARG:O  | 1:f:186:ASN:N   | 2.34                     | 0.57              |
| 1:g:199:TRP:O  | 1:l:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:k:199:TRP:O  | 1:p:81:ARG:NH2  | 2.37                     | 0.57              |
| 1:t:199:TRP:O  | 1:y:81:ARG:NH2  | 2.37                     | 0.57              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:y:182:ARG:O  | 1:y:186:ASN:N    | 2.34                     | 0.57              |
| 1:3:81:ARG:NH2 | 1:y:199:TRP:O    | 2.37                     | 0.57              |
| 1:K:199:TRP:O  | 1:P:81:ARG:NH2   | 2.37                     | 0.57              |
| 1:e:78:ALA:HB1 | 1:e:86:LEU:HD22  | 1.86                     | 0.57              |
| 1:4:182:ARG:O  | 1:4:186:ASN:N    | 2.34                     | 0.56              |
| 1:T:182:ARG:O  | 1:T:186:ASN:N    | 2.34                     | 0.56              |
| 1:V:199:TRP:O  | 1:a:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:H:199:TRP:O  | 1:M:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:O:199:TRP:O  | 1:T:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:S:199:TRP:O  | 1:X:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:Y:199:TRP:O  | 1:d:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:f:199:TRP:O  | 1:k:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:p:199:TRP:O  | 1:u:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:z:182:ARG:O  | 1:z:186:ASN:N    | 2.34                     | 0.56              |
| 1:0:199:TRP:O  | 1:5:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:1:81:ARG:NH2 | 1:w:199:TRP:O    | 2.37                     | 0.56              |
| 1:1:182:ARG:O  | 1:1:186:ASN:N    | 2.34                     | 0.56              |
| 1:5:47:LEU:O   | 1:5:50:THR:OG1   | 2.20                     | 0.56              |
| 1:6:47:LEU:O   | 1:6:50:THR:OG1   | 2.20                     | 0.56              |
| 1:Q:182:ARG:O  | 1:Q:186:ASN:N    | 2.34                     | 0.56              |
| 1:U:199:TRP:O  | 1:Z:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:W:182:ARG:O  | 1:W:186:ASN:N    | 2.34                     | 0.56              |
| 1:W:199:TRP:O  | 1:b:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:X:199:TRP:O  | 1:c:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:c:199:TRP:O  | 1:h:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:l:33:LEU:O   | 1:l:129:TYR:OH   | 2.21                     | 0.56              |
| 1:u:47:LEU:O   | 1:u:50:THR:OG1   | 2.20                     | 0.56              |
| 1:Q:199:TRP:O  | 1:V:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:2:199:TRP:O  | 1:7:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:Z:47:LEU:O   | 1:Z:50:THR:OG1   | 2.20                     | 0.56              |
| 1:2:182:ARG:O  | 1:2:186:ASN:N    | 2.34                     | 0.56              |
| 1:R:182:ARG:O  | 1:R:186:ASN:N    | 2.34                     | 0.56              |
| 1:7:33:LEU:O   | 1:7:129:TYR:OH   | 2.21                     | 0.56              |
| 1:W:96:SER:O   | 1:W:100:HIS:ND1  | 2.33                     | 0.56              |
| 1:b:199:TRP:O  | 1:g:81:ARG:NH2   | 2.37                     | 0.56              |
| 1:A:47:LEU:O   | 1:A:50:THR:OG1   | 2.20                     | 0.56              |
| 1:k:47:LEU:O   | 1:k:50:THR:OG1   | 2.20                     | 0.56              |
| 1:E:39:GLU:HG2 | 1:I:155:ILE:HD12 | 1.88                     | 0.55              |
| 1:U:182:ARG:O  | 1:U:186:ASN:N    | 2.34                     | 0.55              |
| 1:3:182:ARG:O  | 1:3:186:ASN:N    | 2.34                     | 0.55              |
| 1:a:182:ARG:O  | 1:a:186:ASN:N    | 2.34                     | 0.55              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:4:96:SER:O   | 1:4:100:HIS:ND1 | 2.33                     | 0.55              |
| 1:L:47:LEU:O   | 1:L:50:THR:OG1  | 2.20                     | 0.55              |
| 1:S:96:SER:O   | 1:S:100:HIS:ND1 | 2.33                     | 0.55              |
| 1:I:177:GLU:CG | 1:R:49:GLN:HA   | 2.36                     | 0.55              |
| 1:6:182:ARG:O  | 1:6:186:ASN:N   | 2.34                     | 0.55              |
| 1:u:33:LEU:O   | 1:u:129:TYR:OH  | 2.21                     | 0.55              |
| 1:V:182:ARG:O  | 1:V:186:ASN:N   | 2.34                     | 0.55              |
| 1:L:33:LEU:O   | 1:L:129:TYR:OH  | 2.21                     | 0.55              |
| 1:O:33:LEU:O   | 1:O:129:TYR:OH  | 2.21                     | 0.55              |
| 1:V:33:LEU:O   | 1:V:129:TYR:OH  | 2.21                     | 0.54              |
| 1:Y:182:ARG:O  | 1:Y:186:ASN:N   | 2.34                     | 0.54              |
| 1:d:47:LEU:O   | 1:d:50:THR:OG1  | 2.20                     | 0.54              |
| 1:Q:47:LEU:O   | 1:Q:50:THR:OG1  | 2.20                     | 0.54              |
| 1:m:69:GLN:NE2 | 1:m:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:n:69:GLN:NE2 | 1:n:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:0:69:GLN:NE2 | 1:0:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:A:69:GLN:NE2 | 1:A:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:E:69:GLN:NE2 | 1:E:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:H:69:GLN:NE2 | 1:H:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:O:69:GLN:NE2 | 1:O:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:U:69:GLN:NE2 | 1:U:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:h:33:LEU:O   | 1:h:129:TYR:OH  | 2.21                     | 0.54              |
| 1:i:69:GLN:NE2 | 1:i:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:t:69:GLN:NE2 | 1:t:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:2:69:GLN:NE2 | 1:2:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:F:69:GLN:NE2 | 1:F:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:J:69:GLN:NE2 | 1:J:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:U:42:GLU:OE2 | 1:U:45:ARG:NH2  | 2.41                     | 0.54              |
| 1:h:69:GLN:NE2 | 1:h:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:q:69:GLN:NE2 | 1:q:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:r:69:GLN:NE2 | 1:r:73:GLU:OE2  | 2.41                     | 0.54              |
| 1:6:69:GLN:NE2 | 1:6:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:B:69:GLN:NE2 | 1:B:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:H:42:GLU:OE2 | 1:H:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:I:69:GLN:NE2 | 1:I:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:K:42:GLU:OE2 | 1:K:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:S:42:GLU:OE2 | 1:S:45:ARG:NH2  | 2.41                     | 0.53              |
| 1:S:69:GLN:NE2 | 1:S:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:X:69:GLN:NE2 | 1:X:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:Y:66:LEU:O   | 1:Y:70:ARG:N    | 2.35                     | 0.53              |
| 1:b:69:GLN:NE2 | 1:b:73:GLU:OE2  | 2.41                     | 0.53              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:d:69:GLN:NE2 | 1:d:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:g:69:GLN:NE2 | 1:g:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:l:69:GLN:NE2 | 1:l:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:p:69:GLN:NE2 | 1:p:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:v:69:GLN:NE2 | 1:v:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:w:42:GLU:OE2 | 1:w:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:w:69:GLN:NE2 | 1:w:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:4:42:GLU:OE2 | 1:4:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:6:42:GLU:OE2 | 1:6:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:C:42:GLU:OE2 | 1:C:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:F:42:GLU:OE2 | 1:F:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:L:69:GLN:NE2 | 1:L:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:P:42:GLU:OE2 | 1:P:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:a:69:GLN:NE2 | 1:a:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:c:42:GLU:OE2 | 1:c:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:e:69:GLN:NE2 | 1:e:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:k:69:GLN:NE2 | 1:k:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:p:42:GLU:OE2 | 1:p:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:3:33:LEU:O   | 1:3:129:TYR:OH | 2.21                     | 0.53              |
| 1:5:69:GLN:NE2 | 1:5:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:7:42:GLU:OE2 | 1:7:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:I:33:LEU:O   | 1:I:129:TYR:OH | 2.21                     | 0.53              |
| 1:N:69:GLN:NE2 | 1:N:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:Q:69:GLN:NE2 | 1:Q:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:R:69:GLN:NE2 | 1:R:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:X:42:GLU:OE2 | 1:X:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:u:69:GLN:NE2 | 1:u:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:z:42:GLU:OE2 | 1:z:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:1:42:GLU:OE2 | 1:1:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:3:69:GLN:NE2 | 1:3:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:A:42:GLU:OE2 | 1:A:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:C:69:GLN:NE2 | 1:C:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:D:69:GLN:NE2 | 1:D:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:K:69:GLN:NE2 | 1:K:73:GLU:OE2 | 2.41                     | 0.53              |
| 1:M:42:GLU:OE2 | 1:M:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:a:42:GLU:OE2 | 1:a:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:e:42:GLU:OE2 | 1:e:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:f:42:GLU:OE2 | 1:f:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:h:42:GLU:OE2 | 1:h:45:ARG:NH2 | 2.42                     | 0.53              |
| 1:j:42:GLU:OE2 | 1:j:45:ARG:NH2 | 2.41                     | 0.53              |
| 1:m:33:LEU:O   | 1:m:129:TYR:OH | 2.21                     | 0.53              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:m:42:GLU:OE2 | 1:m:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:n:42:GLU:OE2 | 1:n:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:z:69:GLN:NE2 | 1:z:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:I:42:GLU:OE2 | 1:I:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:J:42:GLU:OE2 | 1:J:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:R:42:GLU:OE2 | 1:R:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:T:42:GLU:OE2 | 1:T:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:Y:69:GLN:NE2 | 1:Y:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:Z:69:GLN:NE2 | 1:Z:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:k:42:GLU:OE2 | 1:k:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:o:42:GLU:OE2 | 1:o:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:x:42:GLU:OE2 | 1:x:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:x:69:GLN:NE2 | 1:x:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:y:42:GLU:OE2 | 1:y:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:O:66:LEU:O   | 1:O:70:ARG:N     | 2.35                     | 0.53              |
| 1:2:42:GLU:OE2 | 1:2:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:2:47:LEU:O   | 1:2:50:THR:OG1   | 2.20                     | 0.53              |
| 1:4:69:GLN:NE2 | 1:4:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:I:25:PRO:HB3 | 1:M:167:LEU:HD13 | 1.91                     | 0.53              |
| 1:O:66:LEU:O   | 1:O:70:ARG:N     | 2.35                     | 0.53              |
| 1:T:69:GLN:NE2 | 1:T:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:V:42:GLU:OE2 | 1:V:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:b:42:GLU:OE2 | 1:b:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:j:69:GLN:NE2 | 1:j:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:r:42:GLU:OE2 | 1:r:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:7:69:GLN:NE2 | 1:7:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:M:69:GLN:NE2 | 1:M:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:N:42:GLU:OE2 | 1:N:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:b:101:THR:O  | 1:b:105:GLY:N    | 2.40                     | 0.53              |
| 1:c:69:GLN:NE2 | 1:c:73:GLU:OE2   | 2.41                     | 0.53              |
| 1:i:42:GLU:OE2 | 1:i:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:q:42:GLU:OE2 | 1:q:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:s:42:GLU:OE2 | 1:s:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:t:33:LEU:O   | 1:t:129:TYR:OH   | 2.21                     | 0.53              |
| 1:t:42:GLU:OE2 | 1:t:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:u:42:GLU:OE2 | 1:u:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:v:42:GLU:OE2 | 1:v:45:ARG:NH2   | 2.41                     | 0.53              |
| 1:w:66:LEU:O   | 1:w:70:ARG:N     | 2.35                     | 0.53              |
| 1:3:42:GLU:OE2 | 1:3:45:ARG:NH2   | 2.42                     | 0.53              |
| 1:6:66:LEU:O   | 1:6:70:ARG:N     | 2.35                     | 0.53              |
| 1:E:42:GLU:OE2 | 1:E:45:ARG:NH2   | 2.41                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:V:69:GLN:NE2  | 1:V:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:W:42:GLU:OE2  | 1:W:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:d:42:GLU:OE2  | 1:d:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:f:69:GLN:NE2  | 1:f:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:l:42:GLU:OE2  | 1:l:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:o:69:GLN:NE2  | 1:o:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:y:69:GLN:NE2  | 1:y:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:0:42:GLU:OE2  | 1:0:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:K:66:LEU:O    | 1:K:70:ARG:N    | 2.35                     | 0.53              |
| 1:Z:42:GLU:OE2  | 1:Z:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:s:69:GLN:NE2  | 1:s:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:4:33:LEU:O    | 1:4:129:TYR:OH  | 2.21                     | 0.53              |
| 1:5:42:GLU:OE2  | 1:5:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:O:42:GLU:OE2  | 1:O:45:ARG:NH2  | 2.41                     | 0.53              |
| 1:P:69:GLN:NE2  | 1:P:73:GLU:OE2  | 2.41                     | 0.53              |
| 1:Q:42:GLU:OE2  | 1:Q:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:S:66:LEU:O    | 1:S:70:ARG:N    | 2.35                     | 0.53              |
| 1:g:42:GLU:OE2  | 1:g:45:ARG:NH2  | 2.42                     | 0.53              |
| 1:g:101:THR:O   | 1:g:105:GLY:N   | 2.40                     | 0.53              |
| 1:1:69:GLN:NE2  | 1:1:73:GLU:OE2  | 2.41                     | 0.52              |
| 1:B:33:LEU:O    | 1:B:129:TYR:OH  | 2.21                     | 0.52              |
| 1:B:42:GLU:OE2  | 1:B:45:ARG:NH2  | 2.42                     | 0.52              |
| 1:D:42:GLU:OE2  | 1:D:45:ARG:NH2  | 2.42                     | 0.52              |
| 1:W:69:GLN:NE2  | 1:W:73:GLU:OE2  | 2.41                     | 0.52              |
| 1:B:66:LEU:O    | 1:B:70:ARG:N    | 2.35                     | 0.52              |
| 1:G:69:GLN:NE2  | 1:G:73:GLU:OE2  | 2.41                     | 0.52              |
| 1:H:33:LEU:HD22 | 1:H:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:h:33:LEU:HD22 | 1:h:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:n:66:LEU:O    | 1:n:70:ARG:N    | 2.35                     | 0.52              |
| 1:7:33:LEU:HD22 | 1:7:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:G:42:GLU:OE2  | 1:G:45:ARG:NH2  | 2.42                     | 0.52              |
| 1:U:33:LEU:O    | 1:U:129:TYR:OH  | 2.21                     | 0.52              |
| 1:U:33:LEU:HD22 | 1:U:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:Z:33:LEU:HD22 | 1:Z:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:j:66:LEU:O    | 1:j:70:ARG:N    | 2.35                     | 0.52              |
| 1:s:66:LEU:O    | 1:s:70:ARG:N    | 2.35                     | 0.52              |
| 1:4:66:LEU:O    | 1:4:70:ARG:N    | 2.35                     | 0.52              |
| 1:5:33:LEU:O    | 1:5:129:TYR:OH  | 2.21                     | 0.52              |
| 1:A:33:LEU:HD22 | 1:A:136:LYS:HD3 | 1.92                     | 0.52              |
| 1:I:203:GLN:N   | 1:N:81:ARG:NH2  | 2.57                     | 0.52              |
| 1:M:33:LEU:HD22 | 1:M:136:LYS:HD3 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:33:LEU:HD22  | 1:N:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:P:33:LEU:HD22  | 1:P:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:Y:42:GLU:OE2   | 1:Y:45:ARG:NH2   | 2.42                     | 0.52              |
| 1:c:33:LEU:HD22  | 1:c:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:f:101:THR:O    | 1:f:105:GLY:N    | 2.40                     | 0.52              |
| 1:m:33:LEU:HD22  | 1:m:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:p:33:LEU:HD22  | 1:p:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:u:33:LEU:HD22  | 1:u:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:z:33:LEU:HD22  | 1:z:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:1:33:LEU:HD22  | 1:1:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:C:33:LEU:HD22  | 1:C:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:F:66:LEU:O     | 1:F:70:ARG:N     | 2.35                     | 0.52              |
| 1:K:33:LEU:O     | 1:K:129:TYR:OH   | 2.21                     | 0.52              |
| 1:L:42:GLU:OE2   | 1:L:45:ARG:NH2   | 2.42                     | 0.52              |
| 1:b:66:LEU:O     | 1:b:70:ARG:N     | 2.35                     | 0.52              |
| 1:2:33:LEU:HD22  | 1:2:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:6:33:LEU:HD22  | 1:6:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:U:66:LEU:O     | 1:U:70:ARG:N     | 2.35                     | 0.52              |
| 1:e:33:LEU:HD22  | 1:e:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:6:130:LEU:HD12 | 1:6:130:LEU:C    | 2.35                     | 0.52              |
| 1:F:33:LEU:HD22  | 1:F:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:H:130:LEU:C    | 1:H:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:Q:130:LEU:HD12 | 1:Q:130:LEU:C    | 2.35                     | 0.52              |
| 1:R:33:LEU:O     | 1:R:129:TYR:OH   | 2.21                     | 0.52              |
| 1:R:33:LEU:HD22  | 1:R:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:c:130:LEU:C    | 1:c:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:r:66:LEU:O     | 1:r:70:ARG:N     | 2.35                     | 0.52              |
| 1:t:33:LEU:HD22  | 1:t:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:4:33:LEU:HD22  | 1:4:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:E:33:LEU:HD22  | 1:E:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:E:94:ARG:O     | 1:E:98:GLN:N     | 2.38                     | 0.52              |
| 1:F:130:LEU:HD12 | 1:F:130:LEU:C    | 2.35                     | 0.52              |
| 1:G:66:LEU:O     | 1:G:70:ARG:N     | 2.35                     | 0.52              |
| 1:Q:94:ARG:O     | 1:Q:98:GLN:N     | 2.38                     | 0.52              |
| 1:V:33:LEU:HD22  | 1:V:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:X:33:LEU:HD22  | 1:X:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:X:66:LEU:O     | 1:X:70:ARG:N     | 2.35                     | 0.52              |
| 1:k:33:LEU:HD22  | 1:k:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:l:130:LEU:C    | 1:l:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:r:33:LEU:HD22  | 1:r:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:u:130:LEU:C    | 1:u:130:LEU:HD12 | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:33:LEU:HD22  | 1:x:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:x:130:LEU:C    | 1:x:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:5:130:LEU:C    | 1:5:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:I:33:LEU:HD22  | 1:I:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:K:33:LEU:HD22  | 1:K:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:T:130:LEU:C    | 1:T:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:W:66:LEU:O     | 1:W:70:ARG:N     | 2.35                     | 0.52              |
| 1:Z:130:LEU:C    | 1:Z:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:g:33:LEU:O     | 1:g:129:TYR:OH   | 2.21                     | 0.52              |
| 1:g:33:LEU:HD22  | 1:g:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:l:94:ARG:O     | 1:l:98:GLN:N     | 2.38                     | 0.52              |
| 1:n:130:LEU:C    | 1:n:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:o:33:LEU:HD22  | 1:o:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:r:130:LEU:C    | 1:r:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:w:33:LEU:HD22  | 1:w:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:G:130:LEU:C    | 1:G:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:P:130:LEU:C    | 1:P:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:a:33:LEU:HD22  | 1:a:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:i:33:LEU:HD22  | 1:i:136:LYS:HD3  | 1.92                     | 0.52              |
| 1:j:101:THR:O    | 1:j:105:GLY:N    | 2.40                     | 0.52              |
| 1:k:130:LEU:C    | 1:k:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:o:130:LEU:C    | 1:o:130:LEU:HD12 | 2.35                     | 0.52              |
| 1:5:66:LEU:O     | 1:5:70:ARG:N     | 2.35                     | 0.51              |
| 1:B:130:LEU:C    | 1:B:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:E:130:LEU:C    | 1:E:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:J:130:LEU:C    | 1:J:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:S:33:LEU:HD22  | 1:S:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:f:66:LEU:O     | 1:f:70:ARG:N     | 2.35                     | 0.51              |
| 1:j:33:LEU:HD22  | 1:j:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:v:130:LEU:C    | 1:v:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:w:130:LEU:C    | 1:w:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:2:94:ARG:O     | 1:2:98:GLN:N     | 2.38                     | 0.51              |
| 1:D:94:ARG:O     | 1:D:98:GLN:N     | 2.38                     | 0.51              |
| 1:b:130:LEU:C    | 1:b:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:k:101:THR:O    | 1:k:105:GLY:N    | 2.40                     | 0.51              |
| 1:m:94:ARG:O     | 1:m:98:GLN:N     | 2.38                     | 0.51              |
| 1:t:130:LEU:HD12 | 1:t:130:LEU:C    | 2.35                     | 0.51              |
| 1:7:130:LEU:C    | 1:7:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:A:130:LEU:C    | 1:A:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:B:101:THR:O    | 1:B:105:GLY:N    | 2.40                     | 0.51              |
| 1:D:130:LEU:C    | 1:D:130:LEU:HD12 | 2.35                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:66:LEU:O     | 1:J:70:ARG:N     | 2.35                     | 0.51              |
| 1:N:130:LEU:C    | 1:N:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:Q:72:TYR:O     | 1:Q:76:GLN:N     | 2.44                     | 0.51              |
| 1:Y:130:LEU:HD12 | 1:Y:130:LEU:C    | 2.35                     | 0.51              |
| 1:a:33:LEU:O     | 1:a:129:TYR:OH   | 2.21                     | 0.51              |
| 1:b:33:LEU:HD22  | 1:b:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:d:63:ALA:O     | 1:d:67:ILE:N     | 2.38                     | 0.51              |
| 1:i:130:LEU:C    | 1:i:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:j:33:LEU:O     | 1:j:129:TYR:OH   | 2.21                     | 0.51              |
| 1:u:72:TYR:O     | 1:u:76:GLN:N     | 2.44                     | 0.51              |
| 1:y:33:LEU:HD22  | 1:y:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:y:72:TYR:O     | 1:y:76:GLN:N     | 2.44                     | 0.51              |
| 1:2:66:LEU:O     | 1:2:70:ARG:N     | 2.35                     | 0.51              |
| 1:2:130:LEU:C    | 1:2:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:3:130:LEU:C    | 1:3:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:7:94:ARG:O     | 1:7:98:GLN:N     | 2.38                     | 0.51              |
| 1:D:33:LEU:HD22  | 1:D:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:D:101:THR:O    | 1:D:105:GLY:N    | 2.40                     | 0.51              |
| 1:I:72:TYR:O     | 1:I:76:GLN:N     | 2.44                     | 0.51              |
| 1:I:130:LEU:C    | 1:I:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:J:33:LEU:HD22  | 1:J:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:K:130:LEU:C    | 1:K:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:M:72:TYR:O     | 1:M:76:GLN:N     | 2.44                     | 0.51              |
| 1:R:130:LEU:C    | 1:R:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:S:130:LEU:C    | 1:S:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:T:66:LEU:O     | 1:T:70:ARG:N     | 2.35                     | 0.51              |
| 1:V:94:ARG:O     | 1:V:98:GLN:N     | 2.38                     | 0.51              |
| 1:W:33:LEU:HD22  | 1:W:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:Y:63:ALA:O     | 1:Y:67:ILE:N     | 2.38                     | 0.51              |
| 1:Z:72:TYR:O     | 1:Z:76:GLN:N     | 2.44                     | 0.51              |
| 1:d:130:LEU:C    | 1:d:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:f:33:LEU:HD22  | 1:f:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:h:130:LEU:C    | 1:h:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:j:130:LEU:C    | 1:j:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:l:33:LEU:HD22  | 1:l:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:m:130:LEU:C    | 1:m:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:n:33:LEU:HD22  | 1:n:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:y:130:LEU:C    | 1:y:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:2:72:TYR:O     | 1:2:76:GLN:N     | 2.44                     | 0.51              |
| 1:3:94:ARG:O     | 1:3:98:GLN:N     | 2.38                     | 0.51              |
| 1:7:72:TYR:O     | 1:7:76:GLN:N     | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:33:LEU:HD22  | 1:Q:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:T:33:LEU:HD22  | 1:T:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:U:72:TYR:O     | 1:U:76:GLN:N     | 2.44                     | 0.51              |
| 1:U:130:LEU:C    | 1:U:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:V:72:TYR:O     | 1:V:76:GLN:N     | 2.44                     | 0.51              |
| 1:Y:33:LEU:HD22  | 1:Y:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:d:33:LEU:HD22  | 1:d:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:f:72:TYR:O     | 1:f:76:GLN:N     | 2.44                     | 0.51              |
| 1:o:66:LEU:O     | 1:o:70:ARG:N     | 2.35                     | 0.51              |
| 1:p:94:ARG:O     | 1:p:98:GLN:N     | 2.38                     | 0.51              |
| 1:q:72:TYR:O     | 1:q:76:GLN:N     | 2.44                     | 0.51              |
| 1:s:33:LEU:HD22  | 1:s:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:z:130:LEU:C    | 1:z:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:0:130:LEU:C    | 1:0:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:6:72:TYR:O     | 1:6:76:GLN:N     | 2.44                     | 0.51              |
| 1:C:101:THR:O    | 1:C:105:GLY:N    | 2.40                     | 0.51              |
| 1:E:72:TYR:O     | 1:E:76:GLN:N     | 2.44                     | 0.51              |
| 1:M:130:LEU:C    | 1:M:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:O:130:LEU:C    | 1:O:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:Z:94:ARG:O     | 1:Z:98:GLN:N     | 2.38                     | 0.51              |
| 1:b:72:TYR:O     | 1:b:76:GLN:N     | 2.44                     | 0.51              |
| 1:e:130:LEU:C    | 1:e:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:m:72:TYR:O     | 1:m:76:GLN:N     | 2.44                     | 0.51              |
| 1:v:33:LEU:HD22  | 1:v:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:3:72:TYR:O     | 1:3:76:GLN:N     | 2.44                     | 0.51              |
| 1:5:33:LEU:HD22  | 1:5:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:A:94:ARG:O     | 1:A:98:GLN:N     | 2.38                     | 0.51              |
| 1:E:63:ALA:O     | 1:E:67:ILE:N     | 2.38                     | 0.51              |
| 1:H:33:LEU:O     | 1:H:129:TYR:OH   | 2.21                     | 0.51              |
| 1:L:130:LEU:C    | 1:L:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:R:94:ARG:O     | 1:R:98:GLN:N     | 2.38                     | 0.51              |
| 1:a:130:LEU:HD12 | 1:a:130:LEU:C    | 2.35                     | 0.51              |
| 1:d:72:TYR:O     | 1:d:76:GLN:N     | 2.44                     | 0.51              |
| 1:f:130:LEU:C    | 1:f:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:j:72:TYR:O     | 1:j:76:GLN:N     | 2.44                     | 0.51              |
| 1:n:101:THR:O    | 1:n:105:GLY:N    | 2.40                     | 0.51              |
| 1:p:130:LEU:C    | 1:p:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:0:72:TYR:O     | 1:0:76:GLN:N     | 2.44                     | 0.51              |
| 1:4:130:LEU:C    | 1:4:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:B:72:TYR:O     | 1:B:76:GLN:N     | 2.44                     | 0.51              |
| 1:L:33:LEU:HD22  | 1:L:136:LYS:HD3  | 1.92                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:33:LEU:HD22 | 1:O:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:U:94:ARG:O    | 1:U:98:GLN:N     | 2.38                     | 0.51              |
| 1:X:72:TYR:O    | 1:X:76:GLN:N     | 2.44                     | 0.51              |
| 1:Y:72:TYR:O    | 1:Y:76:GLN:N     | 2.44                     | 0.51              |
| 1:q:130:LEU:C   | 1:q:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:v:66:LEU:O    | 1:v:70:ARG:N     | 2.35                     | 0.51              |
| 1:3:33:LEU:HD22 | 1:3:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:4:72:TYR:O    | 1:4:76:GLN:N     | 2.44                     | 0.51              |
| 1:A:72:TYR:O    | 1:A:76:GLN:N     | 2.44                     | 0.51              |
| 1:H:94:ARG:O    | 1:H:98:GLN:N     | 2.38                     | 0.51              |
| 1:O:72:TYR:O    | 1:O:76:GLN:N     | 2.44                     | 0.51              |
| 1:R:72:TYR:O    | 1:R:76:GLN:N     | 2.44                     | 0.51              |
| 1:S:72:TYR:O    | 1:S:76:GLN:N     | 2.44                     | 0.51              |
| 1:W:72:TYR:O    | 1:W:76:GLN:N     | 2.44                     | 0.51              |
| 1:g:130:LEU:C   | 1:g:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:h:72:TYR:O    | 1:h:76:GLN:N     | 2.44                     | 0.51              |
| 1:p:101:THR:O   | 1:p:105:GLY:N    | 2.40                     | 0.51              |
| 1:q:33:LEU:HD22 | 1:q:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:q:101:THR:O   | 1:q:105:GLY:N    | 2.40                     | 0.51              |
| 1:s:130:LEU:C   | 1:s:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:1:66:LEU:O    | 1:1:70:ARG:N     | 2.35                     | 0.51              |
| 1:1:130:LEU:C   | 1:1:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:5:72:TYR:O    | 1:5:76:GLN:N     | 2.44                     | 0.51              |
| 1:C:130:LEU:C   | 1:C:130:LEU:HD12 | 2.35                     | 0.51              |
| 1:G:33:LEU:HD22 | 1:G:136:LYS:HD3  | 1.92                     | 0.51              |
| 1:Q:66:LEU:O    | 1:Q:70:ARG:N     | 2.35                     | 0.51              |
| 1:T:33:LEU:O    | 1:T:129:TYR:OH   | 2.21                     | 0.51              |
| 1:c:63:ALA:O    | 1:c:67:ILE:N     | 2.38                     | 0.51              |
| 1:n:72:TYR:O    | 1:n:76:GLN:N     | 2.44                     | 0.51              |
| 1:x:66:LEU:O    | 1:x:70:ARG:N     | 2.35                     | 0.51              |
| 1:z:94:ARG:O    | 1:z:98:GLN:N     | 2.38                     | 0.51              |
| 1:0:33:LEU:HD22 | 1:0:136:LYS:HD3  | 1.92                     | 0.50              |
| 1:B:33:LEU:HD22 | 1:B:136:LYS:HD3  | 1.92                     | 0.50              |
| 1:F:47:LEU:O    | 1:F:50:THR:OG1   | 2.20                     | 0.50              |
| 1:F:101:THR:O   | 1:F:105:GLY:N    | 2.40                     | 0.50              |
| 1:a:66:LEU:O    | 1:a:70:ARG:N     | 2.35                     | 0.50              |
| 1:i:72:TYR:O    | 1:i:76:GLN:N     | 2.44                     | 0.50              |
| 1:w:72:TYR:O    | 1:w:76:GLN:N     | 2.44                     | 0.50              |
| 1:2:33:LEU:O    | 1:2:129:TYR:OH   | 2.21                     | 0.50              |
| 1:F:72:TYR:O    | 1:F:76:GLN:N     | 2.44                     | 0.50              |
| 1:T:72:TYR:O    | 1:T:76:GLN:N     | 2.44                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:c:72:TYR:O    | 1:c:76:GLN:N     | 2.44                     | 0.50              |
| 1:d:94:ARG:O    | 1:d:98:GLN:N     | 2.38                     | 0.50              |
| 1:o:33:LEU:O    | 1:o:129:TYR:OH   | 2.21                     | 0.50              |
| 1:z:72:TYR:O    | 1:z:76:GLN:N     | 2.44                     | 0.50              |
| 1:6:94:ARG:O    | 1:6:98:GLN:N     | 2.38                     | 0.50              |
| 1:D:72:TYR:O    | 1:D:76:GLN:N     | 2.44                     | 0.50              |
| 1:H:72:TYR:O    | 1:H:76:GLN:N     | 2.44                     | 0.50              |
| 1:M:101:THR:O   | 1:M:105:GLY:N    | 2.40                     | 0.50              |
| 1:N:33:LEU:O    | 1:N:129:TYR:OH   | 2.21                     | 0.50              |
| 1:W:130:LEU:C   | 1:W:130:LEU:HD12 | 2.35                     | 0.50              |
| 1:X:130:LEU:C   | 1:X:130:LEU:HD12 | 2.35                     | 0.50              |
| 1:a:72:TYR:O    | 1:a:76:GLN:N     | 2.44                     | 0.50              |
| 1:i:94:ARG:O    | 1:i:98:GLN:N     | 2.38                     | 0.50              |
| 1:l:72:TYR:O    | 1:l:76:GLN:N     | 2.44                     | 0.50              |
| 1:o:101:THR:O   | 1:o:105:GLY:N    | 2.40                     | 0.50              |
| 1:p:72:TYR:O    | 1:p:76:GLN:N     | 2.44                     | 0.50              |
| 1:s:33:LEU:O    | 1:s:129:TYR:OH   | 2.21                     | 0.50              |
| 1:t:72:TYR:O    | 1:t:76:GLN:N     | 2.44                     | 0.50              |
| 1:u:101:THR:O   | 1:u:105:GLY:N    | 2.40                     | 0.50              |
| 1:y:101:THR:O   | 1:y:105:GLY:N    | 2.40                     | 0.50              |
| 1:l:72:TYR:O    | 1:l:76:GLN:N     | 2.44                     | 0.50              |
| 1:C:66:LEU:O    | 1:C:70:ARG:N     | 2.35                     | 0.50              |
| 1:I:101:THR:O   | 1:I:105:GLY:N    | 2.40                     | 0.50              |
| 1:K:72:TYR:O    | 1:K:76:GLN:N     | 2.44                     | 0.50              |
| 1:r:72:TYR:O    | 1:r:76:GLN:N     | 2.44                     | 0.50              |
| 1:r:101:THR:O   | 1:r:105:GLY:N    | 2.40                     | 0.50              |
| 1:t:94:ARG:O    | 1:t:98:GLN:N     | 2.38                     | 0.50              |
| 1:z:63:ALA:O    | 1:z:67:ILE:N     | 2.38                     | 0.50              |
| 1:H:101:THR:O   | 1:H:105:GLY:N    | 2.40                     | 0.50              |
| 1:N:72:TYR:O    | 1:N:76:GLN:N     | 2.44                     | 0.50              |
| 1:N:94:ARG:O    | 1:N:98:GLN:N     | 2.38                     | 0.50              |
| 1:Q:101:THR:O   | 1:Q:105:GLY:N    | 2.40                     | 0.50              |
| 1:V:130:LEU:C   | 1:V:130:LEU:HD12 | 2.35                     | 0.50              |
| 1:e:66:LEU:O    | 1:e:70:ARG:N     | 2.35                     | 0.50              |
| 1:6:33:LEU:HD21 | 1:6:132:LEU:HG   | 1.94                     | 0.50              |
| 1:E:33:LEU:O    | 1:E:129:TYR:OH   | 2.21                     | 0.50              |
| 1:L:72:TYR:O    | 1:L:76:GLN:N     | 2.44                     | 0.50              |
| 1:N:66:LEU:O    | 1:N:70:ARG:N     | 2.35                     | 0.50              |
| 1:d:33:LEU:O    | 1:d:129:TYR:OH   | 2.21                     | 0.50              |
| 1:q:63:ALA:O    | 1:q:67:ILE:N     | 2.38                     | 0.50              |
| 1:P:72:TYR:O    | 1:P:76:GLN:N     | 2.44                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:e:72:TYR:O    | 1:e:76:GLN:N    | 2.44                     | 0.50              |
| 1:h:63:ALA:O    | 1:h:67:ILE:N    | 2.38                     | 0.50              |
| 1:l:33:LEU:HD21 | 1:l:132:LEU:HG  | 1.94                     | 0.50              |
| 1:p:33:LEU:O    | 1:p:129:TYR:OH  | 2.21                     | 0.50              |
| 1:s:72:TYR:O    | 1:s:76:GLN:N    | 2.44                     | 0.50              |
| 1:v:72:TYR:O    | 1:v:76:GLN:N    | 2.44                     | 0.50              |
| 1:x:72:TYR:O    | 1:x:76:GLN:N    | 2.44                     | 0.50              |
| 1:2:101:THR:O   | 1:2:105:GLY:N   | 2.40                     | 0.50              |
| 1:H:33:LEU:HD21 | 1:H:132:LEU:HG  | 1.94                     | 0.50              |
| 1:J:72:TYR:O    | 1:J:76:GLN:N    | 2.44                     | 0.50              |
| 1:P:66:LEU:O    | 1:P:70:ARG:N    | 2.35                     | 0.50              |
| 1:c:33:LEU:HD21 | 1:c:132:LEU:HG  | 1.94                     | 0.50              |
| 1:g:72:TYR:O    | 1:g:76:GLN:N    | 2.44                     | 0.50              |
| 1:l:101:THR:O   | 1:l:105:GLY:N   | 2.40                     | 0.50              |
| 1:1:33:LEU:HD21 | 1:1:132:LEU:HG  | 1.94                     | 0.50              |
| 1:7:86:LEU:HD23 | 1:7:86:LEU:C    | 2.37                     | 0.50              |
| 1:C:72:TYR:O    | 1:C:76:GLN:N    | 2.44                     | 0.50              |
| 1:D:86:LEU:HD23 | 1:D:86:LEU:C    | 2.37                     | 0.50              |
| 1:G:101:THR:O   | 1:G:105:GLY:N   | 2.40                     | 0.50              |
| 1:H:86:LEU:HD23 | 1:H:86:LEU:C    | 2.37                     | 0.50              |
| 1:J:101:THR:O   | 1:J:105:GLY:N   | 2.40                     | 0.50              |
| 1:L:66:LEU:O    | 1:L:70:ARG:N    | 2.35                     | 0.50              |
| 1:Y:94:ARG:O    | 1:Y:98:GLN:N    | 2.38                     | 0.50              |
| 1:k:72:TYR:O    | 1:k:76:GLN:N    | 2.44                     | 0.50              |
| 1:o:72:TYR:O    | 1:o:76:GLN:N    | 2.44                     | 0.50              |
| 1:v:94:ARG:O    | 1:v:98:GLN:N    | 2.38                     | 0.50              |
| 1:y:66:LEU:O    | 1:y:70:ARG:N    | 2.35                     | 0.50              |
| 1:3:86:LEU:C    | 1:3:86:LEU:HD23 | 2.37                     | 0.49              |
| 1:6:86:LEU:C    | 1:6:86:LEU:HD23 | 2.38                     | 0.49              |
| 1:C:33:LEU:HD21 | 1:C:132:LEU:HG  | 1.94                     | 0.49              |
| 1:G:72:TYR:O    | 1:G:76:GLN:N    | 2.44                     | 0.49              |
| 1:I:86:LEU:HD23 | 1:I:86:LEU:C    | 2.37                     | 0.49              |
| 1:L:86:LEU:HD23 | 1:L:86:LEU:C    | 2.37                     | 0.49              |
| 1:L:94:ARG:O    | 1:L:98:GLN:N    | 2.38                     | 0.49              |
| 1:Q:33:LEU:HD21 | 1:Q:132:LEU:HG  | 1.94                     | 0.49              |
| 1:Q:86:LEU:HD23 | 1:Q:86:LEU:C    | 2.37                     | 0.49              |
| 1:d:86:LEU:HD23 | 1:d:86:LEU:C    | 2.37                     | 0.49              |
| 1:g:33:LEU:HD21 | 1:g:132:LEU:HG  | 1.94                     | 0.49              |
| 1:g:63:ALA:O    | 1:g:67:ILE:N    | 2.38                     | 0.49              |
| 1:k:66:LEU:O    | 1:k:70:ARG:N    | 2.35                     | 0.49              |
| 1:x:33:LEU:HD21 | 1:x:132:LEU:HG  | 1.94                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:2:86:LEU:HD23 | 1:2:86:LEU:C    | 2.37                     | 0.49              |
| 1:L:33:LEU:HD21 | 1:L:132:LEU:HG  | 1.94                     | 0.49              |
| 1:M:33:LEU:HD21 | 1:M:132:LEU:HG  | 1.94                     | 0.49              |
| 1:h:33:LEU:HD21 | 1:h:132:LEU:HG  | 1.94                     | 0.49              |
| 1:l:86:LEU:HD23 | 1:l:86:LEU:C    | 2.38                     | 0.49              |
| 1:u:86:LEU:HD23 | 1:u:86:LEU:C    | 2.37                     | 0.49              |
| 1:E:101:THR:O   | 1:E:105:GLY:N   | 2.40                     | 0.49              |
| 1:U:101:THR:O   | 1:U:105:GLY:N   | 2.40                     | 0.49              |
| 1:c:86:LEU:HD23 | 1:c:86:LEU:C    | 2.38                     | 0.49              |
| 1:c:94:ARG:O    | 1:c:98:GLN:N    | 2.38                     | 0.49              |
| 1:f:63:ALA:O    | 1:f:67:ILE:N    | 2.38                     | 0.49              |
| 1:h:94:ARG:O    | 1:h:98:GLN:N    | 2.38                     | 0.49              |
| 1:m:86:LEU:HD23 | 1:m:86:LEU:C    | 2.37                     | 0.49              |
| 1:q:86:LEU:C    | 1:q:86:LEU:HD23 | 2.37                     | 0.49              |
| 1:t:101:THR:O   | 1:t:105:GLY:N   | 2.40                     | 0.49              |
| 1:y:86:LEU:C    | 1:y:86:LEU:HD23 | 2.38                     | 0.49              |
| 1:z:86:LEU:HD23 | 1:z:86:LEU:C    | 2.37                     | 0.49              |
| 1:2:33:LEU:HD21 | 1:2:132:LEU:HG  | 1.94                     | 0.49              |
| 1:C:86:LEU:C    | 1:C:86:LEU:HD23 | 2.37                     | 0.49              |
| 1:P:86:LEU:HD23 | 1:P:86:LEU:C    | 2.37                     | 0.49              |
| 1:X:33:LEU:HD21 | 1:X:132:LEU:HG  | 1.94                     | 0.49              |
| 1:Z:86:LEU:HD23 | 1:Z:86:LEU:C    | 2.37                     | 0.49              |
| 1:i:66:LEU:O    | 1:i:70:ARG:N    | 2.35                     | 0.49              |
| 1:p:33:LEU:HD21 | 1:p:132:LEU:HG  | 1.94                     | 0.49              |
| 1:q:33:LEU:HD21 | 1:q:132:LEU:HG  | 1.94                     | 0.49              |
| 1:t:86:LEU:HD23 | 1:t:86:LEU:C    | 2.37                     | 0.49              |
| 1:u:33:LEU:HD21 | 1:u:132:LEU:HG  | 1.94                     | 0.49              |
| 1:x:86:LEU:HD23 | 1:x:86:LEU:C    | 2.37                     | 0.49              |
| 1:A:86:LEU:HD23 | 1:A:86:LEU:C    | 2.37                     | 0.49              |
| 1:J:94:ARG:O    | 1:J:98:GLN:N    | 2.38                     | 0.49              |
| 1:M:66:LEU:O    | 1:M:70:ARG:N    | 2.35                     | 0.49              |
| 1:M:86:LEU:HD23 | 1:M:86:LEU:C    | 2.37                     | 0.49              |
| 1:R:63:ALA:O    | 1:R:67:ILE:N    | 2.38                     | 0.49              |
| 1:R:86:LEU:HD23 | 1:R:86:LEU:C    | 2.37                     | 0.49              |
| 1:U:86:LEU:HD23 | 1:U:86:LEU:C    | 2.37                     | 0.49              |
| 1:V:33:LEU:HD21 | 1:V:132:LEU:HG  | 1.94                     | 0.49              |
| 1:g:66:LEU:O    | 1:g:70:ARG:N    | 2.35                     | 0.49              |
| 1:v:101:THR:O   | 1:v:105:GLY:N   | 2.40                     | 0.49              |
| 1:7:101:THR:O   | 1:7:105:GLY:N   | 2.40                     | 0.49              |
| 1:D:33:LEU:HD21 | 1:D:132:LEU:HG  | 1.94                     | 0.49              |
| 1:G:86:LEU:HD23 | 1:G:86:LEU:C    | 2.37                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:63:ALA:O    | 1:I:67:ILE:N    | 2.39                     | 0.49              |
| 1:Y:86:LEU:C    | 1:Y:86:LEU:HD23 | 2.37                     | 0.49              |
| 1:Z:101:THR:O   | 1:Z:105:GLY:N   | 2.40                     | 0.49              |
| 1:s:101:THR:O   | 1:s:105:GLY:N   | 2.40                     | 0.49              |
| 1:z:66:LEU:O    | 1:z:70:ARG:N    | 2.35                     | 0.49              |
| 1:6:101:THR:O   | 1:6:105:GLY:N   | 2.40                     | 0.49              |
| 1:E:86:LEU:HD23 | 1:E:86:LEU:C    | 2.38                     | 0.49              |
| 1:T:33:LEU:HD21 | 1:T:132:LEU:HG  | 1.94                     | 0.49              |
| 1:e:94:ARG:O    | 1:e:98:GLN:N    | 2.38                     | 0.49              |
| 1:m:101:THR:O   | 1:m:105:GLY:N   | 2.40                     | 0.49              |
| 1:s:33:LEU:HD21 | 1:s:132:LEU:HG  | 1.94                     | 0.49              |
| 1:v:86:LEU:HD23 | 1:v:86:LEU:C    | 2.37                     | 0.49              |
| 1:x:94:ARG:O    | 1:x:98:GLN:N    | 2.38                     | 0.49              |
| 1:D:33:LEU:O    | 1:D:129:TYR:OH  | 2.21                     | 0.49              |
| 1:T:86:LEU:HD23 | 1:T:86:LEU:C    | 2.38                     | 0.49              |
| 1:U:33:LEU:HD21 | 1:U:132:LEU:HG  | 1.94                     | 0.49              |
| 1:V:101:THR:O   | 1:V:105:GLY:N   | 2.40                     | 0.49              |
| 1:Y:33:LEU:HD21 | 1:Y:132:LEU:HG  | 1.94                     | 0.49              |
| 1:Z:33:LEU:HD21 | 1:Z:132:LEU:HG  | 1.94                     | 0.49              |
| 1:a:63:ALA:O    | 1:a:67:ILE:N    | 2.38                     | 0.49              |
| 1:b:33:LEU:HD21 | 1:b:132:LEU:HG  | 1.94                     | 0.49              |
| 1:p:86:LEU:HD23 | 1:p:86:LEU:C    | 2.37                     | 0.49              |
| 1:w:166:SER:O   | 1:w:170:ARG:N   | 2.34                     | 0.49              |
| 1:4:86:LEU:HD23 | 1:4:86:LEU:C    | 2.37                     | 0.49              |
| 1:A:66:LEU:O    | 1:A:70:ARG:N    | 2.35                     | 0.49              |
| 1:G:33:LEU:HD21 | 1:G:132:LEU:HG  | 1.94                     | 0.49              |
| 1:d:101:THR:O   | 1:d:105:GLY:N   | 2.40                     | 0.49              |
| 1:i:86:LEU:C    | 1:i:86:LEU:HD23 | 2.37                     | 0.49              |
| 1:1:86:LEU:HD23 | 1:1:86:LEU:C    | 2.37                     | 0.49              |
| 1:3:101:THR:O   | 1:3:105:GLY:N   | 2.40                     | 0.49              |
| 1:5:33:LEU:HD21 | 1:5:132:LEU:HG  | 1.94                     | 0.49              |
| 1:5:86:LEU:HD23 | 1:5:86:LEU:C    | 2.38                     | 0.49              |
| 1:B:86:LEU:HD23 | 1:B:86:LEU:C    | 2.37                     | 0.49              |
| 1:K:86:LEU:C    | 1:K:86:LEU:HD23 | 2.38                     | 0.49              |
| 1:L:101:THR:O   | 1:L:105:GLY:N   | 2.40                     | 0.49              |
| 1:N:101:THR:O   | 1:N:105:GLY:N   | 2.40                     | 0.49              |
| 1:g:86:LEU:HD23 | 1:g:86:LEU:C    | 2.37                     | 0.49              |
| 1:g:94:ARG:O    | 1:g:98:GLN:N    | 2.38                     | 0.49              |
| 1:r:86:LEU:HD23 | 1:r:86:LEU:C    | 2.37                     | 0.49              |
| 1:r:94:ARG:O    | 1:r:98:GLN:N    | 2.38                     | 0.49              |
| 1:t:66:LEU:O    | 1:t:70:ARG:N    | 2.35                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:w:33:LEU:HD21 | 1:w:132:LEU:HG  | 1.94                     | 0.49              |
| 1:y:33:LEU:O    | 1:y:129:TYR:OH  | 2.21                     | 0.49              |
| 1:0:86:LEU:C    | 1:0:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:7:33:LEU:HD21 | 1:7:132:LEU:HG  | 1.94                     | 0.48              |
| 1:A:33:LEU:HD21 | 1:A:132:LEU:HG  | 1.94                     | 0.48              |
| 1:F:86:LEU:C    | 1:F:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:R:33:LEU:HD21 | 1:R:132:LEU:HG  | 1.94                     | 0.48              |
| 1:V:86:LEU:C    | 1:V:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:W:33:LEU:O    | 1:W:129:TYR:OH  | 2.21                     | 0.48              |
| 1:k:86:LEU:HD23 | 1:k:86:LEU:C    | 2.37                     | 0.48              |
| 1:l:63:ALA:O    | 1:l:67:ILE:N    | 2.39                     | 0.48              |
| 1:m:33:LEU:HD21 | 1:m:132:LEU:HG  | 1.94                     | 0.48              |
| 1:o:86:LEU:HD23 | 1:o:86:LEU:C    | 2.37                     | 0.48              |
| 1:t:33:LEU:HD21 | 1:t:132:LEU:HG  | 1.94                     | 0.48              |
| 1:G:33:LEU:O    | 1:G:129:TYR:OH  | 2.21                     | 0.48              |
| 1:K:101:THR:O   | 1:K:105:GLY:N   | 2.40                     | 0.48              |
| 1:R:101:THR:O   | 1:R:105:GLY:N   | 2.40                     | 0.48              |
| 1:S:88:ARG:O    | 1:S:88:ARG:NE   | 2.43                     | 0.48              |
| 1:X:86:LEU:HD23 | 1:X:86:LEU:C    | 2.38                     | 0.48              |
| 1:e:86:LEU:HD23 | 1:e:86:LEU:C    | 2.37                     | 0.48              |
| 1:f:88:ARG:O    | 1:f:88:ARG:NE   | 2.43                     | 0.48              |
| 1:h:86:LEU:HD23 | 1:h:86:LEU:C    | 2.37                     | 0.48              |
| 1:k:33:LEU:HD21 | 1:k:132:LEU:HG  | 1.94                     | 0.48              |
| 1:I:33:LEU:HD21 | 1:I:132:LEU:HG  | 1.94                     | 0.48              |
| 1:O:86:LEU:HD23 | 1:O:86:LEU:C    | 2.37                     | 0.48              |
| 1:Y:101:THR:O   | 1:Y:105:GLY:N   | 2.40                     | 0.48              |
| 1:a:86:LEU:C    | 1:a:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:c:66:LEU:O    | 1:c:70:ARG:N    | 2.35                     | 0.48              |
| 1:i:88:ARG:O    | 1:i:88:ARG:NE   | 2.43                     | 0.48              |
| 1:k:63:ALA:O    | 1:k:67:ILE:N    | 2.38                     | 0.48              |
| 1:y:33:LEU:HD21 | 1:y:132:LEU:HG  | 1.94                     | 0.48              |
| 1:A:101:THR:O   | 1:A:105:GLY:N   | 2.40                     | 0.48              |
| 1:E:33:LEU:HD21 | 1:E:132:LEU:HG  | 1.94                     | 0.48              |
| 1:J:86:LEU:HD23 | 1:J:86:LEU:C    | 2.38                     | 0.48              |
| 1:P:94:ARG:O    | 1:P:98:GLN:N    | 2.38                     | 0.48              |
| 1:m:66:LEU:O    | 1:m:70:ARG:N    | 2.35                     | 0.48              |
| 1:o:33:LEU:HD21 | 1:o:132:LEU:HG  | 1.94                     | 0.48              |
| 1:u:66:LEU:O    | 1:u:70:ARG:N    | 2.35                     | 0.48              |
| 1:w:86:LEU:HD23 | 1:w:86:LEU:C    | 2.37                     | 0.48              |
| 1:B:33:LEU:HD21 | 1:B:132:LEU:HG  | 1.94                     | 0.48              |
| 1:F:33:LEU:HD21 | 1:F:132:LEU:HG  | 1.94                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:166:SER:O   | 1:H:170:ARG:N   | 2.34                     | 0.48              |
| 1:N:86:LEU:C    | 1:N:86:LEU:HD23 | 2.38                     | 0.48              |
| 1:P:33:LEU:HD21 | 1:P:132:LEU:HG  | 1.94                     | 0.48              |
| 1:Q:33:LEU:O    | 1:Q:129:TYR:OH  | 2.21                     | 0.48              |
| 1:R:66:LEU:O    | 1:R:70:ARG:N    | 2.35                     | 0.48              |
| 1:S:33:LEU:HD21 | 1:S:132:LEU:HG  | 1.94                     | 0.48              |
| 1:W:33:LEU:HD21 | 1:W:132:LEU:HG  | 1.94                     | 0.48              |
| 1:c:33:LEU:O    | 1:c:129:TYR:OH  | 2.21                     | 0.48              |
| 1:n:86:LEU:C    | 1:n:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:s:88:ARG:O    | 1:s:88:ARG:NE   | 2.43                     | 0.48              |
| 1:v:33:LEU:HD21 | 1:v:132:LEU:HG  | 1.94                     | 0.48              |
| 1:0:33:LEU:HD21 | 1:0:132:LEU:HG  | 1.94                     | 0.48              |
| 1:4:33:LEU:HD21 | 1:4:132:LEU:HG  | 1.94                     | 0.48              |
| 1:A:88:ARG:O    | 1:A:88:ARG:NE   | 2.43                     | 0.48              |
| 1:F:94:ARG:O    | 1:F:98:GLN:N    | 2.38                     | 0.48              |
| 1:W:86:LEU:HD23 | 1:W:86:LEU:C    | 2.37                     | 0.48              |
| 1:a:33:LEU:HD21 | 1:a:132:LEU:HG  | 1.94                     | 0.48              |
| 1:d:33:LEU:HD21 | 1:d:132:LEU:HG  | 1.94                     | 0.48              |
| 1:f:86:LEU:C    | 1:f:86:LEU:HD23 | 2.37                     | 0.48              |
| 1:h:101:THR:O   | 1:h:105:GLY:N   | 2.40                     | 0.48              |
| 1:r:33:LEU:HD21 | 1:r:132:LEU:HG  | 1.94                     | 0.48              |
| 1:r:166:SER:O   | 1:r:170:ARG:N   | 2.34                     | 0.48              |
| 1:y:166:SER:O   | 1:y:170:ARG:N   | 2.34                     | 0.48              |
| 1:z:101:THR:O   | 1:z:105:GLY:N   | 2.40                     | 0.48              |
| 1:1:33:LEU:O    | 1:1:129:TYR:OH  | 2.21                     | 0.48              |
| 1:3:63:ALA:O    | 1:3:67:ILE:N    | 2.38                     | 0.48              |
| 1:D:63:ALA:O    | 1:D:67:ILE:N    | 2.38                     | 0.48              |
| 1:F:88:ARG:O    | 1:F:88:ARG:NE   | 2.43                     | 0.48              |
| 1:K:166:SER:O   | 1:K:170:ARG:N   | 2.34                     | 0.48              |
| 1:L:47:LEU:O    | 1:L:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:X:88:ARG:O    | 1:X:88:ARG:NE   | 2.43                     | 0.48              |
| 1:a:94:ARG:O    | 1:a:98:GLN:N    | 2.38                     | 0.48              |
| 1:b:86:LEU:HD23 | 1:b:86:LEU:C    | 2.37                     | 0.48              |
| 1:f:33:LEU:O    | 1:f:129:TYR:OH  | 2.21                     | 0.48              |
| 1:i:33:LEU:O    | 1:i:129:TYR:OH  | 2.21                     | 0.48              |
| 1:k:94:ARG:O    | 1:k:98:GLN:N    | 2.38                     | 0.48              |
| 1:t:47:LEU:HD23 | 1:t:47:LEU:O    | 2.14                     | 0.48              |
| 1:x:47:LEU:O    | 1:x:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:x:101:THR:O   | 1:x:105:GLY:N   | 2.40                     | 0.48              |
| 1:J:33:LEU:HD21 | 1:J:132:LEU:HG  | 1.94                     | 0.48              |
| 1:P:47:LEU:O    | 1:P:47:LEU:HD23 | 2.14                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:e:88:ARG:O    | 1:e:88:ARG:NE   | 2.43                     | 0.48              |
| 1:j:33:LEU:HD21 | 1:j:132:LEU:HG  | 1.94                     | 0.48              |
| 1:n:33:LEU:HD21 | 1:n:132:LEU:HG  | 1.94                     | 0.48              |
| 1:w:101:THR:O   | 1:w:105:GLY:N   | 2.40                     | 0.48              |
| 1:z:33:LEU:HD21 | 1:z:132:LEU:HG  | 1.94                     | 0.48              |
| 1:5:47:LEU:O    | 1:5:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:H:66:LEU:O    | 1:H:70:ARG:N    | 2.35                     | 0.48              |
| 1:S:86:LEU:C    | 1:S:86:LEU:HD23 | 2.38                     | 0.48              |
| 1:e:33:LEU:HD21 | 1:e:132:LEU:HG  | 1.94                     | 0.48              |
| 1:f:33:LEU:HD21 | 1:f:132:LEU:HG  | 1.94                     | 0.48              |
| 1:n:33:LEU:O    | 1:n:129:TYR:OH  | 2.21                     | 0.48              |
| 1:s:86:LEU:HD23 | 1:s:86:LEU:C    | 2.38                     | 0.48              |
| 1:u:63:ALA:O    | 1:u:67:ILE:N    | 2.39                     | 0.48              |
| 1:1:47:LEU:O    | 1:1:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:1:94:ARG:O    | 1:1:98:GLN:N    | 2.38                     | 0.48              |
| 1:C:63:ALA:O    | 1:C:67:ILE:N    | 2.38                     | 0.48              |
| 1:H:47:LEU:O    | 1:H:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:I:66:LEU:O    | 1:I:70:ARG:N    | 2.35                     | 0.48              |
| 1:N:33:LEU:HD21 | 1:N:132:LEU:HG  | 1.94                     | 0.48              |
| 1:O:33:LEU:HD21 | 1:O:132:LEU:HG  | 1.94                     | 0.48              |
| 1:T:47:LEU:O    | 1:T:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:Y:47:LEU:HD23 | 1:Y:47:LEU:O    | 2.14                     | 0.48              |
| 1:j:86:LEU:HD23 | 1:j:86:LEU:C    | 2.37                     | 0.48              |
| 1:k:47:LEU:O    | 1:k:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:l:47:LEU:O    | 1:l:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:m:88:ARG:O    | 1:m:88:ARG:NE   | 2.43                     | 0.48              |
| 1:s:47:LEU:O    | 1:s:47:LEU:HD23 | 2.14                     | 0.48              |
| 1:C:94:ARG:O    | 1:C:98:GLN:N    | 2.38                     | 0.47              |
| 1:E:66:LEU:O    | 1:E:70:ARG:N    | 2.35                     | 0.47              |
| 1:E:166:SER:O   | 1:E:170:ARG:N   | 2.34                     | 0.47              |
| 1:X:47:LEU:O    | 1:X:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:Y:33:LEU:O    | 1:Y:129:TYR:OH  | 2.21                     | 0.47              |
| 1:g:47:LEU:O    | 1:g:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:i:101:THR:O   | 1:i:105:GLY:N   | 2.40                     | 0.47              |
| 1:n:94:ARG:O    | 1:n:98:GLN:N    | 2.38                     | 0.47              |
| 1:p:47:LEU:O    | 1:p:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:q:94:ARG:O    | 1:q:98:GLN:N    | 2.38                     | 0.47              |
| 1:0:88:ARG:O    | 1:0:88:ARG:NE   | 2.43                     | 0.47              |
| 1:2:47:LEU:O    | 1:2:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:3:166:SER:O   | 1:3:170:ARG:N   | 2.34                     | 0.47              |
| 1:5:88:ARG:O    | 1:5:88:ARG:NE   | 2.43                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:6:47:LEU:O    | 1:6:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:G:47:LEU:O    | 1:G:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:K:33:LEU:HD21 | 1:K:132:LEU:HG  | 1.94                     | 0.47              |
| 1:K:47:LEU:HD23 | 1:K:47:LEU:O    | 2.14                     | 0.47              |
| 1:p:166:SER:O   | 1:p:170:ARG:N   | 2.34                     | 0.47              |
| 1:w:47:LEU:O    | 1:w:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:M:166:SER:O   | 1:M:170:ARG:N   | 2.34                     | 0.47              |
| 1:O:47:LEU:O    | 1:O:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:O:101:THR:O   | 1:O:105:GLY:N   | 2.40                     | 0.47              |
| 1:Q:47:LEU:O    | 1:Q:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:U:47:LEU:O    | 1:U:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:W:94:ARG:O    | 1:W:98:GLN:N    | 2.38                     | 0.47              |
| 1:i:33:LEU:HD21 | 1:i:132:LEU:HG  | 1.94                     | 0.47              |
| 1:j:63:ALA:O    | 1:j:67:ILE:N    | 2.38                     | 0.47              |
| 1:o:47:LEU:O    | 1:o:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:3:33:LEU:HD21 | 1:3:132:LEU:HG  | 1.94                     | 0.47              |
| 1:D:47:LEU:O    | 1:D:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:G:88:ARG:O    | 1:G:88:ARG:NE   | 2.43                     | 0.47              |
| 1:f:47:LEU:HD23 | 1:f:47:LEU:O    | 2.14                     | 0.47              |
| 1:o:94:ARG:O    | 1:o:98:GLN:N    | 2.38                     | 0.47              |
| 1:y:47:LEU:O    | 1:y:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:B:94:ARG:O    | 1:B:98:GLN:N    | 2.38                     | 0.47              |
| 1:C:47:LEU:HD23 | 1:C:47:LEU:O    | 2.14                     | 0.47              |
| 1:E:88:ARG:O    | 1:E:88:ARG:NE   | 2.43                     | 0.47              |
| 1:P:101:THR:O   | 1:P:105:GLY:N   | 2.40                     | 0.47              |
| 1:c:101:THR:O   | 1:c:105:GLY:N   | 2.40                     | 0.47              |
| 1:p:63:ALA:O    | 1:p:67:ILE:N    | 2.38                     | 0.47              |
| 1:s:166:SER:O   | 1:s:170:ARG:N   | 2.34                     | 0.47              |
| 1:v:33:LEU:O    | 1:v:129:TYR:OH  | 2.21                     | 0.47              |
| 1:0:47:LEU:HD23 | 1:0:47:LEU:O    | 2.14                     | 0.47              |
| 1:3:66:LEU:O    | 1:3:70:ARG:N    | 2.35                     | 0.47              |
| 1:4:94:ARG:O    | 1:4:98:GLN:N    | 2.38                     | 0.47              |
| 1:M:47:LEU:O    | 1:M:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:T:94:ARG:O    | 1:T:98:GLN:N    | 2.38                     | 0.47              |
| 1:3:30:GLU:OE2  | 1:3:136:LYS:NZ  | 2.47                     | 0.47              |
| 1:3:88:ARG:O    | 1:3:88:ARG:NE   | 2.43                     | 0.47              |
| 1:7:66:LEU:O    | 1:7:70:ARG:N    | 2.35                     | 0.47              |
| 1:7:88:ARG:O    | 1:7:88:ARG:NE   | 2.43                     | 0.47              |
| 1:C:88:ARG:O    | 1:C:88:ARG:NE   | 2.43                     | 0.47              |
| 1:F:166:SER:O   | 1:F:170:ARG:N   | 2.34                     | 0.47              |
| 1:G:94:ARG:O    | 1:G:98:GLN:N    | 2.38                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:94:ARG:O     | 1:I:98:GLN:N    | 2.38                     | 0.47              |
| 1:S:47:LEU:HD23  | 1:S:47:LEU:O    | 2.14                     | 0.47              |
| 1:S:94:ARG:O     | 1:S:98:GLN:N    | 2.38                     | 0.47              |
| 1:V:66:LEU:O     | 1:V:70:ARG:N    | 2.35                     | 0.47              |
| 1:V:88:ARG:O     | 1:V:88:ARG:NE   | 2.43                     | 0.47              |
| 1:i:30:GLU:OE2   | 1:i:136:LYS:NZ  | 2.47                     | 0.47              |
| 1:n:88:ARG:O     | 1:n:88:ARG:NE   | 2.43                     | 0.47              |
| 1:o:63:ALA:O     | 1:o:67:ILE:N    | 2.38                     | 0.47              |
| 1:q:66:LEU:O     | 1:q:70:ARG:N    | 2.35                     | 0.47              |
| 1:u:47:LEU:O     | 1:u:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:O:94:ARG:O     | 1:O:98:GLN:N    | 2.38                     | 0.47              |
| 1:4:47:LEU:O     | 1:4:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:C:33:LEU:O     | 1:C:129:TYR:OH  | 2.21                     | 0.47              |
| 1:M:63:ALA:O     | 1:M:67:ILE:N    | 2.38                     | 0.47              |
| 1:T:88:ARG:O     | 1:T:88:ARG:NE   | 2.43                     | 0.47              |
| 1:V:130:LEU:HD12 | 1:V:131:GLU:N   | 2.30                     | 0.47              |
| 1:W:130:LEU:HD12 | 1:W:131:GLU:N   | 2.30                     | 0.47              |
| 1:Z:88:ARG:O     | 1:Z:88:ARG:NE   | 2.43                     | 0.47              |
| 1:f:30:GLU:OE2   | 1:f:136:LYS:NZ  | 2.47                     | 0.47              |
| 1:j:94:ARG:O     | 1:j:98:GLN:N    | 2.38                     | 0.47              |
| 1:k:88:ARG:O     | 1:k:88:ARG:NE   | 2.43                     | 0.47              |
| 1:s:94:ARG:O     | 1:s:98:GLN:N    | 2.38                     | 0.47              |
| 1:z:130:LEU:HD12 | 1:z:131:GLU:N   | 2.30                     | 0.47              |
| 1:O:101:THR:O    | 1:O:105:GLY:N   | 2.40                     | 0.47              |
| 1:O:130:LEU:HD12 | 1:O:131:GLU:N   | 2.30                     | 0.47              |
| 1:D:130:LEU:HD12 | 1:D:131:GLU:N   | 2.30                     | 0.47              |
| 1:D:166:SER:O    | 1:D:170:ARG:N   | 2.34                     | 0.47              |
| 1:F:130:LEU:HD12 | 1:F:131:GLU:N   | 2.30                     | 0.47              |
| 1:H:130:LEU:HD12 | 1:H:131:GLU:N   | 2.30                     | 0.47              |
| 1:I:47:LEU:HD23  | 1:I:47:LEU:O    | 2.14                     | 0.47              |
| 1:R:47:LEU:O     | 1:R:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:V:63:ALA:O     | 1:V:67:ILE:N    | 2.38                     | 0.47              |
| 1:Z:66:LEU:O     | 1:Z:70:ARG:N    | 2.35                     | 0.47              |
| 1:b:47:LEU:O     | 1:b:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:c:47:LEU:HD23  | 1:c:47:LEU:O    | 2.14                     | 0.47              |
| 1:d:47:LEU:O     | 1:d:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:j:130:LEU:HD12 | 1:j:131:GLU:N   | 2.30                     | 0.47              |
| 1:m:166:SER:O    | 1:m:170:ARG:N   | 2.34                     | 0.47              |
| 1:u:166:SER:O    | 1:u:170:ARG:N   | 2.34                     | 0.47              |
| 1:5:94:ARG:O     | 1:5:98:GLN:N    | 2.38                     | 0.47              |
| 1:E:130:LEU:HD12 | 1:E:131:GLU:N   | 2.30                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:47:LEU:O     | 1:F:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:I:130:LEU:HD12 | 1:I:131:GLU:N   | 2.30                     | 0.47              |
| 1:K:94:ARG:O     | 1:K:98:GLN:N    | 2.38                     | 0.47              |
| 1:K:130:LEU:HD12 | 1:K:131:GLU:N   | 2.30                     | 0.47              |
| 1:O:94:ARG:O     | 1:O:98:GLN:N    | 2.38                     | 0.47              |
| 1:X:130:LEU:HD12 | 1:X:131:GLU:N   | 2.30                     | 0.47              |
| 1:b:30:GLU:OE2   | 1:b:136:LYS:NZ  | 2.48                     | 0.47              |
| 1:e:47:LEU:O     | 1:e:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:h:47:LEU:O     | 1:h:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:h:130:LEU:HD12 | 1:h:131:GLU:N   | 2.30                     | 0.47              |
| 1:p:66:LEU:O     | 1:p:70:ARG:N    | 2.35                     | 0.47              |
| 1:w:94:ARG:O     | 1:w:98:GLN:N    | 2.38                     | 0.47              |
| 1:z:47:LEU:O     | 1:z:47:LEU:HD23 | 2.14                     | 0.47              |
| 1:5:130:LEU:HD12 | 1:5:131:GLU:N   | 2.30                     | 0.46              |
| 1:G:166:SER:O    | 1:G:170:ARG:N   | 2.34                     | 0.46              |
| 1:H:63:ALA:O     | 1:H:67:ILE:N    | 2.38                     | 0.46              |
| 1:N:47:LEU:O     | 1:N:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:R:88:ARG:O     | 1:R:88:ARG:NE   | 2.43                     | 0.46              |
| 1:Z:47:LEU:O     | 1:Z:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:e:63:ALA:O     | 1:e:67:ILE:N    | 2.38                     | 0.46              |
| 1:i:130:LEU:HD12 | 1:i:131:GLU:N   | 2.30                     | 0.46              |
| 1:m:130:LEU:HD12 | 1:m:131:GLU:N   | 2.31                     | 0.46              |
| 1:o:130:LEU:HD12 | 1:o:131:GLU:N   | 2.30                     | 0.46              |
| 1:r:30:GLU:OE2   | 1:r:136:LYS:NZ  | 2.47                     | 0.46              |
| 1:v:47:LEU:O     | 1:v:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:w:130:LEU:HD12 | 1:w:131:GLU:N   | 2.30                     | 0.46              |
| 1:y:130:LEU:HD12 | 1:y:131:GLU:N   | 2.30                     | 0.46              |
| 1:1:101:THR:O    | 1:1:105:GLY:N   | 2.40                     | 0.46              |
| 1:1:130:LEU:HD12 | 1:1:131:GLU:N   | 2.30                     | 0.46              |
| 1:6:130:LEU:HD12 | 1:6:131:GLU:N   | 2.30                     | 0.46              |
| 1:B:63:ALA:O     | 1:B:67:ILE:N    | 2.38                     | 0.46              |
| 1:C:130:LEU:HD12 | 1:C:131:GLU:N   | 2.30                     | 0.46              |
| 1:E:47:LEU:O     | 1:E:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:G:130:LEU:HD12 | 1:G:131:GLU:N   | 2.30                     | 0.46              |
| 1:J:130:LEU:HD12 | 1:J:131:GLU:N   | 2.30                     | 0.46              |
| 1:L:130:LEU:HD12 | 1:L:131:GLU:N   | 2.30                     | 0.46              |
| 1:Q:130:LEU:HD12 | 1:Q:131:GLU:N   | 2.30                     | 0.46              |
| 1:S:47:LEU:O     | 1:S:50:THR:OG1  | 2.20                     | 0.46              |
| 1:S:130:LEU:HD12 | 1:S:131:GLU:N   | 2.30                     | 0.46              |
| 1:b:88:ARG:O     | 1:b:88:ARG:NE   | 2.43                     | 0.46              |
| 1:c:130:LEU:HD12 | 1:c:131:GLU:N   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:j:47:LEU:O     | 1:j:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:n:130:LEU:HD12 | 1:n:131:GLU:N   | 2.30                     | 0.46              |
| 1:q:33:LEU:O     | 1:q:129:TYR:OH  | 2.21                     | 0.46              |
| 1:r:47:LEU:O     | 1:r:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:u:94:ARG:O     | 1:u:98:GLN:N    | 2.38                     | 0.46              |
| 1:u:130:LEU:HD12 | 1:u:131:GLU:N   | 2.30                     | 0.46              |
| 1:v:130:LEU:HD12 | 1:v:131:GLU:N   | 2.30                     | 0.46              |
| 1:6:52:ALA:HB3   | 1:x:177:GLU:OE2 | 2.16                     | 0.46              |
| 1:H:177:GLU:OE2  | 1:Q:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:J:47:LEU:O     | 1:J:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:Q:177:GLU:OE2  | 1:Z:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:R:166:SER:O    | 1:R:170:ARG:N   | 2.34                     | 0.46              |
| 1:Z:130:LEU:HD12 | 1:Z:131:GLU:N   | 2.30                     | 0.46              |
| 1:c:177:GLU:OE2  | 1:l:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:d:66:LEU:O     | 1:d:70:ARG:N    | 2.35                     | 0.46              |
| 1:l:177:GLU:OE2  | 1:u:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:m:47:LEU:O     | 1:m:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:o:88:ARG:O     | 1:o:88:ARG:NE   | 2.43                     | 0.46              |
| 1:q:47:LEU:O     | 1:q:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:q:88:ARG:O     | 1:q:88:ARG:NE   | 2.43                     | 0.46              |
| 1:v:30:GLU:OE2   | 1:v:136:LYS:NZ  | 2.47                     | 0.46              |
| 1:x:130:LEU:HD12 | 1:x:131:GLU:N   | 2.30                     | 0.46              |
| 1:0:30:GLU:OE2   | 1:0:136:LYS:NZ  | 2.48                     | 0.46              |
| 1:3:47:LEU:HD23  | 1:3:47:LEU:O    | 2.14                     | 0.46              |
| 1:3:52:ALA:HB3   | 1:u:177:GLU:OE2 | 2.16                     | 0.46              |
| 1:3:130:LEU:HD12 | 1:3:131:GLU:N   | 2.30                     | 0.46              |
| 1:4:52:ALA:HB3   | 1:v:177:GLU:OE2 | 2.16                     | 0.46              |
| 1:A:33:LEU:O     | 1:A:129:TYR:OH  | 2.21                     | 0.46              |
| 1:B:47:LEU:O     | 1:B:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:D:66:LEU:O     | 1:D:70:ARG:N    | 2.35                     | 0.46              |
| 1:K:84:GLU:O     | 1:K:88:ARG:N    | 2.49                     | 0.46              |
| 1:O:88:ARG:O     | 1:O:88:ARG:NE   | 2.43                     | 0.46              |
| 1:P:130:LEU:HD12 | 1:P:131:GLU:N   | 2.30                     | 0.46              |
| 1:P:177:GLU:OE2  | 1:Y:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:S:101:THR:O    | 1:S:105:GLY:N   | 2.40                     | 0.46              |
| 1:U:130:LEU:HD12 | 1:U:131:GLU:N   | 2.30                     | 0.46              |
| 1:W:30:GLU:OE2   | 1:W:136:LYS:NZ  | 2.47                     | 0.46              |
| 1:a:88:ARG:O     | 1:a:88:ARG:NE   | 2.43                     | 0.46              |
| 1:a:177:GLU:OE2  | 1:j:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:e:101:THR:O    | 1:e:105:GLY:N   | 2.40                     | 0.46              |
| 1:g:88:ARG:O     | 1:g:88:ARG:NE   | 2.43                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:h:66:LEU:O     | 1:h:70:ARG:N    | 2.35                     | 0.46              |
| 1:m:30:GLU:OE2   | 1:m:136:LYS:NZ  | 2.48                     | 0.46              |
| 1:n:47:LEU:HD23  | 1:n:47:LEU:O    | 2.14                     | 0.46              |
| 1:n:177:GLU:OE2  | 1:w:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:0:47:LEU:O     | 1:0:50:THR:OG1  | 2.20                     | 0.46              |
| 1:2:130:LEU:HD12 | 1:2:131:GLU:N   | 2.30                     | 0.46              |
| 1:M:130:LEU:HD12 | 1:M:131:GLU:N   | 2.30                     | 0.46              |
| 1:N:177:GLU:OE2  | 1:W:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:R:130:LEU:HD12 | 1:R:131:GLU:N   | 2.30                     | 0.46              |
| 1:S:177:GLU:OE2  | 1:b:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:W:47:LEU:O     | 1:W:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:a:130:LEU:HD12 | 1:a:131:GLU:N   | 2.30                     | 0.46              |
| 1:f:47:LEU:O     | 1:f:50:THR:OG1  | 2.20                     | 0.46              |
| 1:f:94:ARG:O     | 1:f:98:GLN:N    | 2.38                     | 0.46              |
| 1:h:84:GLU:O     | 1:h:88:ARG:N    | 2.49                     | 0.46              |
| 1:i:177:GLU:OE2  | 1:r:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:k:177:GLU:OE2  | 1:t:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:l:66:LEU:O     | 1:l:70:ARG:N    | 2.35                     | 0.46              |
| 1:t:130:LEU:HD12 | 1:t:131:GLU:N   | 2.30                     | 0.46              |
| 1:w:84:GLU:O     | 1:w:88:ARG:N    | 2.49                     | 0.46              |
| 1:0:33:LEU:O     | 1:0:129:TYR:OH  | 2.21                     | 0.46              |
| 1:0:84:GLU:O     | 1:0:88:ARG:N    | 2.49                     | 0.46              |
| 1:1:88:ARG:O     | 1:1:88:ARG:NE   | 2.43                     | 0.46              |
| 1:2:52:ALA:HB3   | 1:t:177:GLU:OE2 | 2.16                     | 0.46              |
| 1:D:84:GLU:O     | 1:D:88:ARG:N    | 2.49                     | 0.46              |
| 1:D:177:GLU:OE2  | 1:M:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:F:33:LEU:HD23  | 1:F:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:G:63:ALA:O     | 1:G:67:ILE:N    | 2.38                     | 0.46              |
| 1:G:177:GLU:OE2  | 1:P:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:O:84:GLU:O     | 1:O:88:ARG:N    | 2.49                     | 0.46              |
| 1:T:177:GLU:OE2  | 1:c:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:V:47:LEU:O     | 1:V:47:LEU:HD23 | 2.14                     | 0.46              |
| 1:X:94:ARG:O     | 1:X:98:GLN:N    | 2.38                     | 0.46              |
| 1:b:130:LEU:HD12 | 1:b:131:GLU:N   | 2.30                     | 0.46              |
| 1:f:177:GLU:OE2  | 1:o:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:l:84:GLU:O     | 1:l:88:ARG:N    | 2.49                     | 0.46              |
| 1:n:166:SER:O    | 1:n:170:ARG:N   | 2.34                     | 0.46              |
| 1:o:177:GLU:OE2  | 1:x:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:s:84:GLU:O     | 1:s:88:ARG:N    | 2.49                     | 0.46              |
| 1:y:33:LEU:HD23  | 1:y:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:6:33:LEU:HD23  | 1:6:129:TYR:CE1 | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:7:47:LEU:O     | 1:7:47:LEU:HD23  | 2.14                     | 0.46              |
| 1:7:130:LEU:HD12 | 1:7:131:GLU:N    | 2.30                     | 0.46              |
| 1:B:84:GLU:O     | 1:B:88:ARG:N     | 2.49                     | 0.46              |
| 1:E:84:GLU:O     | 1:E:88:ARG:N     | 2.49                     | 0.46              |
| 1:F:84:GLU:O     | 1:F:88:ARG:N     | 2.49                     | 0.46              |
| 1:I:177:GLU:OE2  | 1:R:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:N:33:LEU:HD23  | 1:N:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:N:130:LEU:HD12 | 1:N:131:GLU:N    | 2.30                     | 0.46              |
| 1:O:63:ALA:O     | 1:O:67:ILE:N     | 2.38                     | 0.46              |
| 1:S:33:LEU:HD23  | 1:S:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:Y:177:GLU:OE2  | 1:h:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:Z:177:GLU:OE2  | 1:i:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:a:33:LEU:HD23  | 1:a:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:d:84:GLU:O     | 1:d:88:ARG:N     | 2.49                     | 0.46              |
| 1:f:33:LEU:HD23  | 1:f:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:f:130:LEU:HD12 | 1:f:131:GLU:N    | 2.30                     | 0.46              |
| 1:k:130:LEU:HD12 | 1:k:131:GLU:N    | 2.30                     | 0.46              |
| 1:l:166:SER:O    | 1:l:170:ARG:N    | 2.34                     | 0.46              |
| 1:m:33:LEU:HD23  | 1:m:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:n:47:LEU:O     | 1:n:50:THR:OG1   | 2.20                     | 0.46              |
| 1:n:84:GLU:O     | 1:n:88:ARG:N     | 2.49                     | 0.46              |
| 1:p:84:GLU:O     | 1:p:88:ARG:N     | 2.48                     | 0.46              |
| 1:r:33:LEU:HD23  | 1:r:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:t:33:LEU:HD23  | 1:t:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:z:33:LEU:HD23  | 1:z:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:4:33:LEU:HD23  | 1:4:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:4:130:LEU:HD12 | 1:4:131:GLU:N    | 2.30                     | 0.46              |
| 1:5:33:LEU:HD23  | 1:5:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:A:33:LEU:HD23  | 1:A:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:A:47:LEU:O     | 1:A:47:LEU:HD23  | 2.14                     | 0.46              |
| 1:A:177:GLU:OE2  | 1:J:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:B:177:GLU:OE2  | 1:K:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:D:33:LEU:HD23  | 1:D:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:F:177:GLU:OE2  | 1:O:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:I:33:LEU:HD11  | 1:M:159:LEU:HD21 | 1.96                     | 0.46              |
| 1:I:84:GLU:O     | 1:I:88:ARG:N     | 2.49                     | 0.46              |
| 1:L:33:LEU:HD23  | 1:L:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:M:33:LEU:HD23  | 1:M:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:N:30:GLU:OE2   | 1:N:136:LYS:NZ   | 2.47                     | 0.46              |
| 1:R:33:LEU:HD23  | 1:R:129:TYR:CE1  | 2.51                     | 0.46              |
| 1:T:101:THR:O    | 1:T:105:GLY:N    | 2.40                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:T:130:LEU:HD12 | 1:T:131:GLU:N   | 2.30                     | 0.46              |
| 1:X:33:LEU:O     | 1:X:129:TYR:OH  | 2.21                     | 0.46              |
| 1:Y:33:LEU:HD23  | 1:Y:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:Y:130:LEU:HD12 | 1:Y:131:GLU:N   | 2.31                     | 0.46              |
| 1:Z:33:LEU:HD23  | 1:Z:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:a:47:LEU:HD23  | 1:a:47:LEU:O    | 2.14                     | 0.46              |
| 1:b:177:GLU:OE2  | 1:k:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:d:130:LEU:HD12 | 1:d:131:GLU:N   | 2.30                     | 0.46              |
| 1:j:84:GLU:O     | 1:j:88:ARG:N    | 2.49                     | 0.46              |
| 1:l:33:LEU:HD23  | 1:l:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:n:30:GLU:OE2   | 1:n:136:LYS:NZ  | 2.48                     | 0.46              |
| 1:p:130:LEU:HD12 | 1:p:131:GLU:N   | 2.30                     | 0.46              |
| 1:q:84:GLU:O     | 1:q:88:ARG:N    | 2.49                     | 0.46              |
| 1:s:33:LEU:HD23  | 1:s:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:y:63:ALA:O     | 1:y:67:ILE:N    | 2.38                     | 0.46              |
| 1:z:88:ARG:O     | 1:z:88:ARG:NE   | 2.43                     | 0.46              |
| 1:0:63:ALA:O     | 1:0:67:ILE:N    | 2.38                     | 0.46              |
| 1:4:101:THR:O    | 1:4:105:GLY:N   | 2.40                     | 0.46              |
| 1:7:33:LEU:HD23  | 1:7:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:A:166:SER:O    | 1:A:170:ARG:N   | 2.34                     | 0.46              |
| 1:B:130:LEU:HD12 | 1:B:131:GLU:N   | 2.30                     | 0.46              |
| 1:E:177:GLU:OE2  | 1:N:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:F:58:GLU:OE2   | 1:F:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:G:84:GLU:O     | 1:G:88:ARG:N    | 2.49                     | 0.46              |
| 1:I:88:ARG:O     | 1:I:88:ARG:NE   | 2.43                     | 0.46              |
| 1:L:58:GLU:OE2   | 1:L:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:M:94:ARG:O     | 1:M:98:GLN:N    | 2.38                     | 0.46              |
| 1:P:33:LEU:O     | 1:P:129:TYR:OH  | 2.21                     | 0.46              |
| 1:P:166:SER:O    | 1:P:170:ARG:N   | 2.34                     | 0.46              |
| 1:Q:33:LEU:HD23  | 1:Q:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:S:84:GLU:O     | 1:S:88:ARG:N    | 2.49                     | 0.46              |
| 1:T:33:LEU:HD23  | 1:T:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:V:177:GLU:OE2  | 1:e:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:b:94:ARG:O     | 1:b:98:GLN:N    | 2.38                     | 0.46              |
| 1:d:88:ARG:O     | 1:d:88:ARG:NE   | 2.43                     | 0.46              |
| 1:e:33:LEU:HD23  | 1:e:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:e:58:GLU:OE2   | 1:e:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:e:130:LEU:HD12 | 1:e:131:GLU:N   | 2.30                     | 0.46              |
| 1:g:33:LEU:HD23  | 1:g:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:h:177:GLU:OE2  | 1:q:52:ALA:HB3  | 2.16                     | 0.46              |
| 1:l:130:LEU:HD12 | 1:l:131:GLU:N   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:m:84:GLU:O     | 1:m:88:ARG:N    | 2.49                     | 0.46              |
| 1:n:33:LEU:HD23  | 1:n:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:o:166:SER:O    | 1:o:170:ARG:N   | 2.34                     | 0.46              |
| 1:r:58:GLU:OE2   | 1:r:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:r:84:GLU:O     | 1:r:88:ARG:N    | 2.49                     | 0.46              |
| 1:t:63:ALA:O     | 1:t:67:ILE:N    | 2.38                     | 0.46              |
| 1:u:84:GLU:O     | 1:u:88:ARG:N    | 2.49                     | 0.46              |
| 1:v:33:LEU:HD23  | 1:v:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:0:33:LEU:HD23  | 1:0:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:1:166:SER:O    | 1:1:170:ARG:N   | 2.34                     | 0.46              |
| 1:5:52:ALA:HB3   | 1:w:177:GLU:OE2 | 2.16                     | 0.46              |
| 1:5:84:GLU:O     | 1:5:88:ARG:N    | 2.49                     | 0.46              |
| 1:6:58:GLU:OE2   | 1:6:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:84:GLU:O     | 1:A:88:ARG:N    | 2.49                     | 0.46              |
| 1:B:88:ARG:O     | 1:B:88:ARG:NE   | 2.43                     | 0.46              |
| 1:E:33:LEU:HD23  | 1:E:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:G:33:LEU:HD23  | 1:G:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:J:58:GLU:OE2   | 1:J:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:J:84:GLU:O     | 1:J:88:ARG:N    | 2.49                     | 0.46              |
| 1:M:84:GLU:O     | 1:M:88:ARG:N    | 2.49                     | 0.46              |
| 1:M:88:ARG:O     | 1:M:88:ARG:NE   | 2.43                     | 0.46              |
| 1:U:33:LEU:HD23  | 1:U:129:TYR:CE1 | 2.51                     | 0.46              |
| 1:U:58:GLU:OE2   | 1:U:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:Y:58:GLU:OE2   | 1:Y:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:q:130:LEU:HD12 | 1:q:131:GLU:N   | 2.30                     | 0.46              |
| 1:t:58:GLU:OE2   | 1:t:61:ARG:NH2  | 2.49                     | 0.46              |
| 1:w:63:ALA:O     | 1:w:67:ILE:N    | 2.38                     | 0.46              |
| 1:x:166:SER:O    | 1:x:170:ARG:N   | 2.34                     | 0.46              |
| 1:1:52:ALA:HB3   | 1:s:177:GLU:OE2 | 2.16                     | 0.45              |
| 1:3:58:GLU:OE2   | 1:3:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:H:84:GLU:O     | 1:H:88:ARG:N    | 2.49                     | 0.45              |
| 1:I:58:GLU:OE2   | 1:I:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:I:166:SER:O    | 1:I:170:ARG:N   | 2.34                     | 0.45              |
| 1:J:33:LEU:O     | 1:J:129:TYR:OH  | 2.21                     | 0.45              |
| 1:J:177:GLU:OE2  | 1:S:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:L:166:SER:O    | 1:L:170:ARG:N   | 2.34                     | 0.45              |
| 1:M:177:GLU:OE2  | 1:V:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:O:130:LEU:HD12 | 1:O:131:GLU:N   | 2.30                     | 0.45              |
| 1:S:58:GLU:OE2   | 1:S:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:T:84:GLU:O     | 1:T:88:ARG:N    | 2.49                     | 0.45              |
| 1:V:58:GLU:OE2   | 1:V:61:ARG:NH2  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:W:47:LEU:O     | 1:W:50:THR:OG1  | 2.20                     | 0.45              |
| 1:X:84:GLU:O     | 1:X:88:ARG:N    | 2.49                     | 0.45              |
| 1:a:101:THR:O    | 1:a:105:GLY:N   | 2.40                     | 0.45              |
| 1:h:58:GLU:OE2   | 1:h:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:i:33:LEU:HD23  | 1:i:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:i:58:GLU:OE2   | 1:i:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:k:58:GLU:OE2   | 1:k:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:n:63:ALA:O     | 1:n:67:ILE:N    | 2.39                     | 0.45              |
| 1:o:84:GLU:O     | 1:o:88:ARG:N    | 2.49                     | 0.45              |
| 1:q:177:GLU:OE2  | 1:z:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:s:130:LEU:HD12 | 1:s:131:GLU:N   | 2.30                     | 0.45              |
| 1:u:58:GLU:OE2   | 1:u:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:u:88:ARG:O     | 1:u:88:ARG:NE   | 2.43                     | 0.45              |
| 1:x:58:GLU:OE2   | 1:x:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:x:88:ARG:O     | 1:x:88:ARG:NE   | 2.43                     | 0.45              |
| 1:0:58:GLU:OE2   | 1:0:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:1:84:GLU:O     | 1:1:88:ARG:N    | 2.49                     | 0.45              |
| 1:C:58:GLU:OE2   | 1:C:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:H:33:LEU:HD23  | 1:H:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:H:58:GLU:OE2   | 1:H:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:K:33:LEU:HD23  | 1:K:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:K:177:GLU:OE2  | 1:T:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:L:88:ARG:O     | 1:L:88:ARG:NE   | 2.43                     | 0.45              |
| 1:X:33:LEU:HD23  | 1:X:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:c:84:GLU:O     | 1:c:88:ARG:N    | 2.49                     | 0.45              |
| 1:d:33:LEU:HD23  | 1:d:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:d:177:GLU:OE2  | 1:m:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:g:130:LEU:HD12 | 1:g:131:GLU:N   | 2.30                     | 0.45              |
| 1:h:33:LEU:HD23  | 1:h:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:k:33:LEU:HD23  | 1:k:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:n:58:GLU:OE2   | 1:n:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:t:166:SER:O    | 1:t:170:ARG:N   | 2.34                     | 0.45              |
| 1:y:88:ARG:O     | 1:y:88:ARG:NE   | 2.43                     | 0.45              |
| 1:2:33:LEU:HD23  | 1:2:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:2:58:GLU:OE2   | 1:2:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:4:58:GLU:OE2   | 1:4:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:4:84:GLU:O     | 1:4:88:ARG:N    | 2.49                     | 0.45              |
| 1:7:52:ALA:HB3   | 1:y:177:GLU:OE2 | 2.16                     | 0.45              |
| 1:7:63:ALA:O     | 1:7:67:ILE:N    | 2.38                     | 0.45              |
| 1:A:130:LEU:HD12 | 1:A:131:GLU:N   | 2.30                     | 0.45              |
| 1:O:58:GLU:OE2   | 1:O:61:ARG:NH2  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:P:88:ARG:O     | 1:P:88:ARG:NE   | 2.43                     | 0.45              |
| 1:Q:88:ARG:O     | 1:Q:88:ARG:NE   | 2.43                     | 0.45              |
| 1:R:58:GLU:OE2   | 1:R:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:R:177:GLU:OE2  | 1:a:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:S:63:ALA:O     | 1:S:67:ILE:N    | 2.38                     | 0.45              |
| 1:U:177:GLU:OE2  | 1:d:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:W:177:GLU:OE2  | 1:f:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:a:30:GLU:OE2   | 1:a:136:LYS:NZ  | 2.48                     | 0.45              |
| 1:b:58:GLU:OE2   | 1:b:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:g:58:GLU:OE2   | 1:g:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:i:47:LEU:O     | 1:i:47:LEU:HD23 | 2.14                     | 0.45              |
| 1:i:84:GLU:O     | 1:i:88:ARG:N    | 2.49                     | 0.45              |
| 1:m:177:GLU:OE2  | 1:v:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:p:33:LEU:HD23  | 1:p:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:q:58:GLU:OE2   | 1:q:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:r:130:LEU:HD12 | 1:r:131:GLU:N   | 2.30                     | 0.45              |
| 1:t:88:ARG:O     | 1:t:88:ARG:NE   | 2.43                     | 0.45              |
| 1:u:33:LEU:HD23  | 1:u:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:v:84:GLU:O     | 1:v:88:ARG:N    | 2.49                     | 0.45              |
| 1:x:33:LEU:HD23  | 1:x:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:1:33:LEU:HD23  | 1:1:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:5:101:THR:O    | 1:5:105:GLY:N   | 2.40                     | 0.45              |
| 1:7:58:GLU:OE2   | 1:7:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:B:33:LEU:HD23  | 1:B:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:F:63:ALA:O     | 1:F:67:ILE:N    | 2.38                     | 0.45              |
| 1:H:88:ARG:O     | 1:H:88:ARG:NE   | 2.43                     | 0.45              |
| 1:J:33:LEU:HD23  | 1:J:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:K:47:LEU:O     | 1:K:50:THR:OG1  | 2.20                     | 0.45              |
| 1:K:63:ALA:O     | 1:K:67:ILE:N    | 2.38                     | 0.45              |
| 1:O:177:GLU:OE2  | 1:X:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:P:84:GLU:O     | 1:P:88:ARG:N    | 2.49                     | 0.45              |
| 1:S:33:LEU:O     | 1:S:129:TYR:OH  | 2.21                     | 0.45              |
| 1:W:33:LEU:HD23  | 1:W:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:X:177:GLU:OE2  | 1:g:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:a:166:SER:O    | 1:a:170:ARG:N   | 2.34                     | 0.45              |
| 1:b:63:ALA:O     | 1:b:67:ILE:N    | 2.38                     | 0.45              |
| 1:c:33:LEU:HD23  | 1:c:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:p:177:GLU:OE2  | 1:y:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:y:84:GLU:O     | 1:y:88:ARG:N    | 2.49                     | 0.45              |
| 1:7:84:GLU:O     | 1:7:88:ARG:N    | 2.49                     | 0.45              |
| 1:B:30:GLU:OE2   | 1:B:136:LYS:NZ  | 2.47                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:84:GLU:O    | 1:C:88:ARG:N    | 2.49                     | 0.45              |
| 1:L:177:GLU:OE2 | 1:U:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:M:58:GLU:OE2  | 1:M:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:P:58:GLU:OE2  | 1:P:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:W:58:GLU:OE2  | 1:W:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:X:58:GLU:OE2  | 1:X:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:Z:84:GLU:O    | 1:Z:88:ARG:N    | 2.49                     | 0.45              |
| 1:b:84:GLU:O    | 1:b:88:ARG:N    | 2.48                     | 0.45              |
| 1:e:84:GLU:O    | 1:e:88:ARG:N    | 2.48                     | 0.45              |
| 1:g:84:GLU:O    | 1:g:88:ARG:N    | 2.49                     | 0.45              |
| 1:g:177:GLU:OE2 | 1:p:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:j:33:LEU:HD23 | 1:j:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:l:58:GLU:OE2  | 1:l:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:o:33:LEU:HD23 | 1:o:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:o:58:GLU:OE2  | 1:o:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:q:33:LEU:HD23 | 1:q:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:s:47:LEU:O    | 1:s:50:THR:OG1  | 2.20                     | 0.45              |
| 1:s:63:ALA:O    | 1:s:67:ILE:N    | 2.38                     | 0.45              |
| 1:t:84:GLU:O    | 1:t:88:ARG:N    | 2.49                     | 0.45              |
| 1:v:58:GLU:OE2  | 1:v:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:w:47:LEU:O    | 1:w:50:THR:OG1  | 2.20                     | 0.45              |
| 1:3:33:LEU:HD23 | 1:3:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:B:166:SER:O   | 1:B:170:ARG:N   | 2.34                     | 0.45              |
| 1:E:58:GLU:OE2  | 1:E:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:N:88:ARG:O    | 1:N:88:ARG:NE   | 2.43                     | 0.45              |
| 1:O:33:LEU:HD23 | 1:O:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:V:33:LEU:HD23 | 1:V:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:V:84:GLU:O    | 1:V:88:ARG:N    | 2.49                     | 0.45              |
| 1:W:101:THR:O   | 1:W:105:GLY:N   | 2.40                     | 0.45              |
| 1:b:33:LEU:HD23 | 1:b:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:c:88:ARG:O    | 1:c:88:ARG:NE   | 2.43                     | 0.45              |
| 1:d:58:GLU:OE2  | 1:d:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:j:177:GLU:OE2 | 1:s:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:p:58:GLU:OE2  | 1:p:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:z:166:SER:O   | 1:z:170:ARG:N   | 2.34                     | 0.45              |
| 1:2:88:ARG:O    | 1:2:88:ARG:NE   | 2.43                     | 0.45              |
| 1:3:84:GLU:O    | 1:3:88:ARG:N    | 2.49                     | 0.45              |
| 1:5:58:GLU:OE2  | 1:5:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:A:58:GLU:OE2  | 1:A:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:B:58:GLU:OE2  | 1:B:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:C:166:SER:O   | 1:C:170:ARG:N   | 2.34                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:63:ALA:O    | 1:L:67:ILE:N    | 2.38                     | 0.45              |
| 1:P:33:LEU:HD23 | 1:P:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:Q:84:GLU:O    | 1:Q:88:ARG:N    | 2.49                     | 0.45              |
| 1:W:84:GLU:O    | 1:W:88:ARG:N    | 2.49                     | 0.45              |
| 1:a:58:GLU:OE2  | 1:a:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:b:47:LEU:O    | 1:b:50:THR:OG1  | 2.20                     | 0.45              |
| 1:f:58:GLU:OE2  | 1:f:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:p:88:ARG:O    | 1:p:88:ARG:NE   | 2.43                     | 0.45              |
| 1:w:33:LEU:HD23 | 1:w:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:w:58:GLU:OE2  | 1:w:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:x:84:GLU:O    | 1:x:88:ARG:N    | 2.49                     | 0.45              |
| 1:z:58:GLU:OE2  | 1:z:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:0:52:ALA:HB3  | 1:r:177:GLU:OE2 | 2.16                     | 0.45              |
| 1:U:88:ARG:O    | 1:U:88:ARG:NE   | 2.43                     | 0.45              |
| 1:s:58:GLU:OE2  | 1:s:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:y:94:ARG:O    | 1:y:98:GLN:N    | 2.38                     | 0.45              |
| 1:4:63:ALA:O    | 1:4:67:ILE:N    | 2.38                     | 0.45              |
| 1:C:177:GLU:OE2 | 1:L:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:D:88:ARG:O    | 1:D:88:ARG:NE   | 2.43                     | 0.45              |
| 1:G:58:GLU:OE2  | 1:G:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:I:33:LEU:HD23 | 1:I:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:K:58:GLU:OE2  | 1:K:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:L:84:GLU:O    | 1:L:88:ARG:N    | 2.49                     | 0.45              |
| 1:N:84:GLU:O    | 1:N:88:ARG:N    | 2.49                     | 0.45              |
| 1:O:30:GLU:OE2  | 1:O:136:LYS:NZ  | 2.47                     | 0.45              |
| 1:Q:58:GLU:OE2  | 1:Q:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:Q:63:ALA:O    | 1:Q:67:ILE:N    | 2.38                     | 0.45              |
| 1:Z:58:GLU:OE2  | 1:Z:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:a:47:LEU:O    | 1:a:50:THR:OG1  | 2.20                     | 0.45              |
| 1:i:166:SER:O   | 1:i:170:ARG:N   | 2.34                     | 0.45              |
| 1:q:166:SER:O   | 1:q:170:ARG:N   | 2.34                     | 0.45              |
| 1:l:58:GLU:OE2  | 1:l:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:2:84:GLU:O    | 1:2:88:ARG:N    | 2.49                     | 0.45              |
| 1:6:33:LEU:O    | 1:6:129:TYR:OH  | 2.21                     | 0.45              |
| 1:C:33:LEU:HD23 | 1:C:129:TYR:CE1 | 2.51                     | 0.45              |
| 1:c:58:GLU:OE2  | 1:c:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:e:177:GLU:OE2 | 1:n:52:ALA:HB3  | 2.16                     | 0.45              |
| 1:k:84:GLU:O    | 1:k:88:ARG:N    | 2.49                     | 0.45              |
| 1:w:88:ARG:O    | 1:w:88:ARG:NE   | 2.43                     | 0.45              |
| 1:y:58:GLU:OE2  | 1:y:61:ARG:NH2  | 2.49                     | 0.45              |
| 1:6:88:ARG:O    | 1:6:88:ARG:NE   | 2.43                     | 0.44              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:D:58:GLU:OE2  | 1:D:61:ARG:NH2 | 2.49                     | 0.44              |
| 1:G:47:LEU:O    | 1:G:50:THR:OG1 | 2.20                     | 0.44              |
| 1:N:58:GLU:OE2  | 1:N:61:ARG:NH2 | 2.49                     | 0.44              |
| 1:R:84:GLU:O    | 1:R:88:ARG:N   | 2.49                     | 0.44              |
| 1:T:58:GLU:OE2  | 1:T:61:ARG:NH2 | 2.49                     | 0.44              |
| 1:X:101:THR:O   | 1:X:105:GLY:N  | 2.40                     | 0.44              |
| 1:h:88:ARG:O    | 1:h:88:ARG:NE  | 2.43                     | 0.44              |
| 1:l:88:ARG:O    | 1:l:88:ARG:NE  | 2.43                     | 0.44              |
| 1:x:96:SER:O    | 1:x:99:SER:OG  | 2.33                     | 0.44              |
| 1:X:63:ALA:O    | 1:X:67:ILE:N   | 2.38                     | 0.44              |
| 1:h:96:SER:O    | 1:h:99:SER:OG  | 2.33                     | 0.44              |
| 1:j:58:GLU:OE2  | 1:j:61:ARG:NH2 | 2.49                     | 0.44              |
| 1:m:58:GLU:OE2  | 1:m:61:ARG:NH2 | 2.49                     | 0.44              |
| 1:r:63:ALA:O    | 1:r:67:ILE:N   | 2.38                     | 0.44              |
| 1:z:84:GLU:O    | 1:z:88:ARG:N   | 2.49                     | 0.44              |
| 1:W:63:ALA:O    | 1:W:67:ILE:N   | 2.38                     | 0.44              |
| 1:Y:88:ARG:O    | 1:Y:88:ARG:NE  | 2.43                     | 0.44              |
| 1:r:96:SER:O    | 1:r:99:SER:OG  | 2.33                     | 0.44              |
| 1:2:137:ASN:OD1 | 1:2:138:LEU:N  | 2.51                     | 0.44              |
| 1:3:137:ASN:OD1 | 1:3:138:LEU:N  | 2.51                     | 0.44              |
| 1:4:137:ASN:OD1 | 1:4:138:LEU:N  | 2.51                     | 0.44              |
| 1:6:137:ASN:OD1 | 1:6:138:LEU:N  | 2.51                     | 0.44              |
| 1:7:137:ASN:OD1 | 1:7:138:LEU:N  | 2.51                     | 0.44              |
| 1:A:137:ASN:OD1 | 1:A:138:LEU:N  | 2.51                     | 0.44              |
| 1:C:137:ASN:OD1 | 1:C:138:LEU:N  | 2.51                     | 0.44              |
| 1:E:137:ASN:OD1 | 1:E:138:LEU:N  | 2.51                     | 0.44              |
| 1:U:84:GLU:O    | 1:U:88:ARG:N   | 2.49                     | 0.44              |
| 1:X:137:ASN:OD1 | 1:X:138:LEU:N  | 2.51                     | 0.44              |
| 1:Y:84:GLU:O    | 1:Y:88:ARG:N   | 2.49                     | 0.44              |
| 1:f:84:GLU:O    | 1:f:88:ARG:N   | 2.49                     | 0.44              |
| 1:f:137:ASN:OD1 | 1:f:138:LEU:N  | 2.51                     | 0.44              |
| 1:h:166:SER:O   | 1:h:170:ARG:N  | 2.34                     | 0.44              |
| 1:j:88:ARG:O    | 1:j:88:ARG:NE  | 2.43                     | 0.44              |
| 1:j:137:ASN:OD1 | 1:j:138:LEU:N  | 2.51                     | 0.44              |
| 1:k:166:SER:O   | 1:k:170:ARG:N  | 2.34                     | 0.44              |
| 1:n:137:ASN:OD1 | 1:n:138:LEU:N  | 2.51                     | 0.44              |
| 1:6:84:GLU:O    | 1:6:88:ARG:N   | 2.49                     | 0.44              |
| 1:D:137:ASN:OD1 | 1:D:138:LEU:N  | 2.51                     | 0.44              |
| 1:G:137:ASN:OD1 | 1:G:138:LEU:N  | 2.51                     | 0.44              |
| 1:I:137:ASN:OD1 | 1:I:138:LEU:N  | 2.51                     | 0.44              |
| 1:b:137:ASN:OD1 | 1:b:138:LEU:N  | 2.51                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:r:137:ASN:OD1 | 1:r:138:LEU:N    | 2.51                     | 0.44              |
| 1:x:63:ALA:O    | 1:x:67:ILE:N     | 2.38                     | 0.44              |
| 1:y:137:ASN:OD1 | 1:y:138:LEU:N    | 2.51                     | 0.44              |
| 1:0:137:ASN:OD1 | 1:0:138:LEU:N    | 2.51                     | 0.44              |
| 1:H:137:ASN:OD1 | 1:H:138:LEU:N    | 2.51                     | 0.44              |
| 1:K:137:ASN:OD1 | 1:K:138:LEU:N    | 2.51                     | 0.44              |
| 1:T:137:ASN:OD1 | 1:T:138:LEU:N    | 2.51                     | 0.44              |
| 1:Z:63:ALA:O    | 1:Z:67:ILE:N     | 2.38                     | 0.44              |
| 1:b:33:LEU:O    | 1:b:129:TYR:OH   | 2.21                     | 0.44              |
| 1:v:137:ASN:OD1 | 1:v:138:LEU:N    | 2.51                     | 0.44              |
| 1:z:137:ASN:OD1 | 1:z:138:LEU:N    | 2.51                     | 0.44              |
| 1:1:137:ASN:OD1 | 1:1:138:LEU:N    | 2.51                     | 0.44              |
| 1:1:201:GLU:O   | 1:1:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:201:GLU:O   | 1:A:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:M:137:ASN:OD1 | 1:M:138:LEU:N    | 2.51                     | 0.44              |
| 1:P:137:ASN:OD1 | 1:P:138:LEU:N    | 2.51                     | 0.44              |
| 1:j:166:SER:O   | 1:j:170:ARG:N    | 2.34                     | 0.44              |
| 1:t:137:ASN:OD1 | 1:t:138:LEU:N    | 2.51                     | 0.44              |
| 1:u:137:ASN:OD1 | 1:u:138:LEU:N    | 2.51                     | 0.44              |
| 1:x:137:ASN:OD1 | 1:x:138:LEU:N    | 2.51                     | 0.44              |
| 1:5:201:GLU:O   | 1:5:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:201:GLU:O   | 1:C:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:L:137:ASN:OD1 | 1:L:138:LEU:N    | 2.51                     | 0.44              |
| 1:L:201:GLU:O   | 1:L:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:O:137:ASN:OD1 | 1:O:138:LEU:N    | 2.51                     | 0.44              |
| 1:V:201:GLU:O   | 1:V:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:a:84:GLU:O    | 1:a:88:ARG:N     | 2.49                     | 0.44              |
| 1:r:33:LEU:O    | 1:r:129:TYR:OH   | 2.21                     | 0.44              |
| 1:w:137:ASN:OD1 | 1:w:138:LEU:N    | 2.51                     | 0.44              |
| 1:5:137:ASN:OD1 | 1:5:138:LEU:N    | 2.51                     | 0.44              |
| 1:F:137:ASN:OD1 | 1:F:138:LEU:N    | 2.51                     | 0.44              |
| 1:G:201:GLU:O   | 1:G:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:J:58:GLU:OE1  | 1:J:108:LEU:HD13 | 2.18                     | 0.44              |
| 1:J:137:ASN:OD1 | 1:J:138:LEU:N    | 2.51                     | 0.44              |
| 1:N:137:ASN:OD1 | 1:N:138:LEU:N    | 2.51                     | 0.44              |
| 1:P:58:GLU:OE1  | 1:P:108:LEU:HD13 | 2.18                     | 0.44              |
| 1:Q:137:ASN:OD1 | 1:Q:138:LEU:N    | 2.51                     | 0.44              |
| 1:R:137:ASN:OD1 | 1:R:138:LEU:N    | 2.51                     | 0.44              |
| 1:X:47:LEU:O    | 1:X:50:THR:OG1   | 2.20                     | 0.44              |
| 1:X:201:GLU:O   | 1:X:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:e:201:GLU:O   | 1:e:205:VAL:HG23 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:201:GLU:O    | 1:g:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:i:63:ALA:O     | 1:i:67:ILE:N     | 2.38                     | 0.44              |
| 1:k:58:GLU:OE1   | 1:k:108:LEU:HD13 | 2.18                     | 0.44              |
| 1:n:58:GLU:OE1   | 1:n:108:LEU:HD13 | 2.18                     | 0.44              |
| 1:p:137:ASN:OD1  | 1:p:138:LEU:N    | 2.51                     | 0.44              |
| 1:q:137:ASN:OD1  | 1:q:138:LEU:N    | 2.51                     | 0.44              |
| 1:q:201:GLU:O    | 1:q:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:v:88:ARG:O     | 1:v:88:ARG:NE    | 2.43                     | 0.44              |
| 1:z:201:GLU:O    | 1:z:205:VAL:HG23 | 2.18                     | 0.44              |
| 1:2:63:ALA:O     | 1:2:67:ILE:N     | 2.38                     | 0.43              |
| 1:4:58:GLU:OE1   | 1:4:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:5:63:ALA:O     | 1:5:67:ILE:N     | 2.38                     | 0.43              |
| 1:F:184:LEU:HD23 | 1:F:184:LEU:C    | 2.43                     | 0.43              |
| 1:J:201:GLU:O    | 1:J:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:L:58:GLU:OE1   | 1:L:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:M:33:LEU:O     | 1:M:129:TYR:OH   | 2.21                     | 0.43              |
| 1:N:166:SER:O    | 1:N:170:ARG:N    | 2.34                     | 0.43              |
| 1:O:58:GLU:OE1   | 1:O:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:S:137:ASN:OD1  | 1:S:138:LEU:N    | 2.51                     | 0.43              |
| 1:V:137:ASN:OD1  | 1:V:138:LEU:N    | 2.51                     | 0.43              |
| 1:a:201:GLU:O    | 1:a:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:b:201:GLU:O    | 1:b:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:e:58:GLU:OE1   | 1:e:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:j:58:GLU:OE1   | 1:j:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:k:201:GLU:O    | 1:k:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:l:137:ASN:OD1  | 1:l:138:LEU:N    | 2.51                     | 0.43              |
| 1:p:58:GLU:OE1   | 1:p:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:v:201:GLU:O    | 1:v:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:w:201:GLU:O    | 1:w:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:5:58:GLU:OE1   | 1:5:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:6:201:GLU:O    | 1:6:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:F:201:GLU:O    | 1:F:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:J:63:ALA:O     | 1:J:67:ILE:N     | 2.38                     | 0.43              |
| 1:J:184:LEU:HD23 | 1:J:184:LEU:C    | 2.43                     | 0.43              |
| 1:K:58:GLU:OE1   | 1:K:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:P:201:GLU:O    | 1:P:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:a:96:SER:O     | 1:a:99:SER:OG    | 2.33                     | 0.43              |
| 1:h:201:GLU:O    | 1:h:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:m:137:ASN:OD1  | 1:m:138:LEU:N    | 2.51                     | 0.43              |
| 1:o:58:GLU:OE1   | 1:o:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:s:137:ASN:OD1  | 1:s:138:LEU:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:201:GLU:O    | 1:4:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:7:58:GLU:OE1   | 1:7:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:B:137:ASN:OD1  | 1:B:138:LEU:N    | 2.51                     | 0.43              |
| 1:B:184:LEU:HD23 | 1:B:184:LEU:C    | 2.43                     | 0.43              |
| 1:I:58:GLU:OE1   | 1:I:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:M:201:GLU:O    | 1:M:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:O:201:GLU:O    | 1:O:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:Q:201:GLU:O    | 1:Q:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:U:58:GLU:OE1   | 1:U:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:U:137:ASN:OD1  | 1:U:138:LEU:N    | 2.51                     | 0.43              |
| 1:W:137:ASN:OD1  | 1:W:138:LEU:N    | 2.51                     | 0.43              |
| 1:Z:201:GLU:O    | 1:Z:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:d:58:GLU:OE1   | 1:d:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:h:137:ASN:OD1  | 1:h:138:LEU:N    | 2.51                     | 0.43              |
| 1:i:58:GLU:OE1   | 1:i:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:j:201:GLU:O    | 1:j:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:l:201:GLU:O    | 1:l:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:n:201:GLU:O    | 1:n:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:p:201:GLU:O    | 1:p:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:y:58:GLU:OE1   | 1:y:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:2:201:GLU:O    | 1:2:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:3:58:GLU:OE1   | 1:3:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:D:184:LEU:C    | 1:D:184:LEU:HD23 | 2.44                     | 0.43              |
| 1:F:58:GLU:OE1   | 1:F:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:L:184:LEU:C    | 1:L:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:N:58:GLU:OE1   | 1:N:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:N:184:LEU:HD23 | 1:N:184:LEU:C    | 2.43                     | 0.43              |
| 1:R:58:GLU:OE1   | 1:R:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:R:201:GLU:O    | 1:R:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:S:201:GLU:O    | 1:S:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:W:88:ARG:O     | 1:W:88:ARG:NE    | 2.43                     | 0.43              |
| 1:W:184:LEU:C    | 1:W:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:Y:184:LEU:HD23 | 1:Y:184:LEU:C    | 2.43                     | 0.43              |
| 1:Z:137:ASN:OD1  | 1:Z:138:LEU:N    | 2.51                     | 0.43              |
| 1:f:58:GLU:OE1   | 1:f:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:g:58:GLU:OE1   | 1:g:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:i:137:ASN:OD1  | 1:i:138:LEU:N    | 2.51                     | 0.43              |
| 1:m:58:GLU:OE1   | 1:m:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:n:184:LEU:HD23 | 1:n:184:LEU:C    | 2.43                     | 0.43              |
| 1:o:137:ASN:OD1  | 1:o:138:LEU:N    | 2.51                     | 0.43              |
| 1:s:201:GLU:O    | 1:s:205:VAL:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:201:GLU:O    | 1:u:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:z:58:GLU:OE1   | 1:z:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:2:184:LEU:HD23 | 1:2:184:LEU:C    | 2.43                     | 0.43              |
| 1:E:58:GLU:OE1   | 1:E:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:Q:184:LEU:HD23 | 1:Q:184:LEU:C    | 2.43                     | 0.43              |
| 1:R:184:LEU:HD23 | 1:R:184:LEU:C    | 2.43                     | 0.43              |
| 1:S:58:GLU:OE1   | 1:S:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:S:184:LEU:HD23 | 1:S:184:LEU:C    | 2.43                     | 0.43              |
| 1:T:58:GLU:OE1   | 1:T:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:Y:137:ASN:OD1  | 1:Y:138:LEU:N    | 2.51                     | 0.43              |
| 1:a:137:ASN:OD1  | 1:a:138:LEU:N    | 2.51                     | 0.43              |
| 1:g:184:LEU:C    | 1:g:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:t:58:GLU:OE1   | 1:t:108:LEU:HD13 | 2.19                     | 0.43              |
| 1:7:201:GLU:O    | 1:7:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:G:58:GLU:OE1   | 1:G:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:201:GLU:O    | 1:H:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:P:63:ALA:O     | 1:P:67:ILE:N     | 2.38                     | 0.43              |
| 1:W:201:GLU:O    | 1:W:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:Z:58:GLU:OE1   | 1:Z:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:a:184:LEU:HD23 | 1:a:184:LEU:C    | 2.44                     | 0.43              |
| 1:d:201:GLU:O    | 1:d:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:e:137:ASN:OD1  | 1:e:138:LEU:N    | 2.51                     | 0.43              |
| 1:e:184:LEU:HD23 | 1:e:184:LEU:C    | 2.43                     | 0.43              |
| 1:l:58:GLU:OE1   | 1:l:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:l:184:LEU:HD23 | 1:l:184:LEU:C    | 2.43                     | 0.43              |
| 1:t:184:LEU:HD23 | 1:t:184:LEU:C    | 2.43                     | 0.43              |
| 1:u:58:GLU:OE1   | 1:u:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:4:184:LEU:C    | 1:4:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:6:58:GLU:OE1   | 1:6:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:D:201:GLU:O    | 1:D:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:E:201:GLU:O    | 1:E:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:I:201:GLU:O    | 1:I:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:K:88:ARG:O     | 1:K:88:ARG:NE    | 2.43                     | 0.43              |
| 1:K:184:LEU:HD23 | 1:K:184:LEU:C    | 2.43                     | 0.43              |
| 1:K:201:GLU:O    | 1:K:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:O:184:LEU:C    | 1:O:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:Q:58:GLU:OE1   | 1:Q:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:U:201:GLU:O    | 1:U:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:V:184:LEU:HD23 | 1:V:184:LEU:C    | 2.43                     | 0.43              |
| 1:a:58:GLU:OE1   | 1:a:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:c:137:ASN:OD1  | 1:c:138:LEU:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:201:GLU:O    | 1:c:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:d:137:ASN:OD1  | 1:d:138:LEU:N    | 2.51                     | 0.43              |
| 1:k:137:ASN:OD1  | 1:k:138:LEU:N    | 2.51                     | 0.43              |
| 1:m:201:GLU:O    | 1:m:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:s:58:GLU:OE1   | 1:s:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:w:58:GLU:OE1   | 1:w:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:x:33:LEU:O     | 1:x:129:TYR:OH   | 2.21                     | 0.43              |
| 1:0:58:GLU:OE1   | 1:0:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:1:58:GLU:OE1   | 1:1:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:A:58:GLU:OE1   | 1:A:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:Y:58:GLU:OE1   | 1:Y:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:b:58:GLU:OE1   | 1:b:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:f:201:GLU:O    | 1:f:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:g:137:ASN:OD1  | 1:g:138:LEU:N    | 2.51                     | 0.43              |
| 1:i:184:LEU:HD23 | 1:i:184:LEU:C    | 2.43                     | 0.43              |
| 1:p:184:LEU:HD23 | 1:p:184:LEU:C    | 2.43                     | 0.43              |
| 1:r:58:GLU:OE1   | 1:r:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:v:184:LEU:HD23 | 1:v:184:LEU:C    | 2.43                     | 0.43              |
| 1:0:184:LEU:HD23 | 1:0:184:LEU:C    | 2.43                     | 0.43              |
| 1:1:184:LEU:C    | 1:1:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:3:201:GLU:O    | 1:3:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:6:184:LEU:HD23 | 1:6:184:LEU:C    | 2.43                     | 0.43              |
| 1:A:184:LEU:C    | 1:A:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:C:47:LEU:O     | 1:C:50:THR:OG1   | 2.20                     | 0.43              |
| 1:H:58:GLU:OE1   | 1:H:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:184:LEU:HD23 | 1:H:184:LEU:C    | 2.43                     | 0.43              |
| 1:I:33:LEU:HD11  | 1:M:159:LEU:CD2  | 2.49                     | 0.43              |
| 1:I:96:SER:O     | 1:I:99:SER:OG    | 2.33                     | 0.43              |
| 1:M:58:GLU:OE1   | 1:M:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:S:96:SER:O     | 1:S:99:SER:OG    | 2.33                     | 0.43              |
| 1:T:184:LEU:C    | 1:T:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:U:96:SER:O     | 1:U:99:SER:OG    | 2.33                     | 0.43              |
| 1:h:184:LEU:HD23 | 1:h:184:LEU:C    | 2.43                     | 0.43              |
| 1:r:201:GLU:O    | 1:r:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:t:201:GLU:O    | 1:t:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:v:58:GLU:OE1   | 1:v:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:z:184:LEU:C    | 1:z:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:D:58:GLU:OE1   | 1:D:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:E:184:LEU:HD23 | 1:E:184:LEU:C    | 2.43                     | 0.43              |
| 1:G:184:LEU:HD23 | 1:G:184:LEU:C    | 2.43                     | 0.43              |
| 1:I:203:GLN:HB2  | 1:N:81:ARG:NH2   | 2.27                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:212:MET:O    | 1:K:215:ARG:N    | 2.52                     | 0.43              |
| 1:T:63:ALA:O     | 1:T:67:ILE:N     | 2.38                     | 0.43              |
| 1:W:96:SER:O     | 1:W:99:SER:OG    | 2.33                     | 0.43              |
| 1:f:96:SER:O     | 1:f:99:SER:OG    | 2.33                     | 0.43              |
| 1:f:184:LEU:HD23 | 1:f:184:LEU:C    | 2.43                     | 0.43              |
| 1:i:201:GLU:O    | 1:i:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:k:33:LEU:O     | 1:k:129:TYR:OH   | 2.21                     | 0.43              |
| 1:q:58:GLU:OE1   | 1:q:108:LEU:HD13 | 2.18                     | 0.43              |
| 1:u:184:LEU:HD23 | 1:u:184:LEU:C    | 2.43                     | 0.43              |
| 1:w:184:LEU:C    | 1:w:184:LEU:HD23 | 2.43                     | 0.43              |
| 1:w:212:MET:O    | 1:w:215:ARG:N    | 2.52                     | 0.43              |
| 1:x:201:GLU:O    | 1:x:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:y:201:GLU:O    | 1:y:205:VAL:HG23 | 2.18                     | 0.43              |
| 1:z:47:LEU:O     | 1:z:50:THR:OG1   | 2.20                     | 0.43              |
| 1:B:201:GLU:O    | 1:B:205:VAL:HG23 | 2.18                     | 0.42              |
| 1:C:184:LEU:HD23 | 1:C:184:LEU:C    | 2.43                     | 0.42              |
| 1:F:212:MET:O    | 1:F:215:ARG:N    | 2.52                     | 0.42              |
| 1:G:212:MET:O    | 1:G:215:ARG:N    | 2.52                     | 0.42              |
| 1:I:184:LEU:C    | 1:I:184:LEU:HD23 | 2.43                     | 0.42              |
| 1:N:63:ALA:O     | 1:N:67:ILE:N     | 2.38                     | 0.42              |
| 1:N:201:GLU:O    | 1:N:205:VAL:HG23 | 2.18                     | 0.42              |
| 1:O:212:MET:O    | 1:O:215:ARG:N    | 2.52                     | 0.42              |
| 1:V:58:GLU:OE1   | 1:V:108:LEU:HD13 | 2.19                     | 0.42              |
| 1:Z:184:LEU:HD23 | 1:Z:184:LEU:C    | 2.43                     | 0.42              |
| 1:e:166:SER:O    | 1:e:170:ARG:N    | 2.34                     | 0.42              |
| 1:g:166:SER:O    | 1:g:170:ARG:N    | 2.34                     | 0.42              |
| 1:h:58:GLU:OE1   | 1:h:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:m:184:LEU:HD23 | 1:m:184:LEU:C    | 2.43                     | 0.42              |
| 1:s:212:MET:O    | 1:s:215:ARG:N    | 2.52                     | 0.42              |
| 1:v:63:ALA:O     | 1:v:67:ILE:N     | 2.38                     | 0.42              |
| 1:x:184:LEU:HD23 | 1:x:184:LEU:C    | 2.43                     | 0.42              |
| 1:0:212:MET:O    | 1:0:215:ARG:N    | 2.52                     | 0.42              |
| 1:2:58:GLU:OE1   | 1:2:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:B:58:GLU:OE1   | 1:B:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:J:212:MET:O    | 1:J:215:ARG:N    | 2.52                     | 0.42              |
| 1:U:63:ALA:O     | 1:U:67:ILE:N     | 2.38                     | 0.42              |
| 1:W:166:SER:O    | 1:W:170:ARG:N    | 2.34                     | 0.42              |
| 1:X:58:GLU:OE1   | 1:X:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:X:212:MET:O    | 1:X:215:ARG:N    | 2.52                     | 0.42              |
| 1:d:184:LEU:C    | 1:d:184:LEU:HD23 | 2.43                     | 0.42              |
| 1:f:212:MET:O    | 1:f:215:ARG:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:212:MET:O    | 1:n:215:ARG:N    | 2.52                     | 0.42              |
| 1:o:184:LEU:C    | 1:o:184:LEU:HD23 | 2.43                     | 0.42              |
| 1:r:212:MET:O    | 1:r:215:ARG:N    | 2.52                     | 0.42              |
| 1:5:184:LEU:HD23 | 1:5:184:LEU:C    | 2.43                     | 0.42              |
| 1:B:212:MET:O    | 1:B:215:ARG:N    | 2.52                     | 0.42              |
| 1:I:39:GLU:HB2   | 1:M:151:LYS:CD   | 2.50                     | 0.42              |
| 1:M:184:LEU:HD23 | 1:M:184:LEU:C    | 2.43                     | 0.42              |
| 1:U:184:LEU:HD23 | 1:U:184:LEU:C    | 2.43                     | 0.42              |
| 1:W:58:GLU:OE1   | 1:W:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:Y:30:GLU:OE2   | 1:Y:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:b:212:MET:O    | 1:b:215:ARG:N    | 2.52                     | 0.42              |
| 1:c:58:GLU:OE1   | 1:c:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:c:184:LEU:HD23 | 1:c:184:LEU:C    | 2.43                     | 0.42              |
| 1:d:166:SER:O    | 1:d:170:ARG:N    | 2.34                     | 0.42              |
| 1:j:212:MET:O    | 1:j:215:ARG:N    | 2.52                     | 0.42              |
| 1:o:212:MET:O    | 1:o:215:ARG:N    | 2.52                     | 0.42              |
| 1:x:58:GLU:OE1   | 1:x:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:1:212:MET:O    | 1:1:215:ARG:N    | 2.52                     | 0.42              |
| 1:5:212:MET:O    | 1:5:215:ARG:N    | 2.52                     | 0.42              |
| 1:C:58:GLU:OE1   | 1:C:108:LEU:HD13 | 2.18                     | 0.42              |
| 1:D:142:ARG:O    | 1:D:146:ALA:N    | 2.45                     | 0.42              |
| 1:P:184:LEU:HD23 | 1:P:184:LEU:C    | 2.43                     | 0.42              |
| 1:S:212:MET:O    | 1:S:215:ARG:N    | 2.52                     | 0.42              |
| 1:T:201:GLU:O    | 1:T:205:VAL:HG23 | 2.18                     | 0.42              |
| 1:b:184:LEU:HD23 | 1:b:184:LEU:C    | 2.43                     | 0.42              |
| 1:k:184:LEU:HD23 | 1:k:184:LEU:C    | 2.43                     | 0.42              |
| 1:r:184:LEU:C    | 1:r:184:LEU:HD23 | 2.43                     | 0.42              |
| 1:y:184:LEU:HD23 | 1:y:184:LEU:C    | 2.44                     | 0.42              |
| 1:0:201:GLU:O    | 1:0:205:VAL:HG23 | 2.18                     | 0.42              |
| 1:1:63:ALA:O     | 1:1:67:ILE:N     | 2.38                     | 0.42              |
| 1:4:212:MET:O    | 1:4:215:ARG:N    | 2.52                     | 0.42              |
| 1:7:184:LEU:HD23 | 1:7:184:LEU:C    | 2.43                     | 0.42              |
| 1:C:212:MET:O    | 1:C:215:ARG:N    | 2.52                     | 0.42              |
| 1:D:30:GLU:OE2   | 1:D:136:LYS:NZ   | 2.48                     | 0.42              |
| 1:P:212:MET:O    | 1:P:215:ARG:N    | 2.52                     | 0.42              |
| 1:T:212:MET:O    | 1:T:215:ARG:N    | 2.52                     | 0.42              |
| 1:Y:201:GLU:O    | 1:Y:205:VAL:HG23 | 2.18                     | 0.42              |
| 1:d:212:MET:O    | 1:d:215:ARG:N    | 2.52                     | 0.42              |
| 1:h:212:MET:O    | 1:h:215:ARG:N    | 2.52                     | 0.42              |
| 1:l:212:MET:O    | 1:l:215:ARG:N    | 2.52                     | 0.42              |
| 1:o:201:GLU:O    | 1:o:205:VAL:HG23 | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:212:MET:O    | 1:v:215:ARG:N    | 2.52                     | 0.42              |
| 1:A:63:ALA:O     | 1:A:67:ILE:N     | 2.38                     | 0.42              |
| 1:J:88:ARG:O     | 1:J:88:ARG:NE    | 2.43                     | 0.42              |
| 1:L:212:MET:O    | 1:L:215:ARG:N    | 2.52                     | 0.42              |
| 1:Q:30:GLU:OE2   | 1:Q:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:Z:212:MET:O    | 1:Z:215:ARG:N    | 2.52                     | 0.42              |
| 1:j:184:LEU:HD23 | 1:j:184:LEU:C    | 2.43                     | 0.42              |
| 1:l:30:GLU:OE2   | 1:l:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:q:184:LEU:HD23 | 1:q:184:LEU:C    | 2.43                     | 0.42              |
| 1:s:184:LEU:HD23 | 1:s:184:LEU:C    | 2.44                     | 0.42              |
| 1:x:212:MET:O    | 1:x:215:ARG:N    | 2.52                     | 0.42              |
| 1:7:212:MET:O    | 1:7:215:ARG:N    | 2.52                     | 0.42              |
| 1:D:212:MET:O    | 1:D:215:ARG:N    | 2.52                     | 0.42              |
| 1:N:212:MET:O    | 1:N:215:ARG:N    | 2.52                     | 0.42              |
| 1:V:30:GLU:OE2   | 1:V:136:LYS:NZ   | 2.48                     | 0.42              |
| 1:W:212:MET:O    | 1:W:215:ARG:N    | 2.52                     | 0.42              |
| 1:X:184:LEU:HD23 | 1:X:184:LEU:C    | 2.43                     | 0.42              |
| 1:a:212:MET:O    | 1:a:215:ARG:N    | 2.52                     | 0.42              |
| 1:b:39:GLU:HG2   | 1:f:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:o:96:SER:O     | 1:o:99:SER:OG    | 2.33                     | 0.42              |
| 1:p:212:MET:O    | 1:p:215:ARG:N    | 2.52                     | 0.42              |
| 1:v:166:SER:O    | 1:v:170:ARG:N    | 2.34                     | 0.42              |
| 1:2:30:GLU:OE2   | 1:2:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:6:30:GLU:OE2   | 1:6:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:F:33:LEU:O     | 1:F:129:TYR:OH   | 2.21                     | 0.42              |
| 1:L:30:GLU:OE2   | 1:L:136:LYS:NZ   | 2.47                     | 0.42              |
| 1:k:212:MET:O    | 1:k:215:ARG:N    | 2.52                     | 0.42              |
| 1:m:142:ARG:O    | 1:m:146:ALA:N    | 2.45                     | 0.42              |
| 1:p:142:ARG:O    | 1:p:146:ALA:N    | 2.45                     | 0.42              |
| 1:0:39:GLU:HG2   | 1:4:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:H:212:MET:O    | 1:H:215:ARG:N    | 2.52                     | 0.42              |
| 1:K:39:GLU:HG2   | 1:O:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:O:39:GLU:HG2   | 1:S:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:V:212:MET:O    | 1:V:215:ARG:N    | 2.52                     | 0.42              |
| 1:t:30:GLU:OE2   | 1:t:136:LYS:NZ   | 2.48                     | 0.42              |
| 1:z:212:MET:O    | 1:z:215:ARG:N    | 2.52                     | 0.42              |
| 1:2:155:ILE:HD12 | 1:y:39:GLU:HG2   | 2.02                     | 0.42              |
| 1:3:184:LEU:HD23 | 1:3:184:LEU:C    | 2.43                     | 0.42              |
| 1:B:39:GLU:HG2   | 1:F:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:b:166:SER:O    | 1:b:170:ARG:N    | 2.34                     | 0.42              |
| 1:e:212:MET:O    | 1:e:215:ARG:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:39:GLU:HG2   | 1:j:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:f:166:SER:O    | 1:f:170:ARG:N    | 2.34                     | 0.42              |
| 1:h:39:GLU:HG2   | 1:l:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:j:39:GLU:HG2   | 1:n:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:o:39:GLU:HG2   | 1:s:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:p:30:GLU:OE2   | 1:p:136:LYS:NZ   | 2.48                     | 0.42              |
| 1:s:39:GLU:HG2   | 1:w:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:t:212:MET:O    | 1:t:215:ARG:N    | 2.52                     | 0.42              |
| 1:u:39:GLU:HG2   | 1:y:155:ILE:HD12 | 2.02                     | 0.42              |
| 1:0:155:ILE:HD12 | 1:w:39:GLU:HG2   | 2.02                     | 0.41              |
| 1:3:212:MET:O    | 1:3:215:ARG:N    | 2.52                     | 0.41              |
| 1:E:212:MET:O    | 1:E:215:ARG:N    | 2.52                     | 0.41              |
| 1:G:39:GLU:HG2   | 1:K:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:M:212:MET:O    | 1:M:215:ARG:N    | 2.52                     | 0.41              |
| 1:Q:39:GLU:HG2   | 1:U:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:S:39:GLU:HG2   | 1:W:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:U:39:GLU:HG2   | 1:Y:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:X:39:GLU:HG2   | 1:b:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:Y:93:GLN:O     | 1:Y:96:SER:OG    | 2.36                     | 0.41              |
| 1:n:39:GLU:HG2   | 1:r:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:q:212:MET:O    | 1:q:215:ARG:N    | 2.52                     | 0.41              |
| 1:u:212:MET:O    | 1:u:215:ARG:N    | 2.52                     | 0.41              |
| 1:y:212:MET:O    | 1:y:215:ARG:N    | 2.52                     | 0.41              |
| 1:2:212:MET:O    | 1:2:215:ARG:N    | 2.52                     | 0.41              |
| 1:3:47:LEU:O     | 1:3:50:THR:OG1   | 2.20                     | 0.41              |
| 1:A:212:MET:O    | 1:A:215:ARG:N    | 2.52                     | 0.41              |
| 1:H:142:ARG:O    | 1:H:146:ALA:N    | 2.45                     | 0.41              |
| 1:K:96:SER:O     | 1:K:99:SER:OG    | 2.33                     | 0.41              |
| 1:R:212:MET:O    | 1:R:215:ARG:N    | 2.52                     | 0.41              |
| 1:d:39:GLU:HG2   | 1:h:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:i:212:MET:O    | 1:i:215:ARG:N    | 2.52                     | 0.41              |
| 1:l:39:GLU:HG2   | 1:p:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:2:39:GLU:HG2   | 1:6:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:4:88:ARG:O     | 1:4:88:ARG:NE    | 2.43                     | 0.41              |
| 1:6:63:ALA:O     | 1:6:67:ILE:N     | 2.38                     | 0.41              |
| 1:D:39:GLU:HG2   | 1:H:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:F:39:GLU:HG2   | 1:J:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:G:96:SER:O     | 1:G:99:SER:OG    | 2.33                     | 0.41              |
| 1:I:212:MET:O    | 1:I:215:ARG:N    | 2.52                     | 0.41              |
| 1:Q:212:MET:O    | 1:Q:215:ARG:N    | 2.52                     | 0.41              |
| 1:W:39:GLU:HG2   | 1:a:155:ILE:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:39:GLU:HG2   | 1:e:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:g:30:GLU:OE2   | 1:g:136:LYS:NZ   | 2.47                     | 0.41              |
| 1:g:212:MET:O    | 1:g:215:ARG:N    | 2.52                     | 0.41              |
| 1:m:212:MET:O    | 1:m:215:ARG:N    | 2.52                     | 0.41              |
| 1:q:39:GLU:HG2   | 1:u:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:r:39:GLU:HG2   | 1:v:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:r:142:ARG:O    | 1:r:146:ALA:N    | 2.45                     | 0.41              |
| 1:y:30:GLU:OE2   | 1:y:136:LYS:NZ   | 2.47                     | 0.41              |
| 1:0:143:LEU:HD23 | 1:0:143:LEU:C    | 2.46                     | 0.41              |
| 1:1:39:GLU:HG2   | 1:5:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:7:143:LEU:HD23 | 1:7:143:LEU:C    | 2.46                     | 0.41              |
| 1:M:39:GLU:HG2   | 1:Q:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:T:39:GLU:HG2   | 1:X:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:U:212:MET:O    | 1:U:215:ARG:N    | 2.52                     | 0.41              |
| 1:V:39:GLU:HG2   | 1:Z:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:a:143:LEU:HD23 | 1:a:143:LEU:C    | 2.46                     | 0.41              |
| 1:k:39:GLU:HG2   | 1:o:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:x:30:GLU:OE2   | 1:x:136:LYS:NZ   | 2.47                     | 0.41              |
| 1:x:93:GLN:O     | 1:x:96:SER:OG    | 2.36                     | 0.41              |
| 1:6:212:MET:O    | 1:6:215:ARG:N    | 2.52                     | 0.41              |
| 1:A:143:LEU:HD23 | 1:A:143:LEU:C    | 2.46                     | 0.41              |
| 1:B:143:LEU:C    | 1:B:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:D:93:GLN:O     | 1:D:96:SER:OG    | 2.36                     | 0.41              |
| 1:D:96:SER:O     | 1:D:99:SER:OG    | 2.33                     | 0.41              |
| 1:E:43:LEU:HD13  | 1:I:148:ALA:HB1  | 2.03                     | 0.41              |
| 1:E:142:ARG:O    | 1:E:146:ALA:N    | 2.45                     | 0.41              |
| 1:H:39:GLU:HG2   | 1:L:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:K:142:ARG:O    | 1:K:146:ALA:N    | 2.45                     | 0.41              |
| 1:N:143:LEU:HD23 | 1:N:143:LEU:C    | 2.46                     | 0.41              |
| 1:O:143:LEU:HD23 | 1:O:143:LEU:C    | 2.46                     | 0.41              |
| 1:P:47:LEU:O     | 1:P:50:THR:OG1   | 2.20                     | 0.41              |
| 1:Y:39:GLU:HG2   | 1:c:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:Y:212:MET:O    | 1:Y:215:ARG:N    | 2.52                     | 0.41              |
| 1:b:143:LEU:HD23 | 1:b:143:LEU:C    | 2.46                     | 0.41              |
| 1:d:30:GLU:OE2   | 1:d:136:LYS:NZ   | 2.47                     | 0.41              |
| 1:h:143:LEU:HD23 | 1:h:143:LEU:C    | 2.46                     | 0.41              |
| 1:n:143:LEU:HD23 | 1:n:143:LEU:C    | 2.46                     | 0.41              |
| 1:p:39:GLU:HG2   | 1:t:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:u:143:LEU:HD23 | 1:u:143:LEU:C    | 2.46                     | 0.41              |
| 1:C:39:GLU:HG2   | 1:G:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:H:30:GLU:OE2   | 1:H:136:LYS:NZ   | 2.48                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:39:GLU:HG2   | 1:N:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:R:39:GLU:HG2   | 1:V:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:V:143:LEU:HD23 | 1:V:143:LEU:C    | 2.46                     | 0.41              |
| 1:Z:39:GLU:HG2   | 1:d:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:Z:143:LEU:HD23 | 1:Z:143:LEU:C    | 2.46                     | 0.41              |
| 1:i:143:LEU:HD23 | 1:i:143:LEU:C    | 2.46                     | 0.41              |
| 1:k:93:GLN:O     | 1:k:96:SER:OG    | 2.36                     | 0.41              |
| 1:m:143:LEU:C    | 1:m:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:v:39:GLU:HG2   | 1:z:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:v:143:LEU:HD23 | 1:v:143:LEU:C    | 2.46                     | 0.41              |
| 1:l:143:LEU:HD23 | 1:l:143:LEU:C    | 2.46                     | 0.41              |
| 1:3:39:GLU:HG2   | 1:7:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:39:GLU:HG2   | 1:E:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:G:143:LEU:HD23 | 1:G:143:LEU:C    | 2.46                     | 0.41              |
| 1:I:143:LEU:HD23 | 1:I:143:LEU:C    | 2.46                     | 0.41              |
| 1:M:143:LEU:HD23 | 1:M:143:LEU:C    | 2.46                     | 0.41              |
| 1:N:39:GLU:HG2   | 1:R:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:U:30:GLU:OE2   | 1:U:136:LYS:NZ   | 2.48                     | 0.41              |
| 1:U:143:LEU:C    | 1:U:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:W:143:LEU:HD23 | 1:W:143:LEU:C    | 2.46                     | 0.41              |
| 1:c:30:GLU:OE2   | 1:c:136:LYS:NZ   | 2.48                     | 0.41              |
| 1:c:166:SER:O    | 1:c:170:ARG:N    | 2.34                     | 0.41              |
| 1:e:39:GLU:HG2   | 1:i:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:o:143:LEU:HD23 | 1:o:143:LEU:C    | 2.46                     | 0.41              |
| 1:t:142:ARG:O    | 1:t:146:ALA:N    | 2.45                     | 0.41              |
| 1:l:155:ILE:HD12 | 1:x:39:GLU:HG2   | 2.02                     | 0.41              |
| 1:F:143:LEU:HD23 | 1:F:143:LEU:C    | 2.46                     | 0.41              |
| 1:J:143:LEU:C    | 1:J:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:T:143:LEU:HD23 | 1:T:143:LEU:C    | 2.46                     | 0.41              |
| 1:c:212:MET:O    | 1:c:215:ARG:N    | 2.52                     | 0.41              |
| 1:g:47:LEU:O     | 1:g:50:THR:OG1   | 2.20                     | 0.41              |
| 1:t:143:LEU:HD23 | 1:t:143:LEU:C    | 2.46                     | 0.41              |
| 1:z:143:LEU:HD23 | 1:z:143:LEU:C    | 2.46                     | 0.41              |
| 1:2:93:GLN:O     | 1:2:96:SER:OG    | 2.36                     | 0.41              |
| 1:2:143:LEU:C    | 1:2:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:4:143:LEU:C    | 1:4:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:4:166:SER:O    | 1:4:170:ARG:N    | 2.34                     | 0.41              |
| 1:6:143:LEU:HD23 | 1:6:143:LEU:C    | 2.46                     | 0.41              |
| 1:B:96:SER:O     | 1:B:99:SER:OG    | 2.33                     | 0.41              |
| 1:C:143:LEU:HD23 | 1:C:143:LEU:C    | 2.46                     | 0.41              |
| 1:E:43:LEU:HB2   | 1:I:151:LYS:HZ1  | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:143:LEU:C    | 1:E:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:H:143:LEU:HD23 | 1:H:143:LEU:C    | 2.46                     | 0.41              |
| 1:L:143:LEU:C    | 1:L:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:S:143:LEU:HD23 | 1:S:143:LEU:C    | 2.46                     | 0.41              |
| 1:d:93:GLN:O     | 1:d:96:SER:OG    | 2.36                     | 0.41              |
| 1:f:143:LEU:HD23 | 1:f:143:LEU:C    | 2.46                     | 0.41              |
| 1:g:93:GLN:O     | 1:g:96:SER:OG    | 2.36                     | 0.41              |
| 1:g:143:LEU:HD23 | 1:g:143:LEU:C    | 2.46                     | 0.41              |
| 1:i:39:GLU:HG2   | 1:m:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:j:143:LEU:HD23 | 1:j:143:LEU:C    | 2.46                     | 0.41              |
| 1:m:39:GLU:HG2   | 1:q:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:t:39:GLU:HG2   | 1:x:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:w:143:LEU:HD23 | 1:w:143:LEU:C    | 2.46                     | 0.41              |
| 1:C:93:GLN:O     | 1:C:96:SER:OG    | 2.36                     | 0.41              |
| 1:L:39:GLU:HG2   | 1:P:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:R:143:LEU:HD23 | 1:R:143:LEU:C    | 2.46                     | 0.41              |
| 1:c:39:GLU:HG2   | 1:g:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:g:39:GLU:HG2   | 1:k:155:ILE:HD12 | 2.02                     | 0.41              |
| 1:k:143:LEU:C    | 1:k:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:p:143:LEU:C    | 1:p:143:LEU:HD23 | 2.46                     | 0.41              |
| 1:s:143:LEU:HD23 | 1:s:143:LEU:C    | 2.46                     | 0.41              |
| 1:u:30:GLU:OE2   | 1:u:136:LYS:NZ   | 2.48                     | 0.41              |
| 1:I:30:GLU:OE2   | 1:I:136:LYS:NZ   | 2.47                     | 0.40              |
| 1:J:142:ARG:O    | 1:J:146:ALA:N    | 2.45                     | 0.40              |
| 1:L:142:ARG:O    | 1:L:146:ALA:N    | 2.45                     | 0.40              |
| 1:P:39:GLU:HG2   | 1:T:155:ILE:HD12 | 2.02                     | 0.40              |
| 1:P:143:LEU:HD23 | 1:P:143:LEU:C    | 2.46                     | 0.40              |
| 1:e:33:LEU:O     | 1:e:129:TYR:OH   | 2.21                     | 0.40              |
| 1:m:47:LEU:O     | 1:m:50:THR:OG1   | 2.20                     | 0.40              |
| 1:q:143:LEU:HD23 | 1:q:143:LEU:C    | 2.46                     | 0.40              |
| 1:x:143:LEU:C    | 1:x:143:LEU:HD23 | 2.46                     | 0.40              |
| 1:1:30:GLU:OE2   | 1:1:136:LYS:NZ   | 2.48                     | 0.40              |
| 1:3:143:LEU:HD23 | 1:3:143:LEU:C    | 2.46                     | 0.40              |
| 1:3:155:ILE:HD12 | 1:z:39:GLU:HG2   | 2.02                     | 0.40              |
| 1:5:143:LEU:C    | 1:5:143:LEU:HD23 | 2.46                     | 0.40              |
| 1:6:127:ARG:NH2  | 1:6:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:E:39:GLU:O     | 1:I:151:LYS:NZ   | 2.53                     | 0.40              |
| 1:G:127:ARG:NH2  | 1:G:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:I:127:ARG:NH2  | 1:I:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:J:127:ARG:NH2  | 1:J:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:R:127:ARG:NH2  | 1:R:130:LEU:HD11 | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:127:ARG:NH2  | 1:S:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:T:30:GLU:OE2   | 1:T:136:LYS:NZ   | 2.47                     | 0.40              |
| 1:X:143:LEU:C    | 1:X:143:LEU:HD23 | 2.46                     | 0.40              |
| 1:Y:127:ARG:NH2  | 1:Y:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:Y:143:LEU:HD23 | 1:Y:143:LEU:C    | 2.46                     | 0.40              |
| 1:Z:166:SER:O    | 1:Z:170:ARG:N    | 2.34                     | 0.40              |
| 1:b:127:ARG:NH2  | 1:b:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:c:143:LEU:HD23 | 1:c:143:LEU:C    | 2.46                     | 0.40              |
| 1:m:63:ALA:O     | 1:m:67:ILE:N     | 2.39                     | 0.40              |
| 1:o:127:ARG:NH2  | 1:o:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:q:142:ARG:O    | 1:q:146:ALA:N    | 2.45                     | 0.40              |
| 1:r:143:LEU:C    | 1:r:143:LEU:HD23 | 2.46                     | 0.40              |
| 1:w:142:ARG:O    | 1:w:146:ALA:N    | 2.45                     | 0.40              |
| 1:y:143:LEU:HD23 | 1:y:143:LEU:C    | 2.46                     | 0.40              |
| 1:7:127:ARG:NH2  | 1:7:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:I:40:LEU:HA    | 1:M:151:LYS:NZ   | 2.36                     | 0.40              |
| 1:J:166:SER:O    | 1:J:170:ARG:N    | 2.34                     | 0.40              |
| 1:P:127:ARG:NH2  | 1:P:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:d:127:ARG:NH2  | 1:d:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:e:127:ARG:NH2  | 1:e:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:h:127:ARG:NH2  | 1:h:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:l:143:LEU:HD23 | 1:l:143:LEU:C    | 2.46                     | 0.40              |
| 1:m:127:ARG:NH2  | 1:m:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:n:127:ARG:NH2  | 1:n:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:r:88:ARG:O     | 1:r:88:ARG:NE    | 2.43                     | 0.40              |
| 1:w:127:ARG:NH2  | 1:w:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:x:127:ARG:NH2  | 1:x:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:y:127:ARG:NH2  | 1:y:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:1:127:ARG:NH2  | 1:1:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:A:127:ARG:NH2  | 1:A:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:C:127:ARG:NH2  | 1:C:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:I:202:GLN:CB   | 1:N:81:ARG:HH12  | 2.35                     | 0.40              |
| 1:a:127:ARG:NH2  | 1:a:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:d:143:LEU:HD23 | 1:d:143:LEU:C    | 2.46                     | 0.40              |
| 1:e:143:LEU:HD23 | 1:e:143:LEU:C    | 2.46                     | 0.40              |
| 1:f:127:ARG:NH2  | 1:f:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:l:127:ARG:NH2  | 1:l:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:s:127:ARG:NH2  | 1:s:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:v:127:ARG:NH2  | 1:v:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:z:127:ARG:NH2  | 1:z:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:4:127:ARG:NH2  | 1:4:130:LEU:HD11 | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:47:LEU:O     | 1:E:50:THR:OG1   | 2.20                     | 0.40              |
| 1:F:127:ARG:NH2  | 1:F:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:I:39:GLU:HB2   | 1:M:151:LYS:HD3  | 2.02                     | 0.40              |
| 1:L:127:ARG:NH2  | 1:L:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:M:30:GLU:OE2   | 1:M:136:LYS:NZ   | 2.47                     | 0.40              |
| 1:Q:143:LEU:HD23 | 1:Q:143:LEU:C    | 2.46                     | 0.40              |
| 1:U:127:ARG:NH2  | 1:U:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:V:127:ARG:NH2  | 1:V:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:X:93:GLN:O     | 1:X:96:SER:OG    | 2.36                     | 0.40              |
| 1:q:127:ARG:NH2  | 1:q:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:u:93:GLN:O     | 1:u:96:SER:OG    | 2.36                     | 0.40              |
| 1:u:127:ARG:NH2  | 1:u:130:LEU:HD11 | 2.37                     | 0.40              |
| 1:x:47:LEU:O     | 1:x:50:THR:OG1   | 2.20                     | 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   | 0     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 1     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 2     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 3     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 4     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 5     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 6     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 7     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | A     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | B     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | C     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | D     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | E     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | F     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | G     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | H     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | I     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | J     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | K     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | L     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | M     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | N     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | O     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | P     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | R     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | S     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | T     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | U     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | V     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | W     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | X     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | Y     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | Z     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | a     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | b     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | c     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | d     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | e     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | f     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | g     | 194/246 (79%) | 192 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | h     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | i     | 194/246 (79%)     | 191 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | j     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | k     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | l     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | m     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | n     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | o     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | p     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | q     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | r     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | s     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | t     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | u     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | v     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | w     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | x     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | y     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 1   | z     | 194/246 (79%)     | 192 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| All | All   | 11640/14760 (79%) | 11519 (99%) | 121 (1%) | 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   | 0     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 1     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | 2     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 3     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 4     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 5     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 6     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | 7     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | A     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | B     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | C     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | D     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | E     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | F     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | G     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | H     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | I     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | J     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | K     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | L     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | M     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | N     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | O     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | P     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | Q     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | R     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | S     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | T     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | U     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | V     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | W     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | X     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |
| 1   | Y     | 163/208 (78%) | 162 (99%) | 1 (1%)   | 78          | 83 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | Z     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | a     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | b     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | c     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | d     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | e     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | f     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | g     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | h     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | i     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | j     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | k     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | l     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | m     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | n     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | o     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | p     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | q     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | r     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | s     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | t     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | u     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | v     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | w     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | x     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | y     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| 1   | z     | 163/208 (78%)    | 162 (99%)  | 1 (1%)   | 78          | 83 |
| All | All   | 9780/12480 (78%) | 9720 (99%) | 60 (1%)  | 76          | 83 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 177 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 177 | GLU  |
| 1   | 2     | 177 | GLU  |
| 1   | 3     | 177 | GLU  |
| 1   | 4     | 177 | GLU  |
| 1   | 5     | 177 | GLU  |
| 1   | 6     | 177 | GLU  |
| 1   | 7     | 177 | GLU  |
| 1   | A     | 177 | GLU  |
| 1   | B     | 177 | GLU  |
| 1   | C     | 177 | GLU  |
| 1   | D     | 177 | GLU  |
| 1   | E     | 177 | GLU  |
| 1   | F     | 177 | GLU  |
| 1   | G     | 177 | GLU  |
| 1   | H     | 177 | GLU  |
| 1   | I     | 177 | GLU  |
| 1   | J     | 177 | GLU  |
| 1   | K     | 177 | GLU  |
| 1   | L     | 177 | GLU  |
| 1   | M     | 177 | GLU  |
| 1   | N     | 177 | GLU  |
| 1   | O     | 177 | GLU  |
| 1   | P     | 177 | GLU  |
| 1   | Q     | 177 | GLU  |
| 1   | R     | 177 | GLU  |
| 1   | S     | 177 | GLU  |
| 1   | T     | 177 | GLU  |
| 1   | U     | 177 | GLU  |
| 1   | V     | 177 | GLU  |
| 1   | W     | 177 | GLU  |
| 1   | X     | 177 | GLU  |
| 1   | Y     | 177 | GLU  |
| 1   | Z     | 177 | GLU  |
| 1   | a     | 177 | GLU  |
| 1   | b     | 177 | GLU  |
| 1   | c     | 177 | GLU  |
| 1   | d     | 177 | GLU  |
| 1   | e     | 177 | GLU  |
| 1   | f     | 177 | GLU  |
| 1   | g     | 177 | GLU  |
| 1   | h     | 177 | GLU  |
| 1   | i     | 177 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | j     | 177 | GLU  |
| 1   | k     | 177 | GLU  |
| 1   | l     | 177 | GLU  |
| 1   | m     | 177 | GLU  |
| 1   | n     | 177 | GLU  |
| 1   | o     | 177 | GLU  |
| 1   | p     | 177 | GLU  |
| 1   | q     | 177 | GLU  |
| 1   | r     | 177 | GLU  |
| 1   | s     | 177 | GLU  |
| 1   | t     | 177 | GLU  |
| 1   | u     | 177 | GLU  |
| 1   | v     | 177 | GLU  |
| 1   | w     | 177 | GLU  |
| 1   | x     | 177 | GLU  |
| 1   | y     | 177 | GLU  |
| 1   | z     | 177 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (235) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 76  | GLN  |
| 1   | 0     | 85  | GLN  |
| 1   | 0     | 98  | GLN  |
| 1   | 0     | 203 | GLN  |
| 1   | 1     | 76  | GLN  |
| 1   | 1     | 85  | GLN  |
| 1   | 1     | 98  | GLN  |
| 1   | 1     | 203 | GLN  |
| 1   | 2     | 76  | GLN  |
| 1   | 2     | 85  | GLN  |
| 1   | 2     | 98  | GLN  |
| 1   | 2     | 203 | GLN  |
| 1   | 3     | 76  | GLN  |
| 1   | 3     | 85  | GLN  |
| 1   | 3     | 98  | GLN  |
| 1   | 4     | 76  | GLN  |
| 1   | 4     | 85  | GLN  |
| 1   | 4     | 98  | GLN  |
| 1   | 5     | 76  | GLN  |
| 1   | 5     | 85  | GLN  |
| 1   | 5     | 98  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 76  | GLN  |
| 1   | 6     | 85  | GLN  |
| 1   | 6     | 98  | GLN  |
| 1   | 7     | 76  | GLN  |
| 1   | 7     | 85  | GLN  |
| 1   | 7     | 98  | GLN  |
| 1   | A     | 76  | GLN  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 98  | GLN  |
| 1   | A     | 203 | GLN  |
| 1   | B     | 76  | GLN  |
| 1   | B     | 85  | GLN  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 203 | GLN  |
| 1   | C     | 76  | GLN  |
| 1   | C     | 85  | GLN  |
| 1   | C     | 98  | GLN  |
| 1   | C     | 203 | GLN  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 85  | GLN  |
| 1   | D     | 98  | GLN  |
| 1   | D     | 203 | GLN  |
| 1   | E     | 76  | GLN  |
| 1   | E     | 85  | GLN  |
| 1   | E     | 98  | GLN  |
| 1   | E     | 203 | GLN  |
| 1   | F     | 76  | GLN  |
| 1   | F     | 85  | GLN  |
| 1   | F     | 98  | GLN  |
| 1   | F     | 203 | GLN  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 85  | GLN  |
| 1   | G     | 98  | GLN  |
| 1   | G     | 203 | GLN  |
| 1   | H     | 76  | GLN  |
| 1   | H     | 85  | GLN  |
| 1   | H     | 98  | GLN  |
| 1   | H     | 203 | GLN  |
| 1   | I     | 76  | GLN  |
| 1   | I     | 85  | GLN  |
| 1   | I     | 98  | GLN  |
| 1   | J     | 76  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 85  | GLN  |
| 1   | J     | 98  | GLN  |
| 1   | J     | 203 | GLN  |
| 1   | K     | 76  | GLN  |
| 1   | K     | 85  | GLN  |
| 1   | K     | 98  | GLN  |
| 1   | K     | 203 | GLN  |
| 1   | L     | 76  | GLN  |
| 1   | L     | 85  | GLN  |
| 1   | L     | 98  | GLN  |
| 1   | L     | 203 | GLN  |
| 1   | M     | 76  | GLN  |
| 1   | M     | 85  | GLN  |
| 1   | M     | 98  | GLN  |
| 1   | M     | 203 | GLN  |
| 1   | N     | 76  | GLN  |
| 1   | N     | 83  | ASN  |
| 1   | N     | 85  | GLN  |
| 1   | N     | 98  | GLN  |
| 1   | N     | 203 | GLN  |
| 1   | O     | 76  | GLN  |
| 1   | O     | 85  | GLN  |
| 1   | O     | 98  | GLN  |
| 1   | O     | 203 | GLN  |
| 1   | P     | 76  | GLN  |
| 1   | P     | 85  | GLN  |
| 1   | P     | 98  | GLN  |
| 1   | P     | 203 | GLN  |
| 1   | Q     | 76  | GLN  |
| 1   | Q     | 85  | GLN  |
| 1   | Q     | 98  | GLN  |
| 1   | Q     | 203 | GLN  |
| 1   | R     | 76  | GLN  |
| 1   | R     | 85  | GLN  |
| 1   | R     | 98  | GLN  |
| 1   | R     | 203 | GLN  |
| 1   | S     | 76  | GLN  |
| 1   | S     | 85  | GLN  |
| 1   | S     | 98  | GLN  |
| 1   | S     | 203 | GLN  |
| 1   | T     | 76  | GLN  |
| 1   | T     | 85  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 98  | GLN  |
| 1   | T     | 203 | GLN  |
| 1   | U     | 76  | GLN  |
| 1   | U     | 85  | GLN  |
| 1   | U     | 98  | GLN  |
| 1   | U     | 203 | GLN  |
| 1   | V     | 76  | GLN  |
| 1   | V     | 85  | GLN  |
| 1   | V     | 98  | GLN  |
| 1   | V     | 203 | GLN  |
| 1   | W     | 76  | GLN  |
| 1   | W     | 85  | GLN  |
| 1   | W     | 98  | GLN  |
| 1   | W     | 203 | GLN  |
| 1   | X     | 76  | GLN  |
| 1   | X     | 85  | GLN  |
| 1   | X     | 98  | GLN  |
| 1   | X     | 203 | GLN  |
| 1   | Y     | 76  | GLN  |
| 1   | Y     | 85  | GLN  |
| 1   | Y     | 98  | GLN  |
| 1   | Y     | 203 | GLN  |
| 1   | Z     | 76  | GLN  |
| 1   | Z     | 85  | GLN  |
| 1   | Z     | 98  | GLN  |
| 1   | Z     | 203 | GLN  |
| 1   | a     | 76  | GLN  |
| 1   | a     | 85  | GLN  |
| 1   | a     | 98  | GLN  |
| 1   | a     | 203 | GLN  |
| 1   | b     | 76  | GLN  |
| 1   | b     | 85  | GLN  |
| 1   | b     | 98  | GLN  |
| 1   | b     | 203 | GLN  |
| 1   | c     | 76  | GLN  |
| 1   | c     | 85  | GLN  |
| 1   | c     | 98  | GLN  |
| 1   | c     | 203 | GLN  |
| 1   | d     | 76  | GLN  |
| 1   | d     | 85  | GLN  |
| 1   | d     | 98  | GLN  |
| 1   | d     | 203 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 76  | GLN  |
| 1   | e     | 85  | GLN  |
| 1   | e     | 98  | GLN  |
| 1   | e     | 203 | GLN  |
| 1   | f     | 76  | GLN  |
| 1   | f     | 85  | GLN  |
| 1   | f     | 98  | GLN  |
| 1   | f     | 203 | GLN  |
| 1   | g     | 76  | GLN  |
| 1   | g     | 85  | GLN  |
| 1   | g     | 98  | GLN  |
| 1   | g     | 203 | GLN  |
| 1   | h     | 76  | GLN  |
| 1   | h     | 85  | GLN  |
| 1   | h     | 98  | GLN  |
| 1   | h     | 203 | GLN  |
| 1   | i     | 76  | GLN  |
| 1   | i     | 85  | GLN  |
| 1   | i     | 98  | GLN  |
| 1   | i     | 203 | GLN  |
| 1   | j     | 76  | GLN  |
| 1   | j     | 85  | GLN  |
| 1   | j     | 98  | GLN  |
| 1   | j     | 203 | GLN  |
| 1   | k     | 76  | GLN  |
| 1   | k     | 85  | GLN  |
| 1   | k     | 98  | GLN  |
| 1   | k     | 203 | GLN  |
| 1   | l     | 76  | GLN  |
| 1   | l     | 85  | GLN  |
| 1   | l     | 98  | GLN  |
| 1   | l     | 203 | GLN  |
| 1   | m     | 76  | GLN  |
| 1   | m     | 85  | GLN  |
| 1   | m     | 98  | GLN  |
| 1   | m     | 203 | GLN  |
| 1   | n     | 76  | GLN  |
| 1   | n     | 85  | GLN  |
| 1   | n     | 98  | GLN  |
| 1   | n     | 203 | GLN  |
| 1   | o     | 76  | GLN  |
| 1   | o     | 85  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | o     | 98  | GLN  |
| 1   | o     | 203 | GLN  |
| 1   | p     | 76  | GLN  |
| 1   | p     | 85  | GLN  |
| 1   | p     | 98  | GLN  |
| 1   | p     | 203 | GLN  |
| 1   | q     | 76  | GLN  |
| 1   | q     | 85  | GLN  |
| 1   | q     | 98  | GLN  |
| 1   | q     | 203 | GLN  |
| 1   | r     | 76  | GLN  |
| 1   | r     | 85  | GLN  |
| 1   | r     | 98  | GLN  |
| 1   | r     | 203 | GLN  |
| 1   | s     | 76  | GLN  |
| 1   | s     | 85  | GLN  |
| 1   | s     | 98  | GLN  |
| 1   | s     | 203 | GLN  |
| 1   | t     | 76  | GLN  |
| 1   | t     | 85  | GLN  |
| 1   | t     | 98  | GLN  |
| 1   | t     | 203 | GLN  |
| 1   | u     | 76  | GLN  |
| 1   | u     | 85  | GLN  |
| 1   | u     | 98  | GLN  |
| 1   | u     | 203 | GLN  |
| 1   | v     | 76  | GLN  |
| 1   | v     | 85  | GLN  |
| 1   | v     | 98  | GLN  |
| 1   | v     | 203 | GLN  |
| 1   | w     | 76  | GLN  |
| 1   | w     | 85  | GLN  |
| 1   | w     | 98  | GLN  |
| 1   | w     | 203 | GLN  |
| 1   | x     | 76  | GLN  |
| 1   | x     | 85  | GLN  |
| 1   | x     | 98  | GLN  |
| 1   | x     | 203 | GLN  |
| 1   | y     | 76  | GLN  |
| 1   | y     | 85  | GLN  |
| 1   | y     | 98  | GLN  |
| 1   | y     | 203 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | z     | 76  | GLN  |
| 1   | z     | 85  | GLN  |
| 1   | z     | 98  | GLN  |
| 1   | z     | 203 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

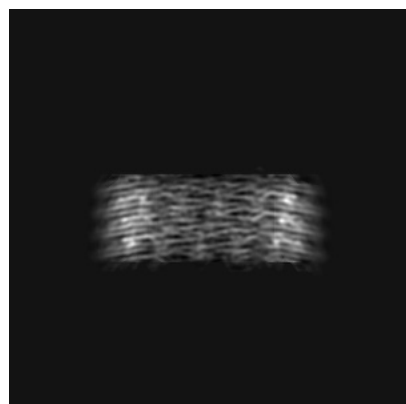
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15496. These allow visual inspection of the internal detail of the map and identification of artifacts.

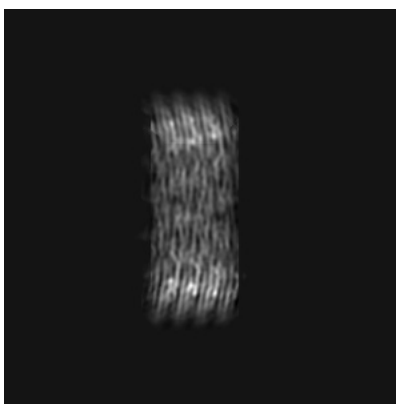
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

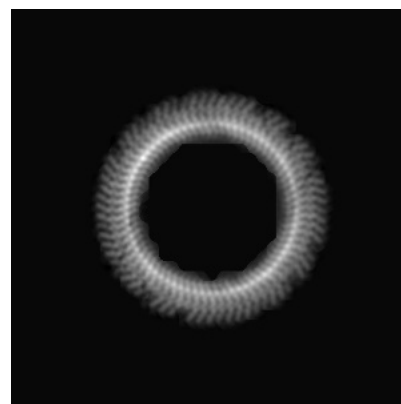
#### 6.1.1 Primary map



X

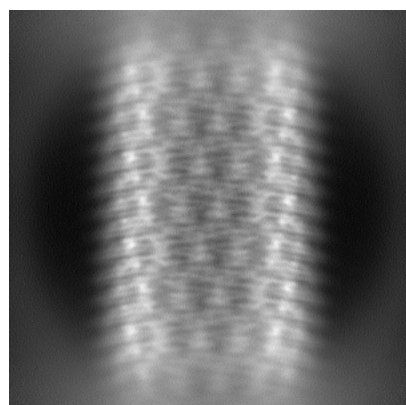


Y

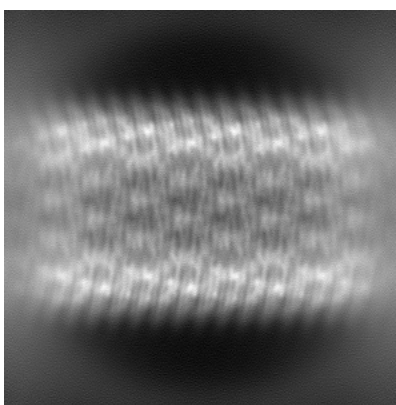


Z

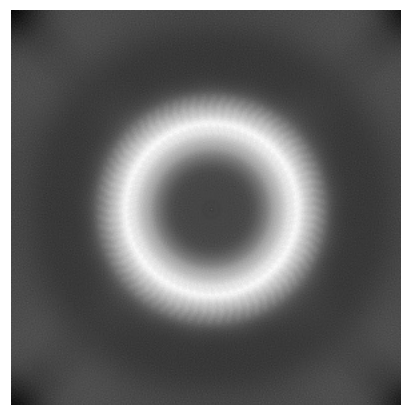
#### 6.1.2 Raw map



X



Y

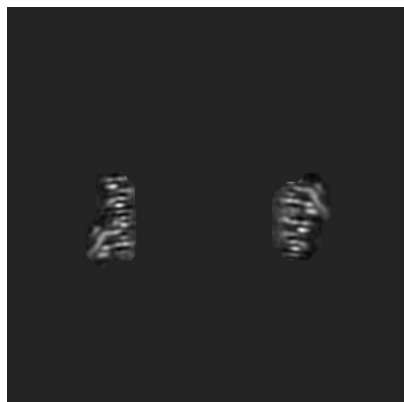


Z

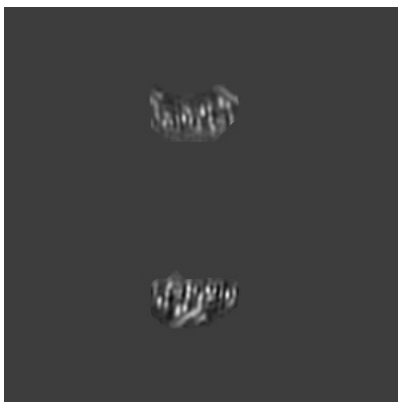
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

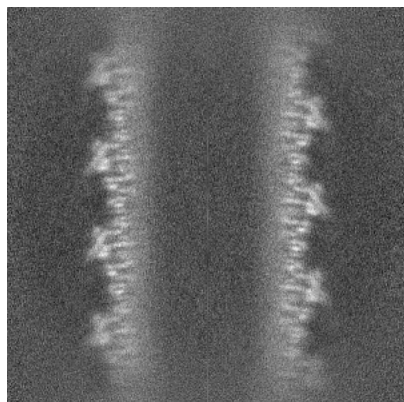


Y Index: 200

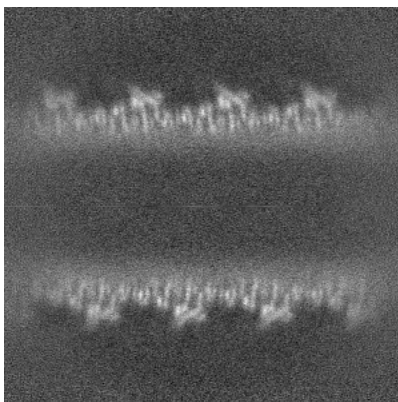


Z Index: 200

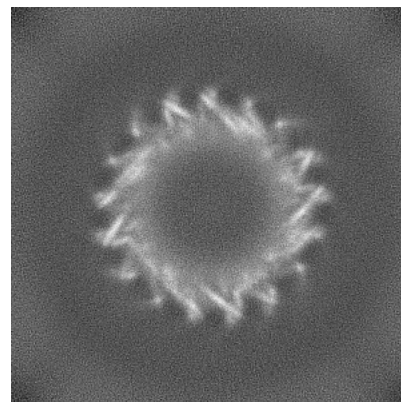
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

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

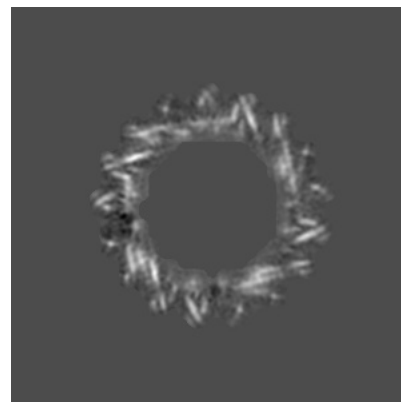
### 6.3.1 Primary map



X Index: 117

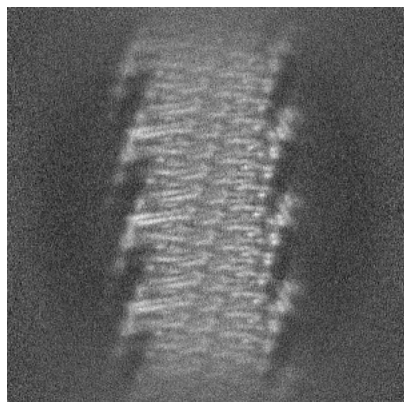


Y Index: 117

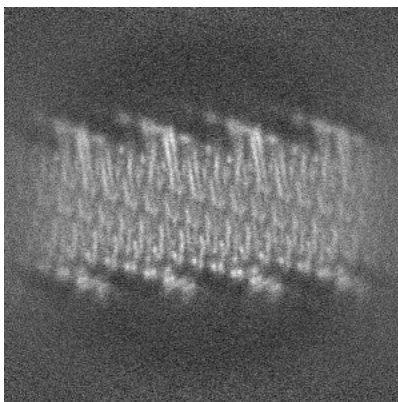


Z Index: 192

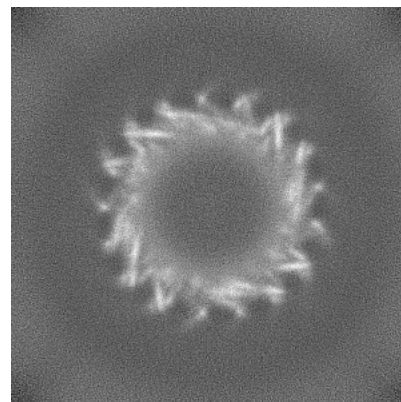
### 6.3.2 Raw map



X Index: 122



Y Index: 122

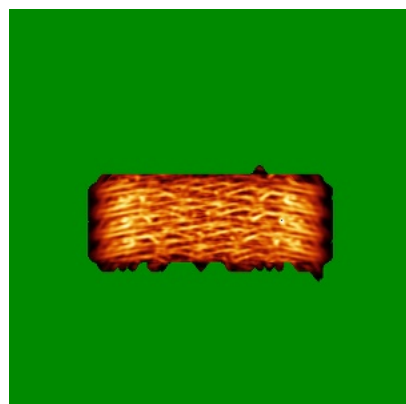


Z Index: 187

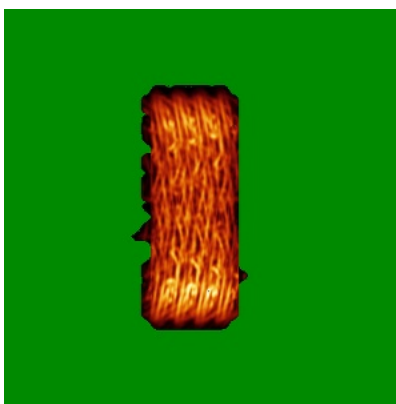
The images above show the largest variance slices of the map in three orthogonal directions.

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

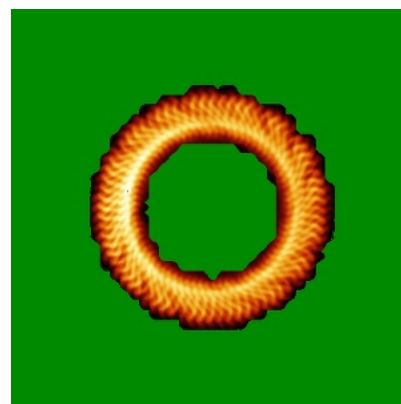
### 6.4.1 Primary map



X

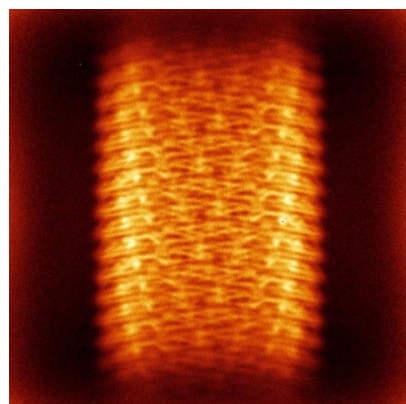


Y

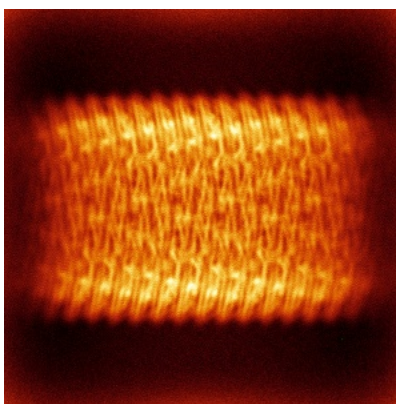


Z

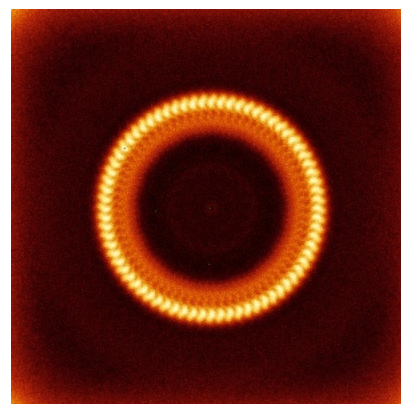
### 6.4.2 Raw map



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.

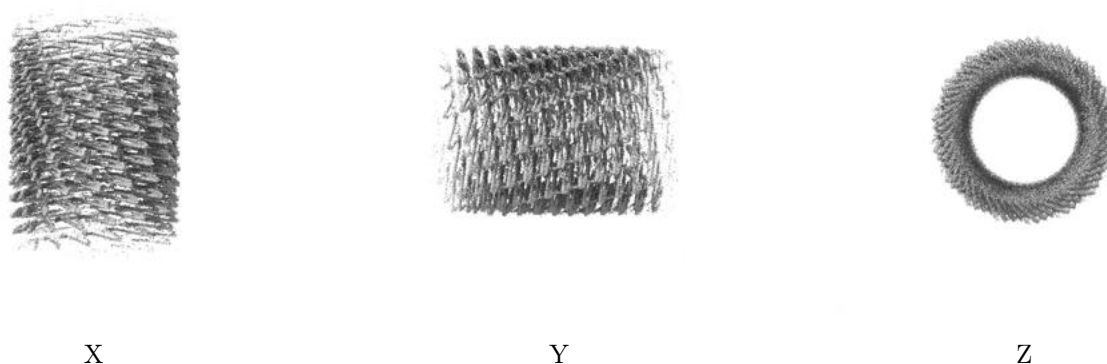
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

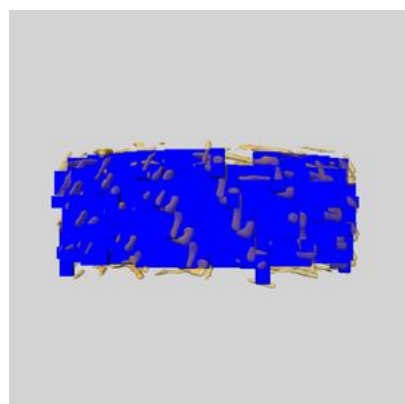
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

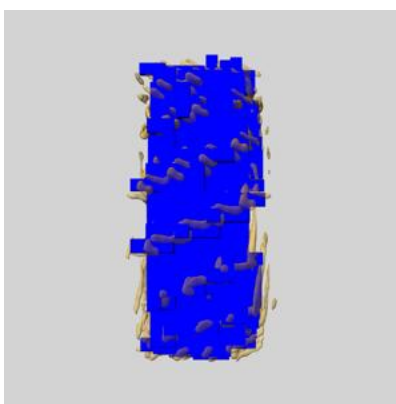
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

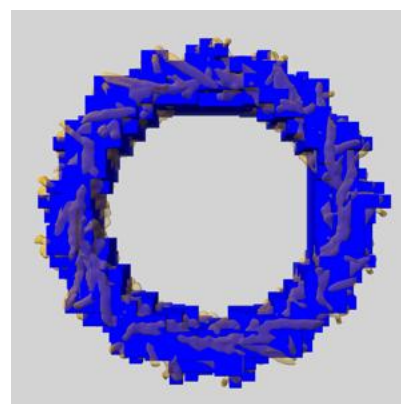
### 6.6.1 emd\_15496\_msk\_1.map [i](#)



X



Y

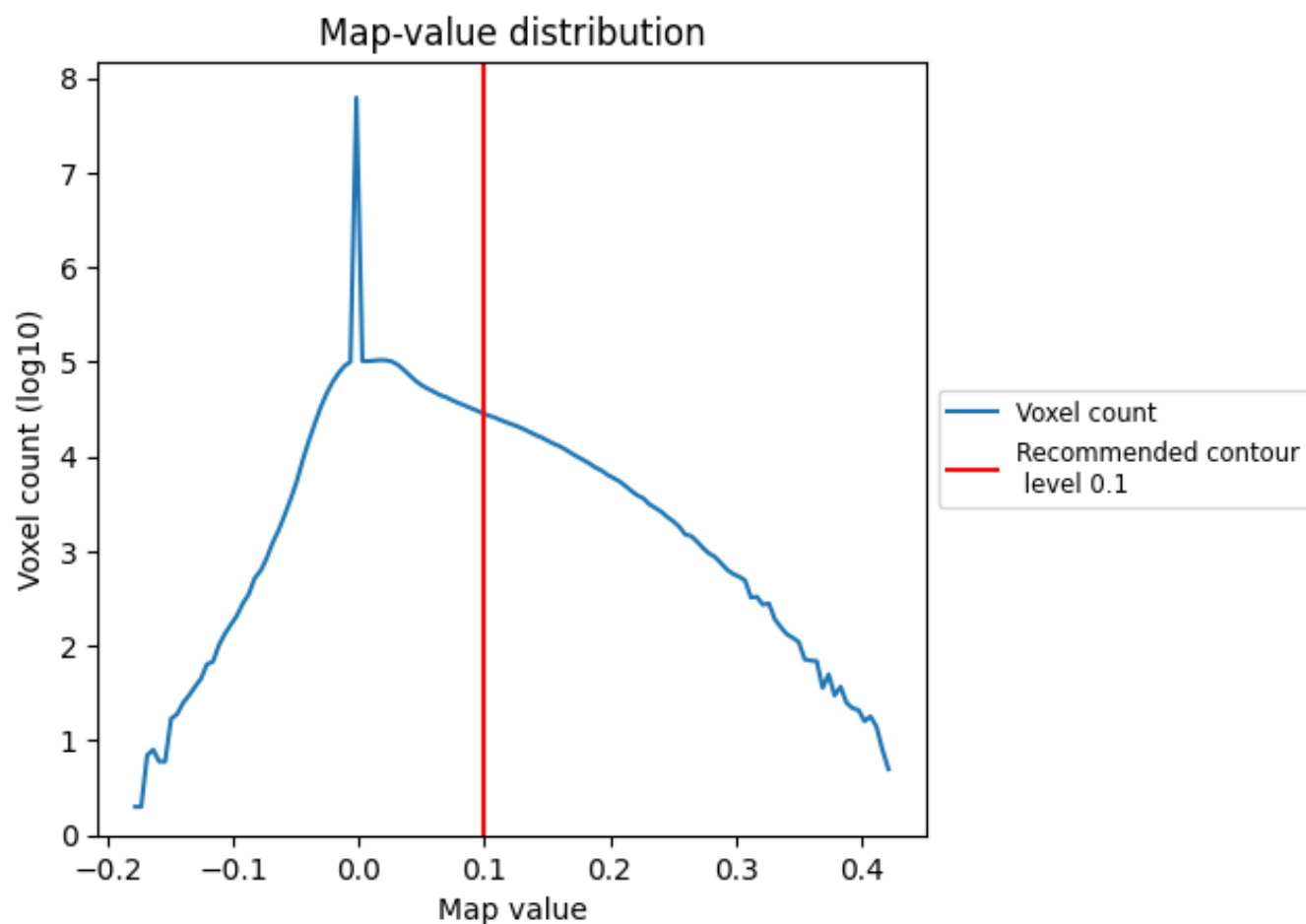


Z

## 7 Map analysis [i](#)

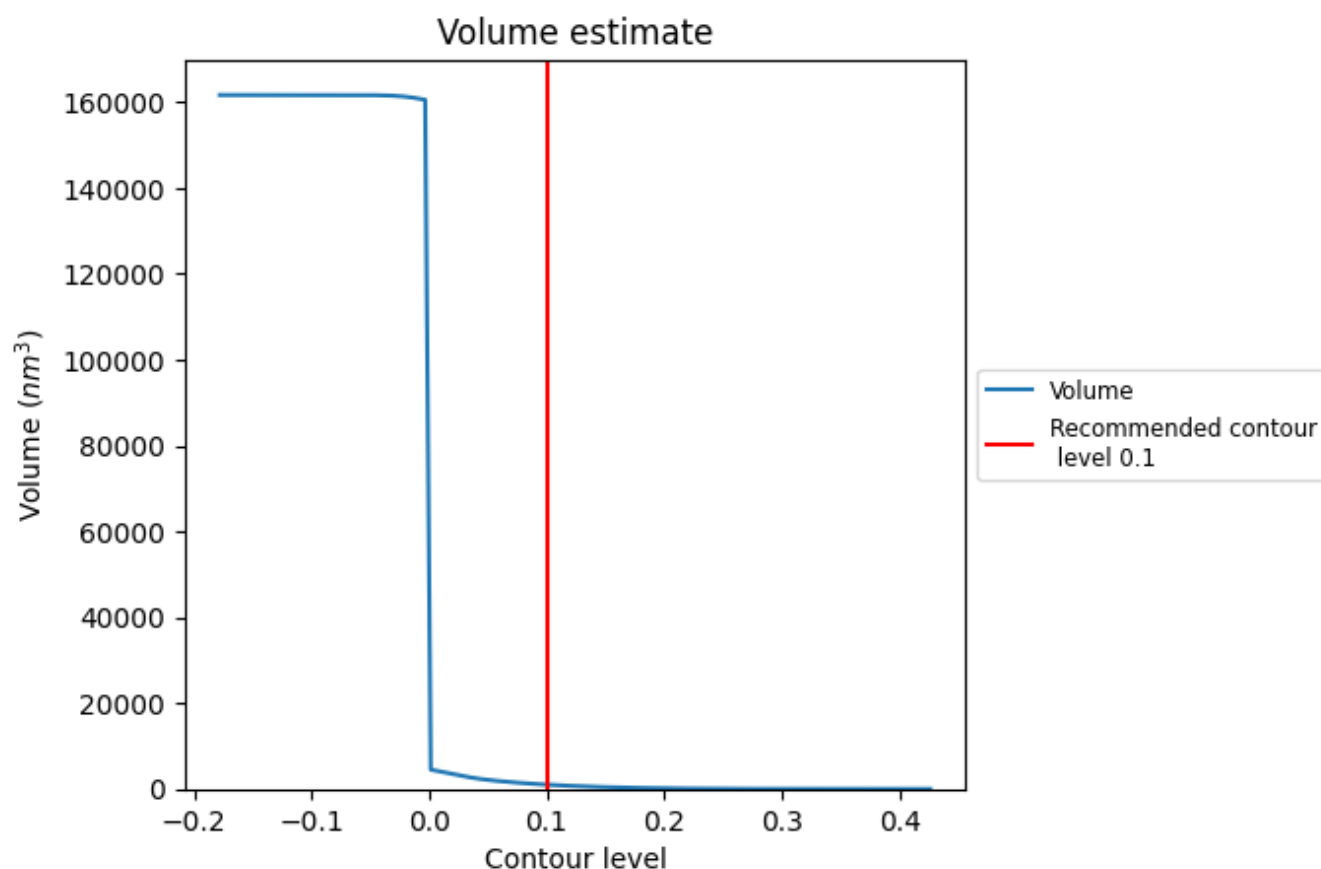
This section contains the results of statistical analysis of the map.

### 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.

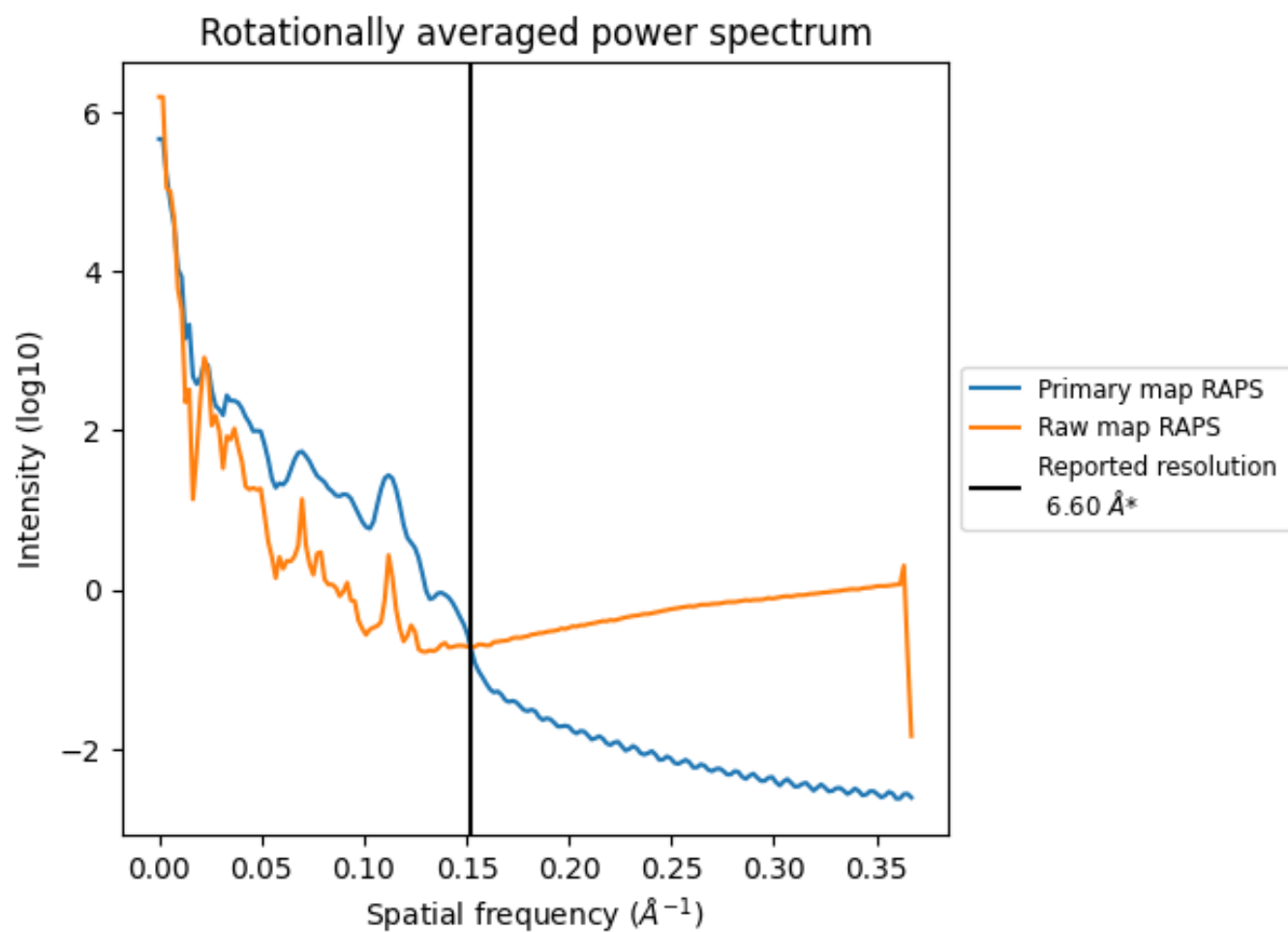
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1009  $\text{nm}^3$ ; this corresponds to an approximate mass of 911 kDa.

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

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

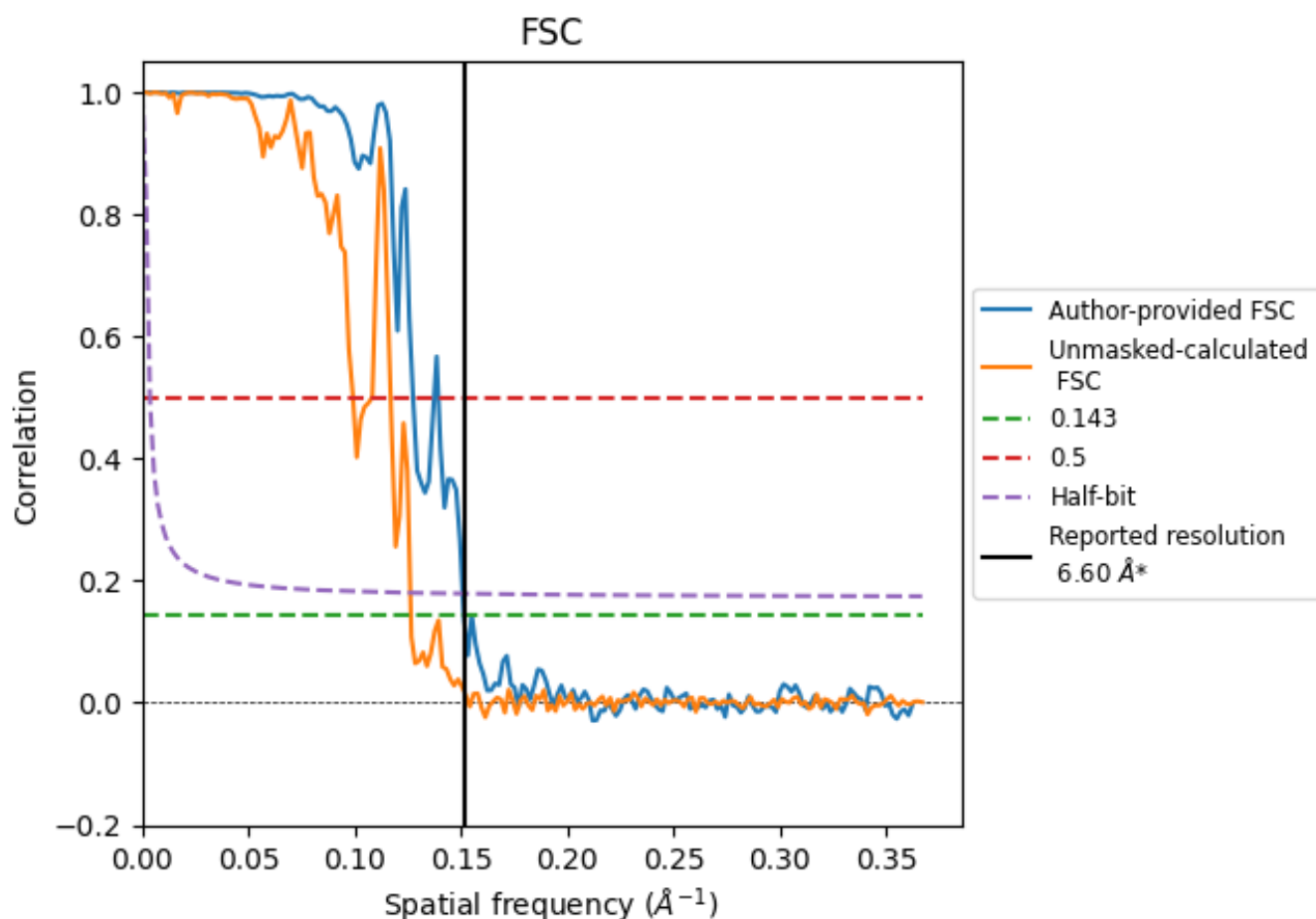


\*Reported resolution corresponds to spatial frequency of  $0.152 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.152  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

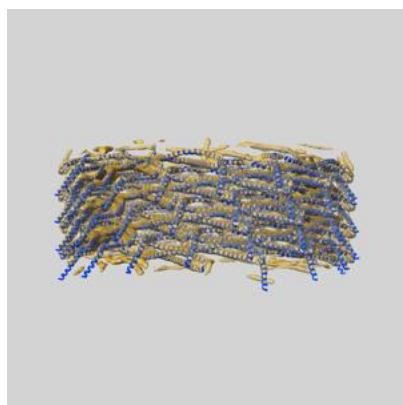
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 6.60                               | -     | -        |
| Author-provided FSC curve | 6.61                               | 7.84  | 6.63     |
| Unmasked-calculated*      | 7.91                               | 10.08 | 7.92     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.91 differs from the reported value 6.6 by more than 10 %

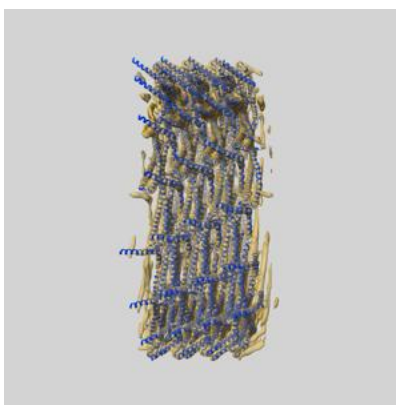
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15496 and PDB model 8AKX. Per-residue inclusion information can be found in section [3](#) on page [42](#).

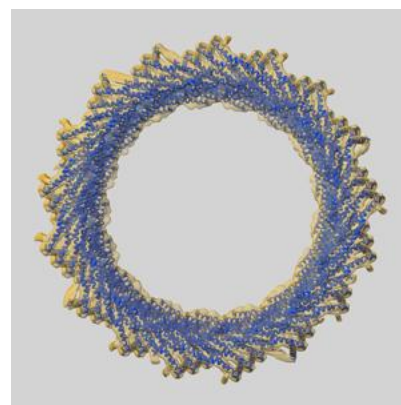
### 9.1 Map-model overlay [i](#)



X



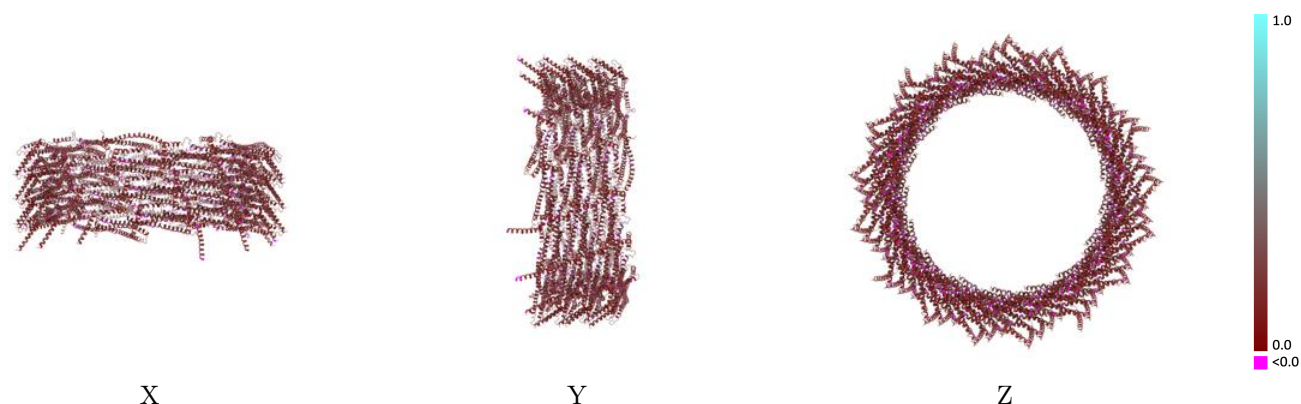
Y



Z

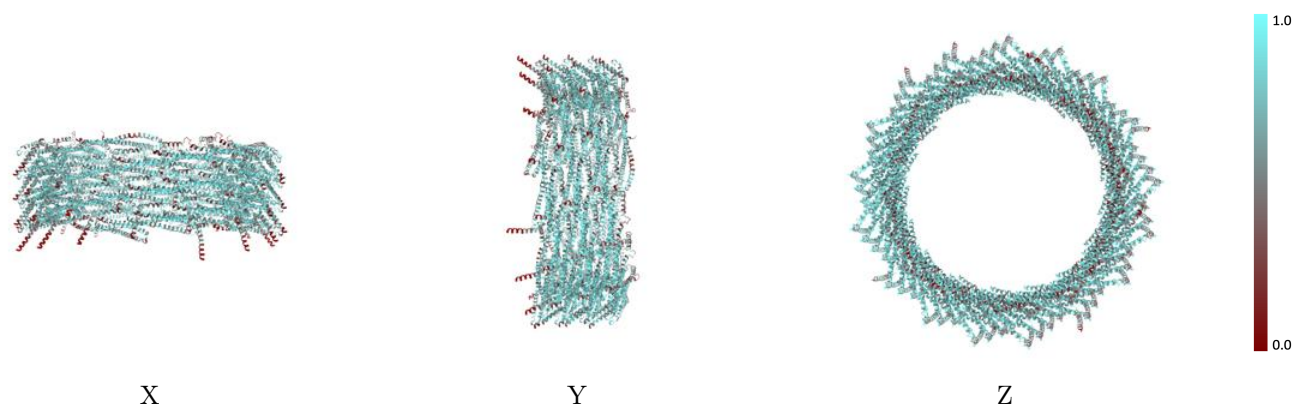
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



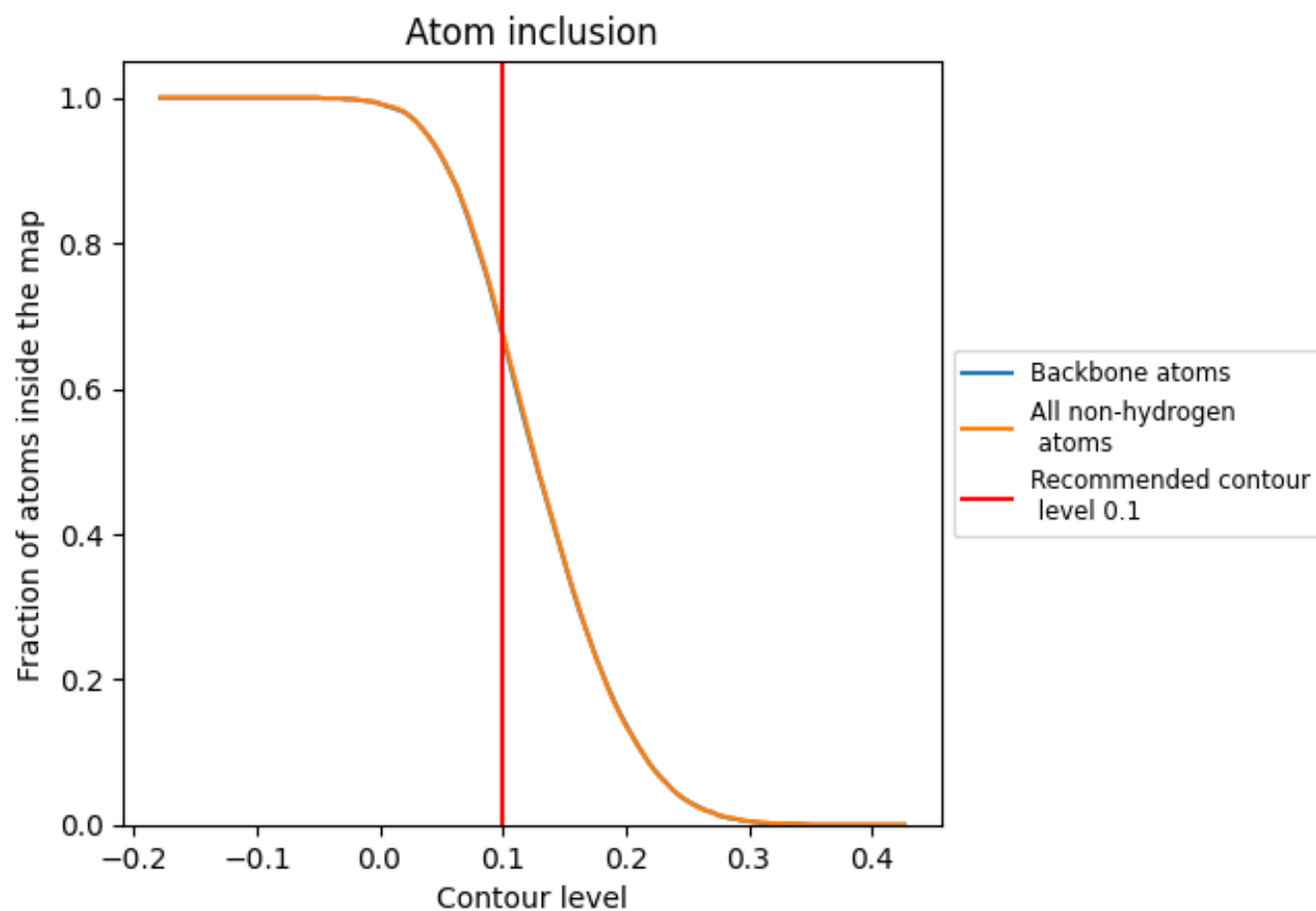
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6770   |  0.1900   |
| 0     |  0.6150   |  0.1890   |
| 1     |  0.6390   |  0.1910   |
| 2     |  0.6710   |  0.1890   |
| 3     |  0.6760   |  0.1890   |
| 4     |  0.5620   |  0.1940   |
| 5     |  0.5610   |  0.1900   |
| 6     |  0.6060   |  0.1900   |
| 7     |  0.6400   |  0.1910   |
| A     |  0.6160   |  0.1880   |
| B     |  0.5700   |  0.1900   |
| C     |  0.5710   |  0.1910   |
| D     |  0.6160   |  0.1860   |
| E     |  0.6690   |  0.1860   |
| F     |  0.6210  |  0.1920  |
| G     |  0.6080 |  0.1900 |
| H     |  0.6400 |  0.1890 |
| I     |  0.6990 |  0.1830 |
| J     |  0.6790 |  0.1870 |
| K     |  0.6470 |  0.1910 |
| L     |  0.6820 |  0.1880 |
| M     |  0.7330 |  0.1880 |
| N     |  0.7110 |  0.1890 |
| O     |  0.6730 |  0.1870 |
| P     |  0.7040 |  0.1910 |
| Q     |  0.7290 |  0.1880 |
| R     |  0.7470 |  0.1890 |
| S     |  0.7170 |  0.1900 |
| T     |  0.7150 |  0.1900 |
| U     |  0.7390 |  0.1890 |
| V     |  0.7510 |  0.1900 |
| W     |  0.7180 |  0.1930 |
| X     |  0.7070 |  0.1910 |
| Y     |  0.7310 |  0.1890 |
| Z     |  0.7550 |  0.1900 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.7330   |  0.1900   |
| b     |  0.7050   |  0.1910   |
| c     |  0.7300   |  0.1890   |
| d     |  0.7580   |  0.1870   |
| e     |  0.7400   |  0.1910   |
| f     |  0.7070   |  0.1890   |
| g     |  0.7180   |  0.1910   |
| h     |  0.7490   |  0.1870   |
| i     |  0.7420   |  0.1900   |
| j     |  0.7110   |  0.1900   |
| k     |  0.7180   |  0.1910   |
| l     |  0.7420   |  0.1870   |
| m     |  0.7560   |  0.1890   |
| n     |  0.7140   |  0.1940   |
| o     |  0.7020   |  0.1910   |
| p     |  0.7270   |  0.1880   |
| q     |  0.7500   |  0.1890   |
| r     |  0.7120   |  0.1900   |
| s     |  0.6840   |  0.1930   |
| t     |  0.7160  |  0.1900  |
| u     |  0.7460 |  0.1890 |
| v     |  0.6950 |  0.1900 |
| w     |  0.6580 |  0.1900 |
| x     |  0.6660 |  0.1910 |
| y     |  0.7140 |  0.1880 |
| z     |  0.6670 |  0.1900 |