



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:51 PM UTC

PDB ID : 9K89 / pdb\_00009k89  
EMDB ID : EMD-62165  
Title : Cryo-EM structure of designed zinc-induced icosahedron Cage-i53-Zn1-HEHE-6  
Authors : Qu, Y.N.; Cao, L.X.  
Deposited on : 2024-10-24  
Resolution : 3.17 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

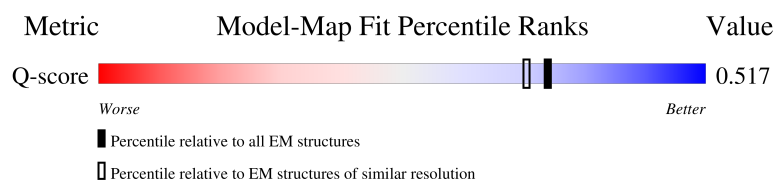
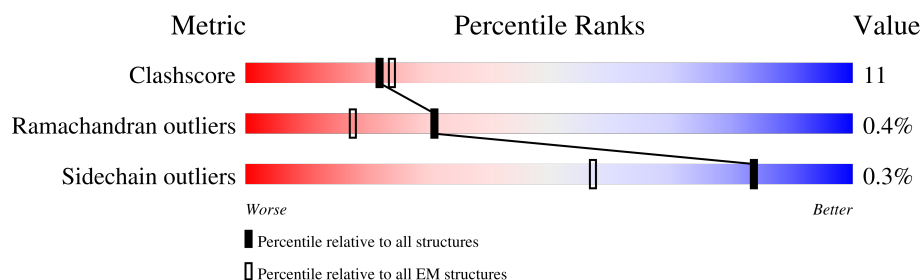
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.17 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.



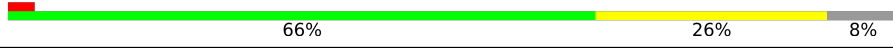
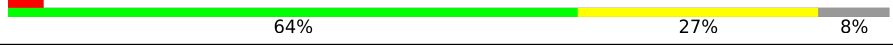
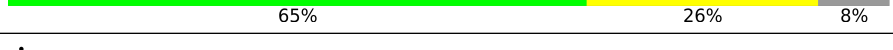
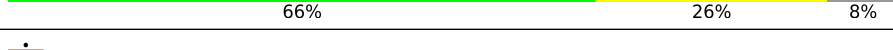
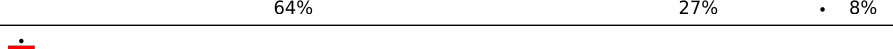
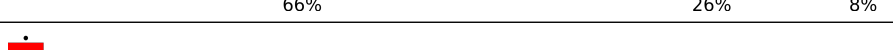
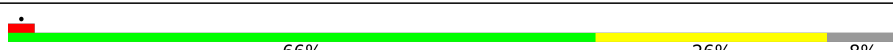
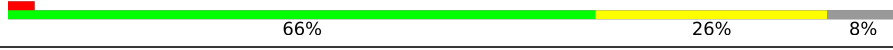
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14465 ( 2.67 - 3.67 )                                    |

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     | 281    |                  |
| 1   | 1     | 281    |                  |
| 1   | 2     | 281    |                  |
| 1   | 3     | 281    |                  |

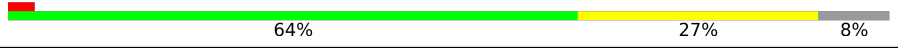
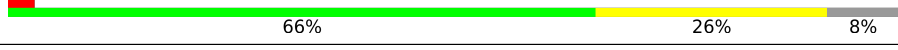
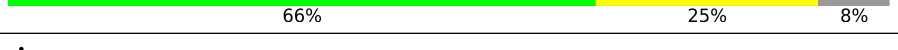
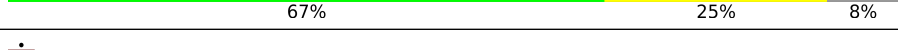
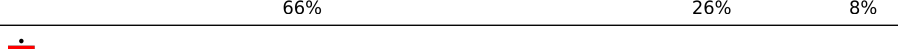
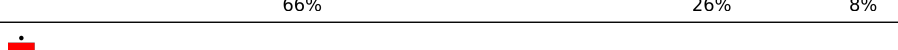
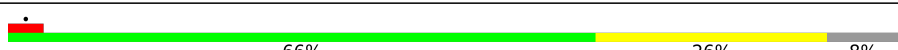
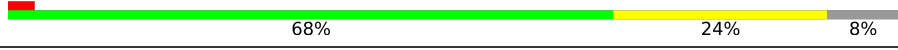
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 4     | 281    |    |
| 1   | 5     | 281    |    |
| 1   | 6     | 281    |    |
| 1   | 7     | 281    |    |
| 1   | A     | 281    |    |
| 1   | B     | 281    |    |
| 1   | C     | 281    |    |
| 1   | D     | 281    |    |
| 1   | E     | 281    |    |
| 1   | F     | 281    |    |
| 1   | G     | 281    |    |
| 1   | H     | 281    |  |
| 1   | I     | 281    |  |
| 1   | J     | 281    |  |
| 1   | K     | 281    |  |
| 1   | L     | 281    |  |
| 1   | M     | 281    |  |
| 1   | N     | 281    |  |
| 1   | O     | 281    |  |
| 1   | P     | 281    |  |
| 1   | Q     | 281    |  |
| 1   | R     | 281    |  |
| 1   | S     | 281    |  |
| 1   | T     | 281    |  |
| 1   | U     | 281    |  |

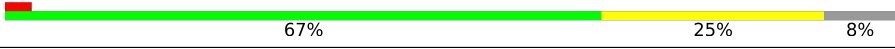
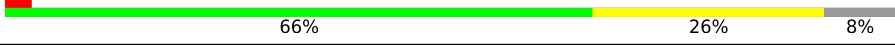
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | V     | 281    |    |
| 1   | W     | 281    |    |
| 1   | X     | 281    |    |
| 1   | Y     | 281    |    |
| 1   | Z     | 281    |    |
| 1   | a     | 281    |    |
| 1   | b     | 281    |    |
| 1   | c     | 281    |    |
| 1   | d     | 281    |    |
| 1   | e     | 281    |    |
| 1   | f     | 281    |    |
| 1   | g     | 281    |  |
| 1   | h     | 281    |  |
| 1   | i     | 281    |  |
| 1   | j     | 281    |  |
| 1   | k     | 281    |  |
| 1   | l     | 281    |  |
| 1   | m     | 281    |  |
| 1   | n     | 281    |  |
| 1   | o     | 281    |  |
| 1   | p     | 281    |  |
| 1   | q     | 281    |  |
| 1   | r     | 281    |  |
| 1   | s     | 281    |  |
| 1   | t     | 281    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | u     | 281    |  |
| 1   | v     | 281    |  |
| 1   | w     | 281    |  |
| 1   | x     | 281    |  |
| 1   | y     | 281    |  |
| 1   | z     | 281    |  |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 122160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cage-i53-Zn1-HEHE-6.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | A     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | B     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | C     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | D     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | E     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | F     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | Q     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | b     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | m     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | x     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | G     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | R     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | c     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | n     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | y     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | H     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | S     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | d     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | o     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | z     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | I     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | T     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | e     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | p     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 0     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | J     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | U     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | f     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | q     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 1     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | K     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | V     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | g     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | r     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 2     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | L     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | W     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | h     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | s     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 3     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | M     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | X     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | i     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | t     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 4     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | N     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | Y     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | j     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | u     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 5     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | O     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | Z     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | k     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | v     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | 6     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | P     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | a     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | l     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |
| 1   | w     | 258      | Total<br>2034 | C<br>1284 | N<br>382 | O<br>365 | S<br>3 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | 7     | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2034  | 1284 | 382 | 365 | 3 |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | A     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |
| 2   | B     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | C     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | D     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | F     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |
| 2   | Q     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | b     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | m     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |
| 2   | x     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | G     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | R     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |
| 2   | c     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | n     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | H     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | S     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 2   | d     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 2   | o     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | z     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | I     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | T     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | e     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | p     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 0     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | J     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | U     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | f     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | q     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 1     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | K     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | V     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | g     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | r     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 2     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | L     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | W     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | h     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | s     | 1        | Total<br>1 | Zn<br>1 | 0       |

*Continued on next page...*

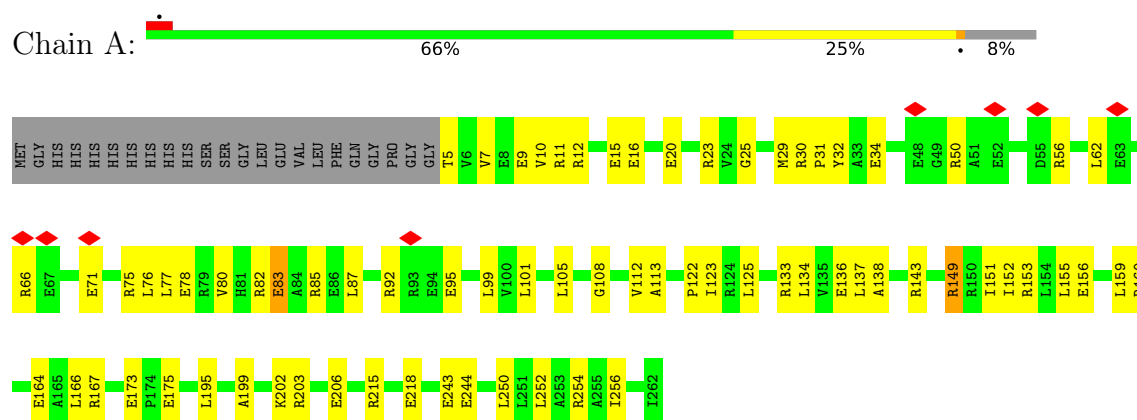
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 2   | 3     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | M     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | X     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | i     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | t     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 4     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | N     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | Y     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | j     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | u     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 5     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | O     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | Z     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | k     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | v     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | 6     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | P     | 3        | Total<br>3 | Zn<br>3 | 0       |
| 2   | a     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | l     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 2   | w     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | 7     | 2        | Total<br>2 | Zn<br>2 | 0       |

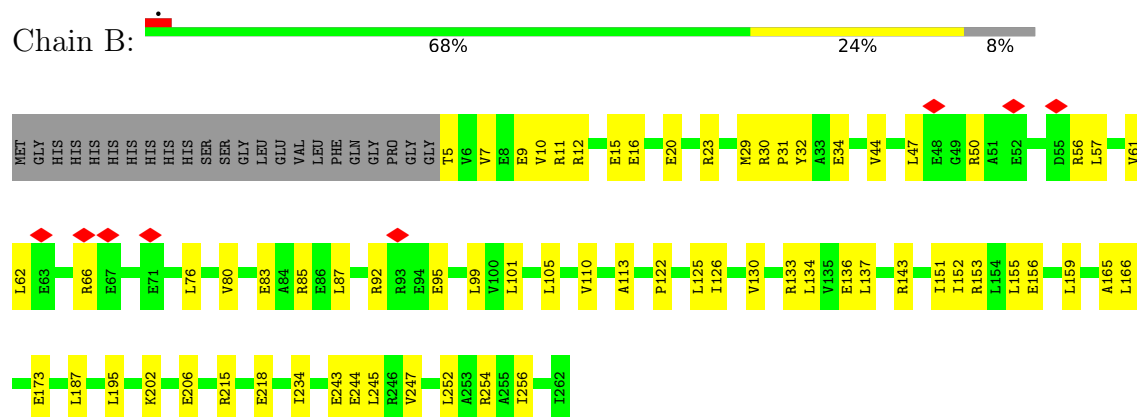
### 3 Residue-property plots

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

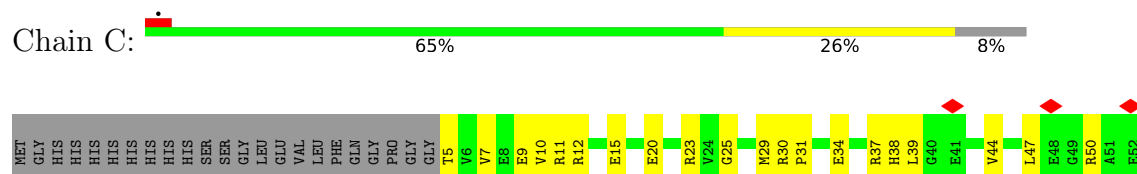
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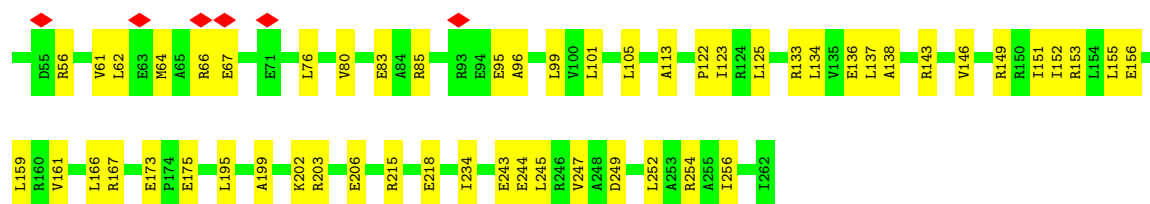


#### • Molecule 1: Cage-i53-Zn1-HEHE-6

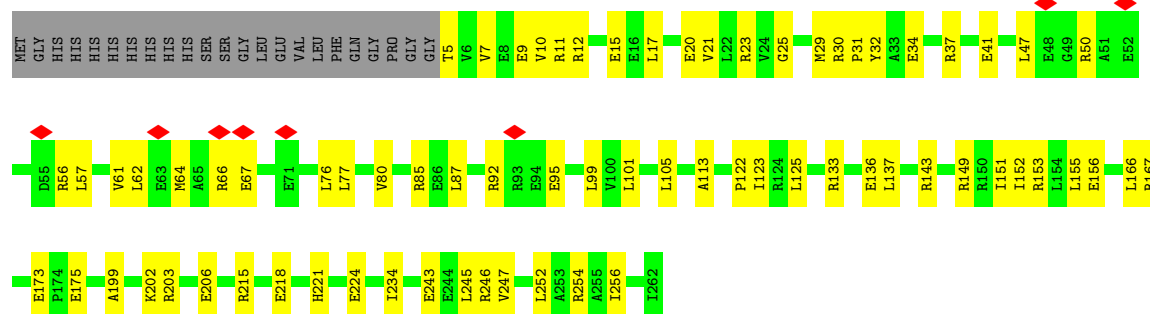


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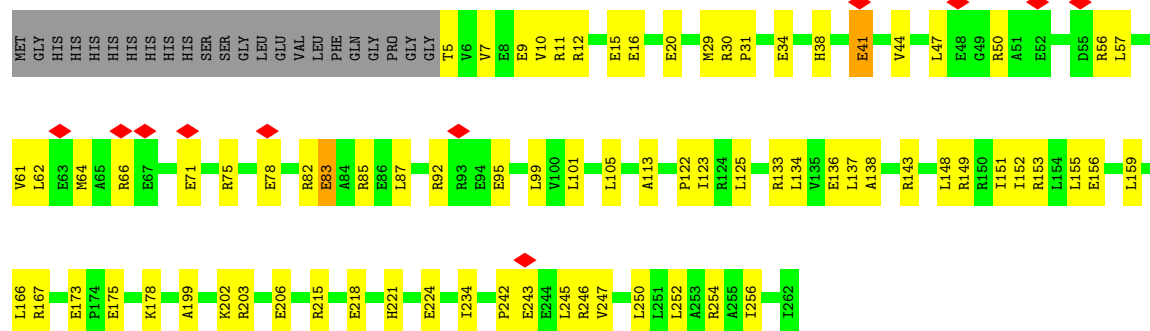




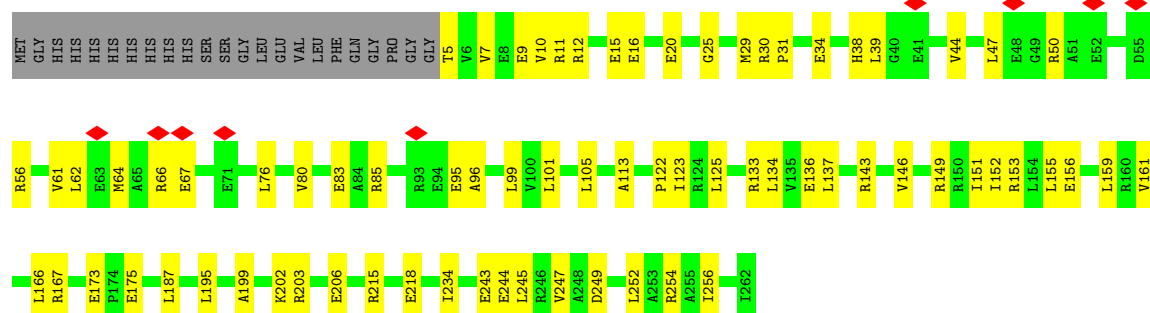
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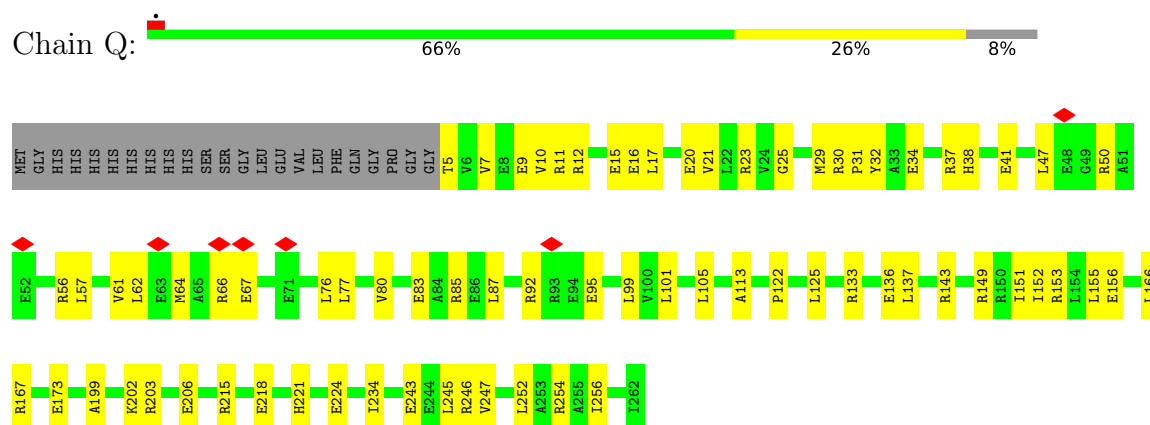
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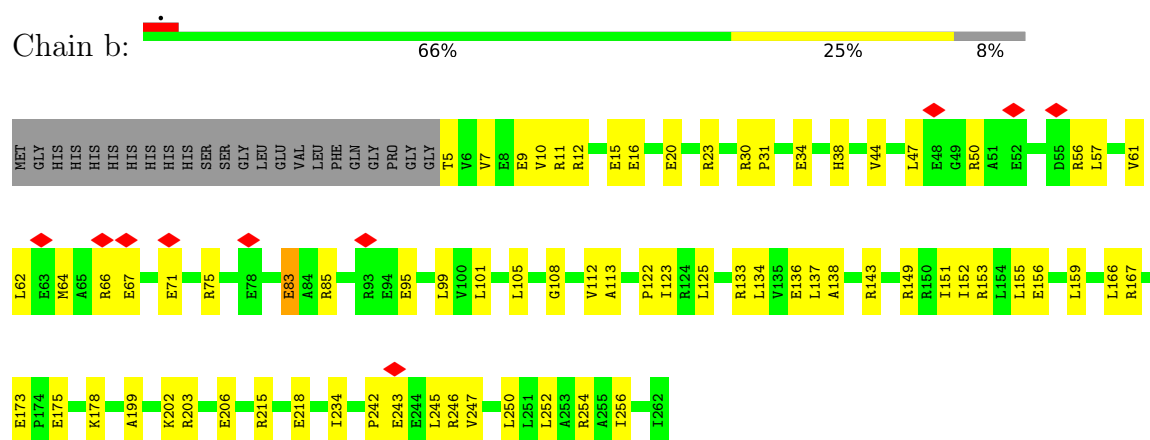
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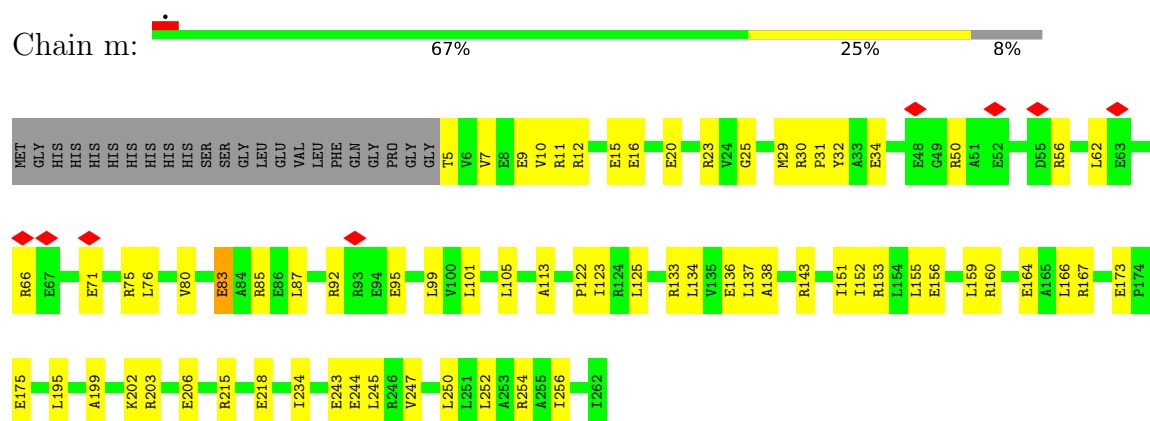
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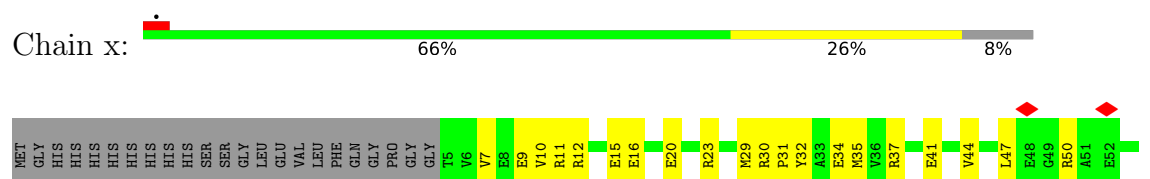
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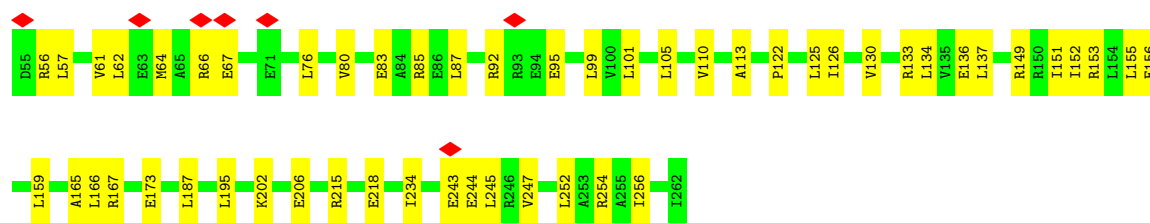


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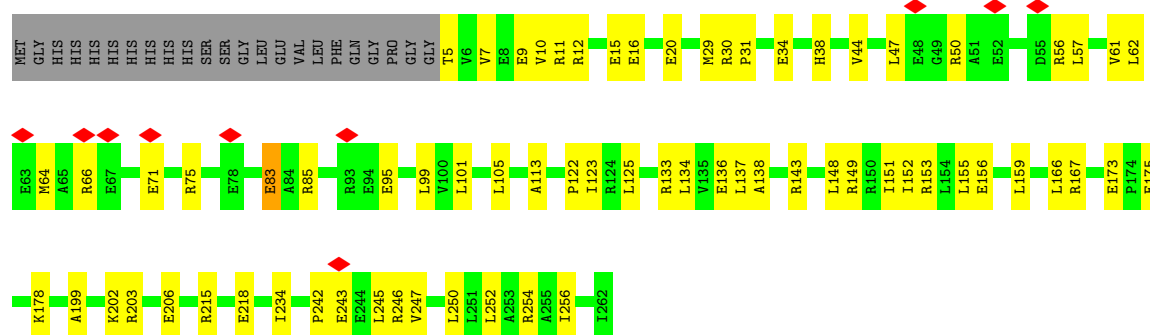


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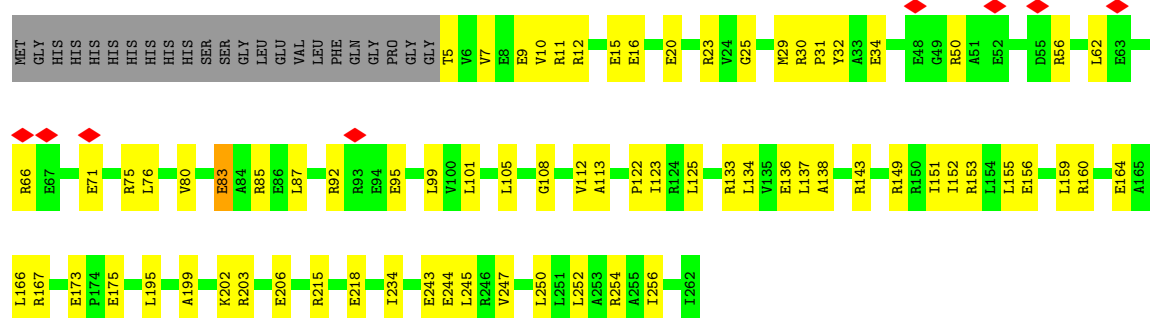




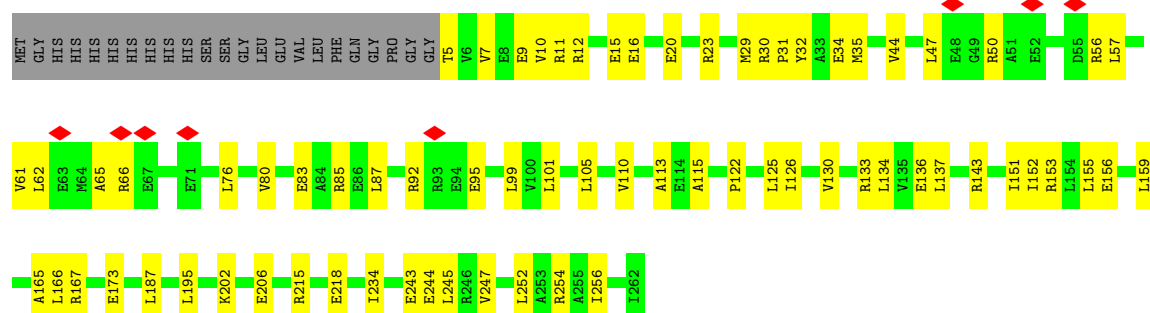
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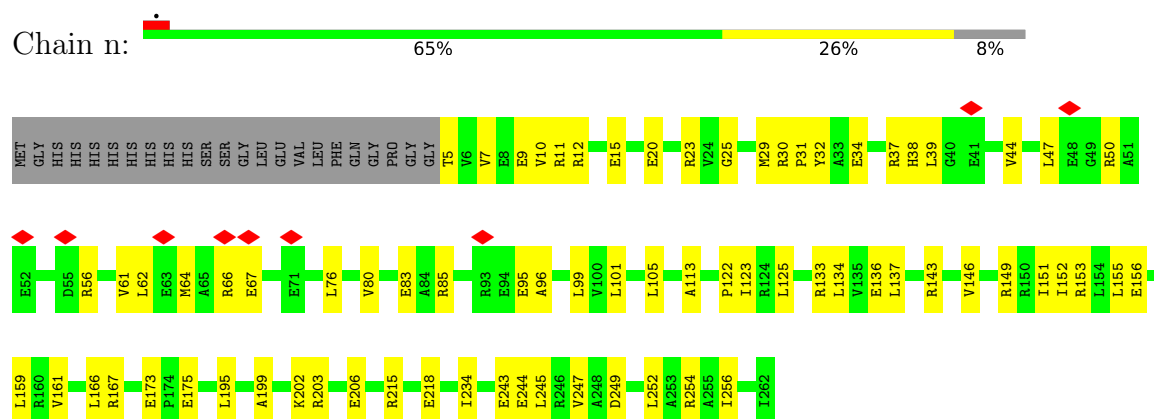
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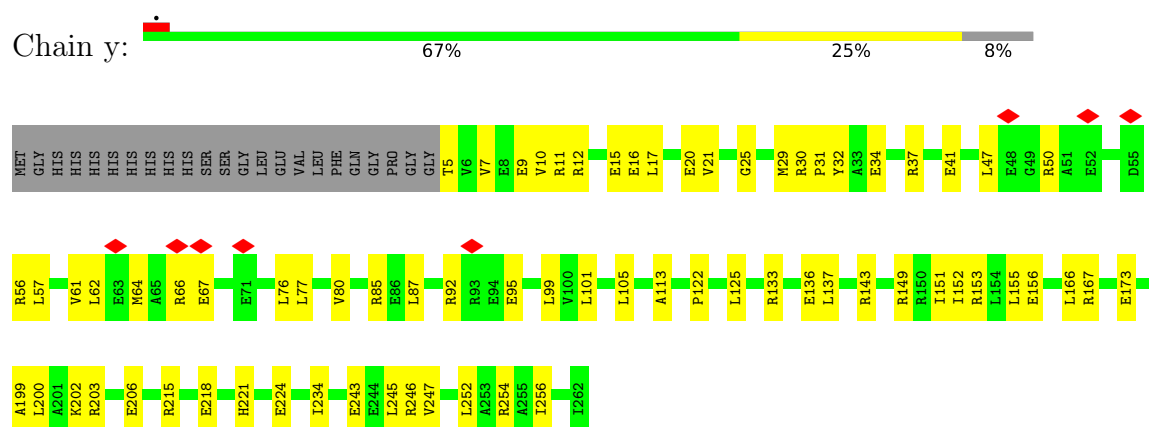
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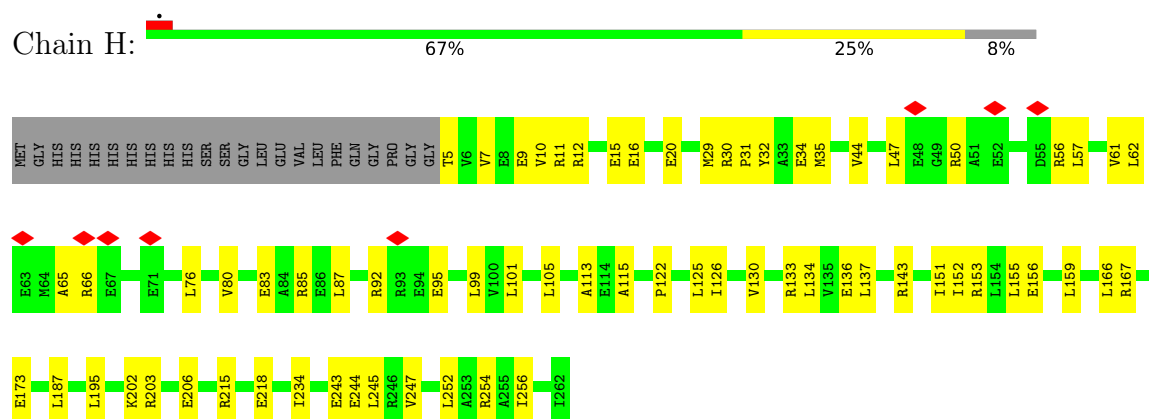
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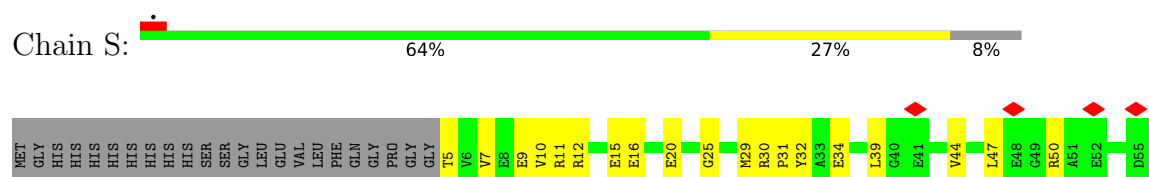
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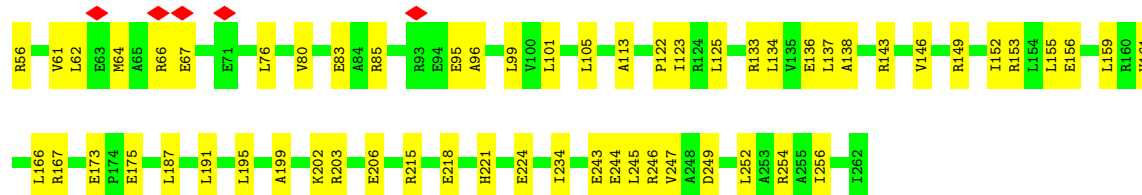


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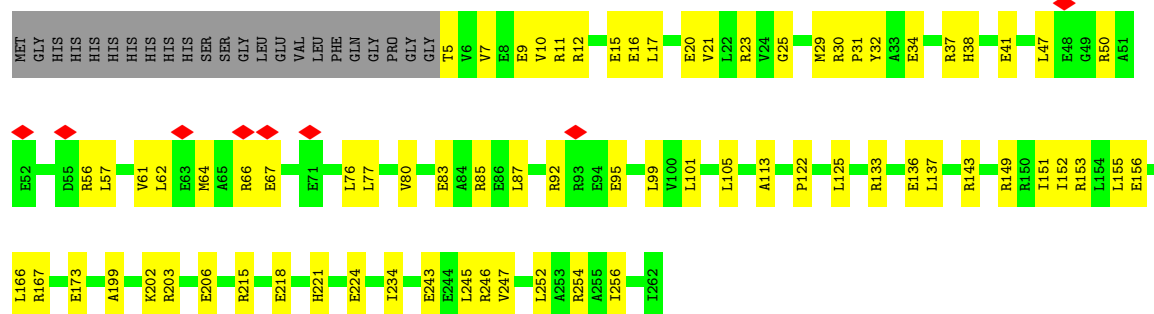


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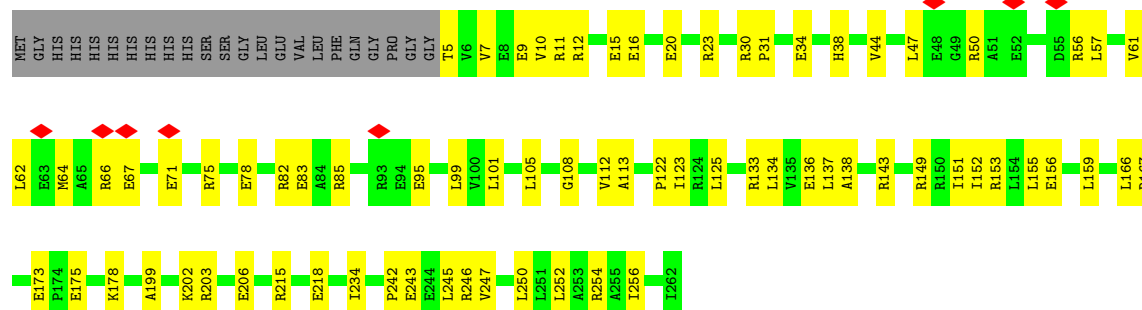




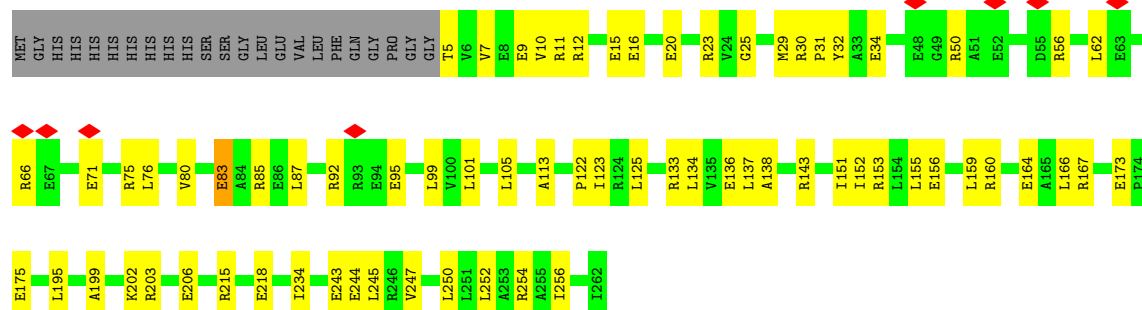
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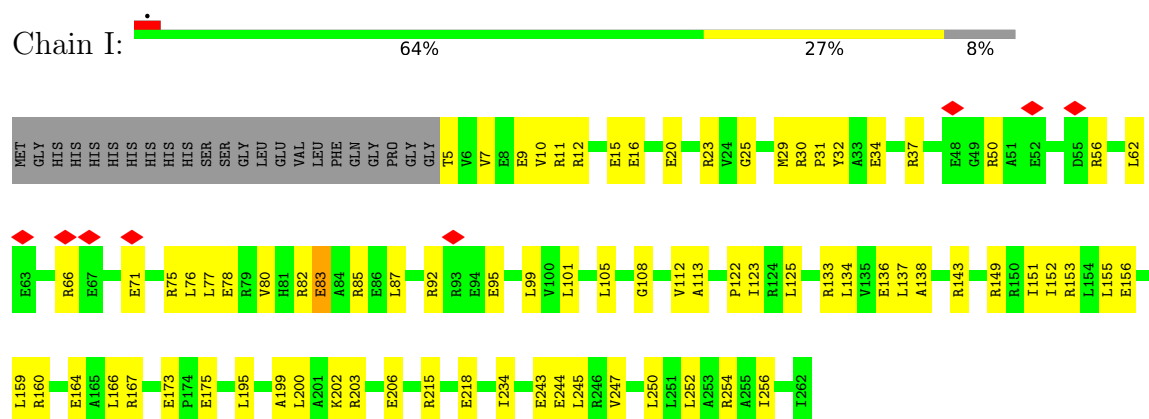
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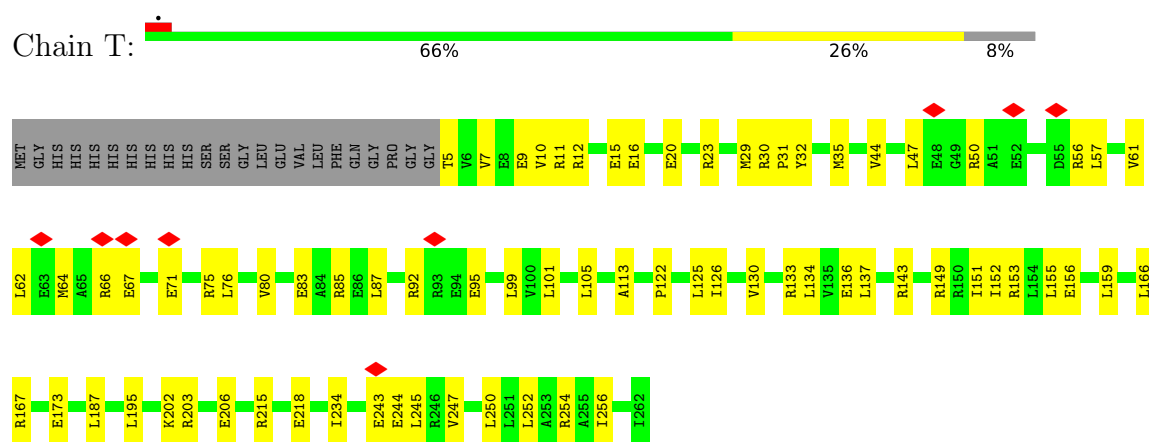
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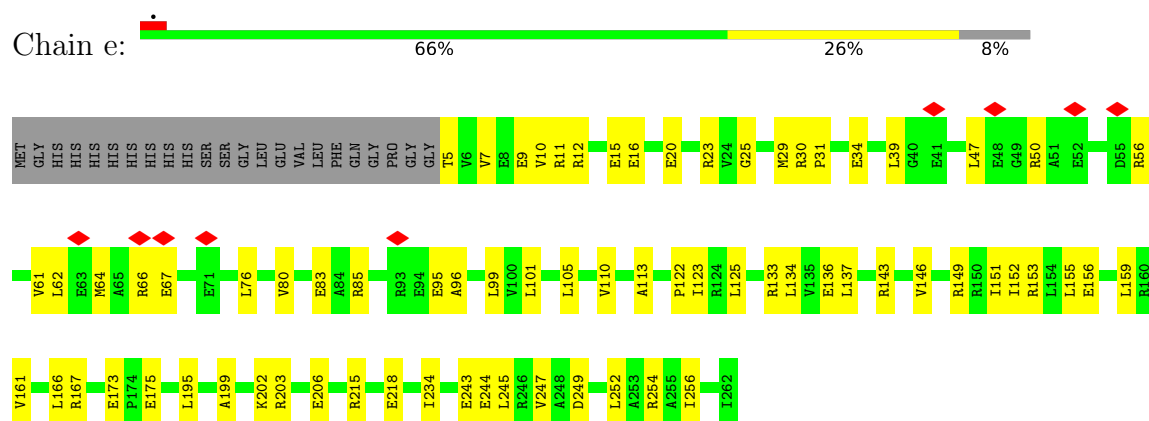
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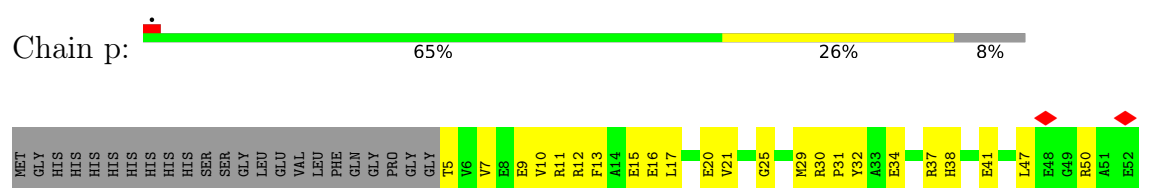
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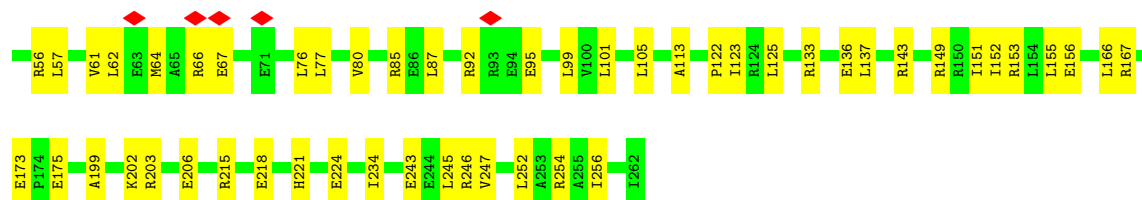


• Molecule 1: Cage-i53-Zn1-HEHE-6



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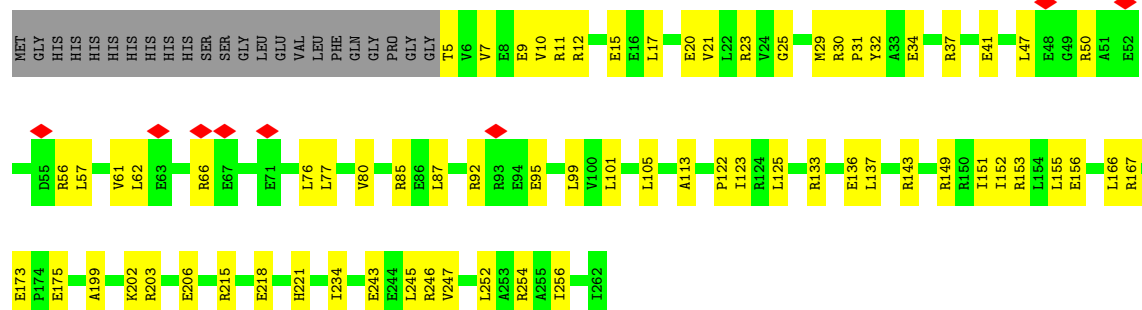




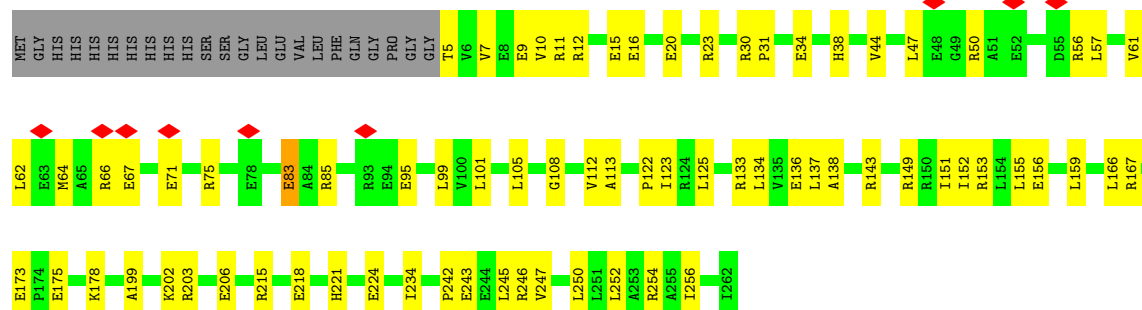
## • Molecule 1: Cage-i53-Zn1-HEHE-6



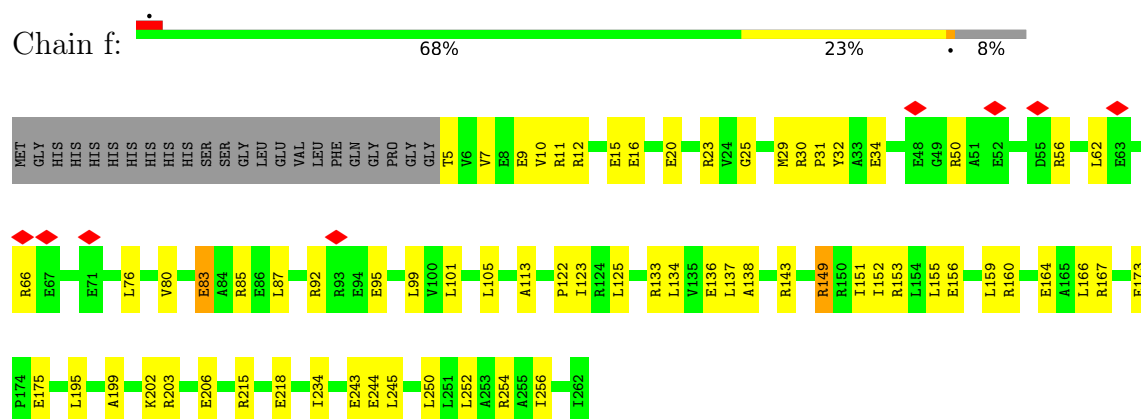
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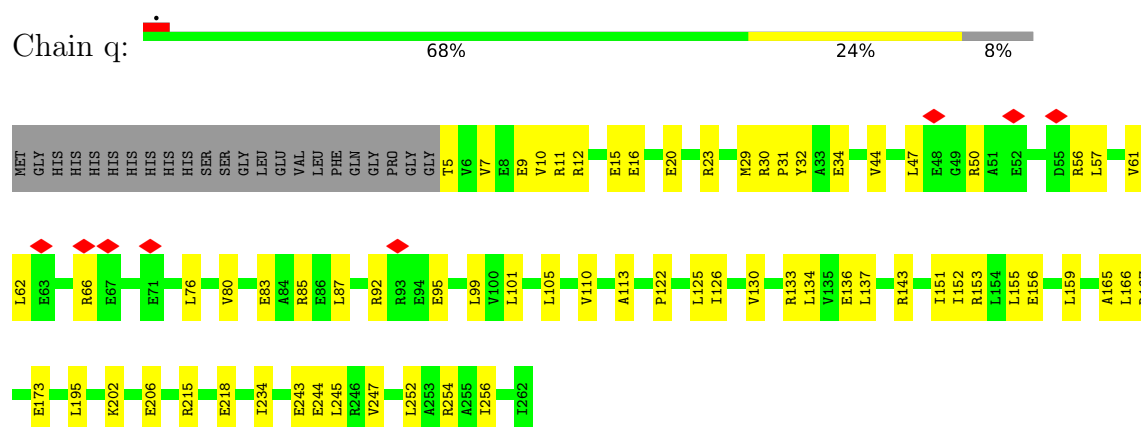
## • Molecule 1: Cage-i53-Zn1-HEHE-6



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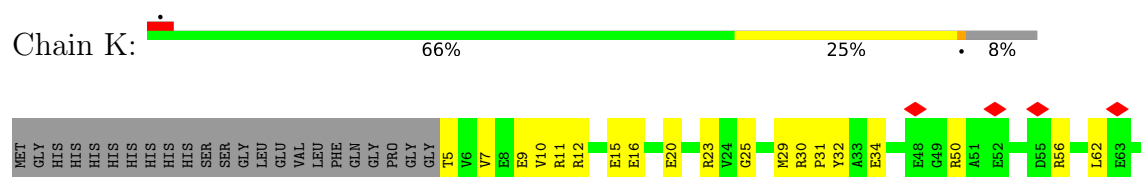
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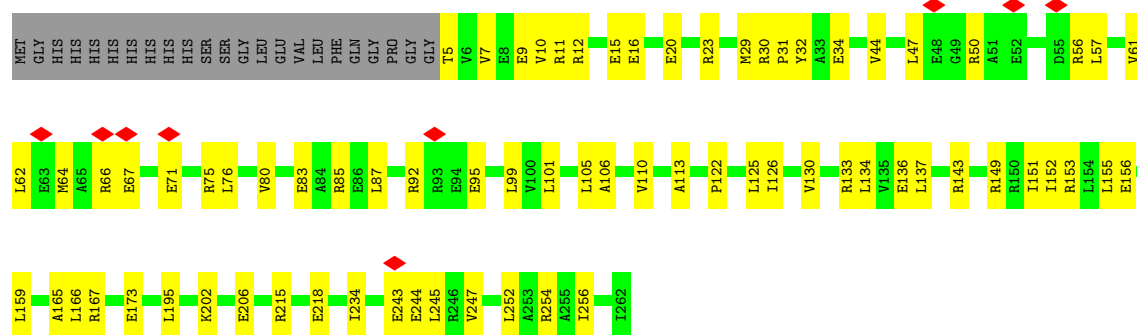


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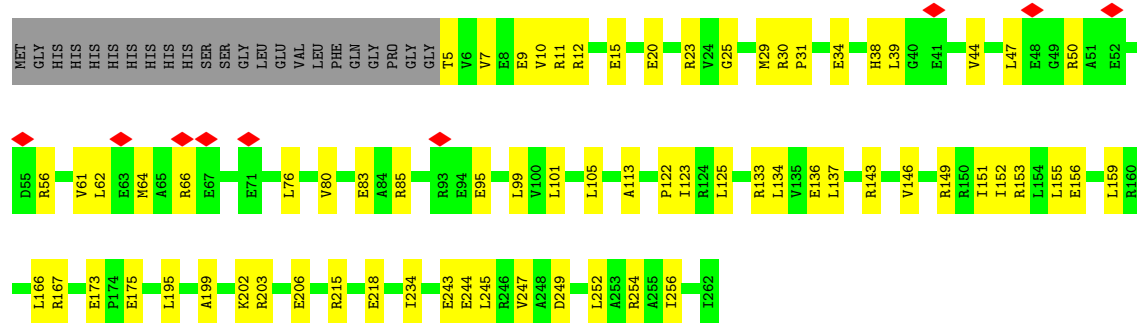




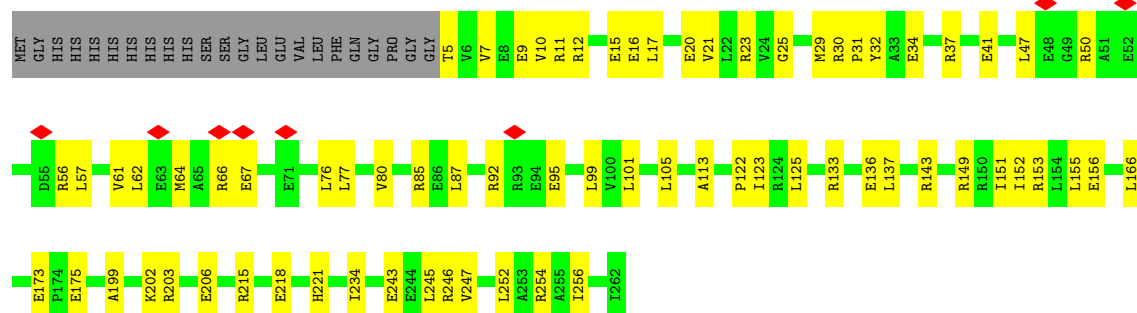
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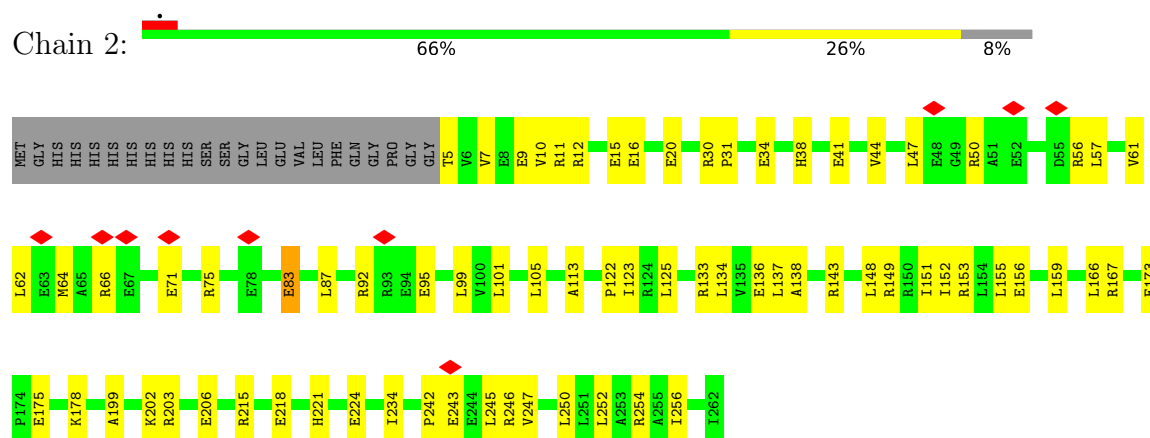
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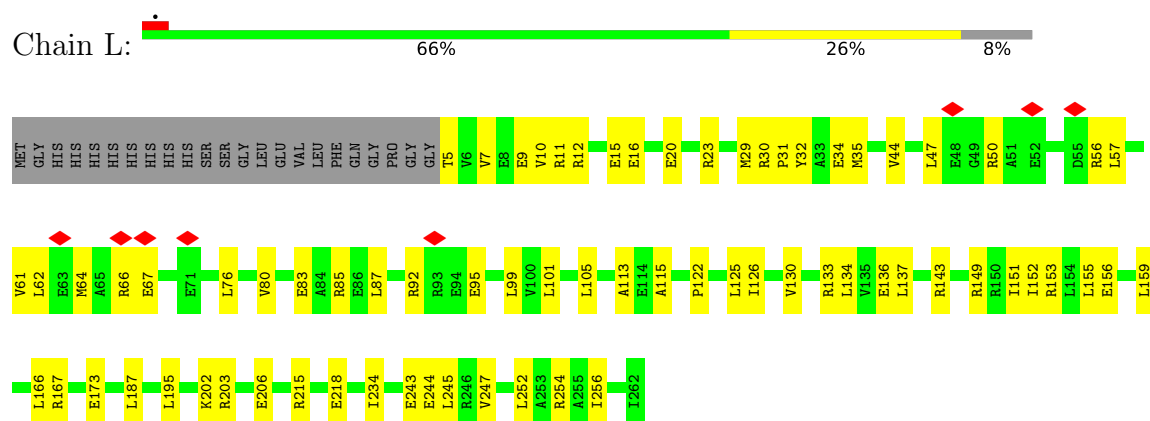
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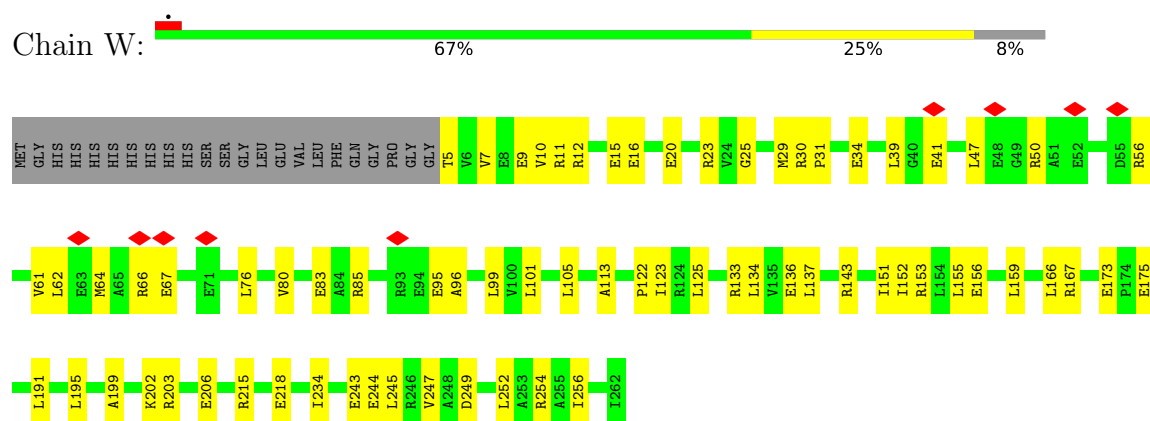
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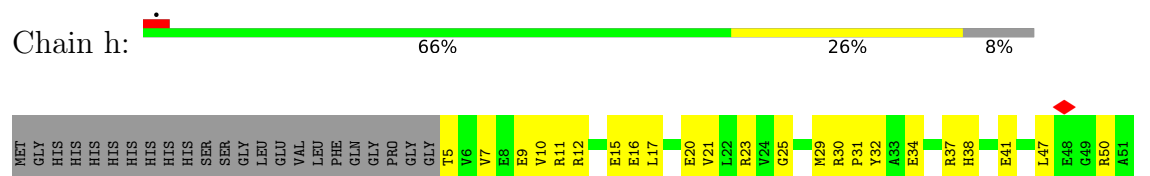
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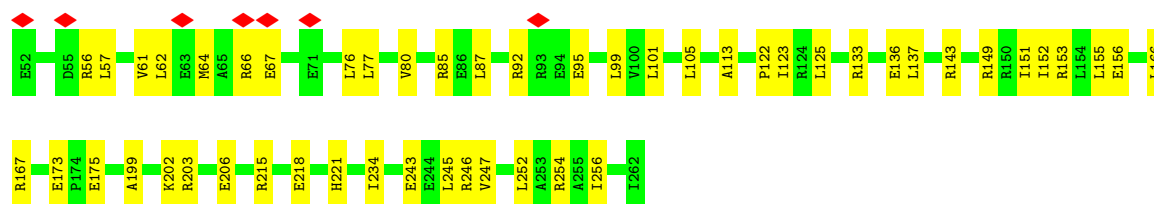


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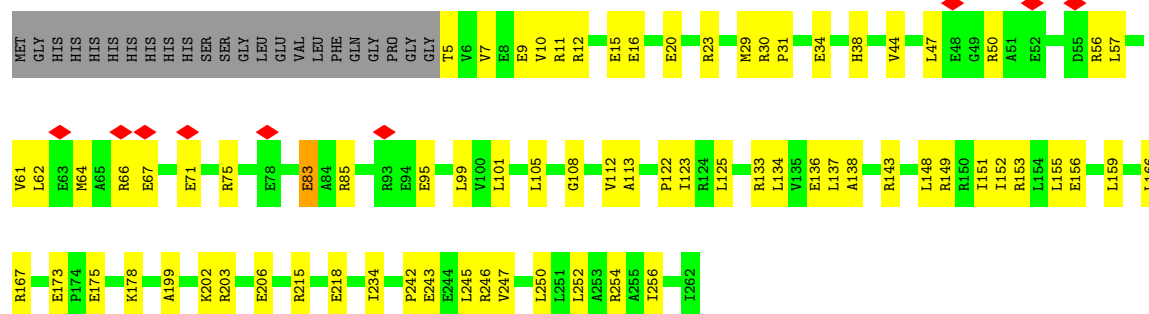


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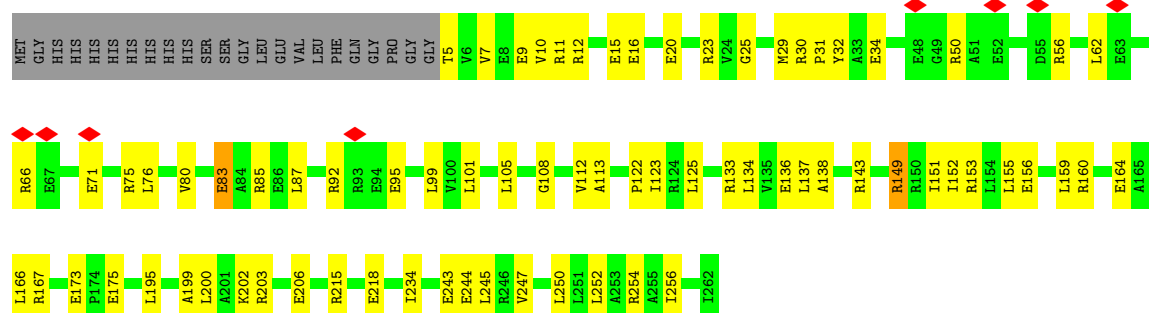




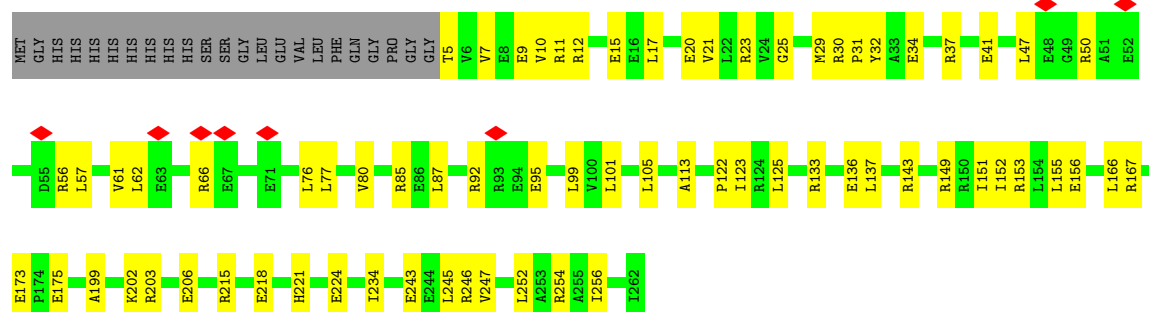
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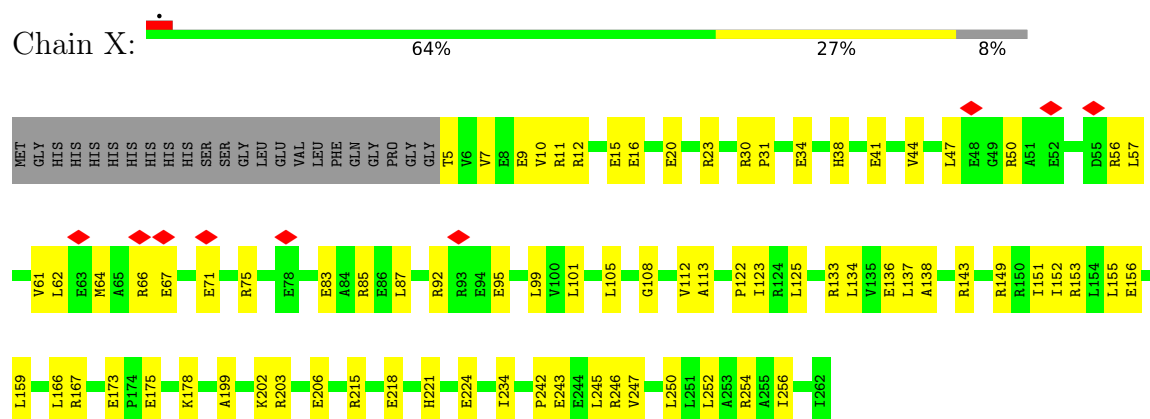
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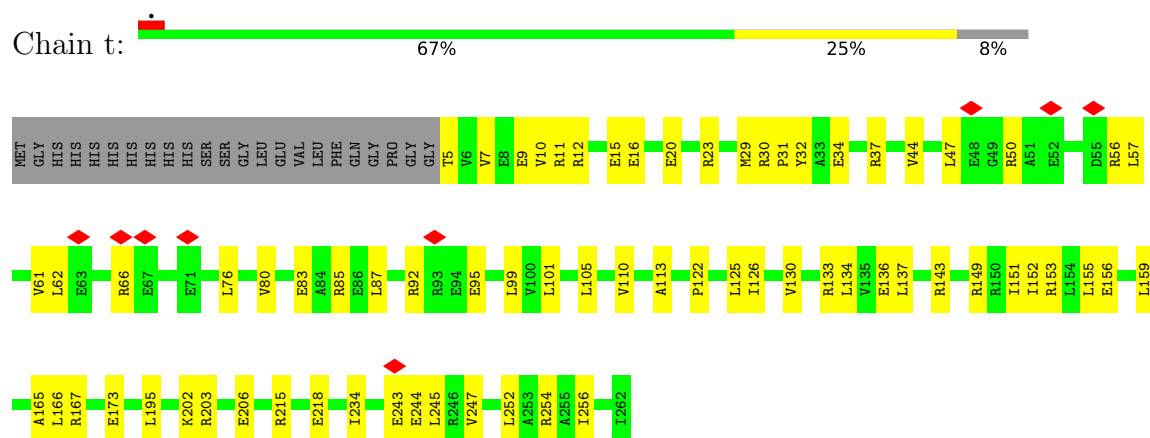
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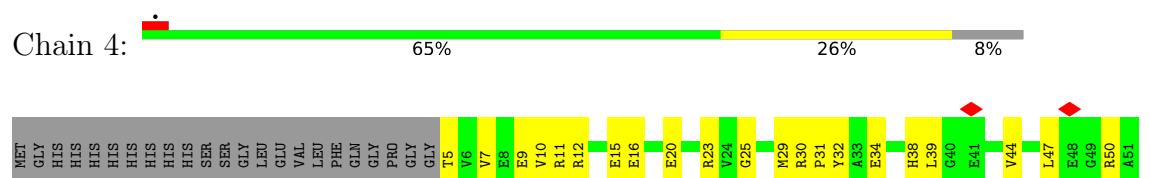
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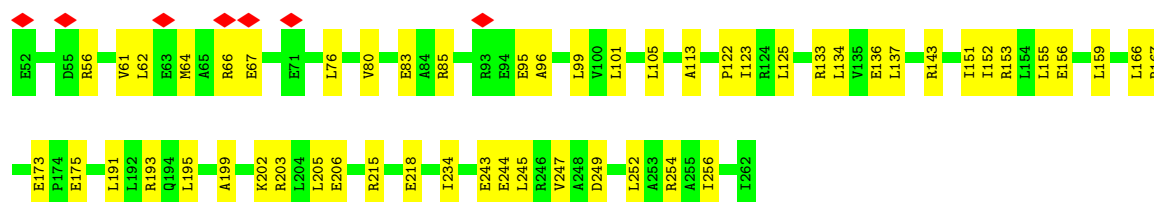


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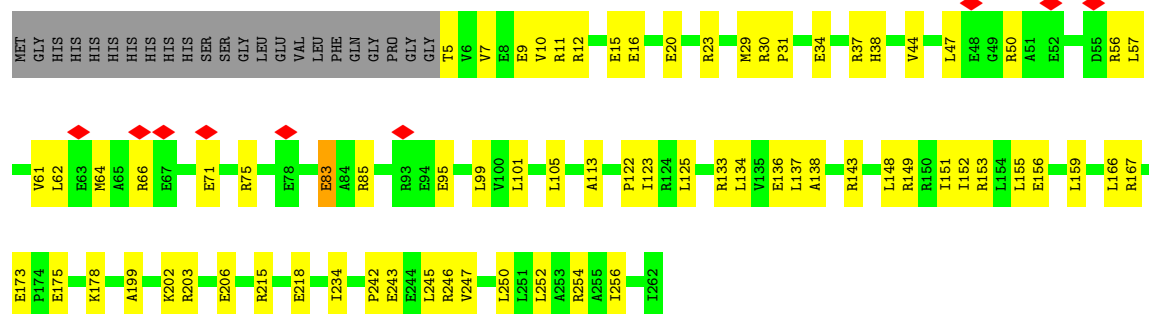


- Molecule 1: Cage-i53-Zn1-HEHE-6





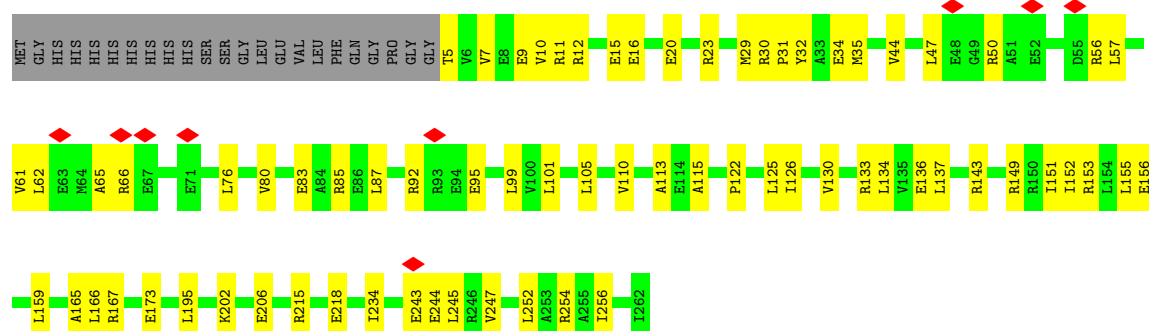
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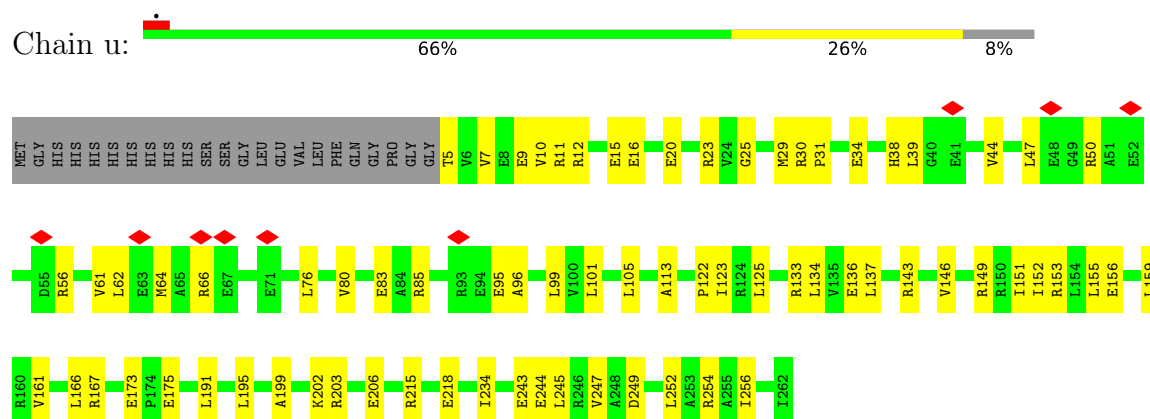
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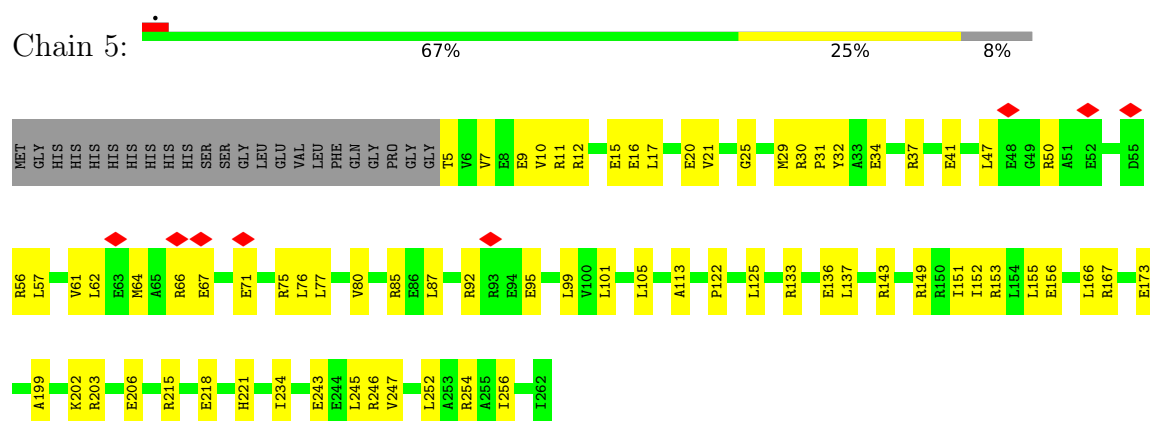
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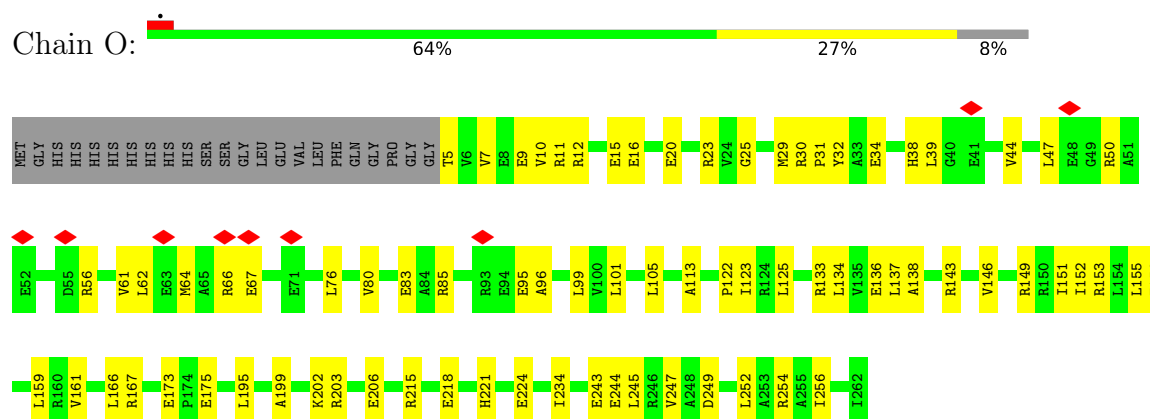
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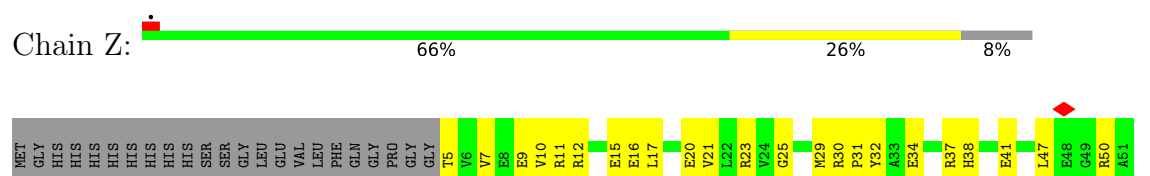
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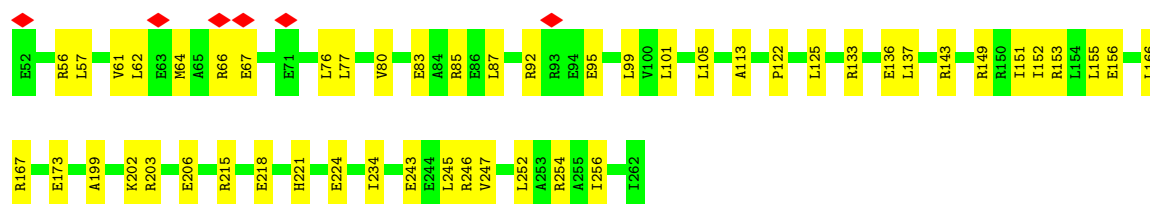


- Molecule 1: Cage-i53-Zn1-HEHE-6



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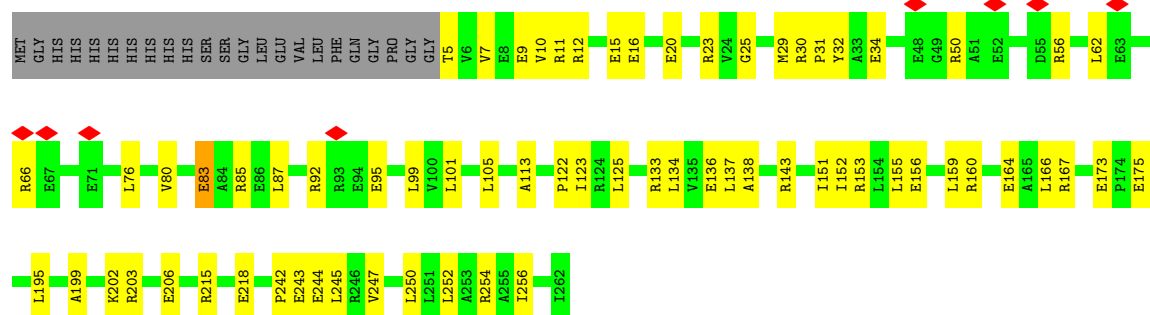




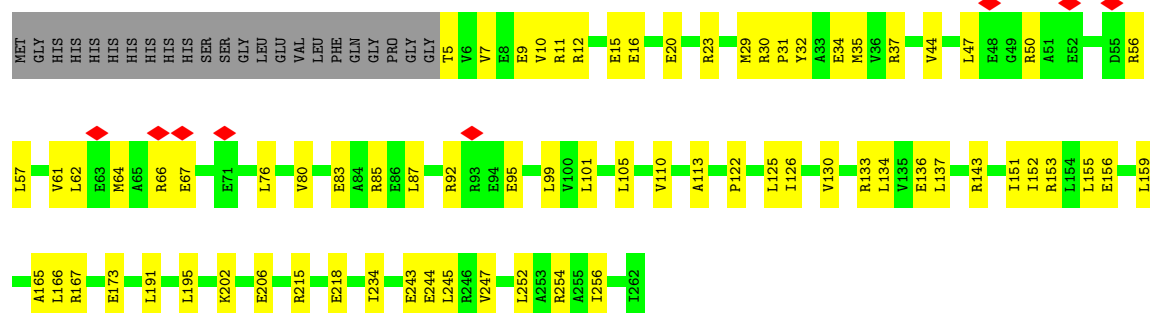
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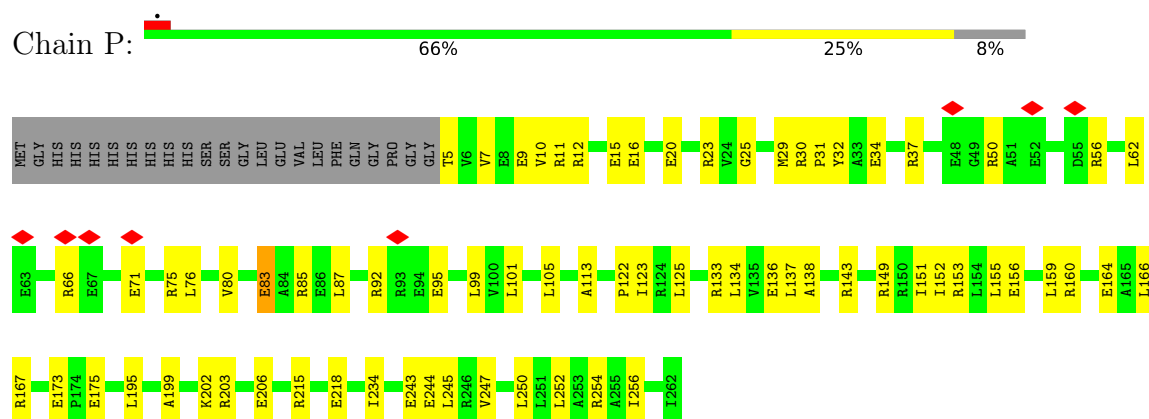
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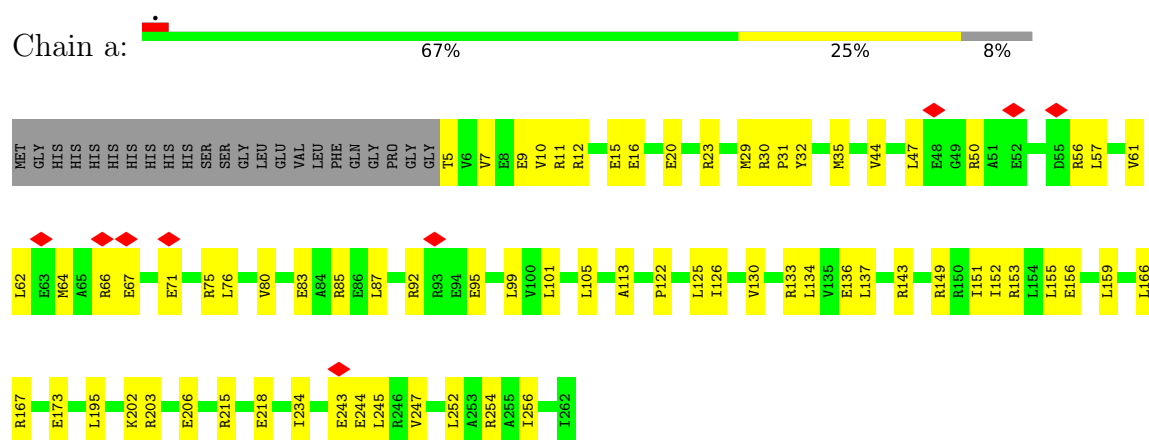
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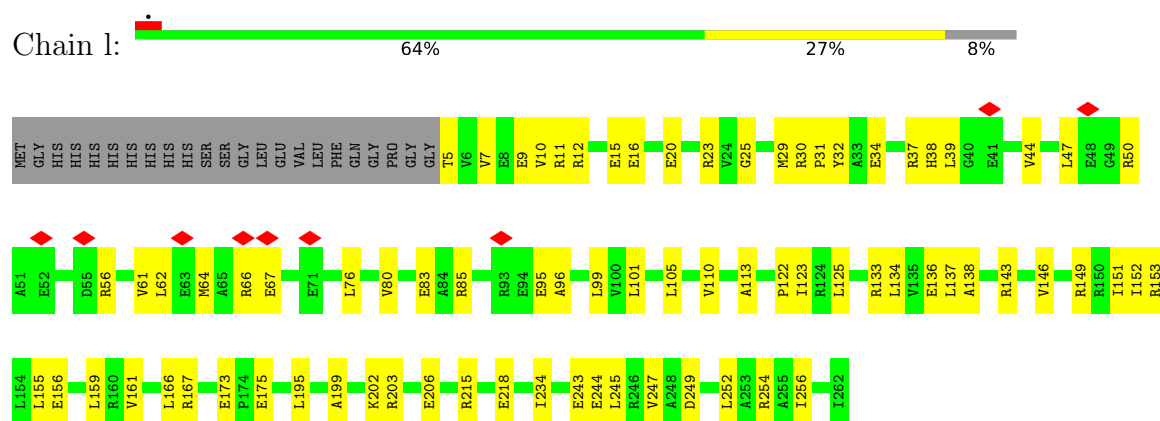
- Molecule 1: Cage-i53-Zn1-HEHE-6



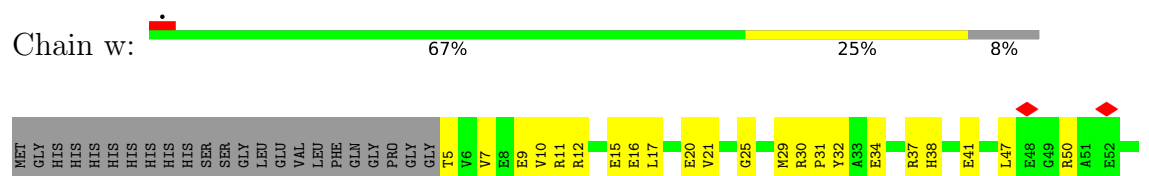
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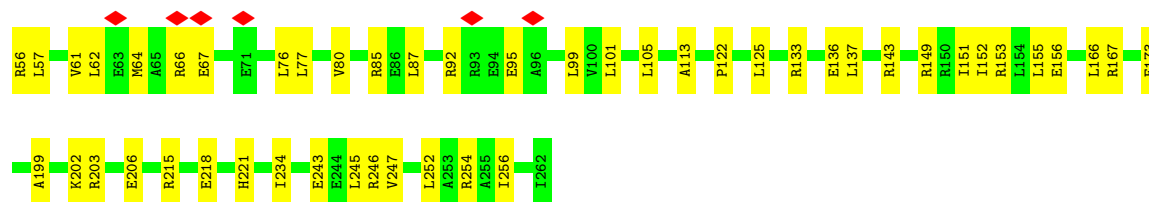


- Molecule 1: Cage-i53-Zn1-HEHE-6

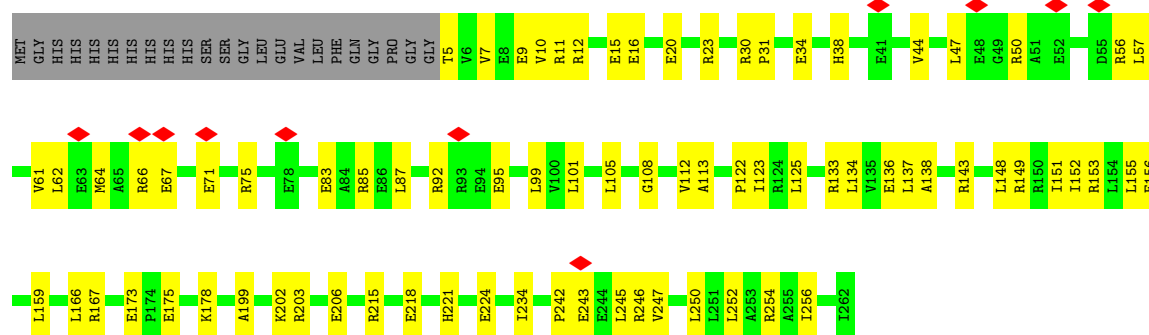


- Molecule 1: Cage-i53-Zn1-HEHE-6





• Molecule 1: Cage-i53-Zn1-HEHE-6



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 66846                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.643                                   | Depositor |
| Minimum map value                    | -0.385                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.025                                   | Depositor |
| Recommended contour level            | 0.09                                    | Depositor |
| Map size (Å)                         | 432.00003, 432.00003, 432.00003         | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.2, 1.2, 1.2                           | Depositor |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 0     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | 1     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | 2     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | 3     | 0.26         | 0/2053      | 0.34        | 0/2768      |
| 1   | 4     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | 5     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | 6     | 0.25         | 0/2053      | 0.35        | 0/2768      |
| 1   | 7     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | A     | 0.26         | 0/2053      | 0.35        | 0/2768      |
| 1   | B     | 0.25         | 0/2053      | 0.36        | 0/2768      |
| 1   | C     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | D     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | E     | 0.25         | 0/2053      | 0.35        | 0/2768      |
| 1   | F     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | G     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | H     | 0.25         | 0/2053      | 0.35        | 0/2768      |
| 1   | I     | 0.26         | 0/2053      | 0.35        | 0/2768      |
| 1   | J     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | K     | 0.26         | 0/2053      | 0.34        | 0/2768      |
| 1   | L     | 0.25         | 0/2053      | 0.35        | 0/2768      |
| 1   | M     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | N     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | O     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | P     | 0.26         | 0/2053      | 0.35        | 0/2768      |
| 1   | Q     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | R     | 0.26         | 0/2053      | 0.34        | 0/2768      |
| 1   | S     | 0.25         | 0/2053      | 0.34        | 0/2768      |
| 1   | T     | 0.25         | 0/2053      | 0.36        | 0/2768      |
| 1   | U     | 0.25         | 0/2053      | 0.33        | 0/2768      |
| 1   | V     | 0.25         | 0/2053      | 0.36        | 0/2768      |
| 1   | W     | 0.25         | 0/2053      | 0.35        | 0/2768      |
| 1   | X     | 0.25         | 0/2053      | 0.34        | 0/2768      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 1   | Y     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | Z     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | a     | 0.25         | 0/2053   | 0.35        | 0/2768   |
| 1   | b     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | c     | 0.25         | 0/2053   | 0.35        | 0/2768   |
| 1   | d     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | e     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | f     | 0.26         | 0/2053   | 0.34        | 0/2768   |
| 1   | g     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | h     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | i     | 0.26         | 0/2053   | 0.35        | 0/2768   |
| 1   | j     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | k     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | l     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | m     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | n     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | o     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | p     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | q     | 0.25         | 0/2053   | 0.35        | 0/2768   |
| 1   | r     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | s     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | t     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | u     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | v     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| 1   | w     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | x     | 0.25         | 0/2053   | 0.36        | 0/2768   |
| 1   | y     | 0.25         | 0/2053   | 0.33        | 0/2768   |
| 1   | z     | 0.25         | 0/2053   | 0.34        | 0/2768   |
| All | All   | 0.25         | 0/123180 | 0.34        | 0/166080 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | 1     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | 2     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | 3     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | 4     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | 5     | 2034  | 0        | 2135     | 48      | 0            |
| 1   | 6     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | 7     | 2034  | 0        | 2135     | 57      | 0            |
| 1   | A     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | B     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | C     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | D     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | E     | 2034  | 0        | 2135     | 60      | 0            |
| 1   | F     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | G     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | H     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | I     | 2034  | 0        | 2135     | 55      | 0            |
| 1   | J     | 2034  | 0        | 2135     | 46      | 0            |
| 1   | K     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | L     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | M     | 2034  | 0        | 2135     | 48      | 0            |
| 1   | N     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | O     | 2034  | 0        | 2135     | 55      | 0            |
| 1   | P     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | Q     | 2034  | 0        | 2135     | 50      | 0            |
| 1   | R     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | S     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | T     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | U     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | V     | 2034  | 0        | 2135     | 55      | 0            |
| 1   | W     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | X     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | Y     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | Z     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | a     | 2034  | 0        | 2135     | 50      | 0            |
| 1   | b     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | c     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | d     | 2034  | 0        | 2135     | 50      | 0            |
| 1   | e     | 2034  | 0        | 2135     | 54      | 0            |
| 1   | f     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | g     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | h     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | i     | 2034  | 0        | 2135     | 51      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | j     | 2034  | 0        | 2135     | 50      | 0            |
| 1   | k     | 2034  | 0        | 2135     | 55      | 0            |
| 1   | l     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | m     | 2034  | 0        | 2135     | 47      | 0            |
| 1   | n     | 2034  | 0        | 2135     | 56      | 0            |
| 1   | o     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | p     | 2034  | 0        | 2135     | 52      | 0            |
| 1   | q     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | r     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | s     | 2034  | 0        | 2135     | 57      | 0            |
| 1   | t     | 2034  | 0        | 2135     | 50      | 0            |
| 1   | u     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | v     | 2034  | 0        | 2135     | 47      | 0            |
| 1   | w     | 2034  | 0        | 2135     | 51      | 0            |
| 1   | x     | 2034  | 0        | 2135     | 53      | 0            |
| 1   | y     | 2034  | 0        | 2135     | 49      | 0            |
| 1   | z     | 2034  | 0        | 2135     | 47      | 0            |
| 2   | 0     | 2     | 0        | 0        | 0       | 0            |
| 2   | 1     | 3     | 0        | 0        | 0       | 0            |
| 2   | 2     | 2     | 0        | 0        | 0       | 0            |
| 2   | 3     | 3     | 0        | 0        | 0       | 0            |
| 2   | 4     | 3     | 0        | 0        | 0       | 0            |
| 2   | 5     | 3     | 0        | 0        | 0       | 0            |
| 2   | 6     | 2     | 0        | 0        | 0       | 0            |
| 2   | 7     | 2     | 0        | 0        | 0       | 0            |
| 2   | A     | 3     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 3     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 3     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 3     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 2   | M     | 2     | 0        | 0        | 0       | 0            |
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 2     | 0        | 0        | 0       | 0            |
| 2   | P     | 3     | 0        | 0        | 0       | 0            |
| 2   | Q     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | R     | 3      | 0        | 0        | 0       | 0            |
| 2   | S     | 2      | 0        | 0        | 0       | 0            |
| 2   | T     | 2      | 0        | 0        | 0       | 0            |
| 2   | U     | 1      | 0        | 0        | 0       | 0            |
| 2   | V     | 2      | 0        | 0        | 0       | 0            |
| 2   | W     | 2      | 0        | 0        | 0       | 0            |
| 2   | X     | 1      | 0        | 0        | 0       | 0            |
| 2   | Y     | 3      | 0        | 0        | 0       | 0            |
| 2   | Z     | 2      | 0        | 0        | 0       | 0            |
| 2   | a     | 2      | 0        | 0        | 0       | 0            |
| 2   | b     | 1      | 0        | 0        | 0       | 0            |
| 2   | c     | 2      | 0        | 0        | 0       | 0            |
| 2   | d     | 2      | 0        | 0        | 0       | 0            |
| 2   | e     | 2      | 0        | 0        | 0       | 0            |
| 2   | f     | 3      | 0        | 0        | 0       | 0            |
| 2   | g     | 2      | 0        | 0        | 0       | 0            |
| 2   | h     | 2      | 0        | 0        | 0       | 0            |
| 2   | i     | 3      | 0        | 0        | 0       | 0            |
| 2   | j     | 2      | 0        | 0        | 0       | 0            |
| 2   | k     | 1      | 0        | 0        | 0       | 0            |
| 2   | l     | 2      | 0        | 0        | 0       | 0            |
| 2   | m     | 3      | 0        | 0        | 0       | 0            |
| 2   | n     | 2      | 0        | 0        | 0       | 0            |
| 2   | o     | 1      | 0        | 0        | 0       | 0            |
| 2   | p     | 1      | 0        | 0        | 0       | 0            |
| 2   | q     | 1      | 0        | 0        | 0       | 0            |
| 2   | r     | 1      | 0        | 0        | 0       | 0            |
| 2   | s     | 1      | 0        | 0        | 0       | 0            |
| 2   | t     | 1      | 0        | 0        | 0       | 0            |
| 2   | u     | 1      | 0        | 0        | 0       | 0            |
| 2   | v     | 3      | 0        | 0        | 0       | 0            |
| 2   | w     | 1      | 0        | 0        | 0       | 0            |
| 2   | x     | 1      | 0        | 0        | 0       | 0            |
| 2   | y     | 1      | 0        | 0        | 0       | 0            |
| 2   | z     | 3      | 0        | 0        | 0       | 0            |
| All | All   | 122160 | 0        | 128100   | 2867    | 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 11.

All (2867) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 1:1:29:MET:HE3  | 1:1:118:ARG:HH22 | 1.45                     | 0.80              |
| 1:B:122:PRO:HG2 | 1:B:125:LEU:HD23 | 1.65                     | 0.79              |
| 1:q:122:PRO:HG2 | 1:q:125:LEU:HD23 | 1.65                     | 0.79              |
| 1:6:122:PRO:HG2 | 1:6:125:LEU:HD23 | 1.65                     | 0.79              |
| 1:V:122:PRO:HG2 | 1:V:125:LEU:HD23 | 1.65                     | 0.78              |
| 1:c:122:PRO:HG2 | 1:c:125:LEU:HD23 | 1.66                     | 0.78              |
| 1:a:122:PRO:HG2 | 1:a:125:LEU:HD23 | 1.66                     | 0.78              |
| 1:j:122:PRO:HG2 | 1:j:125:LEU:HD23 | 1.66                     | 0.78              |
| 1:t:122:PRO:HG2 | 1:t:125:LEU:HD23 | 1.66                     | 0.77              |
| 1:x:122:PRO:HG2 | 1:x:125:LEU:HD23 | 1.65                     | 0.77              |
| 1:H:122:PRO:HG2 | 1:H:125:LEU:HD23 | 1.66                     | 0.76              |
| 1:L:122:PRO:HG2 | 1:L:125:LEU:HD23 | 1.66                     | 0.76              |
| 1:T:122:PRO:HG2 | 1:T:125:LEU:HD23 | 1.66                     | 0.76              |
| 1:S:122:PRO:HG2 | 1:S:125:LEU:HD23 | 1.68                     | 0.76              |
| 1:1:122:PRO:HG2 | 1:1:125:LEU:HD23 | 1.68                     | 0.75              |
| 1:p:9:GLU:HG3   | 1:p:12:ARG:HH21  | 1.52                     | 0.75              |
| 1:U:122:PRO:HG2 | 1:U:125:LEU:HD23 | 1.69                     | 0.75              |
| 1:K:87:LEU:HB3  | 1:K:92:ARG:HG3   | 1.69                     | 0.74              |
| 1:h:9:GLU:HG3   | 1:h:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:d:9:GLU:HG3   | 1:d:12:ARG:HH21  | 1.52                     | 0.74              |
| 1:Z:9:GLU:HG3   | 1:Z:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:D:9:GLU:HG3   | 1:D:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:m:9:GLU:HG3   | 1:m:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:y:9:GLU:HG3   | 1:y:12:ARG:HH21  | 1.52                     | 0.74              |
| 1:A:9:GLU:HG3   | 1:A:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:X:122:PRO:HG2 | 1:X:125:LEU:HD23 | 1.70                     | 0.74              |
| 1:R:9:GLU:HG3   | 1:R:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:w:9:GLU:HG3   | 1:w:12:ARG:HH21  | 1.53                     | 0.74              |
| 1:s:122:PRO:HG2 | 1:s:125:LEU:HD23 | 1.69                     | 0.73              |
| 1:5:9:GLU:HG3   | 1:5:12:ARG:HH21  | 1.52                     | 0.73              |
| 1:P:9:GLU:HG3   | 1:P:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:z:9:GLU:HG3   | 1:z:12:ARG:HH21  | 1.54                     | 0.73              |
| 1:f:9:GLU:HG3   | 1:f:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:i:9:GLU:HG3   | 1:i:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:I:87:LEU:HB3  | 1:I:92:ARG:HG3   | 1.69                     | 0.73              |
| 1:r:9:GLU:HG3   | 1:r:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:v:9:GLU:HG3   | 1:v:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:Y:9:GLU:HG3   | 1:Y:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:K:9:GLU:HG3   | 1:K:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:O:9:GLU:HG3   | 1:O:12:ARG:HH21  | 1.54                     | 0.73              |
| 1:0:122:PRO:HG2 | 1:0:125:LEU:HD23 | 1.70                     | 0.73              |
| 1:J:9:GLU:HG3   | 1:J:12:ARG:HH21  | 1.52                     | 0.73              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:v:87:LEU:HB3  | 1:v:92:ARG:HG3   | 1.70                     | 0.73              |
| 1:P:87:LEU:HB3  | 1:P:92:ARG:HG3   | 1.71                     | 0.73              |
| 1:Q:9:GLU:HG3   | 1:Q:12:ARG:HH21  | 1.53                     | 0.73              |
| 1:N:122:PRO:HG2 | 1:N:125:LEU:HD23 | 1.70                     | 0.73              |
| 1:l:9:GLU:HG3   | 1:l:12:ARG:HH21  | 1.54                     | 0.73              |
| 1:1:9:GLU:HG3   | 1:1:12:ARG:HH21  | 1.54                     | 0.73              |
| 1:7:122:PRO:HG2 | 1:7:125:LEU:HD23 | 1.70                     | 0.72              |
| 1:A:87:LEU:HB3  | 1:A:92:ARG:HG3   | 1.69                     | 0.72              |
| 1:W:9:GLU:HG3   | 1:W:12:ARG:HH21  | 1.55                     | 0.72              |
| 1:4:9:GLU:HG3   | 1:4:12:ARG:HH21  | 1.54                     | 0.72              |
| 1:2:122:PRO:HG2 | 1:2:125:LEU:HD23 | 1.69                     | 0.72              |
| 1:3:87:LEU:HB3  | 1:3:92:ARG:HG3   | 1.70                     | 0.72              |
| 1:M:9:GLU:HG3   | 1:M:12:ARG:HH21  | 1.53                     | 0.72              |
| 1:e:9:GLU:HG3   | 1:e:12:ARG:HH21  | 1.55                     | 0.72              |
| 1:I:9:GLU:HG3   | 1:I:12:ARG:HH21  | 1.53                     | 0.72              |
| 1:C:9:GLU:HG3   | 1:C:12:ARG:HH21  | 1.54                     | 0.72              |
| 1:m:87:LEU:HB3  | 1:m:92:ARG:HG3   | 1.70                     | 0.72              |
| 1:z:87:LEU:HB3  | 1:z:92:ARG:HG3   | 1.70                     | 0.72              |
| 1:E:122:PRO:HG2 | 1:E:125:LEU:HD23 | 1.70                     | 0.72              |
| 1:n:9:GLU:HG3   | 1:n:12:ARG:HH21  | 1.54                     | 0.71              |
| 1:E:9:GLU:HG3   | 1:E:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:G:9:GLU:HG3   | 1:G:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:3:9:GLU:HG3   | 1:3:12:ARG:HH21  | 1.53                     | 0.71              |
| 1:u:9:GLU:HG3   | 1:u:12:ARG:HH21  | 1.54                     | 0.71              |
| 1:o:9:GLU:HG3   | 1:o:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:0:9:GLU:HG3   | 1:0:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:g:9:GLU:HG3   | 1:g:12:ARG:HH21  | 1.54                     | 0.71              |
| 1:Y:87:LEU:HB3  | 1:Y:92:ARG:HG3   | 1.72                     | 0.71              |
| 1:b:9:GLU:HG3   | 1:b:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:G:122:PRO:HG2 | 1:G:125:LEU:HD23 | 1.71                     | 0.71              |
| 1:R:87:LEU:HB3  | 1:R:92:ARG:HG3   | 1.72                     | 0.71              |
| 1:f:87:LEU:HB3  | 1:f:92:ARG:HG3   | 1.71                     | 0.71              |
| 1:s:9:GLU:HG3   | 1:s:12:ARG:HH21  | 1.56                     | 0.71              |
| 1:i:87:LEU:HB3  | 1:i:92:ARG:HG3   | 1.71                     | 0.70              |
| 1:7:9:GLU:HG3   | 1:7:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:k:9:GLU:HG3   | 1:k:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:2:9:GLU:HG3   | 1:2:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:N:9:GLU:HG3   | 1:N:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:k:122:PRO:HG2 | 1:k:125:LEU:HD23 | 1.71                     | 0.70              |
| 1:F:9:GLU:HG3   | 1:F:12:ARG:HH21  | 1.54                     | 0.70              |
| 1:b:122:PRO:HG2 | 1:b:125:LEU:HD23 | 1.73                     | 0.70              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:S:9:GLU:HG3   | 1:S:12:ARG:HH21  | 1.54                     | 0.70              |
| 1:U:9:GLU:HG3   | 1:U:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:V:87:LEU:HB3  | 1:V:92:ARG:HG3   | 1.74                     | 0.70              |
| 1:X:9:GLU:HG3   | 1:X:12:ARG:HH21  | 1.56                     | 0.70              |
| 1:G:149:ARG:NH1 | 1:G:243:GLU:OE1  | 2.25                     | 0.70              |
| 1:B:87:LEU:HB3  | 1:B:92:ARG:HG3   | 1.74                     | 0.70              |
| 1:x:87:LEU:HB3  | 1:x:92:ARG:HG3   | 1.74                     | 0.70              |
| 1:c:87:LEU:HB3  | 1:c:92:ARG:HG3   | 1.74                     | 0.70              |
| 1:0:215:ARG:NH1 | 1:0:218:GLU:OE2  | 2.25                     | 0.70              |
| 1:X:215:ARG:NH1 | 1:X:218:GLU:OE2  | 2.25                     | 0.70              |
| 1:k:215:ARG:NH1 | 1:k:218:GLU:OE2  | 2.25                     | 0.70              |
| 1:7:215:ARG:NH1 | 1:7:218:GLU:OE2  | 2.25                     | 0.70              |
| 1:H:87:LEU:HB3  | 1:H:92:ARG:HG3   | 1.74                     | 0.69              |
| 1:U:215:ARG:NH1 | 1:U:218:GLU:OE2  | 2.25                     | 0.69              |
| 1:q:87:LEU:HB3  | 1:q:92:ARG:HG3   | 1.74                     | 0.69              |
| 1:s:215:ARG:NH1 | 1:s:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:o:122:PRO:HG2 | 1:o:125:LEU:HD23 | 1.74                     | 0.69              |
| 1:o:149:ARG:NH1 | 1:o:243:GLU:OE1  | 2.26                     | 0.69              |
| 1:E:149:ARG:NH1 | 1:E:243:GLU:OE1  | 2.26                     | 0.69              |
| 1:b:149:ARG:NH1 | 1:b:243:GLU:OE1  | 2.26                     | 0.69              |
| 1:2:215:ARG:NH1 | 1:2:218:GLU:OE2  | 2.25                     | 0.69              |
| 1:6:87:LEU:HB3  | 1:6:92:ARG:HG3   | 1.74                     | 0.69              |
| 1:E:11:ARG:O    | 1:E:15:GLU:HG2   | 1.93                     | 0.69              |
| 1:J:215:ARG:NH1 | 1:J:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:s:149:ARG:NH1 | 1:s:243:GLU:OE1  | 2.25                     | 0.69              |
| 1:w:215:ARG:NH1 | 1:w:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:o:215:ARG:NH1 | 1:o:218:GLU:OE2  | 2.25                     | 0.69              |
| 1:Z:215:ARG:NH1 | 1:Z:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:D:215:ARG:NH1 | 1:D:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:Q:122:PRO:HG2 | 1:Q:125:LEU:HD23 | 1.75                     | 0.69              |
| 1:b:215:ARG:NH1 | 1:b:218:GLU:OE2  | 2.25                     | 0.69              |
| 1:I:215:ARG:NH1 | 1:I:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:0:149:ARG:NH1 | 1:0:243:GLU:OE1  | 2.25                     | 0.69              |
| 1:q:9:GLU:HG3   | 1:q:12:ARG:HH21  | 1.58                     | 0.69              |
| 1:r:215:ARG:NH1 | 1:r:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:t:9:GLU:HG3   | 1:t:12:ARG:HH21  | 1.58                     | 0.69              |
| 1:N:215:ARG:NH1 | 1:N:218:GLU:OE2  | 2.25                     | 0.69              |
| 1:5:215:ARG:NH1 | 1:5:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:k:149:ARG:NH1 | 1:k:243:GLU:OE1  | 2.26                     | 0.69              |
| 1:7:149:ARG:NH1 | 1:7:243:GLU:OE1  | 2.25                     | 0.69              |
| 1:B:9:GLU:HG3   | 1:B:12:ARG:HH21  | 1.58                     | 0.69              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:c:9:GLU:HG3   | 1:c:12:ARG:HH21  | 1.58                     | 0.69              |
| 1:y:215:ARG:NH1 | 1:y:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:H:9:GLU:HG3   | 1:H:12:ARG:HH21  | 1.58                     | 0.69              |
| 1:d:122:PRO:HG2 | 1:d:125:LEU:HD23 | 1.75                     | 0.69              |
| 1:T:9:GLU:HG3   | 1:T:12:ARG:HH21  | 1.58                     | 0.69              |
| 1:f:215:ARG:NH1 | 1:f:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:i:215:ARG:NH1 | 1:i:218:GLU:OE2  | 2.26                     | 0.69              |
| 1:L:9:GLU:HG3   | 1:L:12:ARG:HH21  | 1.58                     | 0.68              |
| 1:3:215:ARG:NH1 | 1:3:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:M:215:ARG:NH1 | 1:M:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:o:11:ARG:O    | 1:o:15:GLU:HG2   | 1.93                     | 0.68              |
| 1:E:215:ARG:NH1 | 1:E:218:GLU:OE2  | 2.25                     | 0.68              |
| 1:p:215:ARG:NH1 | 1:p:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:s:11:ARG:O    | 1:s:15:GLU:HG2   | 1.93                     | 0.68              |
| 1:X:149:ARG:NH1 | 1:X:243:GLU:OE1  | 2.25                     | 0.68              |
| 1:Q:215:ARG:NH1 | 1:Q:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:R:215:ARG:NH1 | 1:R:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:d:215:ARG:NH1 | 1:d:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:p:122:PRO:HG2 | 1:p:125:LEU:HD23 | 1.75                     | 0.68              |
| 1:h:122:PRO:HG2 | 1:h:125:LEU:HD23 | 1.75                     | 0.68              |
| 1:m:215:ARG:NH1 | 1:m:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:G:215:ARG:NH1 | 1:G:218:GLU:OE2  | 2.25                     | 0.68              |
| 1:p:11:ARG:O    | 1:p:15:GLU:HG2   | 1.94                     | 0.68              |
| 1:K:215:ARG:NH1 | 1:K:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:r:122:PRO:HG2 | 1:r:125:LEU:HD23 | 1.75                     | 0.68              |
| 1:5:122:PRO:HG2 | 1:5:125:LEU:HD23 | 1.75                     | 0.68              |
| 1:0:11:ARG:O    | 1:0:15:GLU:HG2   | 1.93                     | 0.68              |
| 1:U:149:ARG:NH1 | 1:U:243:GLU:OE1  | 2.26                     | 0.68              |
| 1:v:215:ARG:NH1 | 1:v:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:Y:215:ARG:NH1 | 1:Y:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:A:215:ARG:NH1 | 1:A:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:j:9:GLU:HG3   | 1:j:12:ARG:HH21  | 1.58                     | 0.68              |
| 1:P:215:ARG:NH1 | 1:P:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:z:215:ARG:NH1 | 1:z:218:GLU:OE2  | 2.26                     | 0.68              |
| 1:1:11:ARG:O    | 1:1:15:GLU:HG2   | 1.94                     | 0.68              |
| 1:4:11:ARG:O    | 1:4:15:GLU:HG2   | 1.94                     | 0.68              |
| 1:b:11:ARG:O    | 1:b:15:GLU:HG2   | 1.94                     | 0.68              |
| 1:U:11:ARG:O    | 1:U:15:GLU:HG2   | 1.93                     | 0.68              |
| 1:V:9:GLU:HG3   | 1:V:12:ARG:HH21  | 1.58                     | 0.68              |
| 1:w:11:ARG:O    | 1:w:15:GLU:HG2   | 1.94                     | 0.68              |
| 1:q:76:LEU:O    | 1:q:80:VAL:HG23  | 1.94                     | 0.67              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:h:11:ARG:O    | 1:h:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:h:215:ARG:NH1 | 1:h:218:GLU:OE2  | 2.27                     | 0.67              |
| 1:X:113:ALA:HB1 | 1:X:166:LEU:HD21 | 1.76                     | 0.67              |
| 1:t:76:LEU:O    | 1:t:80:VAL:HG23  | 1.95                     | 0.67              |
| 1:Z:11:ARG:O    | 1:Z:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:a:9:GLU:HG3   | 1:a:12:ARG:HH21  | 1.58                     | 0.67              |
| 1:d:11:ARG:O    | 1:d:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:U:113:ALA:HB1 | 1:U:166:LEU:HD21 | 1.77                     | 0.67              |
| 1:2:11:ARG:O    | 1:2:15:GLU:HG2   | 1.93                     | 0.67              |
| 1:M:122:PRO:HG2 | 1:M:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:X:11:ARG:O    | 1:X:15:GLU:HG2   | 1.93                     | 0.67              |
| 1:N:149:ARG:NH1 | 1:N:243:GLU:OE1  | 2.25                     | 0.67              |
| 1:j:76:LEU:O    | 1:j:80:VAL:HG23  | 1.95                     | 0.67              |
| 1:0:113:ALA:HB1 | 1:0:166:LEU:HD21 | 1.76                     | 0.67              |
| 1:V:76:LEU:O    | 1:V:80:VAL:HG23  | 1.95                     | 0.67              |
| 1:s:113:ALA:HB1 | 1:s:166:LEU:HD21 | 1.76                     | 0.67              |
| 1:O:11:ARG:O    | 1:O:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:l:11:ARG:O    | 1:l:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:w:122:PRO:HG2 | 1:w:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:D:11:ARG:O    | 1:D:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:c:76:LEU:O    | 1:c:80:VAL:HG23  | 1.94                     | 0.67              |
| 1:J:122:PRO:HG2 | 1:J:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:r:11:ARG:O    | 1:r:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:7:11:ARG:O    | 1:7:15:GLU:HG2   | 1.93                     | 0.67              |
| 1:B:76:LEU:O    | 1:B:80:VAL:HG23  | 1.94                     | 0.67              |
| 1:G:11:ARG:O    | 1:G:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:n:11:ARG:O    | 1:n:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:5:11:ARG:O    | 1:5:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:y:11:ARG:O    | 1:y:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:y:122:PRO:HG2 | 1:y:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:Z:122:PRO:HG2 | 1:Z:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:k:11:ARG:O    | 1:k:15:GLU:HG2   | 1.93                     | 0.67              |
| 1:C:11:ARG:O    | 1:C:15:GLU:HG2   | 1.94                     | 0.67              |
| 1:H:113:ALA:HB1 | 1:H:166:LEU:HD21 | 1.77                     | 0.67              |
| 1:T:76:LEU:O    | 1:T:80:VAL:HG23  | 1.94                     | 0.67              |
| 1:6:9:GLU:HG3   | 1:6:12:ARG:HH21  | 1.58                     | 0.67              |
| 1:D:122:PRO:HG2 | 1:D:125:LEU:HD23 | 1.75                     | 0.67              |
| 1:Q:11:ARG:O    | 1:Q:15:GLU:HG2   | 1.95                     | 0.67              |
| 1:e:215:ARG:NH1 | 1:e:218:GLU:OE2  | 2.28                     | 0.67              |
| 1:g:215:ARG:NH1 | 1:g:218:GLU:OE2  | 2.28                     | 0.67              |
| 1:E:113:ALA:HB1 | 1:E:166:LEU:HD21 | 1.76                     | 0.66              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:S:25:GLY:HA3  | 1:S:29:MET:HE2   | 1.77                     | 0.66              |
| 1:L:76:LEU:O    | 1:L:80:VAL:HG23  | 1.95                     | 0.66              |
| 1:N:113:ALA:HB1 | 1:N:166:LEU:HD21 | 1.76                     | 0.66              |
| 1:u:215:ARG:NH1 | 1:u:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:l:215:ARG:NH1 | 1:l:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:F:215:ARG:NH1 | 1:F:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:2:149:ARG:NH1 | 1:2:243:GLU:OE1  | 2.26                     | 0.66              |
| 1:l:25:GLY:HA3  | 1:l:29:MET:HE2   | 1.78                     | 0.66              |
| 1:x:76:LEU:O    | 1:x:80:VAL:HG23  | 1.95                     | 0.66              |
| 1:H:76:LEU:O    | 1:H:80:VAL:HG23  | 1.95                     | 0.66              |
| 1:S:215:ARG:NH1 | 1:S:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:J:11:ARG:O    | 1:J:15:GLU:HG2   | 1.95                     | 0.66              |
| 1:2:113:ALA:HB1 | 1:2:166:LEU:HD21 | 1.76                     | 0.66              |
| 1:W:215:ARG:NH1 | 1:W:218:GLU:OE2  | 2.29                     | 0.66              |
| 1:M:11:ARG:O    | 1:M:15:GLU:HG2   | 1.95                     | 0.66              |
| 1:F:11:ARG:O    | 1:F:15:GLU:HG2   | 1.94                     | 0.66              |
| 1:O:215:ARG:NH1 | 1:O:218:GLU:OE2  | 2.29                     | 0.66              |
| 1:F:25:GLY:HA3  | 1:F:29:MET:HE2   | 1.78                     | 0.66              |
| 1:G:113:ALA:HB1 | 1:G:166:LEU:HD21 | 1.76                     | 0.66              |
| 1:n:25:GLY:HA3  | 1:n:29:MET:HE2   | 1.77                     | 0.66              |
| 1:S:11:ARG:O    | 1:S:15:GLU:HG2   | 1.94                     | 0.66              |
| 1:i:62:LEU:HD11 | 1:i:66:ARG:HH11  | 1.60                     | 0.66              |
| 1:k:113:ALA:HB1 | 1:k:166:LEU:HD21 | 1.76                     | 0.66              |
| 1:7:113:ALA:HB1 | 1:7:166:LEU:HD21 | 1.76                     | 0.66              |
| 1:E:87:LEU:HB3  | 1:E:92:ARG:HG3   | 1.77                     | 0.66              |
| 1:g:11:ARG:O    | 1:g:15:GLU:HG2   | 1.94                     | 0.66              |
| 1:u:11:ARG:O    | 1:u:15:GLU:HG2   | 1.94                     | 0.66              |
| 1:4:215:ARG:NH1 | 1:4:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:C:215:ARG:NH1 | 1:C:218:GLU:OE2  | 2.29                     | 0.66              |
| 1:O:25:GLY:HA3  | 1:O:29:MET:HE2   | 1.78                     | 0.66              |
| 1:n:215:ARG:NH1 | 1:n:218:GLU:OE2  | 2.28                     | 0.66              |
| 1:J:57:LEU:O    | 1:J:61:VAL:HG23  | 1.96                     | 0.66              |
| 1:M:57:LEU:O    | 1:M:61:VAL:HG23  | 1.96                     | 0.66              |
| 1:a:76:LEU:O    | 1:a:80:VAL:HG23  | 1.94                     | 0.66              |
| 1:7:87:LEU:HB3  | 1:7:92:ARG:HG3   | 1.77                     | 0.66              |
| 1:1:215:ARG:NH1 | 1:1:218:GLU:OE2  | 2.29                     | 0.65              |
| 1:h:57:LEU:O    | 1:h:61:VAL:HG23  | 1.96                     | 0.65              |
| 1:X:87:LEU:HB3  | 1:X:92:ARG:HG3   | 1.77                     | 0.65              |
| 1:V:149:ARG:NH1 | 1:V:243:GLU:OE2  | 2.29                     | 0.65              |
| 1:W:11:ARG:O    | 1:W:15:GLU:HG2   | 1.94                     | 0.65              |
| 1:j:149:ARG:NH1 | 1:j:243:GLU:OE2  | 2.29                     | 0.65              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:6:76:LEU:O    | 1:6:80:VAL:HG23  | 1.95                     | 0.65              |
| 1:b:113:ALA:HB1 | 1:b:166:LEU:HD21 | 1.76                     | 0.65              |
| 1:R:113:ALA:HB1 | 1:R:166:LEU:HD21 | 1.79                     | 0.65              |
| 1:o:113:ALA:HB1 | 1:o:166:LEU:HD21 | 1.76                     | 0.65              |
| 1:V:156:GLU:OE1 | 1:V:254:ARG:NH1  | 2.28                     | 0.65              |
| 1:t:149:ARG:NH1 | 1:t:243:GLU:OE2  | 2.29                     | 0.65              |
| 1:x:215:ARG:NH1 | 1:x:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:e:11:ARG:O    | 1:e:15:GLU:HG2   | 1.94                     | 0.65              |
| 1:5:57:LEU:O    | 1:5:61:VAL:HG23  | 1.96                     | 0.65              |
| 1:A:113:ALA:HB1 | 1:A:166:LEU:HD21 | 1.79                     | 0.65              |
| 1:D:57:LEU:O    | 1:D:61:VAL:HG23  | 1.97                     | 0.65              |
| 1:d:57:LEU:O    | 1:d:61:VAL:HG23  | 1.96                     | 0.65              |
| 1:r:57:LEU:O    | 1:r:61:VAL:HG23  | 1.96                     | 0.65              |
| 1:B:215:ARG:NH1 | 1:B:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:D:149:ARG:NH1 | 1:D:243:GLU:OE2  | 2.30                     | 0.65              |
| 1:V:215:ARG:NH1 | 1:V:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:a:113:ALA:HB1 | 1:a:166:LEU:HD21 | 1.78                     | 0.65              |
| 1:x:149:ARG:NH1 | 1:x:243:GLU:OE2  | 2.29                     | 0.65              |
| 1:y:57:LEU:O    | 1:y:61:VAL:HG23  | 1.97                     | 0.65              |
| 1:H:215:ARG:NH1 | 1:H:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:T:149:ARG:NH1 | 1:T:243:GLU:OE2  | 2.29                     | 0.65              |
| 1:e:25:GLY:HA3  | 1:e:29:MET:HE2   | 1.77                     | 0.65              |
| 1:i:113:ALA:HB1 | 1:i:166:LEU:HD21 | 1.79                     | 0.65              |
| 1:j:215:ARG:NH1 | 1:j:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:c:215:ARG:NH1 | 1:c:218:GLU:OE2  | 2.30                     | 0.65              |
| 1:z:11:ARG:O    | 1:z:15:GLU:HG2   | 1.97                     | 0.65              |
| 1:f:113:ALA:HB1 | 1:f:166:LEU:HD21 | 1.79                     | 0.65              |
| 1:L:113:ALA:HB1 | 1:L:166:LEU:HD21 | 1.77                     | 0.65              |
| 1:W:25:GLY:HA3  | 1:W:29:MET:HE2   | 1.77                     | 0.65              |
| 1:x:113:ALA:HB1 | 1:x:166:LEU:HD21 | 1.80                     | 0.64              |
| 1:y:149:ARG:NH1 | 1:y:243:GLU:OE2  | 2.31                     | 0.64              |
| 1:d:149:ARG:NH1 | 1:d:243:GLU:OE2  | 2.31                     | 0.64              |
| 1:T:215:ARG:NH1 | 1:T:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:L:215:ARG:NH1 | 1:L:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:6:156:GLU:OE1 | 1:6:254:ARG:NH1  | 2.28                     | 0.64              |
| 1:Q:149:ARG:NH1 | 1:Q:243:GLU:OE2  | 2.31                     | 0.64              |
| 1:z:113:ALA:HB1 | 1:z:166:LEU:HD21 | 1.79                     | 0.64              |
| 1:6:215:ARG:NH1 | 1:6:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:T:113:ALA:HB1 | 1:T:166:LEU:HD21 | 1.78                     | 0.64              |
| 1:p:57:LEU:O    | 1:p:61:VAL:HG23  | 1.98                     | 0.64              |
| 1:4:25:GLY:HA3  | 1:4:29:MET:HE2   | 1.78                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:156:GLU:OE1 | 1:A:254:ARG:NH1  | 2.29                     | 0.64              |
| 1:m:11:ARG:O    | 1:m:15:GLU:HG2   | 1.98                     | 0.64              |
| 1:x:44:VAL:HA   | 1:x:47:LEU:HD12  | 1.80                     | 0.64              |
| 1:R:156:GLU:OE1 | 1:R:254:ARG:NH1  | 2.28                     | 0.64              |
| 1:t:215:ARG:NH1 | 1:t:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:B:113:ALA:HB1 | 1:B:166:LEU:HD21 | 1.80                     | 0.64              |
| 1:m:156:GLU:OE1 | 1:m:254:ARG:NH1  | 2.28                     | 0.64              |
| 1:x:57:LEU:O    | 1:x:61:VAL:HG23  | 1.98                     | 0.64              |
| 1:a:149:ARG:NH1 | 1:a:243:GLU:OE2  | 2.29                     | 0.64              |
| 1:m:113:ALA:HB1 | 1:m:166:LEU:HD21 | 1.79                     | 0.64              |
| 1:z:156:GLU:OE1 | 1:z:254:ARG:NH1  | 2.28                     | 0.64              |
| 1:e:149:ARG:NH1 | 1:e:243:GLU:OE1  | 2.30                     | 0.64              |
| 1:q:215:ARG:NH1 | 1:q:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:v:156:GLU:OE1 | 1:v:254:ARG:NH1  | 2.28                     | 0.64              |
| 1:a:215:ARG:NH1 | 1:a:218:GLU:OE2  | 2.30                     | 0.64              |
| 1:c:113:ALA:HB1 | 1:c:166:LEU:HD21 | 1.80                     | 0.64              |
| 1:n:149:ARG:NH1 | 1:n:243:GLU:OE1  | 2.30                     | 0.64              |
| 1:V:44:VAL:HA   | 1:V:47:LEU:HD12  | 1.79                     | 0.64              |
| 1:6:44:VAL:HA   | 1:6:47:LEU:HD12  | 1.80                     | 0.64              |
| 1:l:149:ARG:NH1 | 1:l:243:GLU:OE1  | 2.30                     | 0.64              |
| 1:Q:57:LEU:O    | 1:Q:61:VAL:HG23  | 1.98                     | 0.64              |
| 1:R:62:LEU:HD11 | 1:R:66:ARG:HH11  | 1.62                     | 0.64              |
| 1:O:149:ARG:NH1 | 1:O:243:GLU:OE1  | 2.30                     | 0.64              |
| 1:6:57:LEU:O    | 1:6:61:VAL:HG23  | 1.98                     | 0.64              |
| 1:u:149:ARG:NH1 | 1:u:243:GLU:OE1  | 2.30                     | 0.63              |
| 1:P:113:ALA:HB1 | 1:P:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:P:156:GLU:OE1 | 1:P:254:ARG:NH1  | 2.28                     | 0.63              |
| 1:a:57:LEU:O    | 1:a:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:F:149:ARG:NH1 | 1:F:243:GLU:OE2  | 2.31                     | 0.63              |
| 1:f:11:ARG:O    | 1:f:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:f:156:GLU:OE1 | 1:f:254:ARG:NH1  | 2.28                     | 0.63              |
| 1:j:113:ALA:HB1 | 1:j:166:LEU:HD21 | 1.80                     | 0.63              |
| 1:I:113:ALA:HB1 | 1:I:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:I:156:GLU:OE1 | 1:I:254:ARG:NH1  | 2.28                     | 0.63              |
| 1:3:113:ALA:HB1 | 1:3:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:N:11:ARG:O    | 1:N:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:v:113:ALA:HB1 | 1:v:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:C:149:ARG:NH1 | 1:C:243:GLU:OE2  | 2.31                     | 0.63              |
| 1:K:113:ALA:HB1 | 1:K:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:L:57:LEU:O    | 1:L:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:B:44:VAL:HA   | 1:B:47:LEU:HD12  | 1.80                     | 0.63              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:57:LEU:O    | 1:B:61:VAL:HG23  | 1.99                     | 0.63              |
| 1:R:11:ARG:O    | 1:R:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:c:57:LEU:O    | 1:c:61:VAL:HG23  | 1.99                     | 0.63              |
| 1:K:156:GLU:OE1 | 1:K:254:ARG:NH1  | 2.29                     | 0.63              |
| 1:3:11:ARG:O    | 1:3:15:GLU:HG2   | 1.97                     | 0.63              |
| 1:H:57:LEU:O    | 1:H:61:VAL:HG23  | 1.99                     | 0.63              |
| 1:q:113:ALA:HB1 | 1:q:166:LEU:HD21 | 1.80                     | 0.63              |
| 1:V:113:ALA:HB1 | 1:V:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:L:87:LEU:HB3  | 1:L:92:ARG:HG3   | 1.81                     | 0.63              |
| 1:t:113:ALA:HB1 | 1:t:166:LEU:HD21 | 1.80                     | 0.63              |
| 1:Z:149:ARG:NH1 | 1:Z:243:GLU:OE2  | 2.31                     | 0.63              |
| 1:v:11:ARG:O    | 1:v:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:E:242:PRO:HD2 | 1:E:245:LEU:HD12 | 1.81                     | 0.63              |
| 1:Z:57:LEU:O    | 1:Z:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:w:57:LEU:O    | 1:w:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:G:242:PRO:HD2 | 1:G:245:LEU:HD12 | 1.81                     | 0.63              |
| 1:c:44:VAL:HA   | 1:c:47:LEU:HD12  | 1.81                     | 0.63              |
| 1:T:57:LEU:O    | 1:T:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:T:87:LEU:HB3  | 1:T:92:ARG:HG3   | 1.81                     | 0.63              |
| 1:K:11:ARG:O    | 1:K:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:Y:156:GLU:OE1 | 1:Y:254:ARG:NH1  | 2.28                     | 0.63              |
| 1:w:149:ARG:NH1 | 1:w:243:GLU:OE2  | 2.30                     | 0.63              |
| 1:A:11:ARG:O    | 1:A:15:GLU:HG2   | 1.98                     | 0.63              |
| 1:3:156:GLU:OE1 | 1:3:254:ARG:NH1  | 2.29                     | 0.63              |
| 1:Y:113:ALA:HB1 | 1:Y:166:LEU:HD21 | 1.79                     | 0.63              |
| 1:j:57:LEU:O    | 1:j:61:VAL:HG23  | 1.98                     | 0.63              |
| 1:j:87:LEU:HB3  | 1:j:92:ARG:HG3   | 1.81                     | 0.63              |
| 1:S:113:ALA:HB1 | 1:S:166:LEU:HD21 | 1.81                     | 0.62              |
| 1:q:44:VAL:HA   | 1:q:47:LEU:HD12  | 1.80                     | 0.62              |
| 1:F:113:ALA:HB1 | 1:F:166:LEU:HD21 | 1.82                     | 0.62              |
| 1:i:156:GLU:OE1 | 1:i:254:ARG:NH1  | 2.29                     | 0.62              |
| 1:V:57:LEU:O    | 1:V:61:VAL:HG23  | 1.98                     | 0.62              |
| 1:U:242:PRO:HD2 | 1:U:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:q:57:LEU:O    | 1:q:61:VAL:HG23  | 1.99                     | 0.62              |
| 1:t:57:LEU:O    | 1:t:61:VAL:HG23  | 1.99                     | 0.62              |
| 1:u:113:ALA:HB1 | 1:u:166:LEU:HD21 | 1.81                     | 0.62              |
| 1:a:87:LEU:HB3  | 1:a:92:ARG:HG3   | 1.81                     | 0.62              |
| 1:B:156:GLU:OE1 | 1:B:254:ARG:NH1  | 2.28                     | 0.62              |
| 1:c:156:GLU:OE1 | 1:c:254:ARG:NH1  | 2.28                     | 0.62              |
| 1:p:149:ARG:NH1 | 1:p:243:GLU:OE2  | 2.31                     | 0.62              |
| 1:g:113:ALA:HB1 | 1:g:166:LEU:HD21 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:242:PRO:HD2  | 1:X:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:J:105:LEU:HD23 | 1:J:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:g:149:ARG:NH1  | 1:g:243:GLU:OE2  | 2.31                     | 0.62              |
| 1:r:149:ARG:NH1  | 1:r:243:GLU:OE2  | 2.30                     | 0.62              |
| 1:6:113:ALA:HB1  | 1:6:166:LEU:HD21 | 1.80                     | 0.62              |
| 1:h:149:ARG:NH1  | 1:h:243:GLU:OE2  | 2.30                     | 0.62              |
| 1:3:25:GLY:HA3   | 1:3:29:MET:HE2   | 1.82                     | 0.62              |
| 1:5:105:LEU:HD23 | 1:5:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:2:242:PRO:HD2  | 1:2:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:W:113:ALA:HB1  | 1:W:166:LEU:HD21 | 1.81                     | 0.62              |
| 1:M:105:LEU:HD23 | 1:M:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:5:149:ARG:NH1  | 1:5:243:GLU:OE2  | 2.31                     | 0.62              |
| 1:d:105:LEU:HD23 | 1:d:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:I:25:GLY:HA3   | 1:I:29:MET:HE2   | 1.82                     | 0.62              |
| 1:r:105:LEU:HD23 | 1:r:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:N:242:PRO:HD2  | 1:N:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:D:113:ALA:HB1  | 1:D:166:LEU:HD21 | 1.82                     | 0.62              |
| 1:Q:105:LEU:HD23 | 1:Q:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:d:156:GLU:OE1  | 1:d:254:ARG:NH1  | 2.31                     | 0.62              |
| 1:h:105:LEU:HD23 | 1:h:137:LEU:HD22 | 1.82                     | 0.62              |
| 1:k:242:PRO:HD2  | 1:k:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:7:242:PRO:HD2  | 1:7:245:LEU:HD12 | 1.81                     | 0.62              |
| 1:b:10:VAL:HG13  | 1:b:101:LEU:HD21 | 1.82                     | 0.61              |
| 1:y:113:ALA:HB1  | 1:y:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:o:105:LEU:HD23 | 1:o:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:p:113:ALA:HB1  | 1:p:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:0:242:PRO:HD2  | 1:0:245:LEU:HD12 | 1.81                     | 0.61              |
| 1:J:149:ARG:NH1  | 1:J:243:GLU:OE2  | 2.30                     | 0.61              |
| 1:s:242:PRO:HD2  | 1:s:245:LEU:HD12 | 1.81                     | 0.61              |
| 1:3:76:LEU:O     | 1:3:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:Q:156:GLU:OE1  | 1:Q:254:ARG:NH1  | 2.31                     | 0.61              |
| 1:b:105:LEU:HD23 | 1:b:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:m:25:GLY:HA3   | 1:m:29:MET:HE2   | 1.82                     | 0.61              |
| 1:o:10:VAL:HG13  | 1:o:101:LEU:HD21 | 1.82                     | 0.61              |
| 1:o:242:PRO:HD2  | 1:o:245:LEU:HD12 | 1.81                     | 0.61              |
| 1:G:156:GLU:OE1  | 1:G:254:ARG:NH1  | 2.31                     | 0.61              |
| 1:z:25:GLY:HA3   | 1:z:29:MET:HE2   | 1.82                     | 0.61              |
| 1:q:156:GLU:OE1  | 1:q:254:ARG:NH1  | 2.28                     | 0.61              |
| 1:X:156:GLU:OE1  | 1:X:254:ARG:NH1  | 2.31                     | 0.61              |
| 1:Y:25:GLY:HA3   | 1:Y:29:MET:HE2   | 1.82                     | 0.61              |
| 1:E:156:GLU:OE1  | 1:E:254:ARG:NH1  | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:126:ILE:O    | 1:H:130:VAL:HG23 | 2.01                     | 0.61              |
| 1:e:113:ALA:HB1  | 1:e:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:U:156:GLU:OE1  | 1:U:254:ARG:NH1  | 2.31                     | 0.61              |
| 1:i:76:LEU:O     | 1:i:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:k:10:VAL:HG13  | 1:k:101:LEU:HD21 | 1.82                     | 0.61              |
| 1:b:242:PRO:HD2  | 1:b:245:LEU:HD12 | 1.81                     | 0.61              |
| 1:f:76:LEU:O     | 1:f:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:L:126:ILE:O    | 1:L:130:VAL:HG23 | 2.01                     | 0.61              |
| 1:t:87:LEU:HB3   | 1:t:92:ARG:HG3   | 1.81                     | 0.61              |
| 1:4:113:ALA:HB1  | 1:4:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:Z:105:LEU:HD23 | 1:Z:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:w:105:LEU:HD23 | 1:w:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:7:105:LEU:HD23 | 1:7:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:o:234:ILE:HD11 | 1:o:245:LEU:HB3  | 1.83                     | 0.61              |
| 1:T:126:ILE:O    | 1:T:130:VAL:HG23 | 2.01                     | 0.61              |
| 1:K:25:GLY:HA3   | 1:K:29:MET:HE2   | 1.82                     | 0.61              |
| 1:2:10:VAL:HG13  | 1:2:101:LEU:HD21 | 1.82                     | 0.61              |
| 1:t:156:GLU:OE1  | 1:t:254:ARG:NH1  | 2.28                     | 0.61              |
| 1:N:10:VAL:HG13  | 1:N:101:LEU:HD21 | 1.82                     | 0.61              |
| 1:N:234:ILE:HD11 | 1:N:245:LEU:HB3  | 1.82                     | 0.61              |
| 1:a:126:ILE:O    | 1:a:130:VAL:HG23 | 2.01                     | 0.61              |
| 1:1:113:ALA:HB1  | 1:1:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:r:37:ARG:O     | 1:r:41:GLU:HG2   | 2.01                     | 0.61              |
| 1:5:37:ARG:O     | 1:5:41:GLU:HG2   | 2.01                     | 0.61              |
| 1:5:113:ALA:HB1  | 1:5:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:O:113:ALA:HB1  | 1:O:166:LEU:HD21 | 1.81                     | 0.61              |
| 1:v:76:LEU:O     | 1:v:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:P:76:LEU:O     | 1:P:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:b:234:ILE:HD11 | 1:b:245:LEU:HB3  | 1.83                     | 0.61              |
| 1:y:105:LEU:HD23 | 1:y:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:H:44:VAL:HA    | 1:H:47:LEU:HD12  | 1.82                     | 0.61              |
| 1:M:149:ARG:NH1  | 1:M:243:GLU:OE2  | 2.30                     | 0.61              |
| 1:i:25:GLY:HA3   | 1:i:29:MET:HE2   | 1.82                     | 0.61              |
| 1:Y:76:LEU:O     | 1:Y:80:VAL:HG23  | 2.00                     | 0.61              |
| 1:k:105:LEU:HD23 | 1:k:137:LEU:HD22 | 1.82                     | 0.61              |
| 1:k:234:ILE:HD11 | 1:k:245:LEU:HB3  | 1.83                     | 0.61              |
| 1:v:25:GLY:HA3   | 1:v:29:MET:HE2   | 1.82                     | 0.61              |
| 1:P:25:GLY:HA3   | 1:P:29:MET:HE2   | 1.82                     | 0.61              |
| 1:f:25:GLY:HA3   | 1:f:29:MET:HE2   | 1.82                     | 0.61              |
| 1:r:113:ALA:HB1  | 1:r:166:LEU:HD21 | 1.83                     | 0.61              |
| 1:s:234:ILE:HD11 | 1:s:245:LEU:HB3  | 1.83                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:113:ALA:HB1  | 1:l:166:LEU:HD21 | 1.82                     | 0.61              |
| 1:7:234:ILE:HD11 | 1:7:245:LEU:HB3  | 1.83                     | 0.61              |
| 1:D:37:ARG:O     | 1:D:41:GLU:HG2   | 2.01                     | 0.61              |
| 1:G:10:VAL:HG13  | 1:G:101:LEU:HD21 | 1.83                     | 0.61              |
| 1:D:105:LEU:HD23 | 1:D:137:LEU:HD22 | 1.82                     | 0.60              |
| 1:Q:113:ALA:HB1  | 1:Q:166:LEU:HD21 | 1.83                     | 0.60              |
| 1:y:37:ARG:O     | 1:y:41:GLU:HG2   | 2.01                     | 0.60              |
| 1:0:234:ILE:HD11 | 1:0:245:LEU:HB3  | 1.83                     | 0.60              |
| 1:7:10:VAL:HG13  | 1:7:101:LEU:HD21 | 1.83                     | 0.60              |
| 1:C:113:ALA:HB1  | 1:C:166:LEU:HD21 | 1.81                     | 0.60              |
| 1:n:113:ALA:HB1  | 1:n:166:LEU:HD21 | 1.81                     | 0.60              |
| 1:h:113:ALA:HB1  | 1:h:166:LEU:HD21 | 1.83                     | 0.60              |
| 1:d:113:ALA:HB1  | 1:d:166:LEU:HD21 | 1.83                     | 0.60              |
| 1:1:149:ARG:NH1  | 1:1:243:GLU:OE1  | 2.30                     | 0.60              |
| 1:w:113:ALA:HB1  | 1:w:166:LEU:HD21 | 1.82                     | 0.60              |
| 1:A:25:GLY:HA3   | 1:A:29:MET:HE2   | 1.82                     | 0.60              |
| 1:R:25:GLY:HA3   | 1:R:29:MET:HE2   | 1.82                     | 0.60              |
| 1:R:76:LEU:O     | 1:R:80:VAL:HG23  | 2.00                     | 0.60              |
| 1:S:149:ARG:O    | 1:S:153:ARG:HG2  | 2.00                     | 0.60              |
| 1:o:156:GLU:OE1  | 1:o:254:ARG:NH1  | 2.32                     | 0.60              |
| 1:r:156:GLU:OE1  | 1:r:254:ARG:NH1  | 2.31                     | 0.60              |
| 1:h:37:ARG:O     | 1:h:41:GLU:HG2   | 2.02                     | 0.60              |
| 1:s:83:GLU:OE1   | 1:s:83:GLU:N     | 2.34                     | 0.60              |
| 1:E:105:LEU:HD23 | 1:E:137:LEU:HD22 | 1.83                     | 0.60              |
| 1:p:37:ARG:O     | 1:p:41:GLU:HG2   | 2.02                     | 0.60              |
| 1:K:122:PRO:HG2  | 1:K:125:LEU:HD23 | 1.84                     | 0.60              |
| 1:h:10:VAL:HG13  | 1:h:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:M:10:VAL:HG13  | 1:M:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:M:37:ARG:O     | 1:M:41:GLU:HG2   | 2.01                     | 0.60              |
| 1:Z:113:ALA:HB1  | 1:Z:166:LEU:HD21 | 1.83                     | 0.60              |
| 1:E:10:VAL:HG13  | 1:E:101:LEU:HD21 | 1.83                     | 0.60              |
| 1:b:156:GLU:OE1  | 1:b:254:ARG:NH1  | 2.31                     | 0.60              |
| 1:T:156:GLU:OE1  | 1:T:254:ARG:NH1  | 2.28                     | 0.60              |
| 1:U:105:LEU:HD23 | 1:U:137:LEU:HD22 | 1.82                     | 0.60              |
| 1:2:234:ILE:HD11 | 1:2:245:LEU:HB3  | 1.83                     | 0.60              |
| 1:L:156:GLU:OE1  | 1:L:254:ARG:NH1  | 2.28                     | 0.60              |
| 1:w:156:GLU:OE1  | 1:w:254:ARG:NH1  | 2.31                     | 0.60              |
| 1:m:76:LEU:O     | 1:m:80:VAL:HG23  | 2.00                     | 0.60              |
| 1:G:105:LEU:HD23 | 1:G:137:LEU:HD22 | 1.83                     | 0.60              |
| 1:z:76:LEU:O     | 1:z:80:VAL:HG23  | 2.00                     | 0.60              |
| 1:V:11:ARG:O     | 1:V:15:GLU:HG2   | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:17:LEU:O     | 1:D:21:VAL:HG23  | 2.02                     | 0.60              |
| 1:p:10:VAL:HG13  | 1:p:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:J:37:ARG:O     | 1:J:41:GLU:HG2   | 2.01                     | 0.60              |
| 1:U:10:VAL:HG13  | 1:U:101:LEU:HD21 | 1.82                     | 0.60              |
| 1:L:10:VAL:HG13  | 1:L:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:5:156:GLU:OE1  | 1:5:254:ARG:NH1  | 2.31                     | 0.60              |
| 1:w:17:LEU:O     | 1:w:21:VAL:HG23  | 2.02                     | 0.60              |
| 1:Q:37:ARG:O     | 1:Q:41:GLU:HG2   | 2.02                     | 0.60              |
| 1:T:10:VAL:HG13  | 1:T:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:J:10:VAL:HG13  | 1:J:101:LEU:HD21 | 1.84                     | 0.60              |
| 1:X:105:LEU:HD23 | 1:X:137:LEU:HD22 | 1.82                     | 0.60              |
| 1:Y:122:PRO:HG2  | 1:Y:125:LEU:HD23 | 1.84                     | 0.60              |
| 1:j:11:ARG:O     | 1:j:15:GLU:HG2   | 2.02                     | 0.60              |
| 1:a:156:GLU:OE1  | 1:a:254:ARG:NH1  | 2.28                     | 0.60              |
| 1:d:37:ARG:O     | 1:d:41:GLU:HG2   | 2.02                     | 0.60              |
| 1:s:10:VAL:HG13  | 1:s:101:LEU:HD21 | 1.83                     | 0.60              |
| 1:s:105:LEU:HD23 | 1:s:137:LEU:HD22 | 1.82                     | 0.60              |
| 1:t:11:ARG:O     | 1:t:15:GLU:HG2   | 2.02                     | 0.60              |
| 1:Z:37:ARG:O     | 1:Z:41:GLU:HG2   | 2.02                     | 0.60              |
| 1:Z:156:GLU:OE1  | 1:Z:254:ARG:NH1  | 2.31                     | 0.60              |
| 1:v:122:PRO:HG2  | 1:v:125:LEU:HD23 | 1.84                     | 0.60              |
| 1:X:234:ILE:HD11 | 1:X:245:LEU:HB3  | 1.83                     | 0.59              |
| 1:w:16:GLU:O     | 1:w:20:GLU:HG2   | 2.02                     | 0.59              |
| 1:y:16:GLU:O     | 1:y:20:GLU:HG2   | 2.02                     | 0.59              |
| 1:U:234:ILE:HD11 | 1:U:245:LEU:HB3  | 1.83                     | 0.59              |
| 1:r:17:LEU:O     | 1:r:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:2:105:LEU:HD23 | 1:2:137:LEU:HD22 | 1.82                     | 0.59              |
| 1:X:10:VAL:HG13  | 1:X:101:LEU:HD21 | 1.83                     | 0.59              |
| 1:N:105:LEU:HD23 | 1:N:137:LEU:HD22 | 1.82                     | 0.59              |
| 1:E:234:ILE:HD11 | 1:E:245:LEU:HB3  | 1.83                     | 0.59              |
| 1:G:234:ILE:HD11 | 1:G:245:LEU:HB3  | 1.83                     | 0.59              |
| 1:H:105:LEU:HD23 | 1:H:137:LEU:HD22 | 1.84                     | 0.59              |
| 1:O:105:LEU:HD23 | 1:O:137:LEU:HD22 | 1.82                     | 0.59              |
| 1:J:113:ALA:HB1  | 1:J:166:LEU:HD21 | 1.83                     | 0.59              |
| 1:a:44:VAL:HA    | 1:a:47:LEU:HD12  | 1.84                     | 0.59              |
| 1:w:37:ARG:O     | 1:w:41:GLU:HG2   | 2.02                     | 0.59              |
| 1:B:11:ARG:O     | 1:B:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:c:11:ARG:O     | 1:c:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:T:44:VAL:HA    | 1:T:47:LEU:HD12  | 1.83                     | 0.59              |
| 1:p:16:GLU:O     | 1:p:20:GLU:HG2   | 2.02                     | 0.59              |
| 1:O:10:VAL:HG13  | 1:O:101:LEU:HD21 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:11:ARG:O     | 1:q:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:s:156:GLU:OE1  | 1:s:254:ARG:NH1  | 2.31                     | 0.59              |
| 1:5:16:GLU:O     | 1:5:20:GLU:HG2   | 2.02                     | 0.59              |
| 1:Z:17:LEU:O     | 1:Z:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:H:10:VAL:HG13  | 1:H:101:LEU:HD21 | 1.84                     | 0.59              |
| 1:H:11:ARG:O     | 1:H:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:d:17:LEU:O     | 1:d:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:T:11:ARG:O     | 1:T:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:i:122:PRO:HG2  | 1:i:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:5:10:VAL:HG13  | 1:5:101:LEU:HD21 | 1.85                     | 0.59              |
| 1:Z:10:VAL:HG13  | 1:Z:101:LEU:HD21 | 1.84                     | 0.59              |
| 1:a:11:ARG:O     | 1:a:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:I:122:PRO:HG2  | 1:I:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:3:122:PRO:HG2  | 1:3:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:M:17:LEU:O     | 1:M:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:M:113:ALA:HB1  | 1:M:166:LEU:HD21 | 1.83                     | 0.59              |
| 1:P:11:ARG:O     | 1:P:15:GLU:HG2   | 2.03                     | 0.59              |
| 1:P:122:PRO:HG2  | 1:P:125:LEU:HD23 | 1.85                     | 0.59              |
| 1:a:10:VAL:HG13  | 1:a:101:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:122:PRO:HG2  | 1:A:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:C:105:LEU:HD23 | 1:C:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:Q:17:LEU:O     | 1:Q:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:0:156:GLU:OE1  | 1:0:254:ARG:NH1  | 2.31                     | 0.59              |
| 1:J:17:LEU:O     | 1:J:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:f:122:PRO:HG2  | 1:f:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:G:38:HIS:ND1   | 1:G:64:MET:HE1   | 2.18                     | 0.59              |
| 1:n:105:LEU:HD23 | 1:n:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:z:122:PRO:HG2  | 1:z:125:LEU:HD23 | 1.84                     | 0.59              |
| 1:i:11:ARG:O     | 1:i:15:GLU:HG2   | 2.03                     | 0.59              |
| 1:a:105:LEU:HD23 | 1:a:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:F:105:LEU:HD23 | 1:F:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:c:10:VAL:HG13  | 1:c:101:LEU:HD21 | 1.85                     | 0.59              |
| 1:L:11:ARG:O     | 1:L:15:GLU:HG2   | 2.02                     | 0.59              |
| 1:W:105:LEU:HD23 | 1:W:137:LEU:HD22 | 1.84                     | 0.59              |
| 1:h:17:LEU:O     | 1:h:21:VAL:HG23  | 2.02                     | 0.59              |
| 1:O:105:LEU:HD23 | 1:O:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:l:105:LEU:HD23 | 1:l:137:LEU:HD22 | 1.85                     | 0.59              |
| 1:w:10:VAL:HG13  | 1:w:101:LEU:HD21 | 1.84                     | 0.59              |
| 1:m:122:PRO:HG2  | 1:m:125:LEU:HD23 | 1.84                     | 0.58              |
| 1:x:156:GLU:OE1  | 1:x:254:ARG:NH1  | 2.28                     | 0.58              |
| 1:y:10:VAL:HG13  | 1:y:101:LEU:HD21 | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:105:LEU:HD23 | 1:S:137:LEU:HD22 | 1.85                     | 0.58              |
| 1:r:10:VAL:HG13  | 1:r:101:LEU:HD21 | 1.85                     | 0.58              |
| 1:t:44:VAL:HA    | 1:t:47:LEU:HD12  | 1.85                     | 0.58              |
| 1:R:122:PRO:HG2  | 1:R:125:LEU:HD23 | 1.84                     | 0.58              |
| 1:R:195:LEU:HD21 | 1:R:244:GLU:OE1  | 2.04                     | 0.58              |
| 1:I:11:ARG:O     | 1:I:15:GLU:HG2   | 2.03                     | 0.58              |
| 1:e:10:VAL:HG13  | 1:e:101:LEU:HD21 | 1.85                     | 0.58              |
| 1:e:105:LEU:HD23 | 1:e:137:LEU:HD22 | 1.85                     | 0.58              |
| 1:p:156:GLU:OE1  | 1:p:254:ARG:NH1  | 2.32                     | 0.58              |
| 1:4:105:LEU:HD23 | 1:4:137:LEU:HD22 | 1.84                     | 0.58              |
| 1:H:156:GLU:OE1  | 1:H:254:ARG:NH1  | 2.28                     | 0.58              |
| 1:z:195:LEU:HD21 | 1:z:244:GLU:OE1  | 2.03                     | 0.58              |
| 1:K:10:VAL:HG13  | 1:K:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:L:105:LEU:HD23 | 1:L:137:LEU:HD22 | 1.84                     | 0.58              |
| 1:k:156:GLU:OE1  | 1:k:254:ARG:NH1  | 2.32                     | 0.58              |
| 1:7:156:GLU:OE1  | 1:7:254:ARG:NH1  | 2.31                     | 0.58              |
| 1:B:10:VAL:HG13  | 1:B:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:Q:10:VAL:HG13  | 1:Q:101:LEU:HD21 | 1.84                     | 0.58              |
| 1:V:10:VAL:HG13  | 1:V:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:j:10:VAL:HG13  | 1:j:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:u:105:LEU:HD23 | 1:u:137:LEU:HD22 | 1.85                     | 0.58              |
| 1:m:195:LEU:HD21 | 1:m:244:GLU:OE1  | 2.03                     | 0.58              |
| 1:g:105:LEU:HD23 | 1:g:137:LEU:HD22 | 1.85                     | 0.58              |
| 1:Y:11:ARG:O     | 1:Y:15:GLU:HG2   | 2.03                     | 0.58              |
| 1:j:44:VAL:HA    | 1:j:47:LEU:HD12  | 1.84                     | 0.58              |
| 1:D:10:VAL:HG13  | 1:D:101:LEU:HD21 | 1.85                     | 0.58              |
| 1:I:10:VAL:HG13  | 1:I:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:Y:10:VAL:HG13  | 1:Y:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:A:10:VAL:HG13  | 1:A:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:x:105:LEU:HD23 | 1:x:137:LEU:HD22 | 1.86                     | 0.58              |
| 1:y:156:GLU:OE1  | 1:y:254:ARG:NH1  | 2.31                     | 0.58              |
| 1:d:10:VAL:HG13  | 1:d:101:LEU:HD21 | 1.84                     | 0.58              |
| 1:3:10:VAL:HG13  | 1:3:101:LEU:HD21 | 1.86                     | 0.58              |
| 1:N:44:VAL:HA    | 1:N:47:LEU:HD12  | 1.86                     | 0.58              |
| 1:L:44:VAL:HA    | 1:L:47:LEU:HD12  | 1.85                     | 0.58              |
| 1:P:195:LEU:HD21 | 1:P:244:GLU:OE1  | 2.04                     | 0.58              |
| 1:T:105:LEU:HD23 | 1:T:137:LEU:HD22 | 1.85                     | 0.58              |
| 1:h:156:GLU:OE1  | 1:h:254:ARG:NH1  | 2.31                     | 0.58              |
| 1:D:156:GLU:OE1  | 1:D:254:ARG:NH1  | 2.31                     | 0.57              |
| 1:E:83:GLU:OE1   | 1:E:83:GLU:N     | 2.37                     | 0.57              |
| 1:p:38:HIS:ND1   | 1:p:64:MET:HE1   | 2.20                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:83:GLU:N     | 1:0:83:GLU:OE1   | 2.37                     | 0.57              |
| 1:q:10:VAL:HG13  | 1:q:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:6:105:LEU:HD23 | 1:6:137:LEU:HD22 | 1.86                     | 0.57              |
| 1:w:38:HIS:ND1   | 1:w:64:MET:HE1   | 2.19                     | 0.57              |
| 1:2:83:GLU:OE1   | 1:2:83:GLU:N     | 2.37                     | 0.57              |
| 1:b:83:GLU:OE1   | 1:b:83:GLU:N     | 2.37                     | 0.57              |
| 1:f:10:VAL:HG13  | 1:f:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:1:105:LEU:HD23 | 1:1:137:LEU:HD22 | 1.85                     | 0.57              |
| 1:G:83:GLU:OE1   | 1:G:83:GLU:N     | 2.37                     | 0.57              |
| 1:W:10:VAL:HG13  | 1:W:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:E:44:VAL:HA    | 1:E:47:LEU:HD12  | 1.86                     | 0.57              |
| 1:e:76:LEU:O     | 1:e:80:VAL:HG23  | 2.04                     | 0.57              |
| 1:4:76:LEU:O     | 1:4:80:VAL:HG23  | 2.05                     | 0.57              |
| 1:N:83:GLU:N     | 1:N:83:GLU:OE1   | 2.37                     | 0.57              |
| 1:y:234:ILE:HD11 | 1:y:245:LEU:HB3  | 1.87                     | 0.57              |
| 1:S:249:ASP:OD1  | 1:d:221:HIS:NE2  | 2.38                     | 0.57              |
| 1:z:105:LEU:HD23 | 1:z:137:LEU:HD22 | 1.87                     | 0.57              |
| 1:I:195:LEU:HD21 | 1:I:244:GLU:OE1  | 2.05                     | 0.57              |
| 1:v:83:GLU:N     | 1:v:83:GLU:OE1   | 2.38                     | 0.57              |
| 1:v:195:LEU:HD21 | 1:v:244:GLU:OE1  | 2.03                     | 0.57              |
| 1:b:44:VAL:HA    | 1:b:47:LEU:HD12  | 1.86                     | 0.57              |
| 1:m:105:LEU:HD23 | 1:m:137:LEU:HD22 | 1.87                     | 0.57              |
| 1:R:10:VAL:HG13  | 1:R:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:z:83:GLU:OE1   | 1:z:83:GLU:N     | 2.38                     | 0.57              |
| 1:s:38:HIS:ND1   | 1:s:64:MET:HE1   | 2.20                     | 0.57              |
| 1:t:10:VAL:HG13  | 1:t:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:P:83:GLU:OE1   | 1:P:83:GLU:N     | 2.38                     | 0.57              |
| 1:R:83:GLU:OE1   | 1:R:83:GLU:N     | 2.38                     | 0.57              |
| 1:U:83:GLU:OE1   | 1:U:83:GLU:N     | 2.37                     | 0.57              |
| 1:g:10:VAL:HG13  | 1:g:101:LEU:HD21 | 1.87                     | 0.57              |
| 1:m:83:GLU:OE1   | 1:m:83:GLU:N     | 2.38                     | 0.57              |
| 1:u:10:VAL:HG13  | 1:u:101:LEU:HD21 | 1.87                     | 0.57              |
| 1:u:76:LEU:O     | 1:u:80:VAL:HG23  | 2.05                     | 0.57              |
| 1:P:10:VAL:HG13  | 1:P:101:LEU:HD21 | 1.86                     | 0.57              |
| 1:c:29:MET:HE1   | 1:c:115:ALA:HB2  | 1.87                     | 0.57              |
| 1:Y:105:LEU:HD23 | 1:Y:137:LEU:HD22 | 1.87                     | 0.57              |
| 1:v:105:LEU:HD23 | 1:v:137:LEU:HD22 | 1.86                     | 0.57              |
| 1:6:234:ILE:HD11 | 1:6:245:LEU:HB3  | 1.86                     | 0.57              |
| 1:K:105:LEU:HD23 | 1:K:137:LEU:HD22 | 1.87                     | 0.56              |
| 1:L:29:MET:HE1   | 1:L:115:ALA:HB2  | 1.87                     | 0.56              |
| 1:W:76:LEU:O     | 1:W:80:VAL:HG23  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:10:VAL:HG13  | 1:i:101:LEU:HD21 | 1.87                     | 0.56              |
| 1:k:83:GLU:OE1   | 1:k:83:GLU:N     | 2.37                     | 0.56              |
| 1:v:10:VAL:HG13  | 1:v:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:6:10:VAL:HG13  | 1:6:101:LEU:HD21 | 1.87                     | 0.56              |
| 1:G:44:VAL:HA    | 1:G:47:LEU:HD12  | 1.86                     | 0.56              |
| 1:n:10:VAL:HG13  | 1:n:101:LEU:HD21 | 1.87                     | 0.56              |
| 1:0:167:ARG:NH2  | 1:0:173:GLU:OE1  | 2.36                     | 0.56              |
| 1:f:83:GLU:N     | 1:f:83:GLU:OE1   | 2.38                     | 0.56              |
| 1:h:38:HIS:ND1   | 1:h:64:MET:HE1   | 2.21                     | 0.56              |
| 1:s:167:ARG:NH2  | 1:s:173:GLU:OE1  | 2.36                     | 0.56              |
| 1:P:105:LEU:HD23 | 1:P:137:LEU:HD22 | 1.87                     | 0.56              |
| 1:A:195:LEU:HD21 | 1:A:244:GLU:OE1  | 2.05                     | 0.56              |
| 1:C:10:VAL:HG13  | 1:C:101:LEU:HD21 | 1.87                     | 0.56              |
| 1:S:76:LEU:O     | 1:S:80:VAL:HG23  | 2.05                     | 0.56              |
| 1:d:234:ILE:HD11 | 1:d:245:LEU:HB3  | 1.86                     | 0.56              |
| 1:3:105:LEU:HD23 | 1:3:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:i:83:GLU:N     | 1:i:83:GLU:OE1   | 2.38                     | 0.56              |
| 1:4:10:VAL:HG13  | 1:4:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:j:105:LEU:HD23 | 1:j:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:I:105:LEU:HD23 | 1:I:137:LEU:HD22 | 1.87                     | 0.56              |
| 1:J:156:GLU:OE1  | 1:J:254:ARG:NH1  | 2.31                     | 0.56              |
| 1:q:105:LEU:HD23 | 1:q:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:l:76:LEU:O     | 1:l:80:VAL:HG23  | 2.06                     | 0.56              |
| 1:V:105:LEU:HD23 | 1:V:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:g:76:LEU:O     | 1:g:80:VAL:HG23  | 2.06                     | 0.56              |
| 1:3:195:LEU:HD21 | 1:3:244:GLU:OE1  | 2.05                     | 0.56              |
| 1:t:105:LEU:HD23 | 1:t:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:5:234:ILE:HD11 | 1:5:245:LEU:HB3  | 1.87                     | 0.56              |
| 1:F:10:VAL:HG13  | 1:F:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:F:85:ARG:NH1   | 1:s:64:MET:HE2   | 2.21                     | 0.56              |
| 1:Q:234:ILE:HD11 | 1:Q:245:LEU:HB3  | 1.87                     | 0.56              |
| 1:G:64:MET:HE2   | 1:W:85:ARG:NH1   | 2.20                     | 0.56              |
| 1:c:105:LEU:HD23 | 1:c:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:S:10:VAL:HG13  | 1:S:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:0:44:VAL:HA    | 1:0:47:LEU:HD12  | 1.88                     | 0.56              |
| 1:V:195:LEU:HD21 | 1:V:244:GLU:OE1  | 2.06                     | 0.56              |
| 1:L:234:ILE:HD11 | 1:L:245:LEU:HB3  | 1.86                     | 0.56              |
| 1:M:156:GLU:OE1  | 1:M:254:ARG:NH1  | 2.31                     | 0.56              |
| 1:Y:83:GLU:OE1   | 1:Y:83:GLU:N     | 2.38                     | 0.56              |
| 1:Z:234:ILE:HD11 | 1:Z:245:LEU:HB3  | 1.87                     | 0.56              |
| 1:l:10:VAL:HG13  | 1:l:101:LEU:HD21 | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:83:GLU:OE1   | 1:A:83:GLU:N     | 2.39                     | 0.56              |
| 1:D:234:ILE:HD11 | 1:D:245:LEU:HB3  | 1.88                     | 0.56              |
| 1:h:87:LEU:HB3   | 1:h:92:ARG:HG3   | 1.87                     | 0.56              |
| 1:h:234:ILE:HD11 | 1:h:245:LEU:HB3  | 1.86                     | 0.56              |
| 1:k:44:VAL:HA    | 1:k:47:LEU:HD12  | 1.87                     | 0.56              |
| 1:l:76:LEU:O     | 1:l:80:VAL:HG23  | 2.06                     | 0.56              |
| 1:B:105:LEU:HD23 | 1:B:137:LEU:HD22 | 1.86                     | 0.56              |
| 1:E:56:ARG:HD2   | 1:e:56:ARG:HG3   | 1.88                     | 0.56              |
| 1:m:10:VAL:HG13  | 1:m:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:z:10:VAL:HG13  | 1:z:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:I:83:GLU:OE1   | 1:I:83:GLU:N     | 2.38                     | 0.56              |
| 1:J:87:LEU:HB3   | 1:J:92:ARG:HG3   | 1.88                     | 0.56              |
| 1:1:10:VAL:HG13  | 1:1:101:LEU:HD21 | 1.87                     | 0.56              |
| 1:j:29:MET:HE1   | 1:j:115:ALA:HB2  | 1.87                     | 0.56              |
| 1:Q:167:ARG:NH2  | 1:Q:173:GLU:OE1  | 2.39                     | 0.56              |
| 1:d:87:LEU:HB3   | 1:d:92:ARG:HG3   | 1.88                     | 0.56              |
| 1:K:195:LEU:HD21 | 1:K:244:GLU:OE1  | 2.05                     | 0.56              |
| 1:2:156:GLU:OE1  | 1:2:254:ARG:NH1  | 2.32                     | 0.56              |
| 1:3:83:GLU:N     | 1:3:83:GLU:OE1   | 2.38                     | 0.56              |
| 1:Y:195:LEU:HD21 | 1:Y:244:GLU:OE1  | 2.06                     | 0.56              |
| 1:O:10:VAL:HG13  | 1:O:101:LEU:HD21 | 1.86                     | 0.56              |
| 1:6:62:LEU:HD11  | 1:6:66:ARG:HH11  | 1.71                     | 0.56              |
| 1:E:38:HIS:ND1   | 1:E:64:MET:HE1   | 2.21                     | 0.56              |
| 1:x:195:LEU:HD21 | 1:x:244:GLU:OE1  | 2.06                     | 0.56              |
| 1:d:167:ARG:NH2  | 1:d:173:GLU:OE1  | 2.39                     | 0.56              |
| 1:o:44:VAL:HA    | 1:o:47:LEU:HD12  | 1.88                     | 0.56              |
| 1:O:76:LEU:O     | 1:O:80:VAL:HG23  | 2.06                     | 0.56              |
| 1:D:167:ARG:NH2  | 1:D:173:GLU:OE1  | 2.39                     | 0.56              |
| 1:Q:87:LEU:HB3   | 1:Q:92:ARG:HG3   | 1.88                     | 0.56              |
| 1:n:76:LEU:O     | 1:n:80:VAL:HG23  | 2.05                     | 0.56              |
| 1:H:29:MET:HE1   | 1:H:115:ALA:HB2  | 1.87                     | 0.56              |
| 1:M:87:LEU:HB3   | 1:M:92:ARG:HG3   | 1.88                     | 0.56              |
| 1:N:156:GLU:OE1  | 1:N:254:ARG:NH1  | 2.31                     | 0.56              |
| 1:U:44:VAL:HA    | 1:U:47:LEU:HD12  | 1.87                     | 0.55              |
| 1:f:195:LEU:HD21 | 1:f:244:GLU:OE1  | 2.06                     | 0.55              |
| 1:s:44:VAL:HA    | 1:s:47:LEU:HD12  | 1.88                     | 0.55              |
| 1:Z:87:LEU:HB3   | 1:Z:92:ARG:HG3   | 1.88                     | 0.55              |
| 1:B:195:LEU:HD21 | 1:B:244:GLU:OE1  | 2.07                     | 0.55              |
| 1:F:76:LEU:O     | 1:F:80:VAL:HG23  | 2.06                     | 0.55              |
| 1:x:62:LEU:HD11  | 1:x:66:ARG:HH11  | 1.71                     | 0.55              |
| 1:r:234:ILE:HD11 | 1:r:245:LEU:HB3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:44:VAL:HA    | 1:X:47:LEU:HD12  | 1.88                     | 0.55              |
| 1:5:167:ARG:NH2  | 1:5:173:GLU:OE1  | 2.39                     | 0.55              |
| 1:R:105:LEU:HD23 | 1:R:137:LEU:HD22 | 1.87                     | 0.55              |
| 1:K:83:GLU:N     | 1:K:83:GLU:OE1   | 2.39                     | 0.55              |
| 1:j:156:GLU:OE1  | 1:j:254:ARG:NH1  | 2.28                     | 0.55              |
| 1:j:195:LEU:HD21 | 1:j:244:GLU:OE1  | 2.07                     | 0.55              |
| 1:w:87:LEU:HB3   | 1:w:92:ARG:HG3   | 1.89                     | 0.55              |
| 1:A:105:LEU:HD23 | 1:A:137:LEU:HD22 | 1.87                     | 0.55              |
| 1:d:38:HIS:ND1   | 1:d:64:MET:HE1   | 2.21                     | 0.55              |
| 1:f:105:LEU:HD23 | 1:f:137:LEU:HD22 | 1.87                     | 0.55              |
| 1:M:221:HIS:NE2  | 1:4:249:ASP:OD1  | 2.40                     | 0.55              |
| 1:J:234:ILE:HD11 | 1:J:245:LEU:HB3  | 1.88                     | 0.55              |
| 1:W:156:GLU:CD   | 1:W:254:ARG:HH12 | 2.15                     | 0.55              |
| 1:i:105:LEU:HD23 | 1:i:137:LEU:HD22 | 1.87                     | 0.55              |
| 1:i:195:LEU:HD21 | 1:i:244:GLU:OE1  | 2.07                     | 0.55              |
| 1:5:87:LEU:HB3   | 1:5:92:ARG:HG3   | 1.89                     | 0.55              |
| 1:y:87:LEU:HB3   | 1:y:92:ARG:HG3   | 1.89                     | 0.55              |
| 1:T:195:LEU:HD21 | 1:T:244:GLU:OE1  | 2.06                     | 0.55              |
| 1:p:87:LEU:HB3   | 1:p:92:ARG:HG3   | 1.88                     | 0.55              |
| 1:2:44:VAL:HA    | 1:2:47:LEU:HD12  | 1.89                     | 0.55              |
| 1:M:56:ARG:HG3   | 1:5:56:ARG:HD2   | 1.89                     | 0.54              |
| 1:t:195:LEU:HD21 | 1:t:244:GLU:OE1  | 2.07                     | 0.54              |
| 1:a:195:LEU:HD21 | 1:a:244:GLU:OE1  | 2.06                     | 0.54              |
| 1:C:76:LEU:O     | 1:C:80:VAL:HG23  | 2.06                     | 0.54              |
| 1:R:167:ARG:NH2  | 1:R:173:GLU:OE1  | 2.39                     | 0.54              |
| 1:c:195:LEU:HD21 | 1:c:244:GLU:OE1  | 2.07                     | 0.54              |
| 1:q:167:ARG:NH2  | 1:q:173:GLU:OE1  | 2.39                     | 0.54              |
| 1:O:249:ASP:OD1  | 1:Z:221:HIS:NE2  | 2.41                     | 0.54              |
| 1:l:167:ARG:NH2  | 1:l:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:A:167:ARG:NH2  | 1:A:173:GLU:OE1  | 2.39                     | 0.54              |
| 1:C:167:ARG:NH2  | 1:C:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:b:167:ARG:NH2  | 1:b:173:GLU:OE1  | 2.36                     | 0.54              |
| 1:n:167:ARG:NH2  | 1:n:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:e:156:GLU:OE1  | 1:e:254:ARG:NH1  | 2.37                     | 0.54              |
| 1:o:167:ARG:NH2  | 1:o:173:GLU:OE1  | 2.37                     | 0.54              |
| 1:L:62:LEU:HD11  | 1:L:66:ARG:HH11  | 1.71                     | 0.54              |
| 1:W:249:ASP:OD1  | 1:h:221:HIS:NE2  | 2.41                     | 0.54              |
| 1:7:44:VAL:HA    | 1:7:47:LEU:HD12  | 1.88                     | 0.54              |
| 1:K:76:LEU:O     | 1:K:80:VAL:HG12  | 2.08                     | 0.54              |
| 1:3:167:ARG:NH2  | 1:3:173:GLU:OE1  | 2.39                     | 0.54              |
| 1:t:167:ARG:NH2  | 1:t:173:GLU:OE1  | 2.39                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:167:ARG:NH2  | 1:O:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:Z:38:HIS:ND1   | 1:Z:64:MET:HE1   | 2.23                     | 0.54              |
| 1:q:195:LEU:HD21 | 1:q:244:GLU:OE1  | 2.07                     | 0.54              |
| 1:x:10:VAL:HG13  | 1:x:101:LEU:HD21 | 1.89                     | 0.54              |
| 1:c:62:LEU:HD11  | 1:c:66:ARG:HH11  | 1.73                     | 0.54              |
| 1:e:167:ARG:NH2  | 1:e:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:F:56:ARG:HG3   | 1:s:56:ARG:HD2   | 1.90                     | 0.54              |
| 1:p:105:LEU:HD13 | 1:p:137:LEU:HD22 | 1.89                     | 0.54              |
| 1:1:167:ARG:NH2  | 1:1:173:GLU:OE1  | 2.38                     | 0.54              |
| 1:M:234:ILE:HD11 | 1:M:245:LEU:HB3  | 1.89                     | 0.54              |
| 1:a:62:LEU:HD11  | 1:a:66:ARG:HH11  | 1.72                     | 0.54              |
| 1:w:234:ILE:HD11 | 1:w:245:LEU:HB3  | 1.89                     | 0.54              |
| 1:I:167:ARG:NH2  | 1:I:173:GLU:OE1  | 2.39                     | 0.54              |
| 1:k:167:ARG:NH2  | 1:k:173:GLU:OE1  | 2.36                     | 0.54              |
| 1:l:249:ASP:OD1  | 1:w:221:HIS:NE2  | 2.41                     | 0.54              |
| 1:7:167:ARG:NH2  | 1:7:173:GLU:OE1  | 2.36                     | 0.54              |
| 1:Q:38:HIS:ND1   | 1:Q:64:MET:HE1   | 2.23                     | 0.53              |
| 1:J:221:HIS:NE2  | 1:1:249:ASP:OD1  | 2.42                     | 0.53              |
| 1:4:156:GLU:CD   | 1:4:254:ARG:HH12 | 2.16                     | 0.53              |
| 1:4:167:ARG:NH2  | 1:4:173:GLU:OE1  | 2.38                     | 0.53              |
| 1:e:249:ASP:OD1  | 1:p:221:HIS:NE2  | 2.41                     | 0.53              |
| 1:r:56:ARG:HG3   | 1:Z:56:ARG:HD2   | 1.90                     | 0.53              |
| 1:M:167:ARG:NH2  | 1:M:173:GLU:OE1  | 2.39                     | 0.53              |
| 1:X:83:GLU:OE1   | 1:X:83:GLU:N     | 2.41                     | 0.53              |
| 1:4:56:ARG:HG3   | 1:7:56:ARG:HD2   | 1.90                     | 0.53              |
| 1:4:152:ILE:O    | 1:4:156:GLU:HG3  | 2.08                     | 0.53              |
| 1:N:167:ARG:NH2  | 1:N:173:GLU:OE1  | 2.36                     | 0.53              |
| 1:A:76:LEU:O     | 1:A:80:VAL:HG12  | 2.08                     | 0.53              |
| 1:x:167:ARG:NH2  | 1:x:173:GLU:OE1  | 2.39                     | 0.53              |
| 1:o:83:GLU:OE1   | 1:o:83:GLU:N     | 2.42                     | 0.53              |
| 1:J:167:ARG:NH2  | 1:J:173:GLU:OE1  | 2.39                     | 0.53              |
| 1:2:167:ARG:NH2  | 1:2:173:GLU:OE1  | 2.36                     | 0.53              |
| 1:W:167:ARG:NH2  | 1:W:173:GLU:OE1  | 2.39                     | 0.53              |
| 1:F:249:ASP:OD1  | 1:Q:221:HIS:NE2  | 2.42                     | 0.53              |
| 1:p:13:PHE:HZ    | 1:p:105:LEU:HD12 | 1.73                     | 0.53              |
| 1:g:83:GLU:OE1   | 1:g:83:GLU:N     | 2.42                     | 0.53              |
| 1:X:167:ARG:NH2  | 1:X:173:GLU:OE1  | 2.36                     | 0.53              |
| 1:H:62:LEU:HD11  | 1:H:66:ARG:HH11  | 1.73                     | 0.53              |
| 1:2:56:ARG:HD2   | 1:O:56:ARG:HG3   | 1.90                     | 0.53              |
| 1:D:56:ARG:HG3   | 1:p:56:ARG:HD2   | 1.91                     | 0.53              |
| 1:r:87:LEU:HB3   | 1:r:92:ARG:HG3   | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:56:ARG:HD2   | 1:u:56:ARG:HG3   | 1.89                     | 0.53              |
| 1:Q:56:ARG:HG3   | 1:y:56:ARG:HD2   | 1.91                     | 0.53              |
| 1:7:83:GLU:OE1   | 1:7:83:GLU:N     | 2.41                     | 0.53              |
| 1:n:249:ASP:OD1  | 1:y:221:HIS:NE2  | 2.42                     | 0.53              |
| 1:J:56:ARG:HG3   | 1:r:56:ARG:HD2   | 1.91                     | 0.53              |
| 1:V:62:LEU:HD11  | 1:V:66:ARG:HH11  | 1.72                     | 0.53              |
| 1:5:95:GLU:OE1   | 1:5:95:GLU:N     | 2.42                     | 0.53              |
| 1:P:153:ARG:HD3  | 1:a:215:ARG:HH21 | 1.74                     | 0.53              |
| 1:G:56:ARG:HD2   | 1:W:56:ARG:HG3   | 1.91                     | 0.53              |
| 1:0:138:ALA:HB2  | 1:0:155:LEU:HD11 | 1.91                     | 0.53              |
| 1:U:167:ARG:NH2  | 1:U:173:GLU:OE1  | 2.36                     | 0.53              |
| 1:6:167:ARG:NH2  | 1:6:173:GLU:OE1  | 2.39                     | 0.53              |
| 1:C:249:ASP:OD1  | 1:D:221:HIS:NE2  | 2.42                     | 0.52              |
| 1:Q:56:ARG:HD2   | 1:h:56:ARG:HG3   | 1.90                     | 0.52              |
| 1:S:83:GLU:N     | 1:S:83:GLU:OE1   | 2.42                     | 0.52              |
| 1:p:234:ILE:HD11 | 1:p:245:LEU:HB3  | 1.90                     | 0.52              |
| 1:0:133:ARG:HH21 | 1:0:136:GLU:CD   | 2.18                     | 0.52              |
| 1:g:44:VAL:HA    | 1:g:47:LEU:HD12  | 1.91                     | 0.52              |
| 1:D:87:LEU:HB3   | 1:D:92:ARG:HG3   | 1.91                     | 0.52              |
| 1:b:56:ARG:HD2   | 1:n:56:ARG:HG3   | 1.91                     | 0.52              |
| 1:I:76:LEU:O     | 1:I:80:VAL:HG12  | 2.08                     | 0.52              |
| 1:r:95:GLU:OE1   | 1:r:95:GLU:N     | 2.42                     | 0.52              |
| 1:X:138:ALA:HB2  | 1:X:155:LEU:HD11 | 1.91                     | 0.52              |
| 1:j:167:ARG:NH2  | 1:j:173:GLU:OE1  | 2.39                     | 0.52              |
| 1:u:249:ASP:OD1  | 1:5:221:HIS:NE2  | 2.42                     | 0.52              |
| 1:o:133:ARG:HH21 | 1:o:136:GLU:CD   | 2.18                     | 0.52              |
| 1:q:62:LEU:HD11  | 1:q:66:ARG:HH11  | 1.74                     | 0.52              |
| 1:L:215:ARG:HH21 | 1:3:153:ARG:HD3  | 1.74                     | 0.52              |
| 1:s:133:ARG:HH21 | 1:s:136:GLU:CD   | 2.18                     | 0.52              |
| 1:u:44:VAL:HA    | 1:u:47:LEU:HD12  | 1.91                     | 0.52              |
| 1:l:83:GLU:OE1   | 1:l:83:GLU:N     | 2.42                     | 0.52              |
| 1:F:167:ARG:NH2  | 1:F:173:GLU:OE1  | 2.38                     | 0.52              |
| 1:F:195:LEU:HD21 | 1:F:244:GLU:OE1  | 2.09                     | 0.52              |
| 1:c:167:ARG:NH2  | 1:c:173:GLU:OE1  | 2.39                     | 0.52              |
| 1:e:83:GLU:OE1   | 1:e:83:GLU:N     | 2.42                     | 0.52              |
| 1:p:95:GLU:OE1   | 1:p:95:GLU:N     | 2.42                     | 0.52              |
| 1:g:249:ASP:OD1  | 1:r:221:HIS:NE2  | 2.42                     | 0.52              |
| 1:s:138:ALA:HB2  | 1:s:155:LEU:HD11 | 1.91                     | 0.52              |
| 1:j:30:ARG:N     | 1:j:31:PRO:HD2   | 2.25                     | 0.52              |
| 1:j:153:ARG:HD3  | 1:u:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:E:138:ALA:HB2  | 1:E:155:LEU:HD11 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:215:ARG:HH21 | 1:x:153:ARG:HD3  | 1.74                     | 0.52              |
| 1:b:133:ARG:HH21 | 1:b:136:GLU:CD   | 2.18                     | 0.52              |
| 1:c:30:ARG:N     | 1:c:31:PRO:HD2   | 2.25                     | 0.52              |
| 1:S:56:ARG:HG3   | 1:0:56:ARG:HD2   | 1.92                     | 0.52              |
| 1:S:167:ARG:NH2  | 1:S:173:GLU:OE1  | 2.38                     | 0.52              |
| 1:T:62:LEU:HD11  | 1:T:66:ARG:HH11  | 1.73                     | 0.52              |
| 1:U:56:ARG:HD2   | 1:g:56:ARG:HG3   | 1.91                     | 0.52              |
| 1:l:56:ARG:HG3   | 1:k:56:ARG:HD2   | 1.91                     | 0.52              |
| 1:l:83:GLU:OE1   | 1:l:83:GLU:N     | 2.42                     | 0.52              |
| 1:K:153:ARG:HD3  | 1:V:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:V:167:ARG:NH2  | 1:V:173:GLU:OE1  | 2.39                     | 0.52              |
| 1:O:195:LEU:HD21 | 1:O:244:GLU:OE1  | 2.10                     | 0.52              |
| 1:P:167:ARG:NH2  | 1:P:173:GLU:OE1  | 2.39                     | 0.52              |
| 1:l:44:VAL:HA    | 1:l:47:LEU:HD12  | 1.90                     | 0.52              |
| 1:l:153:ARG:HD3  | 1:T:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:V:153:ARG:HD3  | 1:g:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:k:133:ARG:HH21 | 1:k:136:GLU:CD   | 2.18                     | 0.52              |
| 1:v:153:ARG:HD3  | 1:6:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:B:167:ARG:NH2  | 1:B:173:GLU:OE1  | 2.40                     | 0.52              |
| 1:C:83:GLU:N     | 1:C:83:GLU:OE1   | 2.42                     | 0.52              |
| 1:H:30:ARG:N     | 1:H:31:PRO:HD2   | 2.25                     | 0.52              |
| 1:W:152:ILE:O    | 1:W:156:GLU:HG3  | 2.10                     | 0.52              |
| 1:h:95:GLU:OE1   | 1:h:95:GLU:N     | 2.43                     | 0.52              |
| 1:w:167:ARG:NH2  | 1:w:173:GLU:OE1  | 2.38                     | 0.52              |
| 1:C:195:LEU:HD21 | 1:C:244:GLU:OE1  | 2.10                     | 0.52              |
| 1:x:20:GLU:OE1   | 1:x:23:ARG:NH2   | 2.39                     | 0.52              |
| 1:n:195:LEU:HD21 | 1:n:244:GLU:OE1  | 2.10                     | 0.52              |
| 1:N:56:ARG:HD2   | 1:l:56:ARG:HG3   | 1.90                     | 0.52              |
| 1:N:138:ALA:HB2  | 1:N:155:LEU:HD11 | 1.91                     | 0.52              |
| 1:7:133:ARG:HH21 | 1:7:136:GLU:CD   | 2.18                     | 0.52              |
| 1:Z:76:LEU:O     | 1:Z:80:VAL:HG12  | 2.10                     | 0.52              |
| 1:Z:167:ARG:NH2  | 1:Z:173:GLU:OE1  | 2.39                     | 0.52              |
| 1:l:195:LEU:HD21 | 1:l:244:GLU:OE1  | 2.10                     | 0.52              |
| 1:G:138:ALA:HB2  | 1:G:155:LEU:HD11 | 1.92                     | 0.52              |
| 1:n:83:GLU:N     | 1:n:83:GLU:OE1   | 2.42                     | 0.52              |
| 1:S:44:VAL:HA    | 1:S:47:LEU:HD12  | 1.92                     | 0.52              |
| 1:d:95:GLU:OE1   | 1:d:95:GLU:N     | 2.42                     | 0.52              |
| 1:o:138:ALA:HB2  | 1:o:155:LEU:HD11 | 1.92                     | 0.52              |
| 1:I:215:ARG:HH21 | 1:0:153:ARG:HD3  | 1.75                     | 0.52              |
| 1:U:138:ALA:HB2  | 1:U:155:LEU:HD11 | 1.92                     | 0.52              |
| 1:g:195:LEU:HD21 | 1:g:244:GLU:OE1  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:153:ARG:HD3  | 1:l:215:ARG:HH21 | 1.75                     | 0.52              |
| 1:F:156:GLU:OE1  | 1:F:254:ARG:NH1  | 2.37                     | 0.51              |
| 1:c:153:ARG:HD3  | 1:n:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:n:38:HIS:ND1   | 1:n:64:MET:HE1   | 2.25                     | 0.51              |
| 1:H:153:ARG:HD3  | 1:S:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:Y:167:ARG:NH2  | 1:Y:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:j:62:LEU:HD11  | 1:j:66:ARG:HH11  | 1.73                     | 0.51              |
| 1:7:138:ALA:HB2  | 1:7:155:LEU:HD11 | 1.91                     | 0.51              |
| 1:D:25:GLY:HA3   | 1:D:29:MET:HE2   | 1.92                     | 0.51              |
| 1:D:56:ARG:HD2   | 1:d:56:ARG:HG3   | 1.91                     | 0.51              |
| 1:b:138:ALA:HB2  | 1:b:155:LEU:HD11 | 1.92                     | 0.51              |
| 1:L:5:THR:OG1    | 1:L:143:ARG:NH2  | 2.44                     | 0.51              |
| 1:t:62:LEU:HD11  | 1:t:66:ARG:HH11  | 1.75                     | 0.51              |
| 1:4:38:HIS:ND1   | 1:4:64:MET:HE1   | 2.25                     | 0.51              |
| 1:v:167:ARG:NH2  | 1:v:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:D:62:LEU:O     | 1:D:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:E:133:ARG:HH21 | 1:E:136:GLU:CD   | 2.18                     | 0.51              |
| 1:F:44:VAL:HA    | 1:F:47:LEU:HD12  | 1.92                     | 0.51              |
| 1:Q:76:LEU:O     | 1:Q:80:VAL:HG12  | 2.10                     | 0.51              |
| 1:Q:95:GLU:OE1   | 1:Q:95:GLU:N     | 2.43                     | 0.51              |
| 1:d:76:LEU:O     | 1:d:80:VAL:HG12  | 2.10                     | 0.51              |
| 1:T:20:GLU:OE1   | 1:T:23:ARG:NH2   | 2.38                     | 0.51              |
| 1:q:83:GLU:N     | 1:q:83:GLU:OE1   | 2.44                     | 0.51              |
| 1:2:138:ALA:HB2  | 1:2:155:LEU:HD11 | 1.91                     | 0.51              |
| 1:L:20:GLU:OE1   | 1:L:23:ARG:NH2   | 2.37                     | 0.51              |
| 1:Y:83:GLU:O     | 1:Y:87:LEU:HD12  | 2.11                     | 0.51              |
| 1:w:29:MET:HB3   | 1:w:32:TYR:HD2   | 1.76                     | 0.51              |
| 1:A:215:ARG:HH21 | 1:E:153:ARG:HD3  | 1.75                     | 0.51              |
| 1:F:38:HIS:ND1   | 1:F:64:MET:HE1   | 2.25                     | 0.51              |
| 1:y:62:LEU:O     | 1:y:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:J:56:ARG:HD2   | 1:Z:56:ARG:HG3   | 1.92                     | 0.51              |
| 1:U:153:ARG:HD3  | 1:f:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:1:38:HIS:ND1   | 1:1:64:MET:HE1   | 2.25                     | 0.51              |
| 1:1:195:LEU:HD21 | 1:1:244:GLU:OE1  | 2.10                     | 0.51              |
| 1:K:167:ARG:NH2  | 1:K:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:V:95:GLU:N     | 1:V:95:GLU:OE1   | 2.43                     | 0.51              |
| 1:g:38:HIS:ND1   | 1:g:64:MET:HE1   | 2.25                     | 0.51              |
| 1:s:153:ARG:HD3  | 1:3:215:ARG:HH21 | 1.76                     | 0.51              |
| 1:X:153:ARG:HD3  | 1:i:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:t:153:ARG:HD3  | 1:4:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:Z:95:GLU:OE1   | 1:Z:95:GLU:N     | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:20:GLU:OE1   | 1:6:23:ARG:NH2   | 2.39                     | 0.51              |
| 1:l:62:LEU:O     | 1:l:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:B:83:GLU:OE1   | 1:B:83:GLU:N     | 2.44                     | 0.51              |
| 1:B:153:ARG:HD3  | 1:C:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:C:56:ARG:HG3   | 1:o:56:ARG:HD2   | 1.92                     | 0.51              |
| 1:G:56:ARG:HG3   | 1:t:56:ARG:HD2   | 1.92                     | 0.51              |
| 1:c:83:GLU:N     | 1:c:83:GLU:OE1   | 2.44                     | 0.51              |
| 1:H:215:ARG:HH21 | 1:z:153:ARG:HD3  | 1.75                     | 0.51              |
| 1:z:167:ARG:NH2  | 1:z:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:I:95:GLU:OE1   | 1:I:95:GLU:N     | 2.43                     | 0.51              |
| 1:T:56:ARG:HD2   | 1:k:56:ARG:HG3   | 1.92                     | 0.51              |
| 1:T:153:ARG:HD3  | 1:e:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:f:153:ARG:HD3  | 1:q:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:V:83:GLU:N     | 1:V:83:GLU:OE1   | 2.44                     | 0.51              |
| 1:2:133:ARG:HH21 | 1:2:136:GLU:CD   | 2.18                     | 0.51              |
| 1:L:30:ARG:N     | 1:L:31:PRO:HD2   | 2.25                     | 0.51              |
| 1:3:95:GLU:N     | 1:3:95:GLU:OE1   | 2.43                     | 0.51              |
| 1:N:133:ARG:HH21 | 1:N:136:GLU:CD   | 2.18                     | 0.51              |
| 1:Y:153:ARG:HD3  | 1:j:215:ARG:HH21 | 1.76                     | 0.51              |
| 1:l:156:GLU:OE1  | 1:l:254:ARG:NH1  | 2.37                     | 0.51              |
| 1:F:83:GLU:N     | 1:F:83:GLU:OE1   | 2.44                     | 0.51              |
| 1:G:133:ARG:HH21 | 1:G:136:GLU:CD   | 2.18                     | 0.51              |
| 1:c:95:GLU:OE1   | 1:c:95:GLU:N     | 2.43                     | 0.51              |
| 1:H:195:LEU:HD21 | 1:H:244:GLU:OE1  | 2.10                     | 0.51              |
| 1:w:95:GLU:OE1   | 1:w:95:GLU:N     | 2.43                     | 0.51              |
| 1:B:62:LEU:HD11  | 1:B:66:ARG:HH11  | 1.75                     | 0.51              |
| 1:B:95:GLU:OE1   | 1:B:95:GLU:N     | 2.43                     | 0.51              |
| 1:m:167:ARG:NH2  | 1:m:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:y:25:GLY:HA3   | 1:y:29:MET:HE2   | 1.93                     | 0.51              |
| 1:T:5:THR:OG1    | 1:T:143:ARG:NH2  | 2.44                     | 0.51              |
| 1:r:62:LEU:O     | 1:r:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:4:44:VAL:HA    | 1:4:47:LEU:HD12  | 1.92                     | 0.51              |
| 1:j:95:GLU:OE1   | 1:j:95:GLU:N     | 2.44                     | 0.51              |
| 1:u:62:LEU:O     | 1:u:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:O:215:ARG:HH21 | 1:6:153:ARG:HD3  | 1.75                     | 0.51              |
| 1:k:153:ARG:HD3  | 1:v:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:a:83:GLU:OE1   | 1:a:83:GLU:N     | 2.44                     | 0.51              |
| 1:G:153:ARG:HD3  | 1:R:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:n:62:LEU:O     | 1:n:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:p:17:LEU:O     | 1:p:21:VAL:HG23  | 2.11                     | 0.51              |
| 1:q:153:ARG:HD3  | 1:1:215:ARG:HH21 | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:56:ARG:HD2   | 1:s:56:ARG:HG3   | 1.93                     | 0.51              |
| 1:i:153:ARG:HD3  | 1:t:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:u:156:GLU:OE1  | 1:u:254:ARG:NH1  | 2.37                     | 0.51              |
| 1:P:215:ARG:HH21 | 1:7:153:ARG:HD3  | 1.75                     | 0.51              |
| 1:B:5:THR:OG1    | 1:B:143:ARG:NH2  | 2.44                     | 0.51              |
| 1:m:83:GLU:O     | 1:m:87:LEU:HD12  | 2.11                     | 0.51              |
| 1:G:178:LYS:HB2  | 1:G:178:LYS:NZ   | 2.26                     | 0.51              |
| 1:c:5:THR:OG1    | 1:c:143:ARG:NH2  | 2.44                     | 0.51              |
| 1:H:5:THR:OG1    | 1:H:143:ARG:NH2  | 2.44                     | 0.51              |
| 1:H:56:ARG:HD2   | 1:X:56:ARG:HG3   | 1.92                     | 0.51              |
| 1:H:83:GLU:N     | 1:H:83:GLU:OE1   | 2.44                     | 0.51              |
| 1:z:95:GLU:OE1   | 1:z:95:GLU:N     | 2.43                     | 0.51              |
| 1:U:62:LEU:O     | 1:U:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:U:133:ARG:HH21 | 1:U:136:GLU:CD   | 2.18                     | 0.51              |
| 1:g:62:LEU:O     | 1:g:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:g:156:GLU:OE1  | 1:g:254:ARG:NH1  | 2.37                     | 0.51              |
| 1:h:62:LEU:O     | 1:h:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:h:167:ARG:NH2  | 1:h:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:t:83:GLU:OE1   | 1:t:83:GLU:N     | 2.44                     | 0.51              |
| 1:j:83:GLU:OE1   | 1:j:83:GLU:N     | 2.44                     | 0.51              |
| 1:O:62:LEU:O     | 1:O:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:O:83:GLU:OE1   | 1:O:83:GLU:N     | 2.44                     | 0.51              |
| 1:Z:62:LEU:O     | 1:Z:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:k:138:ALA:HB2  | 1:k:155:LEU:HD11 | 1.92                     | 0.51              |
| 1:Q:153:ARG:HD3  | 1:b:215:ARG:HH21 | 1.76                     | 0.51              |
| 1:b:153:ARG:HD3  | 1:m:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:m:95:GLU:OE1   | 1:m:95:GLU:N     | 2.43                     | 0.51              |
| 1:m:153:ARG:HD3  | 1:x:215:ARG:HH21 | 1.75                     | 0.51              |
| 1:x:56:ARG:HD2   | 1:U:56:ARG:HG3   | 1.92                     | 0.51              |
| 1:H:167:ARG:NH2  | 1:H:173:GLU:OE1  | 2.39                     | 0.51              |
| 1:1:156:GLU:OE1  | 1:1:254:ARG:NH1  | 2.37                     | 0.51              |
| 1:K:83:GLU:O     | 1:K:87:LEU:HD12  | 2.11                     | 0.51              |
| 1:W:62:LEU:O     | 1:W:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:X:95:GLU:OE1   | 1:X:95:GLU:N     | 2.44                     | 0.51              |
| 1:u:195:LEU:HD21 | 1:u:244:GLU:OE1  | 2.11                     | 0.51              |
| 1:Z:29:MET:HB3   | 1:Z:32:TYR:HD2   | 1.76                     | 0.51              |
| 1:6:83:GLU:OE1   | 1:6:83:GLU:N     | 2.44                     | 0.51              |
| 1:x:83:GLU:OE1   | 1:x:83:GLU:N     | 2.44                     | 0.50              |
| 1:R:153:ARG:HD3  | 1:c:215:ARG:HH21 | 1.74                     | 0.50              |
| 1:y:167:ARG:NH2  | 1:y:173:GLU:OE1  | 2.39                     | 0.50              |
| 1:S:202:LYS:O    | 1:S:206:GLU:HG3  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:153:ARG:HD3  | 1:o:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:o:153:ARG:HD3  | 1:z:215:ARG:HH21 | 1.75                     | 0.50              |
| 1:T:56:ARG:HG3   | 1:1:56:ARG:HD2   | 1.93                     | 0.50              |
| 1:e:62:LEU:O     | 1:e:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:p:62:LEU:O     | 1:p:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:p:167:ARG:NH2  | 1:p:173:GLU:OE1  | 2.38                     | 0.50              |
| 1:1:202:LYS:O    | 1:1:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:2:95:GLU:OE1   | 1:2:95:GLU:N     | 2.45                     | 0.50              |
| 1:W:153:ARG:HD3  | 1:h:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:h:25:GLY:HA3   | 1:h:29:MET:HE2   | 1.93                     | 0.50              |
| 1:M:153:ARG:HD3  | 1:X:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:X:133:ARG:HH21 | 1:X:136:GLU:CD   | 2.18                     | 0.50              |
| 1:N:95:GLU:OE1   | 1:N:95:GLU:N     | 2.45                     | 0.50              |
| 1:u:202:LYS:O    | 1:u:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:5:56:ARG:HG3   | 1:w:56:ARG:HD2   | 1.93                     | 0.50              |
| 1:5:62:LEU:O     | 1:5:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:a:5:THR:OG1    | 1:a:143:ARG:NH2  | 2.43                     | 0.50              |
| 1:7:95:GLU:OE1   | 1:7:95:GLU:N     | 2.44                     | 0.50              |
| 1:C:202:LYS:O    | 1:C:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:R:95:GLU:OE1   | 1:R:95:GLU:N     | 2.43                     | 0.50              |
| 1:y:95:GLU:N     | 1:y:95:GLU:OE1   | 2.42                     | 0.50              |
| 1:J:62:LEU:O     | 1:J:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:J:153:ARG:HD3  | 1:U:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:r:167:ARG:NH2  | 1:r:173:GLU:OE1  | 2.39                     | 0.50              |
| 1:W:83:GLU:OE1   | 1:W:83:GLU:N     | 2.44                     | 0.50              |
| 1:W:195:LEU:HD11 | 1:W:244:GLU:HB2  | 1.94                     | 0.50              |
| 1:4:83:GLU:OE1   | 1:4:83:GLU:N     | 2.44                     | 0.50              |
| 1:u:83:GLU:OE1   | 1:u:83:GLU:N     | 2.44                     | 0.50              |
| 1:a:167:ARG:NH2  | 1:a:173:GLU:OE1  | 2.40                     | 0.50              |
| 1:b:62:LEU:HD11  | 1:b:66:ARG:HH11  | 1.77                     | 0.50              |
| 1:n:202:LYS:O    | 1:n:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:T:62:LEU:O     | 1:T:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:T:83:GLU:OE1   | 1:T:83:GLU:N     | 2.44                     | 0.50              |
| 1:e:195:LEU:HD21 | 1:e:244:GLU:OE1  | 2.11                     | 0.50              |
| 1:M:62:LEU:O     | 1:M:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:4:195:LEU:HD21 | 1:4:244:GLU:OE1  | 2.12                     | 0.50              |
| 1:j:5:THR:OG1    | 1:j:143:ARG:NH2  | 2.43                     | 0.50              |
| 1:O:156:GLU:OE1  | 1:O:254:ARG:NH1  | 2.37                     | 0.50              |
| 1:a:62:LEU:O     | 1:a:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:w:62:LEU:O     | 1:w:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:w:153:ARG:HD3  | 1:7:215:ARG:HH21 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:LEU:O     | 1:A:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:A:95:GLU:OE1   | 1:A:95:GLU:N     | 2.43                     | 0.50              |
| 1:C:62:LEU:O     | 1:C:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:E:56:ARG:HG3   | 1:q:56:ARG:HD2   | 1.93                     | 0.50              |
| 1:F:202:LYS:O    | 1:F:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:Q:62:LEU:O     | 1:Q:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:S:156:GLU:OE1  | 1:S:254:ARG:NH1  | 2.37                     | 0.50              |
| 1:U:95:GLU:OE1   | 1:U:95:GLU:N     | 2.44                     | 0.50              |
| 1:r:25:GLY:HA3   | 1:r:29:MET:HE2   | 1.93                     | 0.50              |
| 1:L:83:GLU:OE1   | 1:L:83:GLU:N     | 2.44                     | 0.50              |
| 1:s:95:GLU:OE1   | 1:s:95:GLU:N     | 2.44                     | 0.50              |
| 1:3:5:THR:OG1    | 1:3:143:ARG:NH2  | 2.45                     | 0.50              |
| 1:M:29:MET:HB3   | 1:M:32:TYR:HD2   | 1.77                     | 0.50              |
| 1:i:83:GLU:O     | 1:i:87:LEU:HD12  | 2.11                     | 0.50              |
| 1:5:25:GLY:HA3   | 1:5:29:MET:HE2   | 1.93                     | 0.50              |
| 1:O:202:LYS:O    | 1:O:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:k:62:LEU:HD11  | 1:k:66:ARG:HH11  | 1.77                     | 0.50              |
| 1:E:178:LYS:HB2  | 1:E:178:LYS:NZ   | 2.27                     | 0.50              |
| 1:G:215:ARG:HH21 | 1:y:153:ARG:HD3  | 1.76                     | 0.50              |
| 1:n:44:VAL:HA    | 1:n:47:LEU:HD12  | 1.93                     | 0.50              |
| 1:o:62:LEU:O     | 1:o:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:p:25:GLY:HA3   | 1:p:29:MET:HE2   | 1.93                     | 0.50              |
| 1:0:95:GLU:N     | 1:0:95:GLU:OE1   | 2.44                     | 0.50              |
| 1:g:202:LYS:O    | 1:g:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:L:56:ARG:HG3   | 1:4:56:ARG:HD2   | 1.94                     | 0.50              |
| 1:L:153:ARG:HD3  | 1:W:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:4:62:LEU:O     | 1:4:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:4:202:LYS:O    | 1:4:206:GLU:HG3  | 2.12                     | 0.50              |
| 1:Z:153:ARG:HD3  | 1:k:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:k:95:GLU:OE1   | 1:k:95:GLU:N     | 2.44                     | 0.50              |
| 1:A:153:ARG:HD3  | 1:B:215:ARG:HH21 | 1.75                     | 0.50              |
| 1:B:56:ARG:HD2   | 1:b:56:ARG:HG3   | 1.92                     | 0.50              |
| 1:Q:5:THR:OG1    | 1:Q:143:ARG:NH2  | 2.45                     | 0.50              |
| 1:Q:25:GLY:HA3   | 1:Q:29:MET:HE2   | 1.93                     | 0.50              |
| 1:b:62:LEU:O     | 1:b:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:z:83:GLU:O     | 1:z:87:LEU:HD12  | 2.12                     | 0.50              |
| 1:J:77:LEU:HA    | 1:J:80:VAL:HG12  | 1.94                     | 0.50              |
| 1:r:76:LEU:O     | 1:r:80:VAL:HG12  | 2.11                     | 0.50              |
| 1:L:95:GLU:OE1   | 1:L:95:GLU:N     | 2.43                     | 0.50              |
| 1:M:77:LEU:HA    | 1:M:80:VAL:HG12  | 1.94                     | 0.50              |
| 1:N:62:LEU:O     | 1:N:66:ARG:HG2   | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:215:ARG:HH21 | 1:5:153:ARG:HD3  | 1.76                     | 0.50              |
| 1:O:44:VAL:HA    | 1:O:47:LEU:HD12  | 1.92                     | 0.50              |
| 1:l:202:LYS:O    | 1:l:206:GLU:HG3  | 2.11                     | 0.50              |
| 1:C:25:GLY:HA3   | 1:C:29:MET:HE2   | 1.94                     | 0.50              |
| 1:C:44:VAL:HA    | 1:C:47:LEU:HD12  | 1.93                     | 0.50              |
| 1:H:95:GLU:OE1   | 1:H:95:GLU:N     | 2.43                     | 0.50              |
| 1:d:62:LEU:O     | 1:d:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:O:62:LEU:O     | 1:O:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:f:83:GLU:O     | 1:f:87:LEU:HD12  | 2.12                     | 0.50              |
| 1:K:215:ARG:HH21 | 1:2:153:ARG:HD3  | 1.75                     | 0.50              |
| 1:V:106:ALA:O    | 1:V:110:VAL:HG12 | 2.12                     | 0.50              |
| 1:M:56:ARG:HD2   | 1:w:56:ARG:HG3   | 1.94                     | 0.50              |
| 1:X:62:LEU:O     | 1:X:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:Z:25:GLY:HA3   | 1:Z:29:MET:HE2   | 1.94                     | 0.50              |
| 1:D:20:GLU:OE1   | 1:D:23:ARG:NH2   | 2.37                     | 0.50              |
| 1:E:62:LEU:HD11  | 1:E:66:ARG:HH11  | 1.77                     | 0.50              |
| 1:E:95:GLU:OE1   | 1:E:95:GLU:N     | 2.44                     | 0.50              |
| 1:S:234:ILE:HD11 | 1:S:245:LEU:HB3  | 1.93                     | 0.50              |
| 1:I:62:LEU:O     | 1:I:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:I:83:GLU:O     | 1:I:87:LEU:HD12  | 2.11                     | 0.50              |
| 1:V:5:THR:OG1    | 1:V:143:ARG:NH2  | 2.44                     | 0.50              |
| 1:L:62:LEU:O     | 1:L:66:ARG:HG2   | 2.11                     | 0.50              |
| 1:h:153:ARG:HD3  | 1:s:215:ARG:HH21 | 1.76                     | 0.50              |
| 1:i:5:THR:OG1    | 1:i:143:ARG:NH2  | 2.45                     | 0.50              |
| 1:5:17:LEU:O     | 1:5:21:VAL:HG23  | 2.11                     | 0.50              |
| 1:v:5:THR:OG1    | 1:v:143:ARG:NH2  | 2.45                     | 0.50              |
| 1:P:95:GLU:OE1   | 1:P:95:GLU:N     | 2.43                     | 0.50              |
| 1:l:95:GLU:OE1   | 1:l:95:GLU:N     | 2.44                     | 0.50              |
| 1:B:30:ARG:N     | 1:B:31:PRO:HD2   | 2.27                     | 0.50              |
| 1:C:95:GLU:OE1   | 1:C:95:GLU:N     | 2.44                     | 0.50              |
| 1:D:76:LEU:O     | 1:D:80:VAL:HG12  | 2.11                     | 0.50              |
| 1:D:95:GLU:OE1   | 1:D:95:GLU:N     | 2.42                     | 0.50              |
| 1:x:95:GLU:OE1   | 1:x:95:GLU:N     | 2.43                     | 0.50              |
| 1:H:234:ILE:HD11 | 1:H:245:LEU:HB3  | 1.94                     | 0.50              |
| 1:S:56:ARG:HD2   | 1:j:56:ARG:HG3   | 1.93                     | 0.50              |
| 1:o:38:HIS:ND1   | 1:o:64:MET:HE1   | 2.26                     | 0.50              |
| 1:J:95:GLU:OE1   | 1:J:95:GLU:N     | 2.42                     | 0.50              |
| 1:q:5:THR:OG1    | 1:q:143:ARG:NH2  | 2.44                     | 0.50              |
| 1:1:62:LEU:O     | 1:1:66:ARG:HG2   | 2.12                     | 0.50              |
| 1:V:30:ARG:N     | 1:V:31:PRO:HD2   | 2.27                     | 0.50              |
| 1:r:153:ARG:HD3  | 1:2:215:ARG:HH21 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:56:ARG:HG3   | 1:a:56:ARG:HD2   | 1.93                     | 0.50              |
| 1:t:5:THR:OG1    | 1:t:143:ARG:NH2  | 2.44                     | 0.50              |
| 1:N:38:HIS:ND1   | 1:N:64:MET:HE1   | 2.26                     | 0.50              |
| 1:u:25:GLY:HA3   | 1:u:29:MET:HE2   | 1.93                     | 0.50              |
| 1:v:95:GLU:N     | 1:v:95:GLU:OE1   | 2.43                     | 0.50              |
| 1:D:95:GLU:O     | 1:D:99:LEU:HD12  | 2.12                     | 0.49              |
| 1:m:5:THR:OG1    | 1:m:143:ARG:NH2  | 2.45                     | 0.49              |
| 1:G:95:GLU:OE1   | 1:G:95:GLU:N     | 2.44                     | 0.49              |
| 1:R:83:GLU:O     | 1:R:87:LEU:HD12  | 2.11                     | 0.49              |
| 1:o:62:LEU:HD11  | 1:o:66:ARG:HH11  | 1.77                     | 0.49              |
| 1:p:153:ARG:HD3  | 1:0:215:ARG:HH21 | 1.77                     | 0.49              |
| 1:2:62:LEU:O     | 1:2:66:ARG:HG2   | 2.12                     | 0.49              |
| 1:s:62:LEU:O     | 1:s:66:ARG:HG2   | 2.12                     | 0.49              |
| 1:G:62:LEU:HD11  | 1:G:66:ARG:HH11  | 1.77                     | 0.49              |
| 1:n:95:GLU:OE1   | 1:n:95:GLU:N     | 2.44                     | 0.49              |
| 1:d:25:GLY:HA3   | 1:d:29:MET:HE2   | 1.93                     | 0.49              |
| 1:T:71:GLU:O     | 1:T:75:ARG:HG3   | 2.13                     | 0.49              |
| 1:T:95:GLU:OE1   | 1:T:95:GLU:N     | 2.44                     | 0.49              |
| 1:0:56:ARG:HG3   | 1:j:56:ARG:HD2   | 1.94                     | 0.49              |
| 1:J:25:GLY:HA3   | 1:J:29:MET:HE2   | 1.93                     | 0.49              |
| 1:f:20:GLU:OE1   | 1:f:23:ARG:NH2   | 2.39                     | 0.49              |
| 1:f:62:LEU:O     | 1:f:66:ARG:HG2   | 2.12                     | 0.49              |
| 1:V:62:LEU:O     | 1:V:66:ARG:HG2   | 2.11                     | 0.49              |
| 1:L:56:ARG:HD2   | 1:7:56:ARG:HG3   | 1.94                     | 0.49              |
| 1:s:178:LYS:HB2  | 1:s:178:LYS:NZ   | 2.27                     | 0.49              |
| 1:4:195:LEU:HD11 | 1:4:244:GLU:HB2  | 1.94                     | 0.49              |
| 1:N:153:ARG:HD3  | 1:Y:215:ARG:HH21 | 1.76                     | 0.49              |
| 1:O:95:GLU:OE1   | 1:O:95:GLU:N     | 2.44                     | 0.49              |
| 1:Z:5:THR:OG1    | 1:Z:143:ARG:NH2  | 2.46                     | 0.49              |
| 1:6:5:THR:OG1    | 1:6:143:ARG:NH2  | 2.44                     | 0.49              |
| 1:7:134:LEU:HD11 | 1:7:159:LEU:HG   | 1.94                     | 0.49              |
| 1:A:83:GLU:O     | 1:A:87:LEU:HD12  | 2.11                     | 0.49              |
| 1:C:56:ARG:HD2   | 1:c:56:ARG:HG3   | 1.93                     | 0.49              |
| 1:D:153:ARG:HD3  | 1:E:215:ARG:HH21 | 1.77                     | 0.49              |
| 1:F:62:LEU:O     | 1:F:66:ARG:HG2   | 2.11                     | 0.49              |
| 1:y:17:LEU:O     | 1:y:21:VAL:HG23  | 2.11                     | 0.49              |
| 1:H:56:ARG:HG3   | 1:u:56:ARG:HD2   | 1.95                     | 0.49              |
| 1:I:5:THR:OG1    | 1:I:143:ARG:NH2  | 2.46                     | 0.49              |
| 1:0:38:HIS:ND1   | 1:0:64:MET:HE1   | 2.27                     | 0.49              |
| 1:0:62:LEU:HD11  | 1:0:66:ARG:HH11  | 1.78                     | 0.49              |
| 1:M:95:GLU:OE1   | 1:M:95:GLU:N     | 2.43                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:6:95:GLU:OE1   | 1:6:95:GLU:N    | 2.43                     | 0.49              |
| 1:S:62:LEU:O     | 1:S:66:ARG:HG2  | 2.11                     | 0.49              |
| 1:S:195:LEU:HD11 | 1:S:244:GLU:HB2 | 1.95                     | 0.49              |
| 1:S:195:LEU:HD21 | 1:S:244:GLU:OE1 | 2.11                     | 0.49              |
| 1:z:5:THR:OG1    | 1:z:143:ARG:NH2 | 2.46                     | 0.49              |
| 1:U:38:HIS:ND1   | 1:U:64:MET:HE1  | 2.27                     | 0.49              |
| 1:f:5:THR:OG1    | 1:f:143:ARG:NH2 | 2.45                     | 0.49              |
| 1:K:202:LYS:O    | 1:K:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:g:25:GLY:HA3   | 1:g:29:MET:HE2  | 1.94                     | 0.49              |
| 1:r:95:GLU:O     | 1:r:99:LEU:HD12 | 2.12                     | 0.49              |
| 1:W:202:LYS:O    | 1:W:206:GLU:HG3 | 2.11                     | 0.49              |
| 1:M:10:VAL:HG21  | 1:M:47:LEU:HD11 | 1.93                     | 0.49              |
| 1:M:215:ARG:HH21 | 1:4:153:ARG:HD3 | 1.76                     | 0.49              |
| 1:X:62:LEU:HD11  | 1:X:66:ARG:HH11 | 1.77                     | 0.49              |
| 1:i:202:LYS:O    | 1:i:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:N:56:ARG:HG3   | 1:6:56:ARG:HD2  | 1.93                     | 0.49              |
| 1:Y:202:LYS:O    | 1:Y:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:6:62:LEU:O     | 1:6:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:a:30:ARG:N     | 1:a:31:PRO:HD2  | 2.27                     | 0.49              |
| 1:w:5:THR:OG1    | 1:w:143:ARG:NH2 | 2.46                     | 0.49              |
| 1:w:25:GLY:HA3   | 1:w:29:MET:HE2  | 1.94                     | 0.49              |
| 1:b:134:LEU:HD11 | 1:b:159:LEU:HG  | 1.95                     | 0.49              |
| 1:x:62:LEU:O     | 1:x:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:o:134:LEU:HD11 | 1:o:159:LEU:HG  | 1.95                     | 0.49              |
| 1:f:202:LYS:O    | 1:f:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:K:62:LEU:O     | 1:K:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:3:83:GLU:O     | 1:3:87:LEU:HD12 | 2.11                     | 0.49              |
| 1:4:234:ILE:HD11 | 1:4:245:LEU:HB3 | 1.94                     | 0.49              |
| 1:Y:62:LEU:O     | 1:Y:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:k:134:LEU:HD11 | 1:k:159:LEU:HG  | 1.95                     | 0.49              |
| 1:P:5:THR:OG1    | 1:P:143:ARG:NH2 | 2.46                     | 0.49              |
| 1:7:38:HIS:ND1   | 1:7:64:MET:HE1  | 2.27                     | 0.49              |
| 1:7:62:LEU:HD11  | 1:7:66:ARG:HH11 | 1.78                     | 0.49              |
| 1:R:5:THR:OG1    | 1:R:143:ARG:NH2 | 2.45                     | 0.49              |
| 1:d:56:ARG:HD2   | 1:p:56:ARG:HG3  | 1.93                     | 0.49              |
| 1:z:20:GLU:OE1   | 1:z:23:ARG:NH2  | 2.39                     | 0.49              |
| 1:T:202:LYS:O    | 1:T:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:e:202:LYS:O    | 1:e:206:GLU:HG3 | 2.12                     | 0.49              |
| 1:q:95:GLU:N     | 1:q:95:GLU:OE1  | 2.43                     | 0.49              |
| 1:s:62:LEU:HD11  | 1:s:66:ARG:HH11 | 1.78                     | 0.49              |
| 1:i:20:GLU:OE1   | 1:i:23:ARG:NH2  | 2.39                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:6:30:ARG:N     | 1:6:31:PRO:HD2  | 2.27                     | 0.49              |
| 1:A:202:LYS:O    | 1:A:206:GLU:HG3 | 2.12                     | 0.49              |
| 1:b:38:HIS:ND1   | 1:b:64:MET:HE1  | 2.27                     | 0.49              |
| 1:x:30:ARG:N     | 1:x:31:PRO:HD2  | 2.27                     | 0.49              |
| 1:x:56:ARG:HG3   | 1:g:56:ARG:HD2  | 1.95                     | 0.49              |
| 1:c:56:ARG:HD2   | 1:o:56:ARG:HG3  | 1.93                     | 0.49              |
| 1:P:62:LEU:O     | 1:P:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:a:95:GLU:N     | 1:a:95:GLU:OE1  | 2.44                     | 0.49              |
| 1:b:151:ILE:O    | 1:b:155:LEU:HG  | 2.13                     | 0.49              |
| 1:m:202:LYS:O    | 1:m:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:G:62:LEU:O     | 1:G:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:n:5:THR:OG1    | 1:n:143:ARG:NH2 | 2.46                     | 0.49              |
| 1:1:44:VAL:HA    | 1:1:47:LEU:HD12 | 1.94                     | 0.49              |
| 1:2:134:LEU:HD11 | 1:2:159:LEU:HG  | 1.95                     | 0.49              |
| 1:W:234:ILE:HD11 | 1:W:245:LEU:HB3 | 1.93                     | 0.49              |
| 1:s:57:LEU:O     | 1:s:61:VAL:HG23 | 2.12                     | 0.49              |
| 1:N:134:LEU:HD11 | 1:N:159:LEU:HG  | 1.95                     | 0.49              |
| 1:j:62:LEU:O     | 1:j:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:j:202:LYS:O    | 1:j:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:R:56:ARG:HG3   | 1:z:56:ARG:HD2  | 1.95                     | 0.49              |
| 1:c:62:LEU:O     | 1:c:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:H:202:LYS:O    | 1:H:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:o:151:ILE:O    | 1:o:155:LEU:HG  | 2.13                     | 0.49              |
| 1:T:30:ARG:N     | 1:T:31:PRO:HD2  | 2.27                     | 0.49              |
| 1:q:30:ARG:N     | 1:q:31:PRO:HD2  | 2.27                     | 0.49              |
| 1:3:202:LYS:O    | 1:3:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:4:95:GLU:OE1   | 1:4:95:GLU:N    | 2.44                     | 0.49              |
| 1:Y:5:THR:OG1    | 1:Y:143:ARG:NH2 | 2.45                     | 0.49              |
| 1:P:20:GLU:OE1   | 1:P:23:ARG:NH2  | 2.39                     | 0.49              |
| 1:A:20:GLU:OE1   | 1:A:23:ARG:NH2  | 2.39                     | 0.49              |
| 1:B:83:GLU:O     | 1:B:87:LEU:HD12 | 2.13                     | 0.49              |
| 1:C:5:THR:OG1    | 1:C:143:ARG:NH2 | 2.46                     | 0.49              |
| 1:E:62:LEU:O     | 1:E:66:ARG:HG2  | 2.12                     | 0.49              |
| 1:m:20:GLU:OE1   | 1:m:23:ARG:NH2  | 2.39                     | 0.49              |
| 1:o:95:GLU:OE1   | 1:o:95:GLU:N    | 2.44                     | 0.49              |
| 1:z:202:LYS:O    | 1:z:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:I:202:LYS:O    | 1:I:206:GLU:HG3 | 2.13                     | 0.49              |
| 1:W:195:LEU:HD21 | 1:W:244:GLU:OE1 | 2.12                     | 0.49              |
| 1:h:77:LEU:HA    | 1:h:80:VAL:HG12 | 1.94                     | 0.49              |
| 1:3:62:LEU:O     | 1:3:66:ARG:HG2  | 2.13                     | 0.49              |
| 1:i:167:ARG:NH2  | 1:i:173:GLU:OE1 | 2.39                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:95:GLU:OE1   | 1:t:95:GLU:N     | 2.43                     | 0.49              |
| 1:Y:30:ARG:N     | 1:Y:31:PRO:HD2   | 2.28                     | 0.49              |
| 1:O:56:ARG:HD2   | 1:a:56:ARG:HG3   | 1.95                     | 0.49              |
| 1:k:62:LEU:O     | 1:k:66:ARG:HG2   | 2.12                     | 0.49              |
| 1:7:62:LEU:O     | 1:7:66:ARG:HG2   | 2.12                     | 0.49              |
| 1:B:234:ILE:HD11 | 1:B:245:LEU:HB3  | 1.95                     | 0.48              |
| 1:x:202:LYS:O    | 1:x:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:R:202:LYS:O    | 1:R:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:y:56:ARG:HG3   | 1:h:56:ARG:HD2   | 1.95                     | 0.48              |
| 1:I:218:GLU:HB3  | 1:0:250:LEU:HD22 | 1.95                     | 0.48              |
| 1:K:30:ARG:N     | 1:K:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:7:57:LEU:O     | 1:7:61:VAL:HG23  | 2.13                     | 0.48              |
| 1:E:5:THR:OG1    | 1:E:143:ARG:NH2  | 2.46                     | 0.48              |
| 1:E:57:LEU:O     | 1:E:61:VAL:HG23  | 2.13                     | 0.48              |
| 1:b:95:GLU:OE1   | 1:b:95:GLU:N     | 2.45                     | 0.48              |
| 1:G:57:LEU:O     | 1:G:61:VAL:HG23  | 2.13                     | 0.48              |
| 1:0:57:LEU:O     | 1:0:61:VAL:HG23  | 2.13                     | 0.48              |
| 1:U:62:LEU:HD11  | 1:U:66:ARG:HH11  | 1.78                     | 0.48              |
| 1:K:95:GLU:N     | 1:K:95:GLU:OE1   | 2.43                     | 0.48              |
| 1:L:202:LYS:O    | 1:L:206:GLU:HG3  | 2.14                     | 0.48              |
| 1:X:38:HIS:ND1   | 1:X:64:MET:HE1   | 2.28                     | 0.48              |
| 1:X:151:ILE:O    | 1:X:155:LEU:HG   | 2.13                     | 0.48              |
| 1:t:30:ARG:N     | 1:t:31:PRO:HD2   | 2.27                     | 0.48              |
| 1:Y:95:GLU:OE1   | 1:Y:95:GLU:N     | 2.43                     | 0.48              |
| 1:k:151:ILE:O    | 1:k:155:LEU:HG   | 2.13                     | 0.48              |
| 1:v:20:GLU:OE1   | 1:v:23:ARG:NH2   | 2.39                     | 0.48              |
| 1:7:151:ILE:O    | 1:7:155:LEU:HG   | 2.13                     | 0.48              |
| 1:A:30:ARG:N     | 1:A:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:F:56:ARG:HD2   | 1:V:56:ARG:HG3   | 1.95                     | 0.48              |
| 1:Q:202:LYS:O    | 1:Q:206:GLU:HG3  | 2.14                     | 0.48              |
| 1:m:30:ARG:N     | 1:m:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:R:20:GLU:OE1   | 1:R:23:ARG:NH2   | 2.39                     | 0.48              |
| 1:R:30:ARG:N     | 1:R:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:c:234:ILE:HD11 | 1:c:245:LEU:HB3  | 1.95                     | 0.48              |
| 1:z:30:ARG:N     | 1:z:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:U:151:ILE:O    | 1:U:155:LEU:HG   | 2.13                     | 0.48              |
| 1:f:167:ARG:NH2  | 1:f:173:GLU:OE1  | 2.39                     | 0.48              |
| 1:V:126:ILE:O    | 1:V:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:V:202:LYS:O    | 1:V:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:W:95:GLU:OE1   | 1:W:95:GLU:N     | 2.44                     | 0.48              |
| 1:s:151:ILE:O    | 1:s:155:LEU:HG   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:250:LEU:HD22 | 1:3:218:GLU:HB3  | 1.96                     | 0.48              |
| 1:t:62:LEU:O     | 1:t:66:ARG:HG2   | 2.13                     | 0.48              |
| 1:k:38:HIS:ND1   | 1:k:64:MET:HE1   | 2.27                     | 0.48              |
| 1:a:202:LYS:O    | 1:a:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:B:126:ILE:O    | 1:B:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:n:30:ARG:N     | 1:n:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:H:62:LEU:O     | 1:H:66:ARG:HG2   | 2.12                     | 0.48              |
| 1:T:167:ARG:NH2  | 1:T:173:GLU:OE1  | 2.40                     | 0.48              |
| 1:e:153:ARG:HD3  | 1:p:215:ARG:HH21 | 1.79                     | 0.48              |
| 1:K:56:ARG:HG3   | 1:3:56:ARG:HD2   | 1.94                     | 0.48              |
| 1:g:167:ARG:NH2  | 1:g:173:GLU:OE1  | 2.38                     | 0.48              |
| 1:L:167:ARG:NH2  | 1:L:173:GLU:OE1  | 2.40                     | 0.48              |
| 1:W:56:ARG:HD2   | 1:t:56:ARG:HG3   | 1.95                     | 0.48              |
| 1:j:126:ILE:O    | 1:j:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:O:30:ARG:N     | 1:O:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:v:62:LEU:O     | 1:v:66:ARG:HG2   | 2.13                     | 0.48              |
| 1:A:5:THR:OG1    | 1:A:143:ARG:NH2  | 2.46                     | 0.48              |
| 1:A:56:ARG:HG3   | 1:m:56:ARG:HD2   | 1.95                     | 0.48              |
| 1:F:30:ARG:N     | 1:F:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:x:234:ILE:HD11 | 1:x:245:LEU:HB3  | 1.96                     | 0.48              |
| 1:e:95:GLU:OE1   | 1:e:95:GLU:N     | 2.44                     | 0.48              |
| 1:O:151:ILE:O    | 1:O:155:LEU:HG   | 2.13                     | 0.48              |
| 1:U:250:LEU:HD22 | 1:f:218:GLU:HB3  | 1.95                     | 0.48              |
| 1:q:62:LEU:O     | 1:q:66:ARG:HG2   | 2.13                     | 0.48              |
| 1:1:30:ARG:N     | 1:1:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:1:95:GLU:OE1   | 1:1:95:GLU:N     | 2.44                     | 0.48              |
| 1:g:5:THR:OG1    | 1:g:143:ARG:NH2  | 2.46                     | 0.48              |
| 1:2:62:LEU:HD11  | 1:2:66:ARG:HH11  | 1.78                     | 0.48              |
| 1:N:62:LEU:HD11  | 1:N:66:ARG:HH11  | 1.77                     | 0.48              |
| 1:Y:56:ARG:HD2   | 1:v:56:ARG:HG3   | 1.96                     | 0.48              |
| 1:v:202:LYS:O    | 1:v:206:GLU:HG3  | 2.12                     | 0.48              |
| 1:P:202:LYS:O    | 1:P:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:218:GLU:HB3  | 1:E:250:LEU:HD22 | 1.95                     | 0.48              |
| 1:E:134:LEU:HD11 | 1:E:159:LEU:HG   | 1.94                     | 0.48              |
| 1:m:56:ARG:HG3   | 1:f:56:ARG:HD2   | 1.96                     | 0.48              |
| 1:G:250:LEU:HD22 | 1:R:218:GLU:HB3  | 1.95                     | 0.48              |
| 1:S:30:ARG:N     | 1:S:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:f:30:ARG:N     | 1:f:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:K:5:THR:OG1    | 1:K:143:ARG:NH2  | 2.46                     | 0.48              |
| 1:h:20:GLU:OE1   | 1:h:23:ARG:NH2   | 2.37                     | 0.48              |
| 1:u:153:ARG:HD3  | 1:5:215:ARG:HH21 | 1.79                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:5:THR:OG1    | 1:k:143:ARG:NH2  | 2.47                     | 0.48              |
| 1:v:83:GLU:O     | 1:v:87:LEU:HD12  | 2.12                     | 0.48              |
| 1:a:20:GLU:OE1   | 1:a:23:ARG:NH2   | 2.38                     | 0.48              |
| 1:B:202:LYS:O    | 1:B:206:GLU:HG3  | 2.13                     | 0.48              |
| 1:C:153:ARG:HD3  | 1:D:215:ARG:HH21 | 1.79                     | 0.48              |
| 1:F:153:ARG:HD3  | 1:Q:215:ARG:HH21 | 1.79                     | 0.48              |
| 1:x:7:VAL:O      | 1:x:11:ARG:HG3   | 2.14                     | 0.48              |
| 1:G:134:LEU:HD11 | 1:G:159:LEU:HG   | 1.95                     | 0.48              |
| 1:c:126:ILE:O    | 1:c:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:n:153:ARG:HD3  | 1:y:215:ARG:HH21 | 1.79                     | 0.48              |
| 1:d:95:GLU:O     | 1:d:99:LEU:HD12  | 2.14                     | 0.48              |
| 1:z:56:ARG:HG3   | 1:i:56:ARG:HD2   | 1.96                     | 0.48              |
| 1:z:62:LEU:O     | 1:z:66:ARG:HG2   | 2.13                     | 0.48              |
| 1:l:5:THR:OG1    | 1:l:143:ARG:NH2  | 2.47                     | 0.48              |
| 1:g:153:ARG:HD3  | 1:r:215:ARG:HH21 | 1.79                     | 0.48              |
| 1:t:126:ILE:O    | 1:t:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:u:38:HIS:ND1   | 1:u:64:MET:HE1   | 2.29                     | 0.48              |
| 1:u:167:ARG:NH2  | 1:u:173:GLU:OE1  | 2.39                     | 0.48              |
| 1:5:77:LEU:HA    | 1:5:80:VAL:HG12  | 1.95                     | 0.48              |
| 1:l:30:ARG:N     | 1:l:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:p:95:GLU:O     | 1:p:99:LEU:HD12  | 2.14                     | 0.48              |
| 1:J:202:LYS:O    | 1:J:206:GLU:HG3  | 2.14                     | 0.48              |
| 1:K:56:ARG:HD2   | 1:P:56:ARG:HG3   | 1.96                     | 0.48              |
| 1:h:30:ARG:N     | 1:h:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:h:202:LYS:O    | 1:h:206:GLU:HG3  | 2.14                     | 0.48              |
| 1:s:134:LEU:HD11 | 1:s:159:LEU:HG   | 1.95                     | 0.48              |
| 1:M:30:ARG:N     | 1:M:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:X:134:LEU:HD11 | 1:X:159:LEU:HG   | 1.95                     | 0.48              |
| 1:i:30:ARG:N     | 1:i:31:PRO:HD2   | 2.28                     | 0.48              |
| 1:6:56:ARG:HG3   | 1:l:56:ARG:HD2   | 1.95                     | 0.48              |
| 1:P:83:GLU:O     | 1:P:87:LEU:HD12  | 2.12                     | 0.48              |
| 1:B:56:ARG:HG3   | 1:n:56:ARG:HD2   | 1.95                     | 0.48              |
| 1:Q:30:ARG:N     | 1:Q:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:x:126:ILE:O    | 1:x:130:VAL:HG23 | 2.13                     | 0.48              |
| 1:d:30:ARG:N     | 1:d:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:d:202:LYS:O    | 1:d:206:GLU:HG3  | 2.14                     | 0.48              |
| 1:e:30:ARG:N     | 1:e:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:p:30:ARG:N     | 1:p:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:p:133:ARG:HH21 | 1:p:136:GLU:CD   | 2.22                     | 0.48              |
| 1:q:126:ILE:O    | 1:q:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:q:234:ILE:HD11 | 1:q:245:LEU:HB3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:133:ARG:HH21 | 1:h:136:GLU:CD   | 2.22                     | 0.48              |
| 1:N:151:ILE:O    | 1:N:155:LEU:HG   | 2.13                     | 0.48              |
| 1:5:133:ARG:HH21 | 1:5:136:GLU:CD   | 2.22                     | 0.48              |
| 1:G:151:ILE:O    | 1:G:155:LEU:HG   | 2.13                     | 0.48              |
| 1:0:134:LEU:HD11 | 1:0:159:LEU:HG   | 1.95                     | 0.48              |
| 1:U:5:THR:OG1    | 1:U:143:ARG:NH2  | 2.47                     | 0.48              |
| 1:W:30:ARG:N     | 1:W:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:h:5:THR:OG1    | 1:h:143:ARG:NH2  | 2.46                     | 0.48              |
| 1:X:250:LEU:HD22 | 1:i:218:GLU:HB3  | 1.96                     | 0.48              |
| 1:4:30:ARG:N     | 1:4:31:PRO:HD2   | 2.29                     | 0.48              |
| 1:5:95:GLU:O     | 1:5:99:LEU:HD12  | 2.14                     | 0.48              |
| 1:6:126:ILE:O    | 1:6:130:VAL:HG23 | 2.14                     | 0.48              |
| 1:a:71:GLU:O     | 1:a:75:ARG:HG3   | 2.13                     | 0.48              |
| 1:E:151:ILE:O    | 1:E:155:LEU:HG   | 2.13                     | 0.47              |
| 1:m:62:LEU:O     | 1:m:66:ARG:HG2   | 2.13                     | 0.47              |
| 1:o:250:LEU:HD22 | 1:z:218:GLU:HB3  | 1.95                     | 0.47              |
| 1:I:30:ARG:N     | 1:I:31:PRO:HD2   | 2.28                     | 0.47              |
| 1:e:5:THR:OG1    | 1:e:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:p:202:LYS:O    | 1:p:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:0:152:ILE:HG13 | 1:0:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:J:30:ARG:N     | 1:J:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:U:34:GLU:HG3   | 1:g:85:ARG:NH2   | 2.30                     | 0.47              |
| 1:V:134:LEU:HD11 | 1:V:159:LEU:HG   | 1.96                     | 0.47              |
| 1:r:133:ARG:HH21 | 1:r:136:GLU:CD   | 2.22                     | 0.47              |
| 1:2:151:ILE:O    | 1:2:155:LEU:HG   | 2.13                     | 0.47              |
| 1:2:152:ILE:HG13 | 1:2:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:s:152:ILE:HG13 | 1:s:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:t:202:LYS:O    | 1:t:206:GLU:HG3  | 2.13                     | 0.47              |
| 1:N:152:ILE:HG13 | 1:N:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:Z:202:LYS:O    | 1:Z:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:6:202:LYS:O    | 1:6:206:GLU:HG3  | 2.13                     | 0.47              |
| 1:w:30:ARG:N     | 1:w:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:w:77:LEU:HA    | 1:w:80:VAL:HG12  | 1.95                     | 0.47              |
| 1:C:30:ARG:N     | 1:C:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:D:9:GLU:OE1    | 1:D:143:ARG:NE   | 2.47                     | 0.47              |
| 1:Q:95:GLU:O     | 1:Q:99:LEU:HD12  | 2.14                     | 0.47              |
| 1:c:202:LYS:O    | 1:c:206:GLU:HG3  | 2.13                     | 0.47              |
| 1:y:202:LYS:O    | 1:y:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:o:5:THR:OG1    | 1:o:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:h:29:MET:HB3   | 1:h:32:TYR:HD2   | 1.79                     | 0.47              |
| 1:3:30:ARG:N     | 1:3:31:PRO:HD2   | 2.28                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:5:THR:OG1    | 1:u:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:Z:30:ARG:N     | 1:Z:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:D:5:THR:OG1    | 1:D:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:b:5:THR:OG1    | 1:b:143:ARG:NH2  | 2.46                     | 0.47              |
| 1:y:77:LEU:HA    | 1:y:80:VAL:HG12  | 1.95                     | 0.47              |
| 1:d:133:ARG:HH21 | 1:d:136:GLU:CD   | 2.22                     | 0.47              |
| 1:I:56:ARG:HG3   | 1:v:56:ARG:HD2   | 1.95                     | 0.47              |
| 1:p:29:MET:HB3   | 1:p:32:TYR:HD2   | 1.79                     | 0.47              |
| 1:U:134:LEU:HD11 | 1:U:159:LEU:HG   | 1.95                     | 0.47              |
| 1:V:71:GLU:O     | 1:V:75:ARG:HG3   | 2.13                     | 0.47              |
| 1:r:77:LEU:HA    | 1:r:80:VAL:HG12  | 1.96                     | 0.47              |
| 1:h:10:VAL:HG21  | 1:h:47:LEU:HD11  | 1.96                     | 0.47              |
| 1:M:25:GLY:HA3   | 1:M:29:MET:HE2   | 1.95                     | 0.47              |
| 1:4:5:THR:OG1    | 1:4:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:6:134:LEU:HD11 | 1:6:159:LEU:HG   | 1.96                     | 0.47              |
| 1:7:5:THR:OG1    | 1:7:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:D:30:ARG:N     | 1:D:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:D:133:ARG:HH21 | 1:D:136:GLU:CD   | 2.22                     | 0.47              |
| 1:E:167:ARG:NH2  | 1:E:173:GLU:OE1  | 2.36                     | 0.47              |
| 1:b:250:LEU:HD22 | 1:m:218:GLU:HB3  | 1.95                     | 0.47              |
| 1:G:167:ARG:NH2  | 1:G:173:GLU:OE1  | 2.37                     | 0.47              |
| 1:y:9:GLU:OE1    | 1:y:143:ARG:NE   | 2.47                     | 0.47              |
| 1:J:29:MET:HB3   | 1:J:32:TYR:HD2   | 1.80                     | 0.47              |
| 1:1:234:ILE:HD11 | 1:1:245:LEU:HB3  | 1.96                     | 0.47              |
| 1:K:218:GLU:HB3  | 1:2:250:LEU:HD22 | 1.95                     | 0.47              |
| 1:V:83:GLU:O     | 1:V:87:LEU:HD12  | 2.15                     | 0.47              |
| 1:2:5:THR:OG1    | 1:2:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:s:5:THR:OG1    | 1:s:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:t:29:MET:HB2   | 1:t:32:TYR:HD2   | 1.80                     | 0.47              |
| 1:j:134:LEU:HD11 | 1:j:159:LEU:HG   | 1.97                     | 0.47              |
| 1:a:234:ILE:HD11 | 1:a:245:LEU:HB3  | 1.96                     | 0.47              |
| 1:y:29:MET:HB3   | 1:y:32:TYR:HD2   | 1.79                     | 0.47              |
| 1:y:133:ARG:HH21 | 1:y:136:GLU:CD   | 2.22                     | 0.47              |
| 1:o:57:LEU:O     | 1:o:61:VAL:HG23  | 2.13                     | 0.47              |
| 1:q:202:LYS:O    | 1:q:206:GLU:HG3  | 2.13                     | 0.47              |
| 1:l:85:ARG:NH2   | 1:k:34:GLU:HG3   | 2.30                     | 0.47              |
| 1:V:20:GLU:OE1   | 1:V:23:ARG:NH2   | 2.37                     | 0.47              |
| 1:r:202:LYS:O    | 1:r:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:M:133:ARG:HH21 | 1:M:136:GLU:CD   | 2.22                     | 0.47              |
| 1:M:202:LYS:O    | 1:M:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:X:5:THR:OG1    | 1:X:143:ARG:NH2  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:95:GLU:N     | 1:i:95:GLU:OE1   | 2.43                     | 0.47              |
| 1:u:95:GLU:OE1   | 1:u:95:GLU:N     | 2.44                     | 0.47              |
| 1:k:250:LEU:HD22 | 1:v:218:GLU:HB3  | 1.95                     | 0.47              |
| 1:6:83:GLU:O     | 1:6:87:LEU:HD12  | 2.15                     | 0.47              |
| 1:P:30:ARG:N     | 1:P:31:PRO:HD2   | 2.28                     | 0.47              |
| 1:l:153:ARG:HD3  | 1:w:215:ARG:HH21 | 1.78                     | 0.47              |
| 1:A:56:ARG:HD2   | 1:f:56:ARG:HG3   | 1.96                     | 0.47              |
| 1:F:5:THR:OG1    | 1:F:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:Q:9:GLU:OE1    | 1:Q:143:ARG:NE   | 2.47                     | 0.47              |
| 1:Q:133:ARG:HH21 | 1:Q:136:GLU:CD   | 2.22                     | 0.47              |
| 1:x:9:GLU:HG3    | 1:x:12:ARG:NH2   | 2.30                     | 0.47              |
| 1:c:83:GLU:O     | 1:c:87:LEU:HD12  | 2.15                     | 0.47              |
| 1:y:30:ARG:N     | 1:y:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:d:9:GLU:OE1    | 1:d:143:ARG:NE   | 2.47                     | 0.47              |
| 1:p:9:GLU:OE1    | 1:p:143:ARG:NE   | 2.47                     | 0.47              |
| 1:p:77:LEU:HA    | 1:p:80:VAL:HG12  | 1.95                     | 0.47              |
| 1:J:9:GLU:OE1    | 1:J:143:ARG:NE   | 2.47                     | 0.47              |
| 1:J:95:GLU:O     | 1:J:99:LEU:HD12  | 2.14                     | 0.47              |
| 1:f:95:GLU:N     | 1:f:95:GLU:OE1   | 2.43                     | 0.47              |
| 1:r:30:ARG:N     | 1:r:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:2:38:HIS:ND1   | 1:2:64:MET:HE1   | 2.28                     | 0.47              |
| 1:h:95:GLU:O     | 1:h:99:LEU:HD12  | 2.15                     | 0.47              |
| 1:N:34:GLU:HG3   | 1:l:85:ARG:NH2   | 2.30                     | 0.47              |
| 1:u:195:LEU:HD11 | 1:u:244:GLU:HB2  | 1.96                     | 0.47              |
| 1:5:9:GLU:OE1    | 1:5:143:ARG:NE   | 2.47                     | 0.47              |
| 1:Z:133:ARG:HH21 | 1:Z:136:GLU:CD   | 2.22                     | 0.47              |
| 1:a:134:LEU:HD11 | 1:a:159:LEU:HG   | 1.97                     | 0.47              |
| 1:w:202:LYS:O    | 1:w:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:62:LEU:O     | 1:B:66:ARG:HG2   | 2.13                     | 0.47              |
| 1:B:133:ARG:HH21 | 1:B:136:GLU:CD   | 2.23                     | 0.47              |
| 1:B:134:LEU:HD11 | 1:B:159:LEU:HG   | 1.96                     | 0.47              |
| 1:D:29:MET:HB3   | 1:D:32:TYR:HD2   | 1.80                     | 0.47              |
| 1:D:202:LYS:O    | 1:D:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:E:152:ILE:HG13 | 1:E:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:b:30:ARG:N     | 1:b:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:G:5:THR:OG1    | 1:G:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:G:38:HIS:CE1   | 1:G:64:MET:HE1   | 2.50                     | 0.47              |
| 1:G:152:ILE:HG13 | 1:G:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:n:156:GLU:OE1  | 1:n:254:ARG:NH1  | 2.37                     | 0.47              |
| 1:y:95:GLU:O     | 1:y:99:LEU:HD12  | 2.14                     | 0.47              |
| 1:q:83:GLU:O     | 1:q:87:LEU:HD12  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:133:ARG:HH21 | 1:V:136:GLU:CD   | 2.23                     | 0.47              |
| 1:g:95:GLU:OE1   | 1:g:95:GLU:N     | 2.44                     | 0.47              |
| 1:r:5:THR:OG1    | 1:r:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:r:9:GLU:OE1    | 1:r:143:ARG:NE   | 2.47                     | 0.47              |
| 1:W:5:THR:OG1    | 1:W:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:h:9:GLU:OE1    | 1:h:143:ARG:NE   | 2.47                     | 0.47              |
| 1:s:38:HIS:CE1   | 1:s:64:MET:HE1   | 2.50                     | 0.47              |
| 1:N:250:LEU:HD22 | 1:Y:218:GLU:HB3  | 1.95                     | 0.47              |
| 1:5:30:ARG:N     | 1:5:31:PRO:HD2   | 2.29                     | 0.47              |
| 1:O:5:THR:OG1    | 1:O:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:O:234:ILE:HD11 | 1:O:245:LEU:HB3  | 1.97                     | 0.47              |
| 1:v:30:ARG:N     | 1:v:31:PRO:HD2   | 2.28                     | 0.47              |
| 1:6:133:ARG:HH21 | 1:6:136:GLU:CD   | 2.23                     | 0.47              |
| 1:P:218:GLU:HB3  | 1:7:250:LEU:HD22 | 1.96                     | 0.47              |
| 1:l:5:THR:OG1    | 1:l:143:ARG:NH2  | 2.47                     | 0.47              |
| 1:w:9:GLU:OE1    | 1:w:143:ARG:NE   | 2.47                     | 0.47              |
| 1:w:76:LEU:O     | 1:w:80:VAL:HG12  | 2.15                     | 0.47              |
| 1:w:133:ARG:HH21 | 1:w:136:GLU:CD   | 2.22                     | 0.47              |
| 1:Q:10:VAL:HG21  | 1:Q:47:LEU:HD11  | 1.96                     | 0.47              |
| 1:c:133:ARG:HH21 | 1:c:136:GLU:CD   | 2.23                     | 0.47              |
| 1:H:252:LEU:O    | 1:H:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:d:29:MET:HB3   | 1:d:32:TYR:HD2   | 1.79                     | 0.47              |
| 1:0:5:THR:OG1    | 1:0:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:J:133:ARG:HH21 | 1:J:136:GLU:CD   | 2.22                     | 0.47              |
| 1:J:215:ARG:HH21 | 1:1:153:ARG:HD3  | 1.79                     | 0.47              |
| 1:q:29:MET:HB2   | 1:q:32:TYR:HD2   | 1.80                     | 0.47              |
| 1:M:9:GLU:OE1    | 1:M:143:ARG:NE   | 2.47                     | 0.47              |
| 1:i:62:LEU:HD11  | 1:i:66:ARG:NH1   | 2.29                     | 0.47              |
| 1:j:252:LEU:O    | 1:j:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:O:153:ARG:HD3  | 1:Z:215:ARG:HH21 | 1.79                     | 0.47              |
| 1:Z:9:GLU:OE1    | 1:Z:143:ARG:NE   | 2.47                     | 0.47              |
| 1:B:243:GLU:O    | 1:B:247:VAL:HG23 | 2.15                     | 0.47              |
| 1:C:38:HIS:ND1   | 1:C:64:MET:HE1   | 2.29                     | 0.47              |
| 1:D:77:LEU:HA    | 1:D:80:VAL:HG12  | 1.96                     | 0.47              |
| 1:E:30:ARG:N     | 1:E:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:b:34:GLU:HG3   | 1:n:85:ARG:NH2   | 2.30                     | 0.47              |
| 1:G:30:ARG:N     | 1:G:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:c:134:LEU:HD11 | 1:c:159:LEU:HG   | 1.97                     | 0.47              |
| 1:d:5:THR:OG1    | 1:d:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:o:30:ARG:N     | 1:o:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:0:20:GLU:OE1   | 1:0:23:ARG:NH2   | 2.37                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:252:LEU:O    | 1:q:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:V:234:ILE:HD11 | 1:V:245:LEU:HB3  | 1.96                     | 0.47              |
| 1:r:20:GLU:OE1   | 1:r:23:ARG:NH2   | 2.37                     | 0.47              |
| 1:M:152:ILE:HG13 | 1:M:247:VAL:HG11 | 1.97                     | 0.47              |
| 1:X:152:ILE:HG13 | 1:X:247:VAL:HG11 | 1.96                     | 0.47              |
| 1:t:234:ILE:HD11 | 1:t:245:LEU:HB3  | 1.96                     | 0.47              |
| 1:j:20:GLU:OE1   | 1:j:23:ARG:NH2   | 2.37                     | 0.47              |
| 1:j:133:ARG:HH21 | 1:j:136:GLU:CD   | 2.23                     | 0.47              |
| 1:j:234:ILE:HD11 | 1:j:245:LEU:HB3  | 1.96                     | 0.47              |
| 1:5:202:LYS:O    | 1:5:206:GLU:HG3  | 2.14                     | 0.47              |
| 1:k:57:LEU:O     | 1:k:61:VAL:HG23  | 2.15                     | 0.47              |
| 1:w:10:VAL:HG21  | 1:w:47:LEU:HD11  | 1.96                     | 0.47              |
| 1:C:85:ARG:NH2   | 1:o:34:GLU:HG3   | 2.30                     | 0.47              |
| 1:C:156:GLU:OE1  | 1:C:254:ARG:NH1  | 2.37                     | 0.47              |
| 1:y:5:THR:OG1    | 1:y:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:d:77:LEU:HA    | 1:d:80:VAL:HG12  | 1.97                     | 0.47              |
| 1:I:56:ARG:HD2   | 1:Y:56:ARG:HG3   | 1.96                     | 0.47              |
| 1:T:252:LEU:O    | 1:T:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:p:152:ILE:HG13 | 1:p:247:VAL:HG11 | 1.97                     | 0.47              |
| 1:U:30:ARG:N     | 1:U:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:q:133:ARG:HH21 | 1:q:136:GLU:CD   | 2.23                     | 0.47              |
| 1:q:134:LEU:HD11 | 1:q:159:LEU:HG   | 1.96                     | 0.47              |
| 1:V:252:LEU:O    | 1:V:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:M:95:GLU:O     | 1:M:99:LEU:HD12  | 2.15                     | 0.47              |
| 1:X:30:ARG:N     | 1:X:31:PRO:HD2   | 2.30                     | 0.47              |
| 1:t:134:LEU:HD11 | 1:t:159:LEU:HG   | 1.96                     | 0.47              |
| 1:t:252:LEU:O    | 1:t:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:j:29:MET:HB2   | 1:j:32:TYR:HD2   | 1.80                     | 0.47              |
| 1:u:234:ILE:HD11 | 1:u:245:LEU:HB3  | 1.97                     | 0.47              |
| 1:a:252:LEU:O    | 1:a:256:ILE:HG13 | 2.15                     | 0.47              |
| 1:x:133:ARG:HH21 | 1:x:136:GLU:CD   | 2.23                     | 0.46              |
| 1:x:252:LEU:O    | 1:x:256:ILE:HG13 | 2.15                     | 0.46              |
| 1:c:243:GLU:O    | 1:c:247:VAL:HG23 | 2.15                     | 0.46              |
| 1:c:252:LEU:O    | 1:c:256:ILE:HG13 | 2.15                     | 0.46              |
| 1:e:195:LEU:HD11 | 1:e:244:GLU:HB2  | 1.97                     | 0.46              |
| 1:f:149:ARG:NH2  | 1:f:243:GLU:OE2  | 2.48                     | 0.46              |
| 1:h:152:ILE:HG13 | 1:h:247:VAL:HG11 | 1.97                     | 0.46              |
| 1:s:20:GLU:OE1   | 1:s:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:t:133:ARG:HH21 | 1:t:136:GLU:CD   | 2.23                     | 0.46              |
| 1:N:57:LEU:O     | 1:N:61:VAL:HG23  | 2.15                     | 0.46              |
| 1:5:76:LEU:O     | 1:5:80:VAL:HG12  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:95:GLU:O     | 1:Z:99:LEU:HD12  | 2.15                     | 0.46              |
| 1:w:29:MET:HE3   | 1:w:29:MET:HB2   | 1.86                     | 0.46              |
| 1:w:95:GLU:O     | 1:w:99:LEU:HD12  | 2.15                     | 0.46              |
| 1:Q:29:MET:HB3   | 1:Q:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:y:76:LEU:O     | 1:y:80:VAL:HG12  | 2.15                     | 0.46              |
| 1:T:133:ARG:HH21 | 1:T:136:GLU:CD   | 2.23                     | 0.46              |
| 1:U:57:LEU:O     | 1:U:61:VAL:HG23  | 2.14                     | 0.46              |
| 1:U:152:ILE:HG13 | 1:U:247:VAL:HG11 | 1.96                     | 0.46              |
| 1:f:254:ARG:HE   | 1:f:254:ARG:HB2  | 1.56                     | 0.46              |
| 1:L:252:LEU:O    | 1:L:256:ILE:HG13 | 2.15                     | 0.46              |
| 1:i:254:ARG:HE   | 1:i:254:ARG:HB2  | 1.55                     | 0.46              |
| 1:6:195:LEU:HD21 | 1:6:244:GLU:OE1  | 2.15                     | 0.46              |
| 1:6:252:LEU:O    | 1:6:256:ILE:HG13 | 2.15                     | 0.46              |
| 1:D:243:GLU:O    | 1:D:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:b:152:ILE:HG13 | 1:b:247:VAL:HG11 | 1.96                     | 0.46              |
| 1:S:85:ARG:NH2   | 1:0:34:GLU:HG3   | 2.30                     | 0.46              |
| 1:0:178:LYS:NZ   | 1:0:178:LYS:HB2  | 2.30                     | 0.46              |
| 1:J:152:ILE:HG13 | 1:J:247:VAL:HG11 | 1.98                     | 0.46              |
| 1:X:178:LYS:HB2  | 1:X:178:LYS:NZ   | 2.30                     | 0.46              |
| 1:i:133:ARG:HH21 | 1:i:136:GLU:CD   | 2.24                     | 0.46              |
| 1:k:30:ARG:N     | 1:k:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:7:202:LYS:O    | 1:7:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:B:252:LEU:O    | 1:B:256:ILE:HG13 | 2.15                     | 0.46              |
| 1:F:195:LEU:HD11 | 1:F:244:GLU:HB2  | 1.98                     | 0.46              |
| 1:n:234:ILE:HD11 | 1:n:245:LEU:HB3  | 1.96                     | 0.46              |
| 1:H:10:VAL:HG21  | 1:H:47:LEU:HD11  | 1.97                     | 0.46              |
| 1:d:243:GLU:O    | 1:d:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:o:152:ILE:HG13 | 1:o:247:VAL:HG11 | 1.96                     | 0.46              |
| 1:T:29:MET:HB2   | 1:T:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:J:20:GLU:OE1   | 1:J:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:f:133:ARG:HH21 | 1:f:136:GLU:CD   | 2.24                     | 0.46              |
| 1:g:30:ARG:N     | 1:g:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:L:29:MET:HB2   | 1:L:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:3:56:ARG:HG3   | 1:P:56:ARG:HD2   | 1.97                     | 0.46              |
| 1:X:57:LEU:O     | 1:X:61:VAL:HG23  | 2.15                     | 0.46              |
| 1:u:30:ARG:N     | 1:u:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:O:38:HIS:ND1   | 1:O:64:MET:HE1   | 2.29                     | 0.46              |
| 1:Z:10:VAL:HG21  | 1:Z:47:LEU:HD11  | 1.97                     | 0.46              |
| 1:k:152:ILE:HG13 | 1:k:247:VAL:HG11 | 1.96                     | 0.46              |
| 1:l:38:HIS:ND1   | 1:l:64:MET:HE1   | 2.30                     | 0.46              |
| 1:C:243:GLU:O    | 1:C:247:VAL:HG23 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:243:GLU:O    | 1:H:247:VAL:HG23 | 2.15                     | 0.46              |
| 1:o:20:GLU:OE1   | 1:o:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:T:9:GLU:OE1    | 1:T:143:ARG:NE   | 2.49                     | 0.46              |
| 1:1:195:LEU:HD11 | 1:1:244:GLU:HB2  | 1.98                     | 0.46              |
| 1:V:29:MET:HB2   | 1:V:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:g:243:GLU:O    | 1:g:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:r:152:ILE:HG13 | 1:r:247:VAL:HG11 | 1.98                     | 0.46              |
| 1:L:133:ARG:HH21 | 1:L:136:GLU:CD   | 2.24                     | 0.46              |
| 1:X:202:LYS:O    | 1:X:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:5:29:MET:HB3   | 1:5:32:TYR:HD2   | 1.79                     | 0.46              |
| 1:5:152:ILE:HG13 | 1:5:247:VAL:HG11 | 1.98                     | 0.46              |
| 1:a:29:MET:HB2   | 1:a:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:Q:77:LEU:HA    | 1:Q:80:VAL:HG12  | 1.98                     | 0.46              |
| 1:b:57:LEU:O     | 1:b:61:VAL:HG23  | 2.15                     | 0.46              |
| 1:b:178:LYS:HB2  | 1:b:178:LYS:NZ   | 2.30                     | 0.46              |
| 1:R:133:ARG:HH21 | 1:R:136:GLU:CD   | 2.23                     | 0.46              |
| 1:S:5:THR:OG1    | 1:S:143:ARG:NH2  | 2.48                     | 0.46              |
| 1:p:243:GLU:O    | 1:p:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:5:5:THR:OG1    | 1:5:143:ARG:NH2  | 2.49                     | 0.46              |
| 1:k:202:LYS:O    | 1:k:206:GLU:HG3  | 2.16                     | 0.46              |
| 1:l:234:ILE:HD11 | 1:l:245:LEU:HB3  | 1.98                     | 0.46              |
| 1:7:20:GLU:OE1   | 1:7:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:7:30:ARG:N     | 1:7:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:B:29:MET:HE2   | 1:B:29:MET:HB3   | 1.76                     | 0.46              |
| 1:C:122:PRO:HG2  | 1:C:125:LEU:CD2  | 2.46                     | 0.46              |
| 1:c:29:MET:HB2   | 1:c:32:TYR:HD2   | 1.80                     | 0.46              |
| 1:S:243:GLU:O    | 1:S:247:VAL:HG23 | 2.15                     | 0.46              |
| 1:q:243:GLU:O    | 1:q:247:VAL:HG23 | 2.15                     | 0.46              |
| 1:r:243:GLU:O    | 1:r:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:L:9:GLU:OE1    | 1:L:143:ARG:NE   | 2.49                     | 0.46              |
| 1:M:20:GLU:OE1   | 1:M:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:X:34:GLU:HG3   | 1:u:85:ARG:NH2   | 2.31                     | 0.46              |
| 1:N:20:GLU:OE1   | 1:N:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:Z:29:MET:HE3   | 1:Z:29:MET:HB2   | 1.85                     | 0.46              |
| 1:k:178:LYS:HB2  | 1:k:178:LYS:NZ   | 2.30                     | 0.46              |
| 1:v:133:ARG:HH21 | 1:v:136:GLU:CD   | 2.24                     | 0.46              |
| 1:a:9:GLU:OE1    | 1:a:143:ARG:NE   | 2.49                     | 0.46              |
| 1:a:133:ARG:HH21 | 1:a:136:GLU:CD   | 2.24                     | 0.46              |
| 1:l:122:PRO:HG2  | 1:l:125:LEU:CD2  | 2.46                     | 0.46              |
| 1:7:152:ILE:HG13 | 1:7:247:VAL:HG11 | 1.96                     | 0.46              |
| 1:x:134:LEU:HD11 | 1:x:159:LEU:HG   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:56:ARG:HD2   | 1:i:56:ARG:HG3   | 1.97                     | 0.46              |
| 1:y:243:GLU:O    | 1:y:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:U:202:LYS:O    | 1:U:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:q:29:MET:HE2   | 1:q:29:MET:HB3   | 1.76                     | 0.46              |
| 1:r:252:LEU:O    | 1:r:256:ILE:HG13 | 2.16                     | 0.46              |
| 1:i:149:ARG:NH2  | 1:i:243:GLU:OE2  | 2.48                     | 0.46              |
| 1:N:5:THR:OG1    | 1:N:143:ARG:NH2  | 2.48                     | 0.46              |
| 1:N:30:ARG:N     | 1:N:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:5:252:LEU:O    | 1:5:256:ILE:HG13 | 2.16                     | 0.46              |
| 1:O:252:LEU:O    | 1:O:256:ILE:HG13 | 2.16                     | 0.46              |
| 1:w:152:ILE:HG13 | 1:w:247:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:133:ARG:HH21 | 1:A:136:GLU:CD   | 2.23                     | 0.46              |
| 1:E:202:LYS:O    | 1:E:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:m:133:ARG:HH21 | 1:m:136:GLU:CD   | 2.24                     | 0.46              |
| 1:G:202:LYS:O    | 1:G:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:y:29:MET:HE3   | 1:y:29:MET:HB2   | 1.87                     | 0.46              |
| 1:0:71:GLU:O     | 1:0:75:ARG:HG3   | 2.16                     | 0.46              |
| 1:g:252:LEU:O    | 1:g:256:ILE:HG13 | 2.16                     | 0.46              |
| 1:2:30:ARG:N     | 1:2:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:h:243:GLU:O    | 1:h:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:t:9:GLU:OE1    | 1:t:143:ARG:NE   | 2.49                     | 0.46              |
| 1:N:202:LYS:O    | 1:N:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:u:252:LEU:O    | 1:u:256:ILE:HG13 | 2.16                     | 0.46              |
| 1:5:243:GLU:O    | 1:5:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:k:9:GLU:OE1    | 1:k:143:ARG:NE   | 2.49                     | 0.46              |
| 1:k:20:GLU:OE1   | 1:k:23:ARG:NH2   | 2.37                     | 0.46              |
| 1:k:71:GLU:O     | 1:k:75:ARG:HG3   | 2.16                     | 0.46              |
| 1:P:133:ARG:HH21 | 1:P:136:GLU:CD   | 2.24                     | 0.46              |
| 1:l:254:ARG:HE   | 1:l:254:ARG:HB2  | 1.60                     | 0.46              |
| 1:7:71:GLU:O     | 1:7:75:ARG:HG3   | 2.16                     | 0.46              |
| 1:F:95:GLU:OE1   | 1:F:95:GLU:N     | 2.44                     | 0.46              |
| 1:Q:243:GLU:O    | 1:Q:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:n:122:PRO:HG2  | 1:n:125:LEU:CD2  | 2.46                     | 0.46              |
| 1:z:133:ARG:HH21 | 1:z:136:GLU:CD   | 2.24                     | 0.46              |
| 1:p:76:LEU:O     | 1:p:80:VAL:HG12  | 2.15                     | 0.46              |
| 1:0:9:GLU:OE1    | 1:0:143:ARG:NE   | 2.49                     | 0.46              |
| 1:0:202:LYS:O    | 1:0:206:GLU:HG3  | 2.15                     | 0.46              |
| 1:J:76:LEU:O     | 1:J:80:VAL:HG12  | 2.16                     | 0.46              |
| 1:K:20:GLU:OE1   | 1:K:23:ARG:NH2   | 2.39                     | 0.46              |
| 1:g:234:ILE:HD11 | 1:g:245:LEU:HB3  | 1.97                     | 0.46              |
| 1:2:202:LYS:O    | 1:2:206:GLU:HG3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:243:GLU:O    | 1:W:247:VAL:HG23 | 2.16                     | 0.46              |
| 1:s:9:GLU:OE1    | 1:s:143:ARG:NE   | 2.49                     | 0.46              |
| 1:s:30:ARG:N     | 1:s:31:PRO:HD2   | 2.30                     | 0.46              |
| 1:s:71:GLU:O     | 1:s:75:ARG:HG3   | 2.16                     | 0.46              |
| 1:M:76:LEU:O     | 1:M:80:VAL:HG12  | 2.16                     | 0.46              |
| 1:t:66:ARG:HA    | 1:t:66:ARG:HD2   | 1.85                     | 0.46              |
| 1:Y:20:GLU:OE1   | 1:Y:23:ARG:NH2   | 2.39                     | 0.46              |
| 1:Z:77:LEU:HA    | 1:Z:80:VAL:HG12  | 1.98                     | 0.46              |
| 1:6:9:GLU:OE1    | 1:6:143:ARG:NE   | 2.49                     | 0.46              |
| 1:6:254:ARG:HE   | 1:6:254:ARG:HB2  | 1.58                     | 0.46              |
| 1:C:252:LEU:O    | 1:C:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:Q:20:GLU:OE1   | 1:Q:23:ARG:NH2   | 2.37                     | 0.45              |
| 1:Q:252:LEU:O    | 1:Q:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:y:252:LEU:O    | 1:y:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:H:9:GLU:OE1    | 1:H:143:ARG:NE   | 2.49                     | 0.45              |
| 1:S:95:GLU:OE1   | 1:S:95:GLU:N     | 2.44                     | 0.45              |
| 1:I:149:ARG:NH1  | 1:I:243:GLU:OE1  | 2.49                     | 0.45              |
| 1:q:20:GLU:OE1   | 1:q:23:ARG:NH2   | 2.38                     | 0.45              |
| 1:r:29:MET:HB3   | 1:r:32:TYR:HD2   | 1.80                     | 0.45              |
| 1:L:152:ILE:HG22 | 1:L:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:M:243:GLU:O    | 1:M:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:4:243:GLU:O    | 1:4:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:O:195:LEU:HD11 | 1:O:244:GLU:HB2  | 1.97                     | 0.45              |
| 1:a:254:ARG:HE   | 1:a:254:ARG:HB2  | 1.58                     | 0.45              |
| 1:B:9:GLU:OE1    | 1:B:143:ARG:NE   | 2.49                     | 0.45              |
| 1:F:85:ARG:NH2   | 1:s:34:GLU:HG3   | 2.31                     | 0.45              |
| 1:x:29:MET:HB2   | 1:x:32:TYR:HD2   | 1.80                     | 0.45              |
| 1:c:152:ILE:HG22 | 1:c:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:n:252:LEU:O    | 1:n:256:ILE:HG13 | 2.17                     | 0.45              |
| 1:H:29:MET:HB2   | 1:H:32:TYR:HD2   | 1.81                     | 0.45              |
| 1:H:34:GLU:HG3   | 1:X:85:ARG:NH2   | 2.32                     | 0.45              |
| 1:H:133:ARG:HH21 | 1:H:136:GLU:CD   | 2.24                     | 0.45              |
| 1:H:134:LEU:HD11 | 1:H:159:LEU:HG   | 1.97                     | 0.45              |
| 1:o:202:LYS:O    | 1:o:206:GLU:HG3  | 2.16                     | 0.45              |
| 1:T:234:ILE:HD11 | 1:T:245:LEU:HB3  | 1.97                     | 0.45              |
| 1:e:56:ARG:HD2   | 1:q:56:ARG:HG3   | 1.97                     | 0.45              |
| 1:U:178:LYS:HB2  | 1:U:178:LYS:NZ   | 2.31                     | 0.45              |
| 1:2:9:GLU:OE1    | 1:2:143:ARG:NE   | 2.49                     | 0.45              |
| 1:2:71:GLU:O     | 1:2:75:ARG:HG3   | 2.16                     | 0.45              |
| 1:O:122:PRO:HG2  | 1:O:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:Z:152:ILE:HG13 | 1:Z:247:VAL:HG11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:252:LEU:O    | 1:l:256:ILE:HG13 | 2.17                     | 0.45              |
| 1:w:252:LEU:O    | 1:w:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:7:9:GLU:OE1    | 1:7:143:ARG:NE   | 2.49                     | 0.45              |
| 1:7:178:LYS:HB2  | 1:7:178:LYS:NZ   | 2.30                     | 0.45              |
| 1:B:152:ILE:HG22 | 1:B:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:D:29:MET:HE3   | 1:D:29:MET:HB2   | 1.86                     | 0.45              |
| 1:F:234:ILE:HD11 | 1:F:245:LEU:HB3  | 1.97                     | 0.45              |
| 1:b:9:GLU:OE1    | 1:b:143:ARG:NE   | 2.49                     | 0.45              |
| 1:b:20:GLU:OE1   | 1:b:23:ARG:NH2   | 2.37                     | 0.45              |
| 1:b:243:GLU:O    | 1:b:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:d:252:LEU:O    | 1:d:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:I:20:GLU:OE1   | 1:I:23:ARG:NH2   | 2.39                     | 0.45              |
| 1:e:252:LEU:O    | 1:e:256:ILE:HG13 | 2.17                     | 0.45              |
| 1:q:9:GLU:OE1    | 1:q:143:ARG:NE   | 2.49                     | 0.45              |
| 1:2:34:GLU:HG3   | 1:O:85:ARG:NH2   | 2.31                     | 0.45              |
| 1:4:122:PRO:HG2  | 1:4:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:j:152:ILE:HG22 | 1:j:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:Z:252:LEU:O    | 1:Z:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:6:29:MET:HB2   | 1:6:32:TYR:HD2   | 1.80                     | 0.45              |
| 1:A:149:ARG:NH2  | 1:A:243:GLU:OE2  | 2.48                     | 0.45              |
| 1:F:122:PRO:HG2  | 1:F:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:Q:152:ILE:HG22 | 1:Q:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:c:9:GLU:OE1    | 1:c:143:ARG:NE   | 2.49                     | 0.45              |
| 1:n:9:GLU:OE1    | 1:n:143:ARG:NE   | 2.50                     | 0.45              |
| 1:d:20:GLU:OE1   | 1:d:23:ARG:NH2   | 2.37                     | 0.45              |
| 1:I:133:ARG:HH21 | 1:I:136:GLU:CD   | 2.24                     | 0.45              |
| 1:O:30:ARG:N     | 1:O:31:PRO:HD2   | 2.30                     | 0.45              |
| 1:f:9:GLU:OE1    | 1:f:143:ARG:NE   | 2.50                     | 0.45              |
| 1:g:122:PRO:HG2  | 1:g:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:s:202:LYS:O    | 1:s:206:GLU:HG3  | 2.16                     | 0.45              |
| 1:t:20:GLU:OE1   | 1:t:23:ARG:NH2   | 2.38                     | 0.45              |
| 1:N:178:LYS:HB2  | 1:N:178:LYS:NZ   | 2.30                     | 0.45              |
| 1:u:122:PRO:HG2  | 1:u:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:P:149:ARG:NH1  | 1:P:243:GLU:OE1  | 2.49                     | 0.45              |
| 1:B:95:GLU:O     | 1:B:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:C:9:GLU:OE1    | 1:C:143:ARG:NE   | 2.50                     | 0.45              |
| 1:D:152:ILE:HG13 | 1:D:247:VAL:HG11 | 1.98                     | 0.45              |
| 1:D:252:LEU:O    | 1:D:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:b:71:GLU:O     | 1:b:75:ARG:HG3   | 2.16                     | 0.45              |
| 1:b:202:LYS:O    | 1:b:206:GLU:HG3  | 2.16                     | 0.45              |
| 1:d:152:ILE:HG22 | 1:d:156:GLU:OE2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:9:GLU:OE1    | 1:o:143:ARG:NE   | 2.49                     | 0.45              |
| 1:o:243:GLU:O    | 1:o:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:p:252:LEU:O    | 1:p:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:J:152:ILE:HG22 | 1:J:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:K:133:ARG:HH21 | 1:K:136:GLU:CD   | 2.24                     | 0.45              |
| 1:V:152:ILE:HG22 | 1:V:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:r:7:VAL:O      | 1:r:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:X:95:GLU:O     | 1:X:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:i:9:GLU:OE1    | 1:i:143:ARG:NE   | 2.50                     | 0.45              |
| 1:5:7:VAL:O      | 1:5:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:w:243:GLU:O    | 1:w:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:29:MET:HB2   | 1:B:32:TYR:HD2   | 1.80                     | 0.45              |
| 1:C:234:ILE:HD11 | 1:C:245:LEU:HB3  | 1.97                     | 0.45              |
| 1:F:9:GLU:OE1    | 1:F:143:ARG:NE   | 2.50                     | 0.45              |
| 1:F:243:GLU:O    | 1:F:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:S:9:GLU:OE1    | 1:S:143:ARG:NE   | 2.50                     | 0.45              |
| 1:d:152:ILE:HG13 | 1:d:247:VAL:HG11 | 1.98                     | 0.45              |
| 1:I:95:GLU:O     | 1:I:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:e:243:GLU:O    | 1:e:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:J:252:LEU:O    | 1:J:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:U:243:GLU:O    | 1:U:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:q:152:ILE:HG22 | 1:q:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:1:243:GLU:O    | 1:1:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:K:95:GLU:O     | 1:K:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:K:149:ARG:NH2  | 1:K:243:GLU:OE2  | 2.48                     | 0.45              |
| 1:h:252:LEU:O    | 1:h:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:M:252:LEU:O    | 1:M:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:t:29:MET:HE2   | 1:t:29:MET:HB3   | 1.77                     | 0.45              |
| 1:t:152:ILE:HG22 | 1:t:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:4:85:ARG:NH2   | 1:7:34:GLU:HG3   | 2.31                     | 0.45              |
| 1:l:243:GLU:O    | 1:l:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:m:9:GLU:OE1    | 1:m:143:ARG:NE   | 2.50                     | 0.45              |
| 1:R:62:LEU:O     | 1:R:66:ARG:HG2   | 2.17                     | 0.45              |
| 1:c:95:GLU:O     | 1:c:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:o:71:GLU:O     | 1:o:75:ARG:HG3   | 2.17                     | 0.45              |
| 1:T:134:LEU:HD11 | 1:T:159:LEU:HG   | 1.97                     | 0.45              |
| 1:e:9:GLU:OE1    | 1:e:143:ARG:NE   | 2.50                     | 0.45              |
| 1:W:122:PRO:HG2  | 1:W:125:LEU:CD2  | 2.46                     | 0.45              |
| 1:W:252:LEU:O    | 1:W:256:ILE:HG13 | 2.17                     | 0.45              |
| 1:h:152:ILE:HG22 | 1:h:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:3:133:ARG:HH21 | 1:3:136:GLU:CD   | 2.24                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:234:ILE:HD13 | 1:3:245:LEU:HD23 | 1.99                     | 0.45              |
| 1:M:85:ARG:NH2   | 1:5:34:GLU:HG3   | 2.32                     | 0.45              |
| 1:i:7:VAL:O      | 1:i:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:N:9:GLU:OE1    | 1:N:143:ARG:NE   | 2.50                     | 0.45              |
| 1:Y:133:ARG:HH21 | 1:Y:136:GLU:CD   | 2.24                     | 0.45              |
| 1:G:34:GLU:HG3   | 1:W:85:ARG:NH2   | 2.31                     | 0.45              |
| 1:S:252:LEU:O    | 1:S:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:d:7:VAL:O      | 1:d:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:J:243:GLU:O    | 1:J:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:7:VAL:O      | 1:M:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:M:151:ILE:O    | 1:M:155:LEU:HG   | 2.17                     | 0.45              |
| 1:M:152:ILE:HG22 | 1:M:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:N:71:GLU:O     | 1:N:75:ARG:HG3   | 2.17                     | 0.45              |
| 1:Y:95:GLU:O     | 1:Y:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:k:243:GLU:O    | 1:k:247:VAL:HG23 | 2.16                     | 0.45              |
| 1:v:7:VAL:O      | 1:v:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:l:195:LEU:HD11 | 1:l:244:GLU:HB2  | 1.99                     | 0.45              |
| 1:D:151:ILE:O    | 1:D:155:LEU:HG   | 2.17                     | 0.45              |
| 1:E:83:GLU:O     | 1:E:87:LEU:HD12  | 2.17                     | 0.45              |
| 1:Q:152:ILE:HG13 | 1:Q:247:VAL:HG11 | 1.98                     | 0.45              |
| 1:n:243:GLU:O    | 1:n:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:y:152:ILE:HG13 | 1:y:247:VAL:HG11 | 1.98                     | 0.45              |
| 1:p:152:ILE:HG22 | 1:p:156:GLU:OE2  | 2.17                     | 0.45              |
| 1:J:5:THR:OG1    | 1:J:143:ARG:NH2  | 2.48                     | 0.45              |
| 1:f:7:VAL:O      | 1:f:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:f:250:LEU:HD22 | 1:q:218:GLU:HB3  | 1.99                     | 0.45              |
| 1:V:9:GLU:OE1    | 1:V:143:ARG:NE   | 2.49                     | 0.45              |
| 1:V:95:GLU:O     | 1:V:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:r:10:VAL:HG21  | 1:r:47:LEU:HD11  | 1.99                     | 0.45              |
| 1:L:134:LEU:HD11 | 1:L:159:LEU:HG   | 1.97                     | 0.45              |
| 1:3:95:GLU:O     | 1:3:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:3:149:ARG:NH1  | 1:3:243:GLU:OE1  | 2.50                     | 0.45              |
| 1:X:71:GLU:O     | 1:X:75:ARG:HG3   | 2.16                     | 0.45              |
| 1:X:243:GLU:O    | 1:X:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:Y:243:GLU:O    | 1:Y:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:j:9:GLU:OE1    | 1:j:143:ARG:NE   | 2.49                     | 0.45              |
| 1:O:243:GLU:O    | 1:O:247:VAL:HG23 | 2.17                     | 0.45              |
| 1:v:250:LEU:HD22 | 1:6:218:GLU:HB3  | 1.99                     | 0.45              |
| 1:P:7:VAL:O      | 1:P:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:E:9:GLU:OE1    | 1:E:143:ARG:NE   | 2.49                     | 0.45              |
| 1:E:34:GLU:HG3   | 1:e:85:ARG:NH2   | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:252:LEU:O    | 1:F:256:ILE:HG13 | 2.16                     | 0.45              |
| 1:R:7:VAL:O      | 1:R:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:H:95:GLU:O     | 1:H:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:z:9:GLU:OE1    | 1:z:143:ARG:NE   | 2.50                     | 0.45              |
| 1:U:9:GLU:OE1    | 1:U:143:ARG:NE   | 2.49                     | 0.45              |
| 1:V:29:MET:HE2   | 1:V:29:MET:HB3   | 1.76                     | 0.45              |
| 1:r:151:ILE:O    | 1:r:155:LEU:HG   | 2.17                     | 0.45              |
| 1:h:76:LEU:O     | 1:h:80:VAL:HG12  | 2.16                     | 0.45              |
| 1:h:151:ILE:O    | 1:h:155:LEU:HG   | 2.17                     | 0.45              |
| 1:i:250:LEU:HD22 | 1:t:218:GLU:HB3  | 1.99                     | 0.45              |
| 1:4:9:GLU:OE1    | 1:4:143:ARG:NE   | 2.50                     | 0.45              |
| 1:5:10:VAL:HG21  | 1:5:47:LEU:HD11  | 1.99                     | 0.45              |
| 1:v:95:GLU:O     | 1:v:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:6:152:ILE:HG22 | 1:6:156:GLU:OE2  | 2.16                     | 0.45              |
| 1:P:9:GLU:OE1    | 1:P:143:ARG:NE   | 2.50                     | 0.45              |
| 1:P:95:GLU:O     | 1:P:99:LEU:HD12  | 2.17                     | 0.45              |
| 1:P:250:LEU:HD22 | 1:a:218:GLU:HB3  | 1.99                     | 0.45              |
| 1:C:195:LEU:HD11 | 1:C:244:GLU:HB2  | 1.98                     | 0.44              |
| 1:Q:85:ARG:NH2   | 1:y:34:GLU:HG3   | 2.32                     | 0.44              |
| 1:x:95:GLU:O     | 1:x:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:n:156:GLU:CD   | 1:n:254:ARG:HH12 | 2.25                     | 0.44              |
| 1:T:152:ILE:HG22 | 1:T:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:e:234:ILE:HD11 | 1:e:245:LEU:HB3  | 1.98                     | 0.44              |
| 1:J:151:ILE:O    | 1:J:155:LEU:HG   | 2.17                     | 0.44              |
| 1:U:95:GLU:O     | 1:U:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:1:9:GLU:OE1    | 1:1:143:ARG:NE   | 2.50                     | 0.44              |
| 1:g:195:LEU:HD11 | 1:g:244:GLU:HB2  | 1.99                     | 0.44              |
| 1:2:95:GLU:O     | 1:2:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:u:243:GLU:O    | 1:u:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:Z:243:GLU:O    | 1:Z:247:VAL:HG23 | 2.16                     | 0.44              |
| 1:v:9:GLU:OE1    | 1:v:143:ARG:NE   | 2.50                     | 0.44              |
| 1:7:243:GLU:O    | 1:7:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:7:VAL:O      | 1:A:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:A:9:GLU:OE1    | 1:A:143:ARG:NE   | 2.50                     | 0.44              |
| 1:C:156:GLU:CD   | 1:C:254:ARG:HH12 | 2.25                     | 0.44              |
| 1:E:243:GLU:O    | 1:E:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:Q:34:GLU:HG3   | 1:h:85:ARG:NH2   | 2.32                     | 0.44              |
| 1:b:95:GLU:O     | 1:b:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:y:151:ILE:O    | 1:y:155:LEU:HG   | 2.17                     | 0.44              |
| 1:H:83:GLU:O     | 1:H:87:LEU:HD12  | 2.17                     | 0.44              |
| 1:o:178:LYS:HB2  | 1:o:178:LYS:NZ   | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:p:5:THR:OG1    | 1:p:143:ARG:NH2  | 2.49                     | 0.44              |
| 1:p:10:VAL:HG21  | 1:p:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:0:95:GLU:O     | 1:0:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:U:71:GLU:O     | 1:U:75:ARG:HG3   | 2.17                     | 0.44              |
| 1:K:250:LEU:HD22 | 1:V:218:GLU:HB3  | 1.99                     | 0.44              |
| 1:r:152:ILE:HG22 | 1:r:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:W:9:GLU:OE1    | 1:W:143:ARG:NE   | 2.50                     | 0.44              |
| 1:s:95:GLU:O     | 1:s:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:X:9:GLU:OE1    | 1:X:143:ARG:NE   | 2.49                     | 0.44              |
| 1:5:151:ILE:O    | 1:5:155:LEU:HG   | 2.17                     | 0.44              |
| 1:6:95:GLU:O     | 1:6:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:7:10:VAL:HG21  | 1:7:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:m:95:GLU:O     | 1:m:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:G:9:GLU:OE1    | 1:G:143:ARG:NE   | 2.50                     | 0.44              |
| 1:n:254:ARG:HE   | 1:n:254:ARG:HB2  | 1.60                     | 0.44              |
| 1:H:152:ILE:HG22 | 1:H:156:GLU:OE2  | 2.16                     | 0.44              |
| 1:d:10:VAL:HG21  | 1:d:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:o:95:GLU:O     | 1:o:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:z:7:VAL:O      | 1:z:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:p:151:ILE:O    | 1:p:155:LEU:HG   | 2.17                     | 0.44              |
| 1:2:178:LYS:HB2  | 1:2:178:LYS:NZ   | 2.31                     | 0.44              |
| 1:L:218:GLU:HB3  | 1:3:250:LEU:HD22 | 1.99                     | 0.44              |
| 1:3:20:GLU:OE1   | 1:3:23:ARG:NH2   | 2.39                     | 0.44              |
| 1:X:156:GLU:CD   | 1:X:254:ARG:HH12 | 2.24                     | 0.44              |
| 1:N:95:GLU:O     | 1:N:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:j:66:ARG:HA    | 1:j:66:ARG:HD2   | 1.86                     | 0.44              |
| 1:5:152:ILE:HG22 | 1:5:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:a:152:ILE:HG22 | 1:a:156:GLU:OE2  | 2.16                     | 0.44              |
| 1:w:151:ILE:O    | 1:w:155:LEU:HG   | 2.17                     | 0.44              |
| 1:m:7:VAL:O      | 1:m:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:x:83:GLU:O     | 1:x:87:LEU:HD12  | 2.17                     | 0.44              |
| 1:R:9:GLU:OE1    | 1:R:143:ARG:NE   | 2.50                     | 0.44              |
| 1:c:34:GLU:HG3   | 1:o:85:ARG:NH2   | 2.32                     | 0.44              |
| 1:H:218:GLU:HB3  | 1:z:250:LEU:HD22 | 1.99                     | 0.44              |
| 1:d:151:ILE:O    | 1:d:155:LEU:HG   | 2.17                     | 0.44              |
| 1:p:7:VAL:O      | 1:p:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:J:7:VAL:O      | 1:J:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:J:10:VAL:HG21  | 1:J:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:1:123:ILE:HG13 | 1:1:175:GLU:HG2  | 1.99                     | 0.44              |
| 1:g:9:GLU:OE1    | 1:g:143:ARG:NE   | 2.50                     | 0.44              |
| 1:g:254:ARG:HE   | 1:g:254:ARG:HB2  | 1.60                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:243:GLU:O    | 1:2:247:VAL:HG23 | 2.16                     | 0.44              |
| 1:Y:234:ILE:HD13 | 1:Y:245:LEU:HD23 | 1.99                     | 0.44              |
| 1:u:9:GLU:OE1    | 1:u:143:ARG:NE   | 2.50                     | 0.44              |
| 1:u:134:LEU:HD11 | 1:u:159:LEU:HG   | 2.00                     | 0.44              |
| 1:Z:151:ILE:O    | 1:Z:155:LEU:HG   | 2.17                     | 0.44              |
| 1:l:9:GLU:OE1    | 1:l:143:ARG:NE   | 2.50                     | 0.44              |
| 1:D:34:GLU:HG3   | 1:d:85:ARG:NH2   | 2.33                     | 0.44              |
| 1:E:71:GLU:O     | 1:E:75:ARG:HG3   | 2.16                     | 0.44              |
| 1:Q:151:ILE:O    | 1:Q:155:LEU:HG   | 2.17                     | 0.44              |
| 1:m:243:GLU:O    | 1:m:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:x:10:VAL:HG21  | 1:x:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:x:152:ILE:HG22 | 1:x:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:G:243:GLU:O    | 1:G:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:y:152:ILE:HG22 | 1:y:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:q:95:GLU:O     | 1:q:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:l:252:LEU:O    | 1:l:256:ILE:HG13 | 2.16                     | 0.44              |
| 1:K:29:MET:HB3   | 1:K:32:TYR:HD2   | 1.83                     | 0.44              |
| 1:V:66:ARG:HA    | 1:V:66:ARG:HD2   | 1.86                     | 0.44              |
| 1:V:243:GLU:O    | 1:V:247:VAL:HG23 | 2.18                     | 0.44              |
| 1:g:134:LEU:HD11 | 1:g:159:LEU:HG   | 2.00                     | 0.44              |
| 1:t:95:GLU:O     | 1:t:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:P:29:MET:HB3   | 1:P:32:TYR:HD2   | 1.83                     | 0.44              |
| 1:a:243:GLU:O    | 1:a:247:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:87:LEU:HD23  | 1:B:92:ARG:HD3   | 1.99                     | 0.44              |
| 1:D:152:ILE:HG22 | 1:D:156:GLU:OE2  | 2.17                     | 0.44              |
| 1:E:95:GLU:O     | 1:E:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:b:64:MET:HE2   | 1:n:85:ARG:NH1   | 2.33                     | 0.44              |
| 1:z:95:GLU:O     | 1:z:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:z:243:GLU:O    | 1:z:247:VAL:HG23 | 2.18                     | 0.44              |
| 1:J:85:ARG:NH2   | 1:r:34:GLU:HG3   | 2.32                     | 0.44              |
| 1:U:156:GLU:CD   | 1:U:254:ARG:HH12 | 2.24                     | 0.44              |
| 1:f:134:LEU:HD11 | 1:f:159:LEU:HG   | 2.00                     | 0.44              |
| 1:g:199:ALA:O    | 1:g:203:ARG:HG3  | 2.18                     | 0.44              |
| 1:M:5:THR:OG1    | 1:M:143:ARG:NH2  | 2.49                     | 0.44              |
| 1:M:34:GLU:HG3   | 1:w:85:ARG:NH2   | 2.33                     | 0.44              |
| 1:N:152:ILE:HG22 | 1:N:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:Y:250:LEU:HD22 | 1:j:218:GLU:HB3  | 1.99                     | 0.44              |
| 1:j:243:GLU:O    | 1:j:247:VAL:HG23 | 2.18                     | 0.44              |
| 1:u:39:LEU:HD11  | 1:u:61:VAL:HG11  | 2.00                     | 0.44              |
| 1:O:133:ARG:HH21 | 1:O:136:GLU:CD   | 2.26                     | 0.44              |
| 1:Z:20:GLU:OE1   | 1:Z:23:ARG:NH2   | 2.37                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:29:MET:HB3   | 1:v:32:TYR:HD2   | 1.83                     | 0.44              |
| 1:F:39:LEU:HD11  | 1:F:61:VAL:HG11  | 2.00                     | 0.44              |
| 1:m:152:ILE:HG22 | 1:m:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:x:15:GLU:OE1   | 1:x:37:ARG:HG2   | 2.17                     | 0.44              |
| 1:G:71:GLU:O     | 1:G:75:ARG:HG3   | 2.17                     | 0.44              |
| 1:R:149:ARG:NH1  | 1:R:243:GLU:OE1  | 2.50                     | 0.44              |
| 1:H:7:VAL:O      | 1:H:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:d:34:GLU:HG3   | 1:p:85:ARG:NH2   | 2.32                     | 0.44              |
| 1:z:152:ILE:HG22 | 1:z:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:1:199:ALA:O    | 1:1:203:ARG:HG3  | 2.18                     | 0.44              |
| 1:g:39:LEU:HD11  | 1:g:61:VAL:HG11  | 2.00                     | 0.44              |
| 1:L:195:LEU:HD21 | 1:L:244:GLU:OE1  | 2.17                     | 0.44              |
| 1:W:20:GLU:OE1   | 1:W:23:ARG:NH2   | 2.43                     | 0.44              |
| 1:s:156:GLU:CD   | 1:s:254:ARG:HH12 | 2.24                     | 0.44              |
| 1:4:133:ARG:HH21 | 1:4:136:GLU:CD   | 2.26                     | 0.44              |
| 1:4:252:LEU:O    | 1:4:256:ILE:HG13 | 2.17                     | 0.44              |
| 1:Y:152:ILE:HG22 | 1:Y:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:u:254:ARG:HE   | 1:u:254:ARG:HB2  | 1.60                     | 0.44              |
| 1:k:152:ILE:HG22 | 1:k:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:l:133:ARG:HH21 | 1:l:136:GLU:CD   | 2.26                     | 0.44              |
| 1:7:95:GLU:O     | 1:7:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:7:152:ILE:HG22 | 1:7:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:95:GLU:O     | 1:A:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:D:7:VAL:O      | 1:D:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:m:250:LEU:HD22 | 1:x:218:GLU:HB3  | 1.99                     | 0.44              |
| 1:y:7:VAL:O      | 1:y:11:ARG:HG3   | 2.17                     | 0.44              |
| 1:S:134:LEU:HD11 | 1:S:159:LEU:HG   | 2.00                     | 0.44              |
| 1:d:29:MET:HE3   | 1:d:29:MET:HB2   | 1.86                     | 0.44              |
| 1:o:156:GLU:CD   | 1:o:254:ARG:HH12 | 2.24                     | 0.44              |
| 1:I:9:GLU:OE1    | 1:I:143:ARG:NE   | 2.50                     | 0.44              |
| 1:I:250:LEU:HD22 | 1:T:218:GLU:HB3  | 1.99                     | 0.44              |
| 1:0:243:GLU:O    | 1:0:247:VAL:HG23 | 2.17                     | 0.44              |
| 1:J:34:GLU:HG3   | 1:Z:85:ARG:NH2   | 2.33                     | 0.44              |
| 1:f:252:LEU:O    | 1:f:256:ILE:HG13 | 2.18                     | 0.44              |
| 1:K:9:GLU:OE1    | 1:K:143:ARG:NE   | 2.50                     | 0.44              |
| 1:g:133:ARG:HH21 | 1:g:136:GLU:CD   | 2.26                     | 0.44              |
| 1:2:152:ILE:HG22 | 1:2:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:W:133:ARG:HH21 | 1:W:136:GLU:CD   | 2.26                     | 0.44              |
| 1:X:83:GLU:O     | 1:X:87:LEU:HD12  | 2.18                     | 0.44              |
| 1:i:62:LEU:O     | 1:i:66:ARG:HG2   | 2.18                     | 0.44              |
| 1:i:134:LEU:HD11 | 1:i:159:LEU:HG   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:7:VAL:O      | 1:4:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:Y:29:MET:HB3   | 1:Y:32:TYR:HD2   | 1.83                     | 0.44              |
| 1:j:31:PRO:O     | 1:j:35:MET:HG3   | 2.18                     | 0.44              |
| 1:5:85:ARG:NH2   | 1:w:34:GLU:HG3   | 2.32                     | 0.44              |
| 1:O:9:GLU:OE1    | 1:O:143:ARG:NE   | 2.50                     | 0.44              |
| 1:O:199:ALA:O    | 1:O:203:ARG:HG3  | 2.18                     | 0.44              |
| 1:6:7:VAL:O      | 1:6:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:P:252:LEU:O    | 1:P:256:ILE:HG13 | 2.17                     | 0.44              |
| 1:a:7:VAL:O      | 1:a:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:C:7:VAL:O      | 1:C:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:D:10:VAL:HG21  | 1:D:47:LEU:HD11  | 1.99                     | 0.44              |
| 1:F:133:ARG:HH21 | 1:F:136:GLU:CD   | 2.26                     | 0.44              |
| 1:b:156:GLU:CD   | 1:b:254:ARG:HH12 | 2.24                     | 0.44              |
| 1:G:152:ILE:HG22 | 1:G:156:GLU:OE2  | 2.18                     | 0.44              |
| 1:n:7:VAL:O      | 1:n:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:n:133:ARG:HH21 | 1:n:136:GLU:CD   | 2.26                     | 0.44              |
| 1:y:85:ARG:NH2   | 1:h:34:GLU:HG3   | 2.32                     | 0.44              |
| 1:S:199:ALA:O    | 1:S:203:ARG:HG3  | 2.18                     | 0.44              |
| 1:z:134:LEU:HD11 | 1:z:159:LEU:HG   | 2.00                     | 0.44              |
| 1:T:243:GLU:O    | 1:T:247:VAL:HG23 | 2.18                     | 0.44              |
| 1:f:29:MET:HB3   | 1:f:32:TYR:HD2   | 1.83                     | 0.44              |
| 1:q:10:VAL:HG21  | 1:q:47:LEU:HD11  | 2.00                     | 0.44              |
| 1:l:7:VAL:O      | 1:l:11:ARG:HG3   | 2.18                     | 0.44              |
| 1:3:9:GLU:OE1    | 1:3:143:ARG:NE   | 2.50                     | 0.44              |
| 1:Y:34:GLU:HG3   | 1:v:85:ARG:NH2   | 2.33                     | 0.44              |
| 1:j:95:GLU:O     | 1:j:99:LEU:HD12  | 2.17                     | 0.44              |
| 1:u:133:ARG:HH21 | 1:u:136:GLU:CD   | 2.26                     | 0.44              |
| 1:k:95:GLU:O     | 1:k:99:LEU:HD12  | 2.18                     | 0.44              |
| 1:v:252:LEU:O    | 1:v:256:ILE:HG13 | 2.18                     | 0.44              |
| 1:P:16:GLU:O     | 1:P:20:GLU:HG2   | 2.18                     | 0.44              |
| 1:l:199:ALA:O    | 1:l:203:ARG:HG3  | 2.18                     | 0.44              |
| 1:B:20:GLU:OE1   | 1:B:23:ARG:NH2   | 2.38                     | 0.43              |
| 1:C:62:LEU:HD11  | 1:C:66:ARG:HH11  | 1.83                     | 0.43              |
| 1:F:199:ALA:O    | 1:F:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:F:254:ARG:HE   | 1:F:254:ARG:HB2  | 1.60                     | 0.43              |
| 1:n:195:LEU:HD11 | 1:n:244:GLU:HB2  | 1.99                     | 0.43              |
| 1:S:39:LEU:HD11  | 1:S:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:L:35:MET:HG2   | 1:L:61:VAL:HG13  | 2.00                     | 0.43              |
| 1:i:29:MET:HB3   | 1:i:32:TYR:HD2   | 1.83                     | 0.43              |
| 1:i:252:LEU:O    | 1:i:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:N:243:GLU:O    | 1:N:247:VAL:HG23 | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:20:GLU:OE1   | 1:O:23:ARG:NH2   | 2.43                     | 0.43              |
| 1:Z:152:ILE:HG22 | 1:Z:156:GLU:OE2  | 2.17                     | 0.43              |
| 1:w:152:ILE:HG22 | 1:w:156:GLU:OE2  | 2.17                     | 0.43              |
| 1:C:133:ARG:HH21 | 1:C:136:GLU:CD   | 2.26                     | 0.43              |
| 1:C:199:ALA:O    | 1:C:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:E:152:ILE:HG22 | 1:E:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:m:134:LEU:HD11 | 1:m:159:LEU:HG   | 2.00                     | 0.43              |
| 1:c:7:VAL:O      | 1:c:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:c:20:GLU:OE1   | 1:c:23:ARG:NH2   | 2.37                     | 0.43              |
| 1:y:10:VAL:HG21  | 1:y:47:LEU:HD11  | 1.99                     | 0.43              |
| 1:H:85:ARG:NH2   | 1:u:34:GLU:HG3   | 2.34                     | 0.43              |
| 1:S:254:ARG:HE   | 1:S:254:ARG:HB2  | 1.60                     | 0.43              |
| 1:o:252:LEU:O    | 1:o:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:z:138:ALA:HB2  | 1:z:155:LEU:HD11 | 2.00                     | 0.43              |
| 1:I:234:ILE:HD13 | 1:I:245:LEU:HD23 | 2.01                     | 0.43              |
| 1:e:134:LEU:HD11 | 1:e:159:LEU:HG   | 2.00                     | 0.43              |
| 1:0:156:GLU:CD   | 1:0:254:ARG:HH12 | 2.24                     | 0.43              |
| 1:q:7:VAL:O      | 1:q:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:s:243:GLU:O    | 1:s:247:VAL:HG23 | 2.17                     | 0.43              |
| 1:t:7:VAL:O      | 1:t:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:4:199:ALA:O    | 1:4:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:Y:7:VAL:O      | 1:Y:11:ARG:HG3   | 2.17                     | 0.43              |
| 1:Y:9:GLU:OE1    | 1:Y:143:ARG:NE   | 2.50                     | 0.43              |
| 1:k:252:LEU:O    | 1:k:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:6:243:GLU:O    | 1:6:247:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:7:VAL:O      | 1:B:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:C:39:LEU:HD11  | 1:C:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:F:7:VAL:O      | 1:F:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:m:16:GLU:O     | 1:m:20:GLU:HG2   | 2.18                     | 0.43              |
| 1:m:160:ARG:O    | 1:m:164:GLU:HG3  | 2.19                     | 0.43              |
| 1:R:138:ALA:HB2  | 1:R:155:LEU:HD11 | 2.00                     | 0.43              |
| 1:S:7:VAL:O      | 1:S:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:S:133:ARG:HH21 | 1:S:136:GLU:CD   | 2.26                     | 0.43              |
| 1:z:160:ARG:O    | 1:z:164:GLU:HG3  | 2.19                     | 0.43              |
| 1:I:123:ILE:HG13 | 1:I:175:GLU:HG2  | 2.00                     | 0.43              |
| 1:e:20:GLU:OE1   | 1:e:23:ARG:NH2   | 2.43                     | 0.43              |
| 1:0:10:VAL:HG21  | 1:0:47:LEU:HD11  | 1.99                     | 0.43              |
| 1:1:85:ARG:NH1   | 1:k:64:MET:HE2   | 2.34                     | 0.43              |
| 1:1:133:ARG:HH21 | 1:1:136:GLU:CD   | 2.26                     | 0.43              |
| 1:L:243:GLU:O    | 1:L:247:VAL:HG23 | 2.18                     | 0.43              |
| 1:3:7:VAL:O      | 1:3:11:ARG:HG3   | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:16:GLU:O     | 1:i:20:GLU:HG2   | 2.18                     | 0.43              |
| 1:4:39:LEU:HD11  | 1:4:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:u:199:ALA:O    | 1:u:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:7:156:GLU:CD   | 1:7:254:ARG:HH12 | 2.24                     | 0.43              |
| 1:7:252:LEU:O    | 1:7:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:b:252:LEU:O    | 1:b:256:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:252:LEU:O    | 1:G:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:R:199:ALA:O    | 1:R:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:c:31:PRO:O     | 1:c:35:MET:HG3   | 2.18                     | 0.43              |
| 1:n:39:LEU:HD11  | 1:n:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:y:199:ALA:O    | 1:y:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:H:31:PRO:O     | 1:H:35:MET:HG3   | 2.18                     | 0.43              |
| 1:S:152:ILE:HG22 | 1:S:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:z:16:GLU:O     | 1:z:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:I:7:VAL:O      | 1:I:11:ARG:HG3   | 2.17                     | 0.43              |
| 1:I:29:MET:HB3   | 1:I:32:TYR:HD2   | 1.83                     | 0.43              |
| 1:e:133:ARG:HH21 | 1:e:136:GLU:CD   | 2.26                     | 0.43              |
| 1:f:123:ILE:HG13 | 1:f:175:GLU:HG2  | 2.01                     | 0.43              |
| 1:f:160:ARG:O    | 1:f:164:GLU:HG3  | 2.18                     | 0.43              |
| 1:K:7:VAL:O      | 1:K:11:ARG:HG3   | 2.17                     | 0.43              |
| 1:r:199:ALA:O    | 1:r:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:W:7:VAL:O      | 1:W:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:i:160:ARG:O    | 1:i:164:GLU:HG3  | 2.18                     | 0.43              |
| 1:4:254:ARG:HE   | 1:4:254:ARG:HB2  | 1.56                     | 0.43              |
| 1:Z:199:ALA:O    | 1:Z:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:v:16:GLU:O     | 1:v:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:v:152:ILE:HG22 | 1:v:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:C:34:GLU:HG3   | 1:c:85:ARG:NH2   | 2.34                     | 0.43              |
| 1:F:134:LEU:HD11 | 1:F:159:LEU:HG   | 2.00                     | 0.43              |
| 1:Q:29:MET:HE3   | 1:Q:29:MET:HB2   | 1.86                     | 0.43              |
| 1:Q:199:ALA:O    | 1:Q:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:m:138:ALA:HB2  | 1:m:155:LEU:HD11 | 2.01                     | 0.43              |
| 1:R:95:GLU:O     | 1:R:99:LEU:HD12  | 2.17                     | 0.43              |
| 1:R:250:LEU:HD22 | 1:c:218:GLU:HB3  | 1.99                     | 0.43              |
| 1:n:62:LEU:HD11  | 1:n:66:ARG:HH11  | 1.84                     | 0.43              |
| 1:n:152:ILE:HG22 | 1:n:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:T:95:GLU:O     | 1:T:99:LEU:HD12  | 2.18                     | 0.43              |
| 1:e:7:VAL:O      | 1:e:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:e:10:VAL:HG21  | 1:e:47:LEU:HD11  | 2.01                     | 0.43              |
| 1:J:66:ARG:HA    | 1:J:66:ARG:HD2   | 1.88                     | 0.43              |
| 1:f:234:ILE:HD13 | 1:f:245:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:39:LEU:HD11  | 1:1:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:K:152:ILE:HG22 | 1:K:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:L:95:GLU:O     | 1:L:99:LEU:HD12  | 2.18                     | 0.43              |
| 1:s:252:LEU:O    | 1:s:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:3:29:MET:HB3   | 1:3:32:TYR:HD2   | 1.83                     | 0.43              |
| 1:t:243:GLU:O    | 1:t:247:VAL:HG23 | 2.18                     | 0.43              |
| 1:j:7:VAL:O      | 1:j:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:u:152:ILE:HG22 | 1:u:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:k:156:GLU:CD   | 1:k:254:ARG:HH12 | 2.24                     | 0.43              |
| 1:v:160:ARG:O    | 1:v:164:GLU:HG3  | 2.19                     | 0.43              |
| 1:6:15:GLU:OE1   | 1:6:37:ARG:HG2   | 2.17                     | 0.43              |
| 1:P:123:ILE:HG13 | 1:P:175:GLU:HG2  | 2.00                     | 0.43              |
| 1:P:134:LEU:HD11 | 1:P:159:LEU:HG   | 2.00                     | 0.43              |
| 1:P:160:ARG:O    | 1:P:164:GLU:HG3  | 2.19                     | 0.43              |
| 1:w:199:ALA:O    | 1:w:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:A:29:MET:HB3   | 1:A:32:TYR:HD2   | 1.83                     | 0.43              |
| 1:A:160:ARG:O    | 1:A:164:GLU:HG3  | 2.18                     | 0.43              |
| 1:B:85:ARG:NH2   | 1:n:34:GLU:HG3   | 2.34                     | 0.43              |
| 1:E:252:LEU:O    | 1:E:256:ILE:HG13 | 2.19                     | 0.43              |
| 1:m:85:ARG:NH2   | 1:f:34:GLU:HG3   | 2.33                     | 0.43              |
| 1:H:152:ILE:HG13 | 1:H:247:VAL:HG11 | 2.01                     | 0.43              |
| 1:S:123:ILE:HG13 | 1:S:175:GLU:HG2  | 2.00                     | 0.43              |
| 1:I:16:GLU:O     | 1:I:20:GLU:HG2   | 2.18                     | 0.43              |
| 1:0:85:ARG:NH2   | 1:j:34:GLU:HG3   | 2.33                     | 0.43              |
| 1:0:252:LEU:O    | 1:0:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:V:151:ILE:O    | 1:V:155:LEU:HG   | 2.19                     | 0.43              |
| 1:g:152:ILE:HG22 | 1:g:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:L:7:VAL:O      | 1:L:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:s:152:ILE:HG22 | 1:s:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:3:134:LEU:HD11 | 1:3:159:LEU:HG   | 1.99                     | 0.43              |
| 1:M:66:ARG:HA    | 1:M:66:ARG:HD2   | 1.87                     | 0.43              |
| 1:X:16:GLU:O     | 1:X:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:i:123:ILE:HG13 | 1:i:175:GLU:HG2  | 2.01                     | 0.43              |
| 1:Y:138:ALA:HB2  | 1:Y:155:LEU:HD11 | 2.01                     | 0.43              |
| 1:j:151:ILE:O    | 1:j:155:LEU:HG   | 2.19                     | 0.43              |
| 1:5:199:ALA:O    | 1:5:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:6:152:ILE:HG13 | 1:6:247:VAL:HG11 | 2.01                     | 0.43              |
| 1:l:39:LEU:HD11  | 1:l:61:VAL:HG11  | 2.00                     | 0.43              |
| 1:7:16:GLU:O     | 1:7:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:A:199:ALA:O    | 1:A:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:E:16:GLU:O     | 1:E:20:GLU:HG2   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:34:GLU:HG3   | 1:V:85:ARG:NH2   | 2.34                     | 0.43              |
| 1:m:29:MET:HB3   | 1:m:32:TYR:HD2   | 1.83                     | 0.43              |
| 1:m:123:ILE:HG13 | 1:m:175:GLU:HG2  | 2.01                     | 0.43              |
| 1:n:199:ALA:O    | 1:n:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:I:34:GLU:HG3   | 1:Y:85:ARG:NH2   | 2.34                     | 0.43              |
| 1:I:252:LEU:O    | 1:I:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:e:122:PRO:HG2  | 1:e:125:LEU:CD2  | 2.49                     | 0.43              |
| 1:U:64:MET:HE2   | 1:g:85:ARG:NH1   | 2.33                     | 0.43              |
| 1:U:152:ILE:HG22 | 1:U:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:f:16:GLU:O     | 1:f:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:1:134:LEU:HD11 | 1:1:159:LEU:HG   | 2.00                     | 0.43              |
| 1:K:85:ARG:NH2   | 1:3:34:GLU:HG3   | 2.34                     | 0.43              |
| 1:2:16:GLU:O     | 1:2:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:W:10:VAL:HG21  | 1:W:47:LEU:HD11  | 2.01                     | 0.43              |
| 1:3:16:GLU:O     | 1:3:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:3:252:LEU:O    | 1:3:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:N:199:ALA:O    | 1:N:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:5:254:ARG:HE   | 1:5:254:ARG:HB2  | 1.57                     | 0.43              |
| 1:O:34:GLU:HG3   | 1:a:85:ARG:NH2   | 2.33                     | 0.43              |
| 1:O:152:ILE:HG22 | 1:O:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:v:134:LEU:HD11 | 1:v:159:LEU:HG   | 2.00                     | 0.43              |
| 1:l:152:ILE:HG22 | 1:l:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:A:250:LEU:HD22 | 1:B:218:GLU:HB3  | 1.99                     | 0.43              |
| 1:b:152:ILE:HG22 | 1:b:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:d:199:ALA:O    | 1:d:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:o:152:ILE:HG22 | 1:o:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:z:123:ILE:HG13 | 1:z:175:GLU:HG2  | 2.01                     | 0.43              |
| 1:T:7:VAL:O      | 1:T:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:T:35:MET:HG2   | 1:T:61:VAL:HG13  | 2.01                     | 0.43              |
| 1:f:95:GLU:O     | 1:f:99:LEU:HD12  | 2.17                     | 0.43              |
| 1:f:152:ILE:HG22 | 1:f:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:q:87:LEU:HD23  | 1:q:92:ARG:HD3   | 2.00                     | 0.43              |
| 1:1:156:GLU:CD   | 1:1:254:ARG:HH12 | 2.25                     | 0.43              |
| 1:K:138:ALA:HB2  | 1:K:155:LEU:HD11 | 2.01                     | 0.43              |
| 1:V:7:VAL:O      | 1:V:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:L:152:ILE:HG13 | 1:L:247:VAL:HG11 | 2.01                     | 0.43              |
| 1:W:156:GLU:OE1  | 1:W:254:ARG:NH1  | 2.50                     | 0.43              |
| 1:i:15:GLU:OE2   | 1:i:37:ARG:HG2   | 2.19                     | 0.43              |
| 1:i:152:ILE:HG22 | 1:i:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:4:191:LEU:HD22 | 1:4:244:GLU:HG2  | 2.01                     | 0.43              |
| 1:Y:134:LEU:HD11 | 1:Y:159:LEU:HG   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:252:LEU:O    | 1:Y:256:ILE:HG13 | 2.18                     | 0.43              |
| 1:O:7:VAL:O      | 1:O:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:a:95:GLU:O     | 1:a:99:LEU:HD12  | 2.18                     | 0.43              |
| 1:l:20:GLU:OE1   | 1:l:23:ARG:NH2   | 2.43                     | 0.43              |
| 1:C:20:GLU:OE1   | 1:C:23:ARG:NH2   | 2.43                     | 0.43              |
| 1:C:152:ILE:HG22 | 1:C:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:x:243:GLU:O    | 1:x:247:VAL:HG23 | 2.18                     | 0.43              |
| 1:G:95:GLU:O     | 1:G:99:LEU:HD12  | 2.18                     | 0.43              |
| 1:R:160:ARG:O    | 1:R:164:GLU:HG3  | 2.19                     | 0.43              |
| 1:c:10:VAL:HG21  | 1:c:47:LEU:HD11  | 1.99                     | 0.43              |
| 1:n:134:LEU:HD11 | 1:n:159:LEU:HG   | 2.00                     | 0.43              |
| 1:I:152:ILE:HG22 | 1:I:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:0:16:GLU:O     | 1:0:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:U:16:GLU:O     | 1:U:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:q:151:ILE:O    | 1:q:155:LEU:HG   | 2.19                     | 0.43              |
| 1:1:152:ILE:HG22 | 1:1:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:3:152:ILE:HG22 | 1:3:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:X:152:ILE:HG22 | 1:X:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:X:199:ALA:O    | 1:X:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:i:199:ALA:O    | 1:i:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:t:151:ILE:O    | 1:t:155:LEU:HG   | 2.19                     | 0.43              |
| 1:k:16:GLU:O     | 1:k:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:P:152:ILE:HG22 | 1:P:156:GLU:OE2  | 2.19                     | 0.43              |
| 1:P:199:ALA:O    | 1:P:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:l:7:VAL:O      | 1:l:11:ARG:HG3   | 2.18                     | 0.43              |
| 1:7:83:GLU:O     | 1:7:87:LEU:HD12  | 2.18                     | 0.43              |
| 1:7:199:ALA:O    | 1:7:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:A:138:ALA:HB2  | 1:A:155:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:134:LEU:HD11 | 1:C:159:LEU:HG   | 2.00                     | 0.43              |
| 1:E:85:ARG:NH2   | 1:q:34:GLU:HG3   | 2.34                     | 0.43              |
| 1:m:199:ALA:O    | 1:m:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:x:35:MET:HG2   | 1:x:61:VAL:HG13  | 2.01                     | 0.43              |
| 1:G:16:GLU:O     | 1:G:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:R:85:ARG:NH2   | 1:z:34:GLU:HG3   | 2.33                     | 0.43              |
| 1:R:134:LEU:HD11 | 1:R:159:LEU:HG   | 2.00                     | 0.43              |
| 1:R:252:LEU:O    | 1:R:256:ILE:HG13 | 2.17                     | 0.43              |
| 1:S:246:ARG:NH2  | 1:d:206:GLU:OE1  | 2.50                     | 0.43              |
| 1:z:85:ARG:NH2   | 1:i:34:GLU:HG3   | 2.33                     | 0.43              |
| 1:I:77:LEU:HA    | 1:I:80:VAL:HG12  | 2.01                     | 0.43              |
| 1:I:134:LEU:HD11 | 1:I:159:LEU:HG   | 2.00                     | 0.43              |
| 1:I:254:ARG:HE   | 1:I:254:ARG:HB2  | 1.56                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:20:GLU:OE1   | 1:l:23:ARG:NH2   | 2.42                     | 0.43              |
| 1:r:254:ARG:HE   | 1:r:254:ARG:HB2  | 1.57                     | 0.43              |
| 1:W:199:ALA:O    | 1:W:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:i:95:GLU:O     | 1:i:99:LEU:HD12  | 2.18                     | 0.43              |
| 1:N:16:GLU:O     | 1:N:20:GLU:HG2   | 2.19                     | 0.43              |
| 1:k:199:ALA:O    | 1:k:203:ARG:HG3  | 2.19                     | 0.43              |
| 1:a:151:ILE:O    | 1:a:155:LEU:HG   | 2.19                     | 0.43              |
| 1:a:152:ILE:HG13 | 1:a:247:VAL:HG11 | 2.01                     | 0.43              |
| 1:A:123:ILE:HG13 | 1:A:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:D:199:ALA:O    | 1:D:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:b:123:ILE:HG13 | 1:b:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:x:85:ARG:NH2   | 1:g:34:GLU:HG3   | 2.34                     | 0.42              |
| 1:R:123:ILE:HG13 | 1:R:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:z:29:MET:HB3   | 1:z:32:TYR:HD2   | 1.83                     | 0.42              |
| 1:I:138:ALA:HB2  | 1:I:155:LEU:HD11 | 2.01                     | 0.42              |
| 1:e:152:ILE:HG22 | 1:e:156:GLU:OE2  | 2.19                     | 0.42              |
| 1:e:199:ALA:O    | 1:e:203:ARG:HG3  | 2.18                     | 0.42              |
| 1:p:199:ALA:O    | 1:p:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:K:252:LEU:O    | 1:K:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:W:95:GLU:O     | 1:W:99:LEU:HD12  | 2.19                     | 0.42              |
| 1:3:85:ARG:NH2   | 1:P:34:GLU:HG3   | 2.34                     | 0.42              |
| 1:3:138:ALA:HB2  | 1:3:155:LEU:HD11 | 2.01                     | 0.42              |
| 1:v:138:ALA:HB2  | 1:v:155:LEU:HD11 | 2.01                     | 0.42              |
| 1:v:199:ALA:O    | 1:v:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:P:138:ALA:HB2  | 1:P:155:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:16:GLU:O     | 1:A:20:GLU:HG2   | 2.18                     | 0.42              |
| 1:A:152:ILE:HG22 | 1:A:156:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:151:ILE:O    | 1:B:155:LEU:HG   | 2.19                     | 0.42              |
| 1:D:85:ARG:NH2   | 1:p:34:GLU:HG3   | 2.33                     | 0.42              |
| 1:R:16:GLU:O     | 1:R:20:GLU:HG2   | 2.18                     | 0.42              |
| 1:R:29:MET:HB3   | 1:R:32:TYR:HD2   | 1.83                     | 0.42              |
| 1:c:151:ILE:O    | 1:c:155:LEU:HG   | 2.19                     | 0.42              |
| 1:z:199:ALA:O    | 1:z:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:T:85:ARG:NH2   | 1:l:34:GLU:HG3   | 2.34                     | 0.42              |
| 1:e:156:GLU:CD   | 1:e:254:ARG:HH12 | 2.25                     | 0.42              |
| 1:0:152:ILE:HG22 | 1:0:156:GLU:OE2  | 2.18                     | 0.42              |
| 1:J:199:ALA:O    | 1:J:203:ARG:HG3  | 2.18                     | 0.42              |
| 1:s:16:GLU:O     | 1:s:20:GLU:HG2   | 2.19                     | 0.42              |
| 1:3:123:ILE:HG13 | 1:3:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:3:254:ARG:HE   | 1:3:254:ARG:HB2  | 1.56                     | 0.42              |
| 1:N:123:ILE:HG13 | 1:N:175:GLU:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:35:MET:HE1   | 1:j:65:ALA:HB2   | 2.01                     | 0.42              |
| 1:u:7:VAL:O      | 1:u:11:ARG:HG3   | 2.18                     | 0.42              |
| 1:O:39:LEU:HD11  | 1:O:61:VAL:HG11  | 2.00                     | 0.42              |
| 1:P:15:GLU:OE2   | 1:P:37:ARG:HG2   | 2.19                     | 0.42              |
| 1:P:151:ILE:O    | 1:P:155:LEU:HG   | 2.20                     | 0.42              |
| 1:l:134:LEU:HD11 | 1:l:159:LEU:HG   | 2.00                     | 0.42              |
| 1:C:76:LEU:HD22  | 1:C:161:VAL:HG21 | 2.02                     | 0.42              |
| 1:F:156:GLU:CD   | 1:F:254:ARG:HH12 | 2.25                     | 0.42              |
| 1:R:152:ILE:HG22 | 1:R:156:GLU:OE2  | 2.19                     | 0.42              |
| 1:n:20:GLU:OE1   | 1:n:23:ARG:NH2   | 2.43                     | 0.42              |
| 1:S:156:GLU:CD   | 1:S:254:ARG:HH12 | 2.25                     | 0.42              |
| 1:o:123:ILE:HG13 | 1:o:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:z:252:LEU:O    | 1:z:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:I:243:GLU:O    | 1:I:247:VAL:HG23 | 2.19                     | 0.42              |
| 1:U:252:LEU:O    | 1:U:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:q:110:VAL:HG23 | 1:q:165:ALA:HB1  | 2.02                     | 0.42              |
| 1:V:87:LEU:HD23  | 1:V:92:ARG:HD3   | 2.01                     | 0.42              |
| 1:g:123:ILE:HG13 | 1:g:175:GLU:HG2  | 2.02                     | 0.42              |
| 1:2:123:ILE:HG13 | 1:2:175:GLU:HG2  | 2.02                     | 0.42              |
| 1:2:252:LEU:O    | 1:2:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:4:134:LEU:HD11 | 1:4:159:LEU:HG   | 2.00                     | 0.42              |
| 1:N:252:LEU:O    | 1:N:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:Y:199:ALA:O    | 1:Y:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:u:95:GLU:O     | 1:u:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:v:123:ILE:HG13 | 1:v:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:6:35:MET:HG2   | 1:6:61:VAL:HG13  | 2.01                     | 0.42              |
| 1:6:151:ILE:O    | 1:6:155:LEU:HG   | 2.19                     | 0.42              |
| 1:A:134:LEU:HD11 | 1:A:159:LEU:HG   | 2.00                     | 0.42              |
| 1:m:234:ILE:HD13 | 1:m:245:LEU:HD23 | 2.01                     | 0.42              |
| 1:G:85:ARG:NH2   | 1:t:34:GLU:HG3   | 2.34                     | 0.42              |
| 1:c:87:LEU:HD23  | 1:c:92:ARG:HD3   | 2.00                     | 0.42              |
| 1:H:254:ARG:HE   | 1:H:254:ARG:HB2  | 1.58                     | 0.42              |
| 1:I:85:ARG:NH2   | 1:v:34:GLU:HG3   | 2.35                     | 0.42              |
| 1:I:149:ARG:NH2  | 1:I:243:GLU:OE1  | 2.53                     | 0.42              |
| 1:I:199:ALA:O    | 1:I:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:T:152:ILE:HG13 | 1:T:247:VAL:HG11 | 2.01                     | 0.42              |
| 1:e:95:GLU:O     | 1:e:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:U:123:ILE:HG13 | 1:U:175:GLU:HG2  | 2.02                     | 0.42              |
| 1:1:95:GLU:O     | 1:1:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:K:134:LEU:HD11 | 1:K:159:LEU:HG   | 2.00                     | 0.42              |
| 1:K:199:ALA:O    | 1:K:203:ARG:HG3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:95:GLU:O     | 1:g:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:L:85:ARG:NH2   | 1:4:34:GLU:HG3   | 2.35                     | 0.42              |
| 1:W:134:LEU:HD11 | 1:W:159:LEU:HG   | 2.01                     | 0.42              |
| 1:X:252:LEU:O    | 1:X:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:N:66:ARG:HA    | 1:N:66:ARG:HD2   | 1.86                     | 0.42              |
| 1:O:134:LEU:HD11 | 1:O:159:LEU:HG   | 2.00                     | 0.42              |
| 1:6:10:VAL:HG21  | 1:6:47:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:252:LEU:O    | 1:A:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:m:252:LEU:O    | 1:m:256:ILE:HG13 | 2.18                     | 0.42              |
| 1:x:151:ILE:O    | 1:x:155:LEU:HG   | 2.19                     | 0.42              |
| 1:R:34:GLU:HG3   | 1:i:85:ARG:NH2   | 2.34                     | 0.42              |
| 1:R:151:ILE:O    | 1:R:155:LEU:HG   | 2.20                     | 0.42              |
| 1:n:76:LEU:HD22  | 1:n:161:VAL:HG21 | 2.02                     | 0.42              |
| 1:S:62:LEU:HD11  | 1:S:66:ARG:HH11  | 1.84                     | 0.42              |
| 1:f:199:ALA:O    | 1:f:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:K:34:GLU:HG3   | 1:P:85:ARG:NH2   | 2.34                     | 0.42              |
| 1:K:123:ILE:HG13 | 1:K:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:g:7:VAL:O      | 1:g:11:ARG:HG3   | 2.18                     | 0.42              |
| 1:r:85:ARG:NH2   | 1:Z:34:GLU:HG3   | 2.33                     | 0.42              |
| 1:W:191:LEU:HD22 | 1:W:244:GLU:HG2  | 2.01                     | 0.42              |
| 1:4:95:GLU:O     | 1:4:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:u:123:ILE:HG13 | 1:u:175:GLU:HG2  | 2.02                     | 0.42              |
| 1:v:243:GLU:O    | 1:v:247:VAL:HG23 | 2.18                     | 0.42              |
| 1:6:85:ARG:NH2   | 1:l:34:GLU:HG3   | 2.34                     | 0.42              |
| 1:G:66:ARG:HA    | 1:G:66:ARG:HD2   | 1.86                     | 0.42              |
| 1:n:151:ILE:O    | 1:n:155:LEU:HG   | 2.20                     | 0.42              |
| 1:T:151:ILE:O    | 1:T:155:LEU:HG   | 2.19                     | 0.42              |
| 1:U:20:GLU:OE1   | 1:U:23:ARG:NH2   | 2.37                     | 0.42              |
| 1:U:199:ALA:O    | 1:U:203:ARG:HG3  | 2.20                     | 0.42              |
| 1:1:29:MET:HE2   | 1:1:29:MET:HB3   | 1.94                     | 0.42              |
| 1:K:149:ARG:NH1  | 1:K:243:GLU:OE2  | 2.53                     | 0.42              |
| 1:2:199:ALA:O    | 1:2:203:ARG:HG3  | 2.20                     | 0.42              |
| 1:h:199:ALA:O    | 1:h:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:3:199:ALA:O    | 1:3:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:t:254:ARG:HE   | 1:t:254:ARG:HB2  | 1.58                     | 0.42              |
| 1:Y:15:GLU:OE2   | 1:Y:37:ARG:HG2   | 2.19                     | 0.42              |
| 1:u:20:GLU:OE1   | 1:u:23:ARG:NH2   | 2.43                     | 0.42              |
| 1:l:62:LEU:HD11  | 1:l:66:ARG:HH11  | 1.84                     | 0.42              |
| 1:A:34:GLU:HG3   | 1:f:85:ARG:NH2   | 2.35                     | 0.42              |
| 1:B:34:GLU:HG3   | 1:b:85:ARG:NH2   | 2.34                     | 0.42              |
| 1:G:203:ARG:HH21 | 1:y:246:ARG:CZ   | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:152:ILE:HG13 | 1:c:247:VAL:HG11 | 2.01                     | 0.42              |
| 1:H:16:GLU:O     | 1:H:20:GLU:HG2   | 2.20                     | 0.42              |
| 1:J:246:ARG:CZ   | 1:U:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:q:16:GLU:O     | 1:q:20:GLU:HG2   | 2.20                     | 0.42              |
| 1:q:254:ARG:HE   | 1:q:254:ARG:HB2  | 1.58                     | 0.42              |
| 1:2:66:ARG:HA    | 1:2:66:ARG:HD2   | 1.87                     | 0.42              |
| 1:3:149:ARG:NH2  | 1:3:243:GLU:OE1  | 2.53                     | 0.42              |
| 1:X:123:ILE:HG13 | 1:X:175:GLU:HG2  | 2.02                     | 0.42              |
| 1:t:16:GLU:O     | 1:t:20:GLU:HG2   | 2.20                     | 0.42              |
| 1:O:249:ASP:OD1  | 1:O:249:ASP:C    | 2.63                     | 0.42              |
| 1:k:246:ARG:CZ   | 1:v:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:v:151:ILE:O    | 1:v:155:LEU:HG   | 2.20                     | 0.42              |
| 1:6:87:LEU:HD23  | 1:6:92:ARG:HD3   | 2.01                     | 0.42              |
| 1:A:77:LEU:HA    | 1:A:80:VAL:HG12  | 2.01                     | 0.42              |
| 1:A:254:ARG:HE   | 1:A:254:ARG:HB2  | 1.55                     | 0.42              |
| 1:C:151:ILE:O    | 1:C:155:LEU:HG   | 2.20                     | 0.42              |
| 1:D:246:ARG:CZ   | 1:E:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:E:66:ARG:HA    | 1:E:66:ARG:HD2   | 1.87                     | 0.42              |
| 1:b:16:GLU:O     | 1:b:20:GLU:HG2   | 2.19                     | 0.42              |
| 1:b:246:ARG:CZ   | 1:m:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:R:66:ARG:HA    | 1:R:66:ARG:HD2   | 1.86                     | 0.42              |
| 1:H:35:MET:HE1   | 1:H:65:ALA:HB2   | 2.02                     | 0.42              |
| 1:I:15:GLU:OE2   | 1:I:37:ARG:HG2   | 2.19                     | 0.42              |
| 1:q:152:ILE:HG13 | 1:q:247:VAL:HG11 | 2.01                     | 0.42              |
| 1:2:221:HIS:O    | 1:2:224:GLU:HG2  | 2.20                     | 0.42              |
| 1:3:160:ARG:O    | 1:3:164:GLU:HG3  | 2.19                     | 0.42              |
| 1:X:20:GLU:OE1   | 1:X:23:ARG:NH2   | 2.37                     | 0.42              |
| 1:4:85:ARG:NH1   | 1:7:64:MET:HE2   | 2.35                     | 0.42              |
| 1:A:151:ILE:O    | 1:A:155:LEU:HG   | 2.20                     | 0.42              |
| 1:B:152:ILE:HG13 | 1:B:247:VAL:HG11 | 2.01                     | 0.42              |
| 1:C:85:ARG:NH1   | 1:o:64:MET:HE2   | 2.35                     | 0.42              |
| 1:E:38:HIS:CE1   | 1:E:64:MET:HE1   | 2.55                     | 0.42              |
| 1:F:249:ASP:OD1  | 1:F:249:ASP:C    | 2.63                     | 0.42              |
| 1:b:7:VAL:O      | 1:b:11:ARG:HG3   | 2.20                     | 0.42              |
| 1:x:152:ILE:HG13 | 1:x:247:VAL:HG11 | 2.01                     | 0.42              |
| 1:H:151:ILE:O    | 1:H:155:LEU:HG   | 2.19                     | 0.42              |
| 1:S:34:GLU:HG3   | 1:j:85:ARG:NH2   | 2.35                     | 0.42              |
| 1:S:64:MET:O     | 1:S:67:GLU:HG3   | 2.20                     | 0.42              |
| 1:o:7:VAL:O      | 1:o:11:ARG:HG3   | 2.20                     | 0.42              |
| 1:o:16:GLU:O     | 1:o:20:GLU:HG2   | 2.19                     | 0.42              |
| 1:0:199:ALA:O    | 1:0:203:ARG:HG3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:151:ILE:O    | 1:1:155:LEU:HG   | 2.20                     | 0.42              |
| 1:K:151:ILE:O    | 1:K:155:LEU:HG   | 2.20                     | 0.42              |
| 1:g:62:LEU:HD11  | 1:g:66:ARG:HH11  | 1.83                     | 0.42              |
| 1:L:10:VAL:HG21  | 1:L:47:LEU:HD11  | 2.02                     | 0.42              |
| 1:W:39:LEU:HD11  | 1:W:61:VAL:HG11  | 2.00                     | 0.42              |
| 1:W:123:ILE:HG13 | 1:W:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:M:199:ALA:O    | 1:M:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:Y:151:ILE:O    | 1:Y:155:LEU:HG   | 2.20                     | 0.42              |
| 1:Z:246:ARG:CZ   | 1:k:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:l:96:ALA:HA    | 1:l:99:LEU:HD12  | 2.02                     | 0.42              |
| 1:B:66:ARG:HA    | 1:B:66:ARG:HD2   | 1.85                     | 0.42              |
| 1:F:95:GLU:O     | 1:F:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:x:16:GLU:O     | 1:x:20:GLU:HG2   | 2.20                     | 0.42              |
| 1:x:85:ARG:HD2   | 1:g:38:HIS:CE1   | 2.55                     | 0.42              |
| 1:x:254:ARG:HE   | 1:x:254:ARG:HB2  | 1.58                     | 0.42              |
| 1:G:199:ALA:O    | 1:G:203:ARG:HG3  | 2.19                     | 0.42              |
| 1:R:152:ILE:HG13 | 1:R:247:VAL:HG11 | 2.02                     | 0.42              |
| 1:R:254:ARG:HE   | 1:R:254:ARG:HB2  | 1.56                     | 0.42              |
| 1:n:29:MET:HB3   | 1:n:32:TYR:HD2   | 1.85                     | 0.42              |
| 1:S:95:GLU:O     | 1:S:99:LEU:HD12  | 2.20                     | 0.42              |
| 1:I:71:GLU:O     | 1:I:75:ARG:HG3   | 2.20                     | 0.42              |
| 1:e:76:LEU:HD22  | 1:e:161:VAL:HG21 | 2.02                     | 0.42              |
| 1:K:16:GLU:O     | 1:K:20:GLU:HG2   | 2.19                     | 0.42              |
| 1:K:78:GLU:O     | 1:K:82:ARG:HG3   | 2.20                     | 0.42              |
| 1:2:64:MET:HE2   | 1:O:85:ARG:NH1   | 2.35                     | 0.42              |
| 1:L:151:ILE:O    | 1:L:155:LEU:HG   | 2.19                     | 0.42              |
| 1:h:246:ARG:CZ   | 1:s:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:s:64:MET:O     | 1:s:67:GLU:HG3   | 2.20                     | 0.42              |
| 1:M:246:ARG:CZ   | 1:X:203:ARG:HH21 | 2.33                     | 0.42              |
| 1:t:110:VAL:HG23 | 1:t:165:ALA:HB1  | 2.02                     | 0.42              |
| 1:N:7:VAL:O      | 1:N:11:ARG:HG3   | 2.20                     | 0.42              |
| 1:N:64:MET:HE2   | 1:l:85:ARG:NH1   | 2.35                     | 0.42              |
| 1:Y:123:ILE:HG13 | 1:Y:175:GLU:HG2  | 2.01                     | 0.42              |
| 1:6:191:LEU:HD22 | 1:6:244:GLU:HG2  | 2.02                     | 0.42              |
| 1:P:149:ARG:NH2  | 1:P:243:GLU:OE1  | 2.53                     | 0.42              |
| 1:P:203:ARG:HH21 | 1:7:246:ARG:CZ   | 2.33                     | 0.42              |
| 1:P:234:ILE:HD13 | 1:P:245:LEU:HD23 | 2.01                     | 0.42              |
| 1:P:243:GLU:O    | 1:P:247:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:203:ARG:HH21 | 1:E:246:ARG:CZ   | 2.33                     | 0.41              |
| 1:F:16:GLU:O     | 1:F:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:F:38:HIS:CE1   | 1:V:85:ARG:HD2   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:199:ALA:O    | 1:b:203:ARG:HG3  | 2.20                     | 0.41              |
| 1:R:62:LEU:HD11  | 1:R:66:ARG:NH1   | 2.31                     | 0.41              |
| 1:R:243:GLU:O    | 1:R:247:VAL:HG23 | 2.19                     | 0.41              |
| 1:c:66:ARG:HA    | 1:c:66:ARG:HD2   | 1.85                     | 0.41              |
| 1:S:16:GLU:O     | 1:S:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:o:246:ARG:CZ   | 1:z:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:1:62:LEU:HD11  | 1:1:66:ARG:HH11  | 1.84                     | 0.41              |
| 1:g:20:GLU:OE1   | 1:g:23:ARG:NH2   | 2.43                     | 0.41              |
| 1:2:7:VAL:O      | 1:2:11:ARG:HG3   | 2.20                     | 0.41              |
| 1:3:151:ILE:O    | 1:3:155:LEU:HG   | 2.19                     | 0.41              |
| 1:M:29:MET:HB3   | 1:M:32:TYR:CD2   | 2.55                     | 0.41              |
| 1:4:20:GLU:OE1   | 1:4:23:ARG:NH2   | 2.43                     | 0.41              |
| 1:4:151:ILE:O    | 1:4:155:LEU:HG   | 2.20                     | 0.41              |
| 1:Y:16:GLU:O     | 1:Y:20:GLU:HG2   | 2.18                     | 0.41              |
| 1:F:152:ILE:HG22 | 1:F:156:GLU:OE2  | 2.19                     | 0.41              |
| 1:x:62:LEU:HD11  | 1:x:66:ARG:NH1   | 2.35                     | 0.41              |
| 1:G:29:MET:HE3   | 1:G:29:MET:HB2   | 1.82                     | 0.41              |
| 1:G:246:ARG:CZ   | 1:R:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:y:66:ARG:HD2   | 1:y:66:ARG:HA    | 1.87                     | 0.41              |
| 1:H:87:LEU:HD23  | 1:H:92:ARG:HD3   | 2.03                     | 0.41              |
| 1:S:85:ARG:NH1   | 1:0:64:MET:HE2   | 2.35                     | 0.41              |
| 1:S:187:LEU:HD23 | 1:S:187:LEU:HA   | 1.91                     | 0.41              |
| 1:z:234:ILE:HD13 | 1:z:245:LEU:HD23 | 2.02                     | 0.41              |
| 1:I:151:ILE:O    | 1:I:155:LEU:HG   | 2.20                     | 0.41              |
| 1:I:160:ARG:O    | 1:I:164:GLU:HG3  | 2.19                     | 0.41              |
| 1:I:203:ARG:HH21 | 1:0:246:ARG:CZ   | 2.33                     | 0.41              |
| 1:K:77:LEU:HA    | 1:K:80:VAL:HG12  | 2.01                     | 0.41              |
| 1:g:76:LEU:HD22  | 1:g:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:s:199:ALA:O    | 1:s:203:ARG:HG3  | 2.20                     | 0.41              |
| 1:s:246:ARG:CZ   | 1:3:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:X:64:MET:HE2   | 1:u:85:ARG:NH1   | 2.35                     | 0.41              |
| 1:4:16:GLU:O     | 1:4:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:j:16:GLU:O     | 1:j:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:u:62:LEU:HD11  | 1:u:66:ARG:HH11  | 1.84                     | 0.41              |
| 1:u:151:ILE:O    | 1:u:155:LEU:HG   | 2.20                     | 0.41              |
| 1:Z:64:MET:O     | 1:Z:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:a:35:MET:HG2   | 1:a:61:VAL:HG13  | 2.02                     | 0.41              |
| 1:l:76:LEU:HD22  | 1:l:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:78:GLU:O     | 1:A:82:ARG:HG3   | 2.20                     | 0.41              |
| 1:B:10:VAL:HG21  | 1:B:47:LEU:HD11  | 2.00                     | 0.41              |
| 1:B:110:VAL:HG23 | 1:B:165:ALA:HB1  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:56:ARG:HD2   | 1:e:56:ARG:CG    | 2.50                     | 0.41              |
| 1:E:123:ILE:HG13 | 1:E:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:E:221:HIS:O    | 1:E:224:GLU:HG2  | 2.20                     | 0.41              |
| 1:F:96:ALA:HA    | 1:F:99:LEU:HD12  | 2.02                     | 0.41              |
| 1:F:123:ILE:HG13 | 1:F:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:F:187:LEU:HD23 | 1:F:187:LEU:HA   | 1.91                     | 0.41              |
| 1:n:123:ILE:HG13 | 1:n:175:GLU:HG2  | 2.01                     | 0.41              |
| 1:S:96:ALA:HA    | 1:S:99:LEU:HD12  | 2.02                     | 0.41              |
| 1:e:39:LEU:HD11  | 1:e:61:VAL:HG11  | 2.01                     | 0.41              |
| 1:p:64:MET:O     | 1:p:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:K:160:ARG:O    | 1:K:164:GLU:HG3  | 2.19                     | 0.41              |
| 1:V:16:GLU:O     | 1:V:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:L:16:GLU:O     | 1:L:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:3:71:GLU:O     | 1:3:75:ARG:HG3   | 2.21                     | 0.41              |
| 1:3:243:GLU:O    | 1:3:247:VAL:HG23 | 2.19                     | 0.41              |
| 1:N:15:GLU:OE2   | 1:N:37:ARG:HG2   | 2.21                     | 0.41              |
| 1:O:96:ALA:HA    | 1:O:99:LEU:HD12  | 2.02                     | 0.41              |
| 1:k:123:ILE:HG13 | 1:k:175:GLU:HG2  | 2.01                     | 0.41              |
| 1:w:66:ARG:HA    | 1:w:66:ARG:HD2   | 1.87                     | 0.41              |
| 1:A:66:ARG:HD2   | 1:A:66:ARG:HA    | 1.87                     | 0.41              |
| 1:A:85:ARG:NH2   | 1:m:34:GLU:HG3   | 2.35                     | 0.41              |
| 1:E:41:GLU:HA    | 1:E:44:VAL:HG22  | 2.02                     | 0.41              |
| 1:E:78:GLU:O     | 1:E:82:ARG:HG3   | 2.20                     | 0.41              |
| 1:c:35:MET:HE1   | 1:c:65:ALA:HB2   | 2.01                     | 0.41              |
| 1:U:246:ARG:CZ   | 1:f:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:g:151:ILE:O    | 1:g:155:LEU:HG   | 2.20                     | 0.41              |
| 1:W:34:GLU:HG3   | 1:t:85:ARG:NH2   | 2.35                     | 0.41              |
| 1:W:152:ILE:HG13 | 1:W:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:t:152:ILE:HG13 | 1:t:247:VAL:HG11 | 2.01                     | 0.41              |
| 1:4:29:MET:HB3   | 1:4:32:TYR:HD2   | 1.85                     | 0.41              |
| 1:j:152:ILE:HG13 | 1:j:247:VAL:HG11 | 2.01                     | 0.41              |
| 1:u:76:LEU:HD22  | 1:u:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:O:29:MET:HB3   | 1:O:32:TYR:HD2   | 1.86                     | 0.41              |
| 1:O:95:GLU:O     | 1:O:99:LEU:HD12  | 2.20                     | 0.41              |
| 1:l:95:GLU:O     | 1:l:99:LEU:HD12  | 2.20                     | 0.41              |
| 1:w:64:MET:O     | 1:w:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:w:246:ARG:CZ   | 1:7:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:C:95:GLU:O     | 1:C:99:LEU:HD12  | 2.20                     | 0.41              |
| 1:C:152:ILE:HG13 | 1:C:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:F:62:LEU:HD11  | 1:F:66:ARG:HH11  | 1.86                     | 0.41              |
| 1:x:87:LEU:HD23  | 1:x:92:ARG:HD3   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:123:ILE:HG13 | 1:G:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:c:16:GLU:O     | 1:c:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:S:138:ALA:HB2  | 1:S:155:LEU:HD11 | 2.02                     | 0.41              |
| 1:S:152:ILE:HG13 | 1:S:247:VAL:HG11 | 2.01                     | 0.41              |
| 1:o:64:MET:O     | 1:o:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:o:199:ALA:O    | 1:o:203:ARG:HG3  | 2.20                     | 0.41              |
| 1:e:34:GLU:HG3   | 1:q:85:ARG:NH2   | 2.35                     | 0.41              |
| 1:e:123:ILE:HG13 | 1:e:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:p:66:ARG:HA    | 1:p:66:ARG:HD2   | 1.87                     | 0.41              |
| 1:1:152:ILE:HG13 | 1:1:247:VAL:HG11 | 2.03                     | 0.41              |
| 1:L:62:LEU:HD11  | 1:L:66:ARG:NH1   | 2.35                     | 0.41              |
| 1:M:56:ARG:CG    | 1:5:56:ARG:HD2   | 2.51                     | 0.41              |
| 1:X:64:MET:O     | 1:X:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:i:138:ALA:HB2  | 1:i:155:LEU:HD11 | 2.01                     | 0.41              |
| 1:i:151:ILE:O    | 1:i:155:LEU:HG   | 2.20                     | 0.41              |
| 1:4:152:ILE:HG13 | 1:4:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:Y:160:ARG:O    | 1:Y:164:GLU:HG3  | 2.19                     | 0.41              |
| 1:O:76:LEU:HD22  | 1:O:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:v:152:ILE:HG13 | 1:v:247:VAL:HG11 | 2.03                     | 0.41              |
| 1:a:16:GLU:O     | 1:a:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:l:29:MET:HB3   | 1:l:32:TYR:HD2   | 1.86                     | 0.41              |
| 1:E:199:ALA:O    | 1:E:203:ARG:HG3  | 2.20                     | 0.41              |
| 1:R:234:ILE:HD13 | 1:R:245:LEU:HD23 | 2.02                     | 0.41              |
| 1:n:95:GLU:O     | 1:n:99:LEU:HD12  | 2.20                     | 0.41              |
| 1:z:71:GLU:O     | 1:z:75:ARG:HG3   | 2.21                     | 0.41              |
| 1:e:62:LEU:HD11  | 1:e:66:ARG:HH11  | 1.85                     | 0.41              |
| 1:V:152:ILE:HG13 | 1:V:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:g:95:GLU:HG3   | 1:g:146:VAL:HG13 | 2.03                     | 0.41              |
| 1:r:64:MET:O     | 1:r:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:r:246:ARG:CZ   | 1:2:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:L:64:MET:O     | 1:L:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:L:149:ARG:NH1  | 1:L:243:GLU:HG2  | 2.35                     | 0.41              |
| 1:W:62:LEU:HD11  | 1:W:66:ARG:HH11  | 1.85                     | 0.41              |
| 1:4:62:LEU:HD11  | 1:4:66:ARG:HH11  | 1.85                     | 0.41              |
| 1:4:249:ASP:OD1  | 1:4:249:ASP:C    | 2.64                     | 0.41              |
| 1:O:95:GLU:HG3   | 1:O:146:VAL:HG13 | 2.03                     | 0.41              |
| 1:k:66:ARG:HD2   | 1:k:66:ARG:HA    | 1.87                     | 0.41              |
| 1:6:16:GLU:O     | 1:6:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:6:62:LEU:HD11  | 1:6:66:ARG:NH1   | 2.35                     | 0.41              |
| 1:B:16:GLU:O     | 1:B:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:C:123:ILE:HG13 | 1:C:175:GLU:HG2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:76:LEU:HD22  | 1:F:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:F:151:ILE:O    | 1:F:155:LEU:HG   | 2.20                     | 0.41              |
| 1:S:249:ASP:OD1  | 1:S:249:ASP:C    | 2.64                     | 0.41              |
| 1:d:16:GLU:O     | 1:d:20:GLU:HG2   | 2.21                     | 0.41              |
| 1:e:16:GLU:O     | 1:e:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:e:152:ILE:HG13 | 1:e:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:p:246:ARG:CZ   | 1:0:203:ARG:HH21 | 2.34                     | 0.41              |
| 1:0:221:HIS:O    | 1:0:224:GLU:HG2  | 2.21                     | 0.41              |
| 1:f:151:ILE:O    | 1:f:155:LEU:HG   | 2.20                     | 0.41              |
| 1:1:76:LEU:HD22  | 1:1:161:VAL:HG21 | 2.02                     | 0.41              |
| 1:W:16:GLU:O     | 1:W:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:W:151:ILE:O    | 1:W:155:LEU:HG   | 2.20                     | 0.41              |
| 1:h:16:GLU:O     | 1:h:20:GLU:HG2   | 2.21                     | 0.41              |
| 1:h:64:MET:O     | 1:h:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:s:123:ILE:HG13 | 1:s:175:GLU:HG2  | 2.01                     | 0.41              |
| 1:3:200:LEU:HD12 | 1:3:200:LEU:HA   | 1.94                     | 0.41              |
| 1:X:7:VAL:O      | 1:X:11:ARG:HG3   | 2.20                     | 0.41              |
| 1:X:246:ARG:CZ   | 1:i:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:N:29:MET:HE3   | 1:N:29:MET:HB2   | 1.82                     | 0.41              |
| 1:N:203:ARG:HH21 | 1:5:246:ARG:CZ   | 2.33                     | 0.41              |
| 1:6:64:MET:O     | 1:6:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:a:252:LEU:HD23 | 1:a:252:LEU:HA   | 1.92                     | 0.41              |
| 1:l:16:GLU:O     | 1:l:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:7:64:MET:O     | 1:7:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:B:85:ARG:HD2   | 1:n:38:HIS:CE1   | 2.55                     | 0.41              |
| 1:F:64:MET:O     | 1:F:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:Q:7:VAL:O      | 1:Q:11:ARG:HG3   | 2.21                     | 0.41              |
| 1:b:64:MET:O     | 1:b:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:m:151:ILE:O    | 1:m:155:LEU:HG   | 2.20                     | 0.41              |
| 1:z:151:ILE:O    | 1:z:155:LEU:HG   | 2.20                     | 0.41              |
| 1:T:16:GLU:O     | 1:T:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:T:203:ARG:NH1  | 1:T:206:GLU:OE2  | 2.54                     | 0.41              |
| 1:p:15:GLU:OE1   | 1:p:37:ARG:HG2   | 2.21                     | 0.41              |
| 1:U:7:VAL:O      | 1:U:11:ARG:HG3   | 2.20                     | 0.41              |
| 1:f:138:ALA:HB2  | 1:f:155:LEU:HD11 | 2.01                     | 0.41              |
| 1:1:16:GLU:O     | 1:1:20:GLU:HG2   | 2.21                     | 0.41              |
| 1:2:57:LEU:O     | 1:2:61:VAL:HG23  | 2.20                     | 0.41              |
| 1:W:64:MET:O     | 1:W:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:O:152:ILE:HG13 | 1:O:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:k:64:MET:O     | 1:k:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:P:152:ILE:HG13 | 1:P:247:VAL:HG11 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:149:ARG:NH1  | 1:A:243:GLU:OE2  | 2.52                     | 0.41              |
| 1:B:110:VAL:HG23 | 1:B:165:ALA:CB   | 2.51                     | 0.41              |
| 1:C:64:MET:O     | 1:C:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:E:7:VAL:O      | 1:E:11:ARG:HG3   | 2.20                     | 0.41              |
| 1:F:152:ILE:HG13 | 1:F:247:VAL:HG11 | 2.01                     | 0.41              |
| 1:Q:56:ARG:HD2   | 1:h:56:ARG:CG    | 2.50                     | 0.41              |
| 1:Q:64:MET:O     | 1:Q:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:b:38:HIS:CE1   | 1:b:64:MET:HE1   | 2.56                     | 0.41              |
| 1:m:71:GLU:O     | 1:m:75:ARG:HG3   | 2.21                     | 0.41              |
| 1:x:187:LEU:HD23 | 1:x:187:LEU:HA   | 1.92                     | 0.41              |
| 1:n:64:MET:O     | 1:n:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:H:203:ARG:NH1  | 1:H:206:GLU:OE2  | 2.54                     | 0.41              |
| 1:S:191:LEU:HD22 | 1:S:244:GLU:HG2  | 2.03                     | 0.41              |
| 1:d:246:ARG:CZ   | 1:o:203:ARG:HH21 | 2.33                     | 0.41              |
| 1:I:78:GLU:O     | 1:I:82:ARG:HG3   | 2.20                     | 0.41              |
| 1:T:64:MET:O     | 1:T:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:T:187:LEU:HD23 | 1:T:187:LEU:HA   | 1.93                     | 0.41              |
| 1:e:64:MET:O     | 1:e:67:GLU:HG3   | 2.20                     | 0.41              |
| 1:e:96:ALA:HA    | 1:e:99:LEU:HD12  | 2.02                     | 0.41              |
| 1:U:221:HIS:O    | 1:U:224:GLU:HG2  | 2.20                     | 0.41              |
| 1:l:64:MET:O     | 1:l:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:K:71:GLU:O     | 1:K:75:ARG:HG3   | 2.21                     | 0.41              |
| 1:V:10:VAL:HG21  | 1:V:47:LEU:HD11  | 2.02                     | 0.41              |
| 1:V:110:VAL:HG23 | 1:V:165:ALA:HB1  | 2.02                     | 0.41              |
| 1:r:16:GLU:O     | 1:r:20:GLU:HG2   | 2.21                     | 0.41              |
| 1:W:96:ALA:HA    | 1:W:99:LEU:HD12  | 2.02                     | 0.41              |
| 1:h:66:ARG:HA    | 1:h:66:ARG:HD2   | 1.87                     | 0.41              |
| 1:s:29:MET:HE3   | 1:s:29:MET:HB2   | 1.82                     | 0.41              |
| 1:i:71:GLU:O     | 1:i:75:ARG:HG3   | 2.21                     | 0.41              |
| 1:4:64:MET:O     | 1:4:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:4:123:ILE:HG13 | 1:4:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:4:156:GLU:OE1  | 1:4:254:ARG:NH1  | 2.50                     | 0.41              |
| 1:N:254:ARG:HE   | 1:N:254:ARG:HB2  | 1.57                     | 0.41              |
| 1:u:95:GLU:HG3   | 1:u:146:VAL:HG13 | 2.03                     | 0.41              |
| 1:u:191:LEU:HD22 | 1:u:244:GLU:HG2  | 2.03                     | 0.41              |
| 1:5:64:MET:O     | 1:5:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:O:16:GLU:O     | 1:O:20:GLU:HG2   | 2.20                     | 0.41              |
| 1:O:62:LEU:HD11  | 1:O:66:ARG:HH11  | 1.86                     | 0.41              |
| 1:Z:29:MET:HB3   | 1:Z:32:TYR:CD2   | 2.55                     | 0.41              |
| 1:k:38:HIS:CE1   | 1:k:64:MET:HE1   | 2.56                     | 0.41              |
| 1:k:148:LEU:O    | 1:k:152:ILE:HG12 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:29:MET:HB3   | 1:6:29:MET:HE2   | 1.77                     | 0.41              |
| 1:a:64:MET:O     | 1:a:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:l:64:MET:O     | 1:l:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:l:152:ILE:HG13 | 1:l:247:VAL:HG11 | 2.02                     | 0.41              |
| 1:w:29:MET:HB3   | 1:w:32:TYR:CD2   | 2.55                     | 0.41              |
| 1:7:148:LEU:O    | 1:7:152:ILE:HG12 | 2.21                     | 0.41              |
| 1:7:221:HIS:O    | 1:7:224:GLU:HG2  | 2.21                     | 0.41              |
| 1:D:66:ARG:HD2   | 1:D:66:ARG:HA    | 1.88                     | 0.41              |
| 1:F:95:GLU:HG3   | 1:F:146:VAL:HG13 | 2.03                     | 0.41              |
| 1:0:29:MET:HE3   | 1:0:29:MET:HB2   | 1.81                     | 0.41              |
| 1:0:148:LEU:O    | 1:0:152:ILE:HG12 | 2.21                     | 0.41              |
| 1:U:108:GLY:O    | 1:U:112:VAL:HG23 | 2.21                     | 0.41              |
| 1:f:66:ARG:HD2   | 1:f:66:ARG:HA    | 1.87                     | 0.41              |
| 1:K:203:ARG:HH21 | 1:2:246:ARG:CZ   | 2.33                     | 0.41              |
| 1:h:7:VAL:O      | 1:h:11:ARG:HG3   | 2.21                     | 0.41              |
| 1:s:148:LEU:O    | 1:s:152:ILE:HG12 | 2.21                     | 0.41              |
| 1:X:108:GLY:O    | 1:X:112:VAL:HG23 | 2.21                     | 0.41              |
| 1:X:221:HIS:O    | 1:X:224:GLU:HG2  | 2.21                     | 0.41              |
| 1:N:85:ARG:NH2   | 1:6:34:GLU:HG3   | 2.36                     | 0.41              |
| 1:Y:87:LEU:HD23  | 1:Y:92:ARG:HD3   | 2.03                     | 0.41              |
| 1:O:64:MET:O     | 1:O:67:GLU:HG3   | 2.21                     | 0.41              |
| 1:O:138:ALA:HB2  | 1:O:155:LEU:HD11 | 2.03                     | 0.41              |
| 1:a:203:ARG:NH1  | 1:a:206:GLU:OE2  | 2.54                     | 0.41              |
| 1:7:123:ILE:HG13 | 1:7:175:GLU:HG2  | 2.02                     | 0.41              |
| 1:A:149:ARG:O    | 1:A:153:ARG:HG3  | 2.22                     | 0.40              |
| 1:E:38:HIS:CE1   | 1:e:85:ARG:HD2   | 2.56                     | 0.40              |
| 1:E:148:LEU:O    | 1:E:152:ILE:HG12 | 2.21                     | 0.40              |
| 1:F:56:ARG:CG    | 1:s:56:ARG:HD2   | 2.51                     | 0.40              |
| 1:Q:16:GLU:O     | 1:Q:20:GLU:HG2   | 2.21                     | 0.40              |
| 1:Q:246:ARG:CZ   | 1:b:203:ARG:HH21 | 2.34                     | 0.40              |
| 1:b:108:GLY:O    | 1:b:112:VAL:HG23 | 2.21                     | 0.40              |
| 1:x:110:VAL:HG23 | 1:x:165:ALA:HB1  | 2.03                     | 0.40              |
| 1:G:10:VAL:HG21  | 1:G:47:LEU:HD11  | 2.03                     | 0.40              |
| 1:c:110:VAL:HG23 | 1:c:165:ALA:HB1  | 2.03                     | 0.40              |
| 1:n:11:ARG:HG3   | 1:n:44:VAL:HG11  | 2.03                     | 0.40              |
| 1:y:64:MET:O     | 1:y:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:p:123:ILE:HG13 | 1:p:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:U:64:MET:O     | 1:U:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:f:149:ARG:NH1  | 1:f:243:GLU:OE2  | 2.53                     | 0.40              |
| 1:g:152:ILE:HG13 | 1:g:247:VAL:HG11 | 2.02                     | 0.40              |
| 1:h:254:ARG:HE   | 1:h:254:ARG:HB2  | 1.57                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:234:ILE:HD13 | 1:i:245:LEU:HD23 | 2.02                     | 0.40              |
| 1:u:96:ALA:HA    | 1:u:99:LEU:HD12  | 2.02                     | 0.40              |
| 1:Z:16:GLU:O     | 1:Z:20:GLU:HG2   | 2.21                     | 0.40              |
| 1:k:10:VAL:HG21  | 1:k:47:LEU:HD11  | 2.03                     | 0.40              |
| 1:l:95:GLU:HG3   | 1:l:146:VAL:HG13 | 2.03                     | 0.40              |
| 1:l:138:ALA:HB2  | 1:l:155:LEU:HD11 | 2.03                     | 0.40              |
| 1:w:15:GLU:OE1   | 1:w:37:ARG:HG2   | 2.21                     | 0.40              |
| 1:C:95:GLU:HG3   | 1:C:146:VAL:HG13 | 2.03                     | 0.40              |
| 1:D:123:ILE:HG13 | 1:D:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:x:29:MET:HE2   | 1:x:29:MET:HB3   | 1.77                     | 0.40              |
| 1:G:7:VAL:O      | 1:G:11:ARG:HG3   | 2.20                     | 0.40              |
| 1:G:148:LEU:O    | 1:G:152:ILE:HG12 | 2.21                     | 0.40              |
| 1:R:71:GLU:O     | 1:R:75:ARG:HG3   | 2.21                     | 0.40              |
| 1:c:110:VAL:HG23 | 1:c:165:ALA:CB   | 2.52                     | 0.40              |
| 1:n:15:GLU:OE1   | 1:n:37:ARG:HG2   | 2.22                     | 0.40              |
| 1:n:95:GLU:HG3   | 1:n:146:VAL:HG13 | 2.03                     | 0.40              |
| 1:S:76:LEU:HD22  | 1:S:161:VAL:HG21 | 2.03                     | 0.40              |
| 1:S:95:GLU:HG3   | 1:S:146:VAL:HG13 | 2.03                     | 0.40              |
| 1:d:221:HIS:O    | 1:d:224:GLU:HG2  | 2.21                     | 0.40              |
| 1:o:78:GLU:O     | 1:o:82:ARG:HG3   | 2.21                     | 0.40              |
| 1:T:250:LEU:HD22 | 1:e:218:GLU:HB3  | 2.03                     | 0.40              |
| 1:V:64:MET:O     | 1:V:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:r:56:ARG:CG    | 1:Z:56:ARG:HD2   | 2.51                     | 0.40              |
| 1:2:148:LEU:O    | 1:2:152:ILE:HG12 | 2.21                     | 0.40              |
| 1:L:187:LEU:HD23 | 1:L:187:LEU:HA   | 1.93                     | 0.40              |
| 1:s:7:VAL:O      | 1:s:11:ARG:HG3   | 2.20                     | 0.40              |
| 1:4:96:ALA:HA    | 1:4:99:LEU:HD12  | 2.02                     | 0.40              |
| 1:4:193:ARG:HH12 | 1:4:205:LEU:HD11 | 1.86                     | 0.40              |
| 1:N:148:LEU:O    | 1:N:152:ILE:HG12 | 2.21                     | 0.40              |
| 1:N:246:ARG:CZ   | 1:Y:203:ARG:HH21 | 2.33                     | 0.40              |
| 1:Z:7:VAL:O      | 1:Z:11:ARG:HG3   | 2.21                     | 0.40              |
| 1:Z:66:ARG:HA    | 1:Z:66:ARG:HD2   | 1.88                     | 0.40              |
| 1:k:7:VAL:O      | 1:k:11:ARG:HG3   | 2.20                     | 0.40              |
| 1:k:108:GLY:O    | 1:k:112:VAL:HG23 | 2.21                     | 0.40              |
| 1:w:7:VAL:O      | 1:w:11:ARG:HG3   | 2.20                     | 0.40              |
| 1:w:254:ARG:HE   | 1:w:254:ARG:HB2  | 1.57                     | 0.40              |
| 1:A:71:GLU:O     | 1:A:75:ARG:HG3   | 2.21                     | 0.40              |
| 1:B:187:LEU:HD23 | 1:B:187:LEU:HA   | 1.92                     | 0.40              |
| 1:C:11:ARG:HG3   | 1:C:44:VAL:HG11  | 2.04                     | 0.40              |
| 1:D:221:HIS:O    | 1:D:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:E:64:MET:HE2   | 1:e:85:ARG:NH1   | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:34:GLU:HG3   | 1:U:85:ARG:NH2   | 2.36                     | 0.40              |
| 1:c:187:LEU:HD23 | 1:c:187:LEU:HA   | 1.93                     | 0.40              |
| 1:n:96:ALA:HA    | 1:n:99:LEU:HD12  | 2.02                     | 0.40              |
| 1:n:152:ILE:HG13 | 1:n:247:VAL:HG11 | 2.03                     | 0.40              |
| 1:S:29:MET:HB3   | 1:S:32:TYR:HD2   | 1.85                     | 0.40              |
| 1:o:108:GLY:O    | 1:o:112:VAL:HG23 | 2.21                     | 0.40              |
| 1:I:200:LEU:HD12 | 1:I:200:LEU:HA   | 1.95                     | 0.40              |
| 1:e:95:GLU:HG3   | 1:e:146:VAL:HG13 | 2.03                     | 0.40              |
| 1:e:151:ILE:O    | 1:e:155:LEU:HG   | 2.20                     | 0.40              |
| 1:0:123:ILE:HG13 | 1:0:175:GLU:HG2  | 2.02                     | 0.40              |
| 1:J:123:ILE:HG13 | 1:J:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:K:108:GLY:O    | 1:K:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:V:62:LEU:HD11  | 1:V:66:ARG:NH1   | 2.36                     | 0.40              |
| 1:g:156:GLU:CD   | 1:g:254:ARG:HH12 | 2.25                     | 0.40              |
| 1:2:87:LEU:HD23  | 1:2:92:ARG:HD3   | 2.04                     | 0.40              |
| 1:h:123:ILE:HG13 | 1:h:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:s:66:ARG:HD2   | 1:s:66:ARG:HA    | 1.87                     | 0.40              |
| 1:M:123:ILE:HG13 | 1:M:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:j:110:VAL:HG23 | 1:j:165:ALA:CB   | 2.52                     | 0.40              |
| 1:O:151:ILE:O    | 1:O:155:LEU:HG   | 2.20                     | 0.40              |
| 1:l:123:ILE:HG13 | 1:l:175:GLU:HG2  | 2.02                     | 0.40              |
| 1:A:108:GLY:O    | 1:A:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:C:15:GLU:OE1   | 1:C:37:ARG:HG2   | 2.22                     | 0.40              |
| 1:C:96:ALA:HA    | 1:C:99:LEU:HD12  | 2.02                     | 0.40              |
| 1:C:138:ALA:HB2  | 1:C:155:LEU:HD11 | 2.03                     | 0.40              |
| 1:D:64:MET:O     | 1:D:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:E:10:VAL:HG21  | 1:E:47:LEU:HD11  | 2.03                     | 0.40              |
| 1:E:29:MET:HE3   | 1:E:29:MET:HB2   | 1.81                     | 0.40              |
| 1:x:64:MET:O     | 1:x:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:y:200:LEU:HD23 | 1:y:200:LEU:HA   | 1.92                     | 0.40              |
| 1:S:221:HIS:O    | 1:S:224:GLU:HG2  | 2.21                     | 0.40              |
| 1:d:15:GLU:OE1   | 1:d:37:ARG:HG2   | 2.21                     | 0.40              |
| 1:I:108:GLY:O    | 1:I:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:p:254:ARG:HE   | 1:p:254:ARG:HB2  | 1.57                     | 0.40              |
| 1:0:64:MET:O     | 1:0:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:1:254:ARG:HE   | 1:1:254:ARG:HB2  | 1.60                     | 0.40              |
| 1:K:87:LEU:HD23  | 1:K:92:ARG:HD3   | 2.04                     | 0.40              |
| 1:V:34:GLU:HG3   | 1:s:85:ARG:NH2   | 2.36                     | 0.40              |
| 1:L:34:GLU:HG3   | 1:7:85:ARG:NH2   | 2.37                     | 0.40              |
| 1:L:203:ARG:NH1  | 1:L:206:GLU:OE2  | 2.55                     | 0.40              |
| 1:h:15:GLU:OE1   | 1:h:37:ARG:HG2   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:108:GLY:O    | 1:s:112:VAL:HG23 | 2.21                     | 0.40              |
| 1:t:203:ARG:NH1  | 1:t:206:GLU:OE2  | 2.55                     | 0.40              |
| 1:Y:71:GLU:O     | 1:Y:75:ARG:HG3   | 2.21                     | 0.40              |
| 1:Y:152:ILE:HG13 | 1:Y:247:VAL:HG11 | 2.04                     | 0.40              |
| 1:O:123:ILE:HG13 | 1:O:175:GLU:HG2  | 2.02                     | 0.40              |
| 1:Z:125:LEU:HD13 | 1:Z:125:LEU:HA   | 1.93                     | 0.40              |
| 1:Z:221:HIS:O    | 1:Z:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:v:242:PRO:HD2  | 1:v:245:LEU:HD22 | 2.02                     | 0.40              |
| 1:6:85:ARG:HD2   | 1:l:38:HIS:CE1   | 2.56                     | 0.40              |
| 1:a:29:MET:HB3   | 1:a:29:MET:HE2   | 1.77                     | 0.40              |
| 1:l:15:GLU:OE1   | 1:l:37:ARG:HG2   | 2.22                     | 0.40              |
| 1:l:151:ILE:O    | 1:l:155:LEU:HG   | 2.20                     | 0.40              |
| 1:Q:221:HIS:O    | 1:Q:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:R:108:GLY:O    | 1:R:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:y:221:HIS:O    | 1:y:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:H:62:LEU:HD11  | 1:H:66:ARG:NH1   | 2.37                     | 0.40              |
| 1:H:187:LEU:HD23 | 1:H:187:LEU:HA   | 1.93                     | 0.40              |
| 1:d:64:MET:O     | 1:d:67:GLU:HG3   | 2.21                     | 0.40              |
| 1:p:221:HIS:O    | 1:p:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:0:66:ARG:HD2   | 1:0:66:ARG:HA    | 1.86                     | 0.40              |
| 1:0:108:GLY:O    | 1:0:112:VAL:HG23 | 2.21                     | 0.40              |
| 1:1:15:GLU:OE1   | 1:1:37:ARG:HG2   | 2.22                     | 0.40              |
| 1:r:123:ILE:HG13 | 1:r:175:GLU:HG2  | 2.03                     | 0.40              |
| 1:2:254:ARG:HE   | 1:2:254:ARG:HB2  | 1.57                     | 0.40              |
| 1:3:108:GLY:O    | 1:3:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:X:56:ARG:HD2   | 1:u:56:ARG:CG    | 2.51                     | 0.40              |
| 1:t:15:GLU:OE1   | 1:t:37:ARG:HG2   | 2.22                     | 0.40              |
| 1:Y:108:GLY:O    | 1:Y:112:VAL:HG23 | 2.22                     | 0.40              |
| 1:j:110:VAL:HG23 | 1:j:165:ALA:HB1  | 2.03                     | 0.40              |
| 1:u:16:GLU:O     | 1:u:20:GLU:HG2   | 2.21                     | 0.40              |
| 1:u:156:GLU:CD   | 1:u:254:ARG:HH12 | 2.25                     | 0.40              |
| 1:5:71:GLU:O     | 1:5:75:ARG:HG3   | 2.22                     | 0.40              |
| 1:O:221:HIS:O    | 1:O:224:GLU:HG2  | 2.22                     | 0.40              |
| 1:6:110:VAL:HG23 | 1:6:165:ALA:HB1  | 2.02                     | 0.40              |
| 1:P:71:GLU:O     | 1:P:75:ARG:HG3   | 2.21                     | 0.40              |
| 1:7:7:VAL:O      | 1:7:11:ARG:HG3   | 2.21                     | 0.40              |
| 1:7:108:GLY:O    | 1:7:112:VAL:HG23 | 2.21                     | 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     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | 1     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | 2     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | 3     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | 4     | 256/281 (91%) | 250 (98%) | 5 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | 5     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | 6     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | 7     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | A     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | B     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | C     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | D     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | E     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | F     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | G     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | H     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | I     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | J     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | K     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | L     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | M     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | N     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | O     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | P     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | Q     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | R     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | S     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | T     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | U     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | V     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | W     | 256/281 (91%) | 250 (98%) | 5 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | X     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | Y     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | Z     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | a     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | b     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | c     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | d     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | e     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | f     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | g     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | h     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | i     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | j     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | k     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | l     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | m     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | n     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | o     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | p     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | q     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | r     | 256/281 (91%) | 249 (97%) | 6 (2%)  | 1 (0%)   | 30          | 60 |
| 1   | s     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | t     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | u     | 256/281 (91%) | 248 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | v     | 256/281 (91%) | 247 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|----------|-------------|----|
| 1   | w     | 256/281 (91%)     | 248 (97%)   | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | x     | 256/281 (91%)     | 248 (97%)   | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | y     | 256/281 (91%)     | 248 (97%)   | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | z     | 256/281 (91%)     | 247 (96%)   | 8 (3%)   | 1 (0%)   | 30          | 60 |
| All | All   | 15360/16860 (91%) | 14870 (97%) | 430 (3%) | 60 (0%)  | 31          | 60 |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 50  | ARG  |
| 1   | B     | 50  | ARG  |
| 1   | D     | 50  | ARG  |
| 1   | E     | 50  | ARG  |
| 1   | Q     | 50  | ARG  |
| 1   | b     | 50  | ARG  |
| 1   | x     | 50  | ARG  |
| 1   | G     | 50  | ARG  |
| 1   | R     | 50  | ARG  |
| 1   | c     | 50  | ARG  |
| 1   | y     | 50  | ARG  |
| 1   | H     | 50  | ARG  |
| 1   | d     | 50  | ARG  |
| 1   | o     | 50  | ARG  |
| 1   | z     | 50  | ARG  |
| 1   | T     | 50  | ARG  |
| 1   | p     | 50  | ARG  |
| 1   | 0     | 50  | ARG  |
| 1   | J     | 50  | ARG  |
| 1   | U     | 50  | ARG  |
| 1   | q     | 50  | ARG  |
| 1   | V     | 50  | ARG  |
| 1   | r     | 50  | ARG  |
| 1   | 2     | 50  | ARG  |
| 1   | L     | 50  | ARG  |
| 1   | h     | 50  | ARG  |
| 1   | s     | 50  | ARG  |
| 1   | M     | 50  | ARG  |
| 1   | X     | 50  | ARG  |
| 1   | t     | 50  | ARG  |
| 1   | N     | 50  | ARG  |
| 1   | j     | 50  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 50  | ARG  |
| 1   | Z     | 50  | ARG  |
| 1   | k     | 50  | ARG  |
| 1   | 6     | 50  | ARG  |
| 1   | a     | 50  | ARG  |
| 1   | w     | 50  | ARG  |
| 1   | 7     | 50  | ARG  |
| 1   | C     | 50  | ARG  |
| 1   | F     | 50  | ARG  |
| 1   | m     | 50  | ARG  |
| 1   | n     | 50  | ARG  |
| 1   | S     | 50  | ARG  |
| 1   | I     | 50  | ARG  |
| 1   | e     | 50  | ARG  |
| 1   | f     | 50  | ARG  |
| 1   | 1     | 50  | ARG  |
| 1   | K     | 50  | ARG  |
| 1   | g     | 50  | ARG  |
| 1   | W     | 50  | ARG  |
| 1   | 3     | 50  | ARG  |
| 1   | i     | 50  | ARG  |
| 1   | 4     | 50  | ARG  |
| 1   | Y     | 50  | ARG  |
| 1   | u     | 50  | ARG  |
| 1   | O     | 50  | ARG  |
| 1   | v     | 50  | ARG  |
| 1   | P     | 50  | ARG  |
| 1   | l     | 50  | ARG  |

### 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     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | 1     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | 2     | 195/213 (92%) | 193 (99%)  | 2 (1%)   | 68          | 78  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 3     | 195/213 (92%) | 193 (99%)  | 2 (1%)   | 68          | 78  |
| 1   | 4     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | 5     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | 6     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | 7     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | A     | 195/213 (92%) | 193 (99%)  | 2 (1%)   | 68          | 78  |
| 1   | B     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | C     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | D     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | E     | 195/213 (92%) | 193 (99%)  | 2 (1%)   | 68          | 78  |
| 1   | F     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | G     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | H     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | I     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | J     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | K     | 195/213 (92%) | 193 (99%)  | 2 (1%)   | 68          | 78  |
| 1   | L     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | M     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | N     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | O     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | P     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | Q     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | R     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | S     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | T     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | U     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | V     | 195/213 (92%) | 195 (100%) | 0        | 100         | 100 |
| 1   | W     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | X     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | Y     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |
| 1   | Z     | 195/213 (92%) | 194 (100%) | 1 (0%)   | 81          | 83  |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 1   | a     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | b     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | c     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | d     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | e     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | f     | 195/213 (92%)     | 193 (99%)    | 2 (1%)   | 68          | 78  |
| 1   | g     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | h     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | i     | 195/213 (92%)     | 192 (98%)    | 3 (2%)   | 57          | 73  |
| 1   | j     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | k     | 195/213 (92%)     | 193 (99%)    | 2 (1%)   | 68          | 78  |
| 1   | l     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | m     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | n     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | o     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | p     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | q     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | r     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | s     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | t     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | u     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | v     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | w     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | x     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| 1   | y     | 195/213 (92%)     | 195 (100%)   | 0        | 100         | 100 |
| 1   | z     | 195/213 (92%)     | 194 (100%)   | 1 (0%)   | 81          | 83  |
| All | All   | 11700/12780 (92%) | 11661 (100%) | 39 (0%)  | 84          | 86  |

All (39) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | GLU  |
| 1   | A     | 149 | ARG  |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 41  | GLU  |
| 1   | E     | 83  | GLU  |
| 1   | Q     | 83  | GLU  |
| 1   | b     | 83  | GLU  |
| 1   | m     | 83  | GLU  |
| 1   | x     | 41  | GLU  |
| 1   | G     | 83  | GLU  |
| 1   | R     | 83  | GLU  |
| 1   | d     | 83  | GLU  |
| 1   | z     | 83  | GLU  |
| 1   | I     | 83  | GLU  |
| 1   | e     | 110 | VAL  |
| 1   | 0     | 83  | GLU  |
| 1   | U     | 83  | GLU  |
| 1   | f     | 83  | GLU  |
| 1   | f     | 149 | ARG  |
| 1   | K     | 83  | GLU  |
| 1   | K     | 149 | ARG  |
| 1   | 2     | 41  | GLU  |
| 1   | 2     | 83  | GLU  |
| 1   | W     | 41  | GLU  |
| 1   | s     | 83  | GLU  |
| 1   | 3     | 83  | GLU  |
| 1   | 3     | 149 | ARG  |
| 1   | M     | 224 | GLU  |
| 1   | X     | 41  | GLU  |
| 1   | i     | 83  | GLU  |
| 1   | i     | 149 | ARG  |
| 1   | i     | 231 | HIS  |
| 1   | N     | 83  | GLU  |
| 1   | Y     | 83  | GLU  |
| 1   | Z     | 83  | GLU  |
| 1   | k     | 41  | GLU  |
| 1   | k     | 83  | GLU  |
| 1   | v     | 83  | GLU  |
| 1   | P     | 83  | GLU  |
| 1   | l     | 110 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 231 | HIS  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 121 | GLN  |
| 1   | C     | 231 | HIS  |
| 1   | D     | 231 | HIS  |
| 1   | F     | 121 | GLN  |
| 1   | Q     | 231 | HIS  |
| 1   | b     | 231 | HIS  |
| 1   | x     | 231 | HIS  |
| 1   | c     | 194 | GLN  |
| 1   | c     | 231 | HIS  |
| 1   | n     | 121 | GLN  |
| 1   | y     | 231 | HIS  |
| 1   | H     | 231 | HIS  |
| 1   | d     | 231 | HIS  |
| 1   | o     | 231 | HIS  |
| 1   | e     | 121 | GLN  |
| 1   | J     | 231 | HIS  |
| 1   | U     | 231 | HIS  |
| 1   | V     | 194 | GLN  |
| 1   | g     | 121 | GLN  |
| 1   | r     | 231 | HIS  |
| 1   | 2     | 231 | HIS  |
| 1   | W     | 121 | GLN  |
| 1   | s     | 231 | HIS  |
| 1   | M     | 231 | HIS  |
| 1   | X     | 231 | HIS  |
| 1   | 4     | 121 | GLN  |
| 1   | 4     | 231 | HIS  |
| 1   | N     | 231 | HIS  |
| 1   | j     | 231 | HIS  |
| 1   | u     | 121 | GLN  |
| 1   | 5     | 231 | HIS  |
| 1   | O     | 121 | GLN  |
| 1   | Z     | 231 | HIS  |
| 1   | k     | 231 | HIS  |
| 1   | l     | 121 | GLN  |
| 1   | w     | 231 | HIS  |
| 1   | 7     | 231 | HIS  |

### 5.3.3 RNA ⓘ

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](#)

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

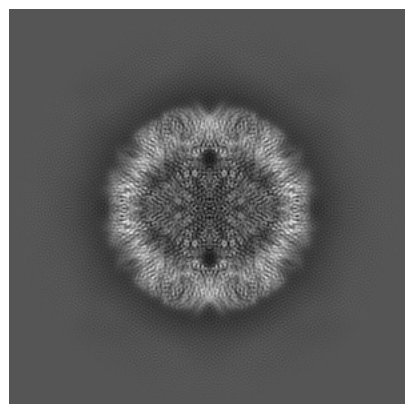
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62165. These allow visual inspection of the internal detail of the map and identification of artifacts.

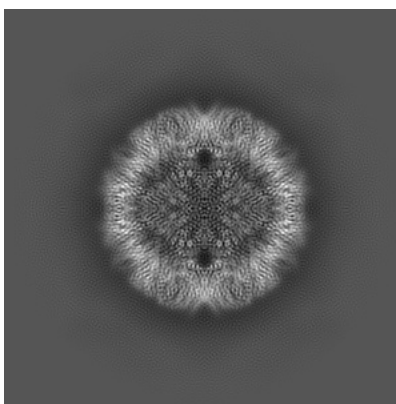
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

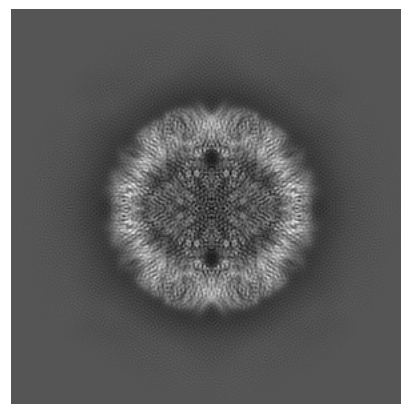
#### 6.1.1 Primary map



X

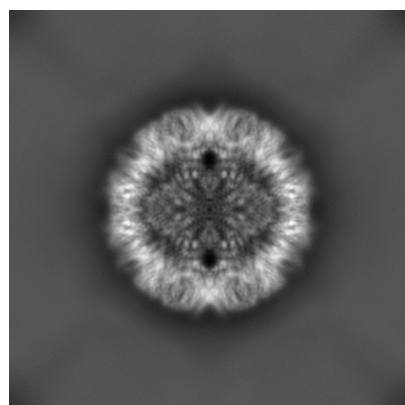


Y

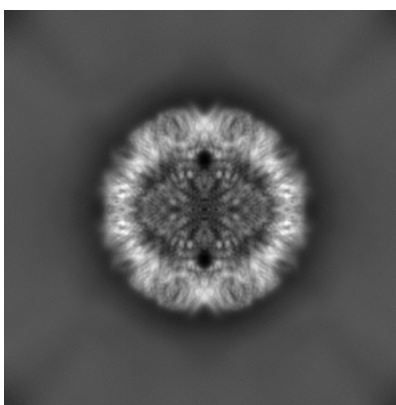


Z

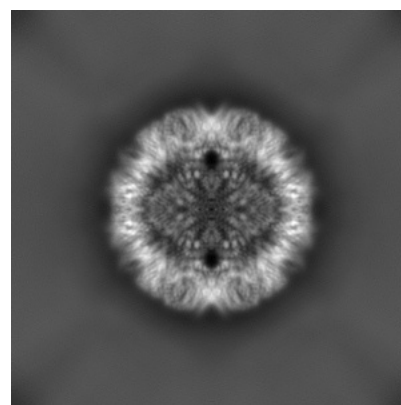
#### 6.1.2 Raw map



X



Y

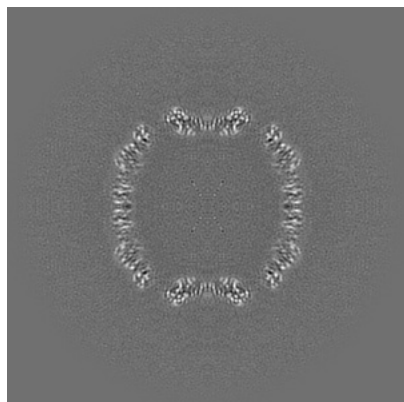


Z

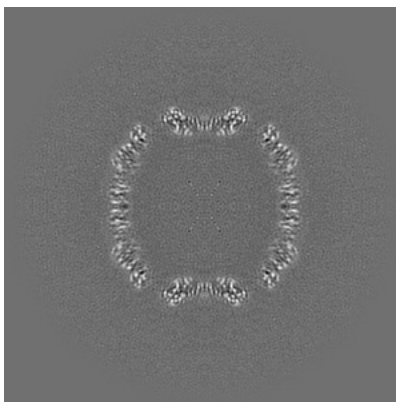
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

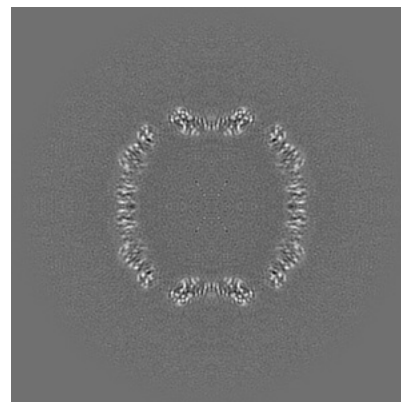
### 6.2.1 Primary map



X Index: 180

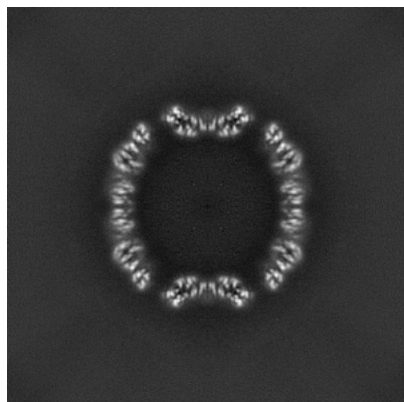


Y Index: 180

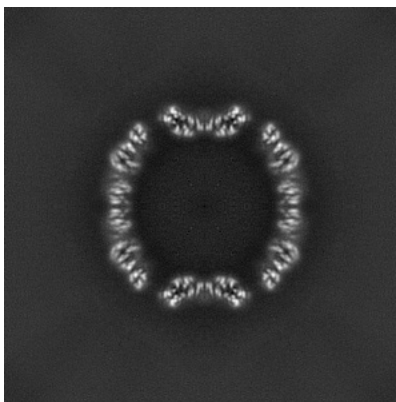


Z Index: 180

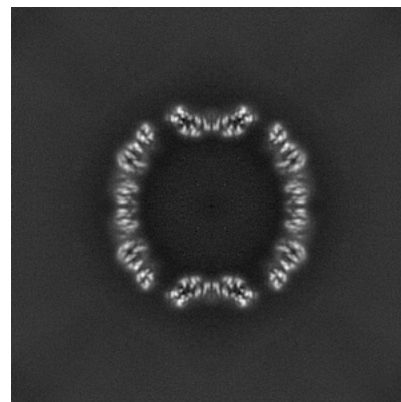
### 6.2.2 Raw map



X Index: 180



Y Index: 180

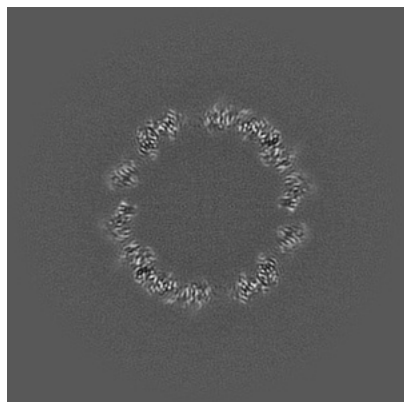


Z Index: 180

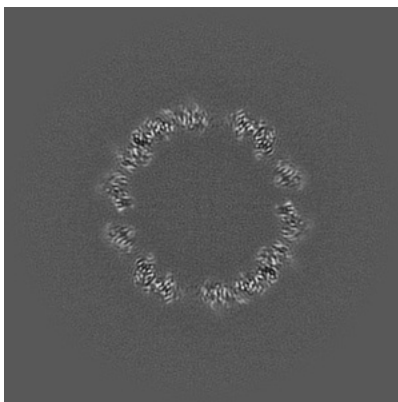
The images above show central slices of the map in three orthogonal directions.

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

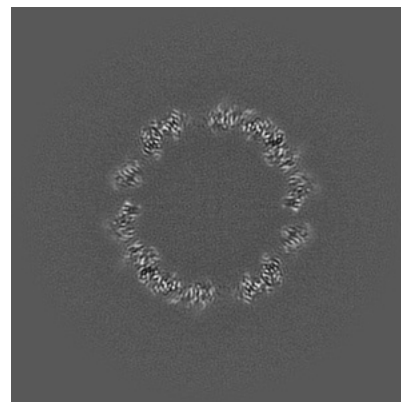
### 6.3.1 Primary map



X Index: 193

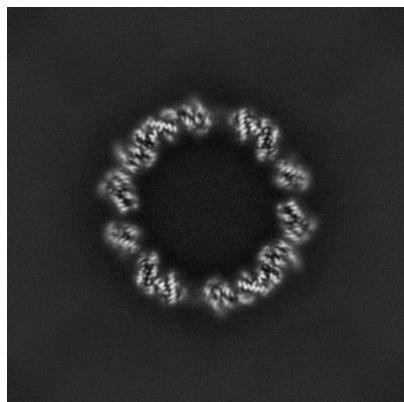


Y Index: 167

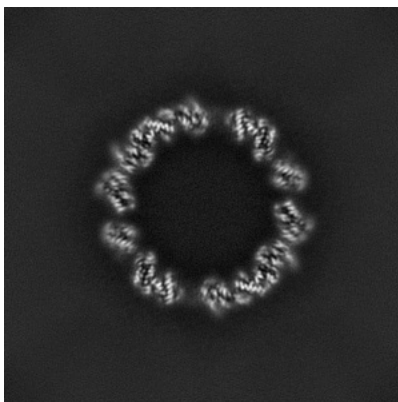


Z Index: 193

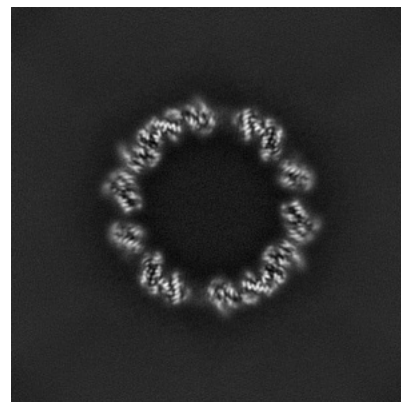
### 6.3.2 Raw map



X Index: 167



Y Index: 167

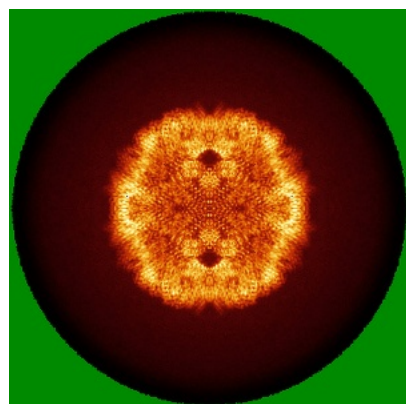


Z Index: 167

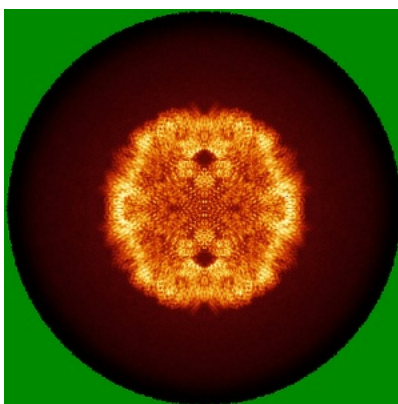
The images above show the largest variance slices of the map in three orthogonal directions.

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

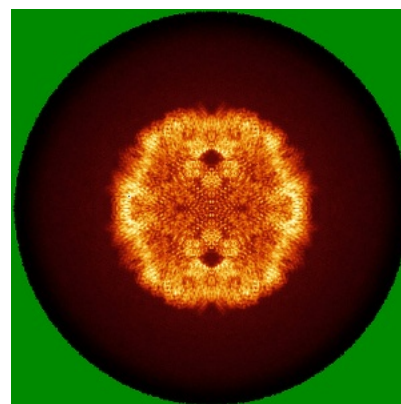
### 6.4.1 Primary map



X

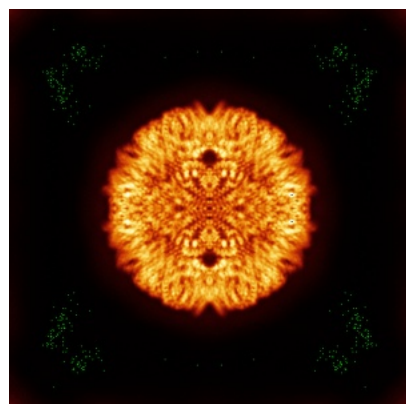


Y

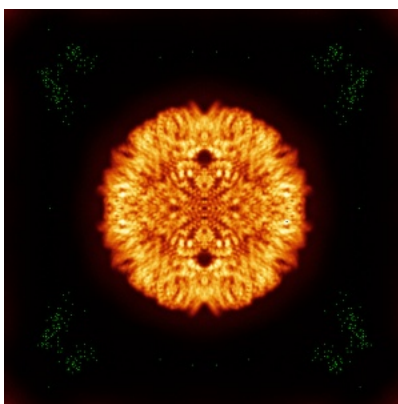


Z

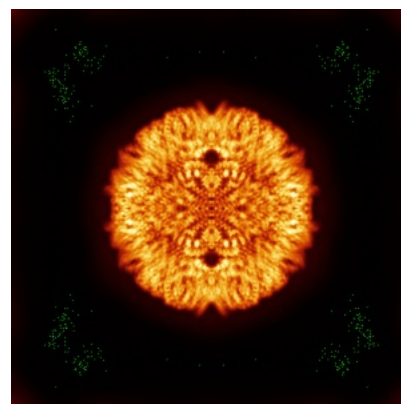
### 6.4.2 Raw map



X



Y

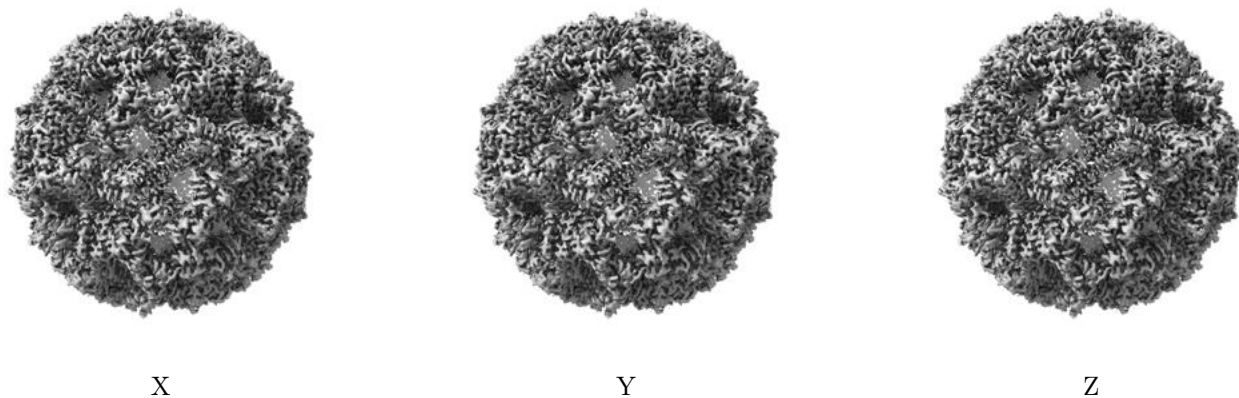


Z

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.

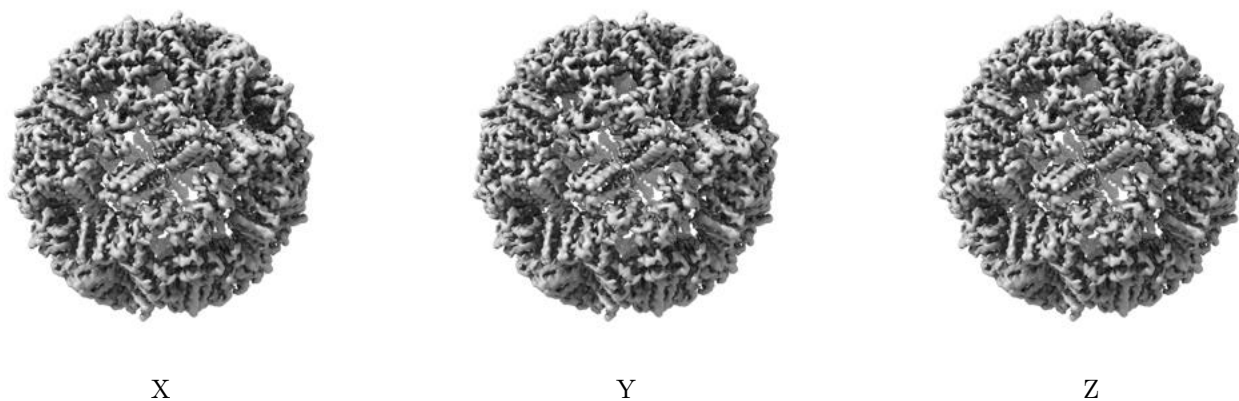
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

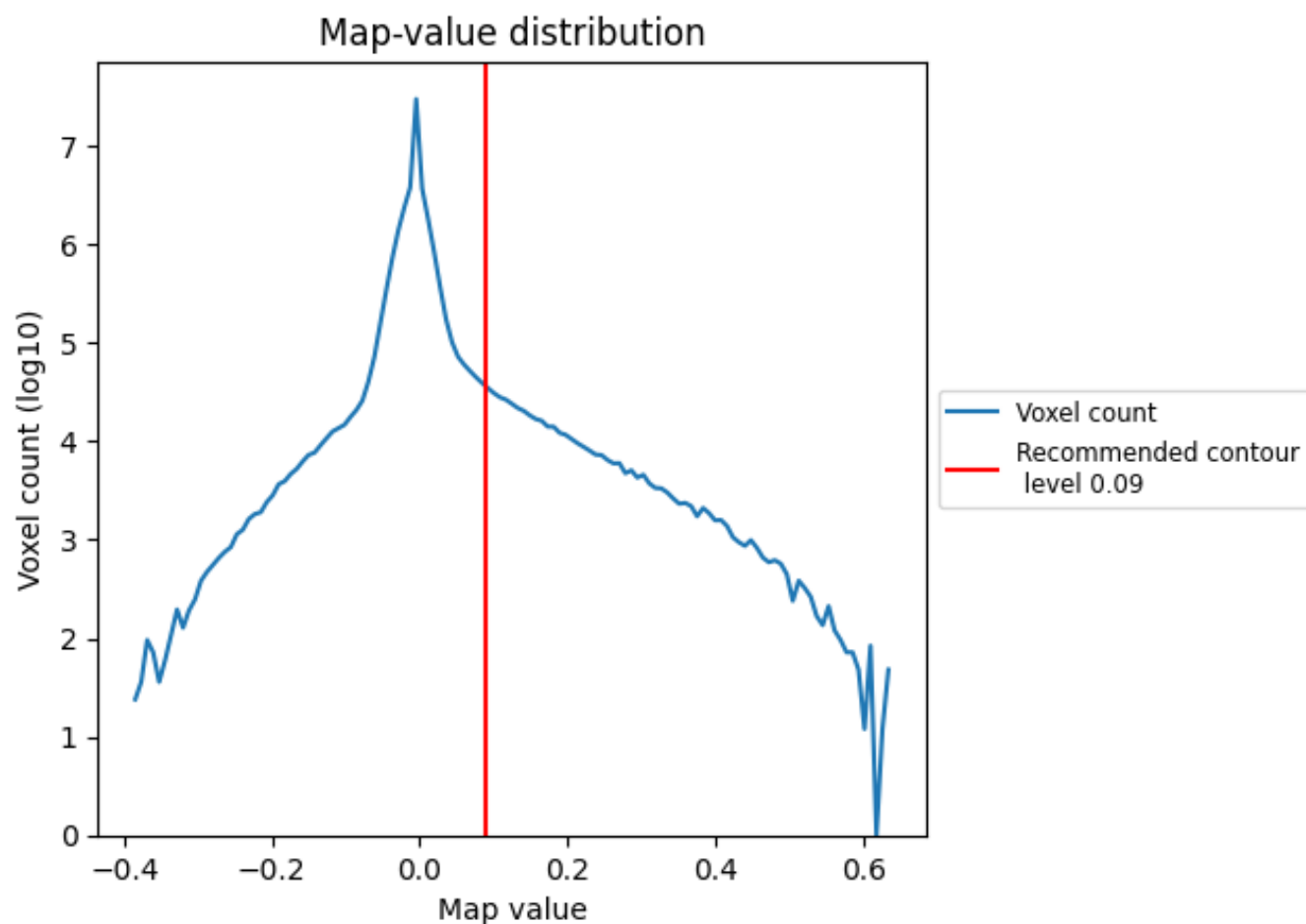
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

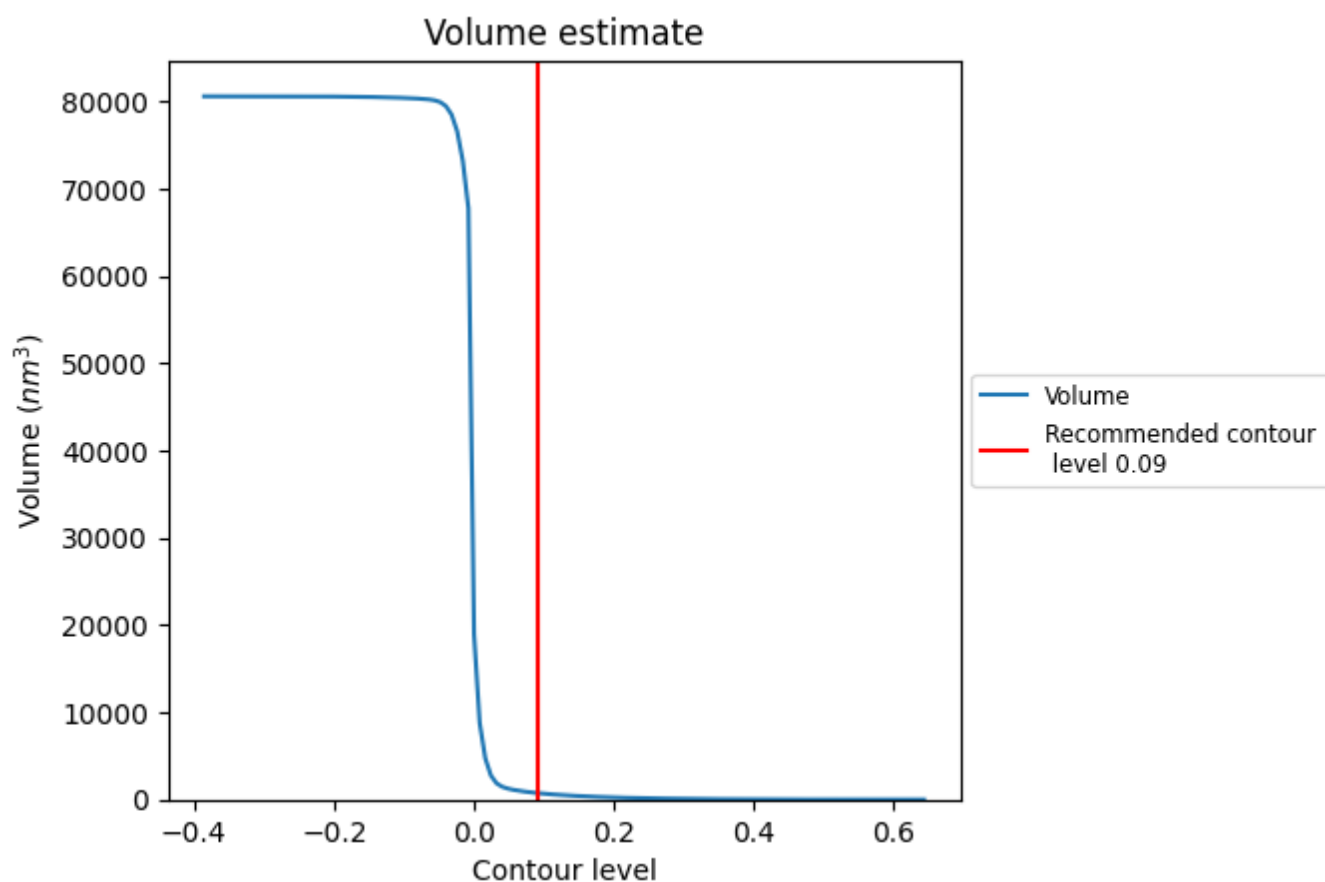
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

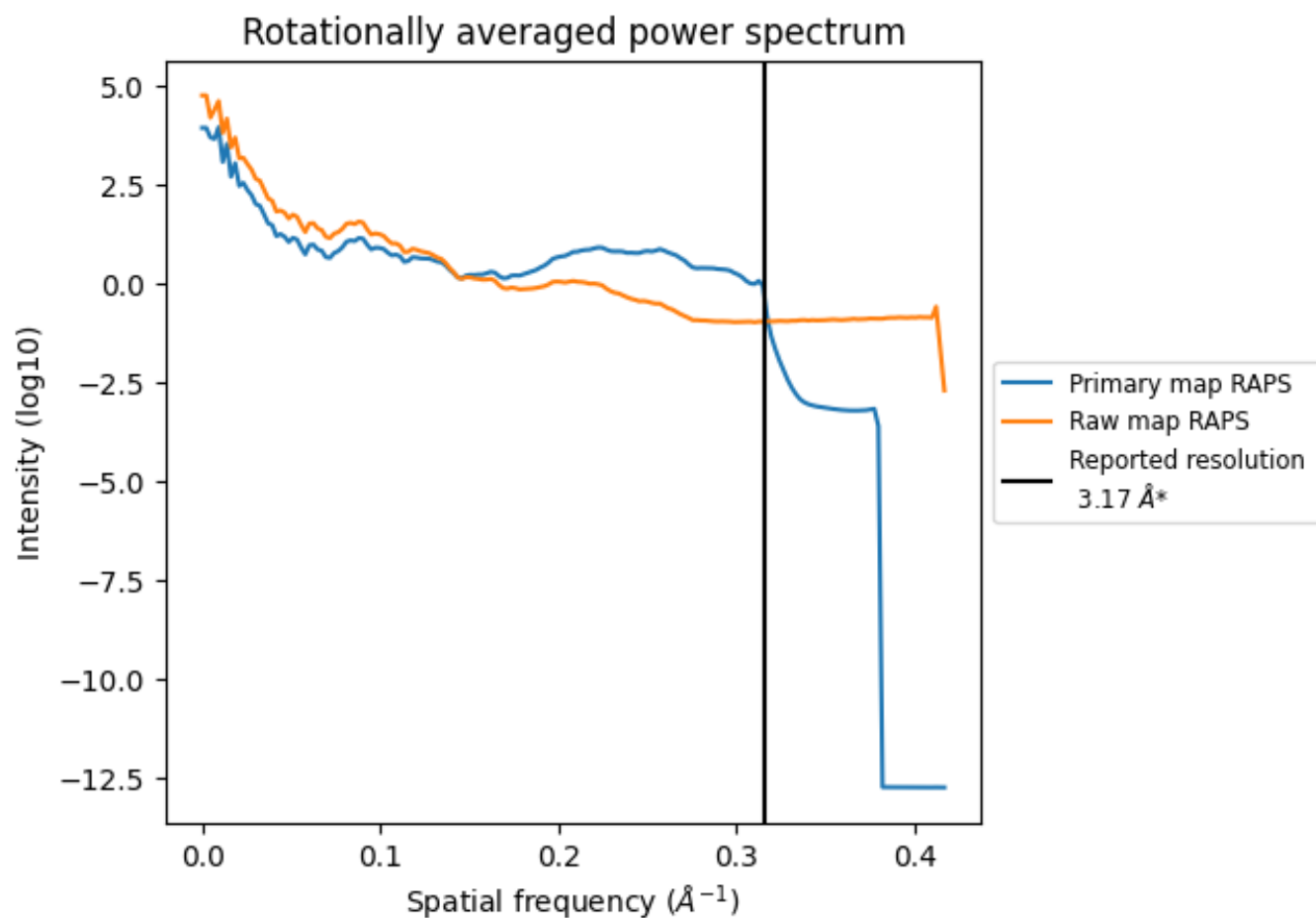
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 749 nm<sup>3</sup>; this corresponds to an approximate mass of 676 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

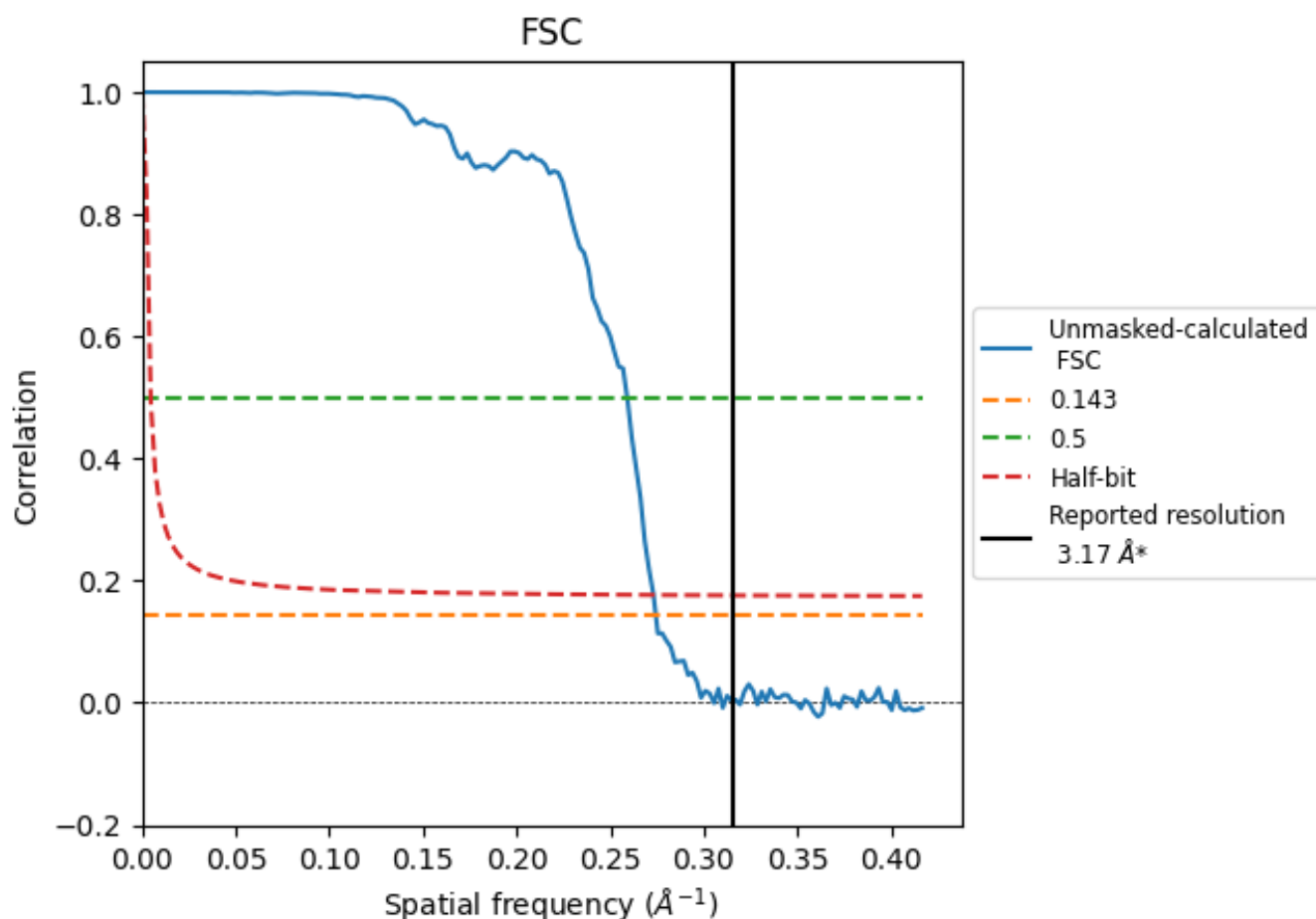


\*Reported resolution corresponds to spatial frequency of  $0.315 \text{ \AA}^{-1}$

## 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  $0.315 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

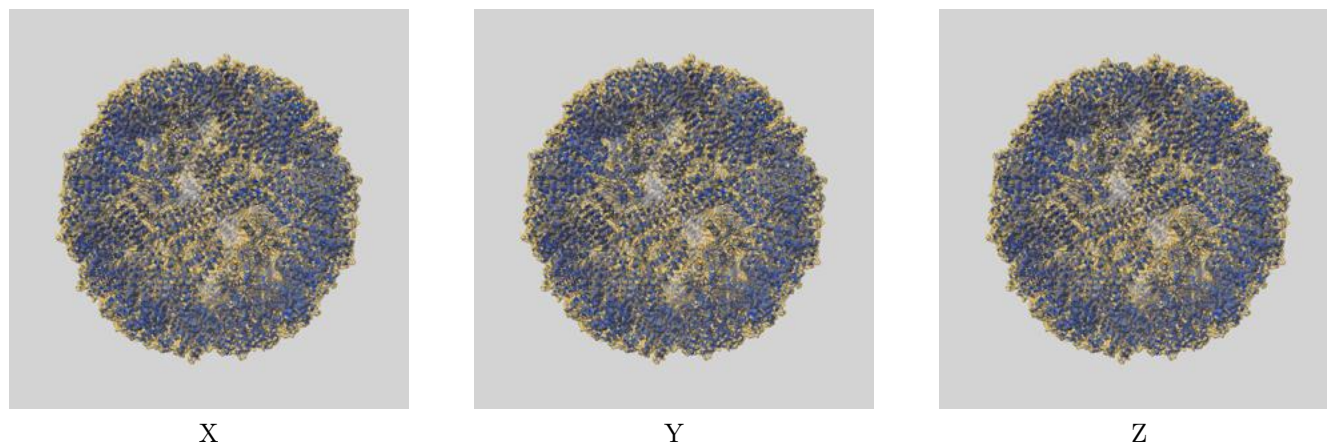
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.17                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.64                               | 3.86 | 3.66     |

\*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 3.64 differs from the reported value 3.17 by more than 10 %

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

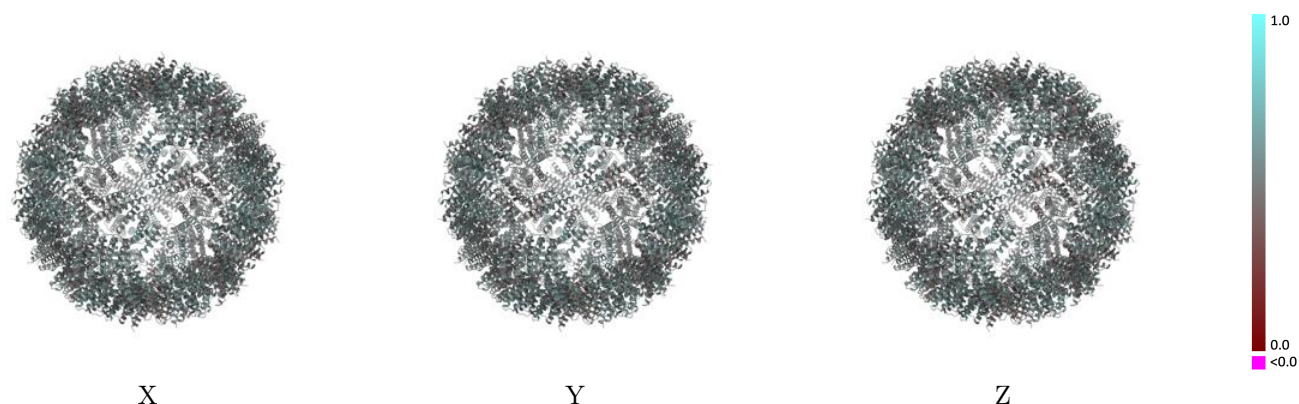
This section contains information regarding the fit between EMDB map EMD-62165 and PDB model 9K89. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



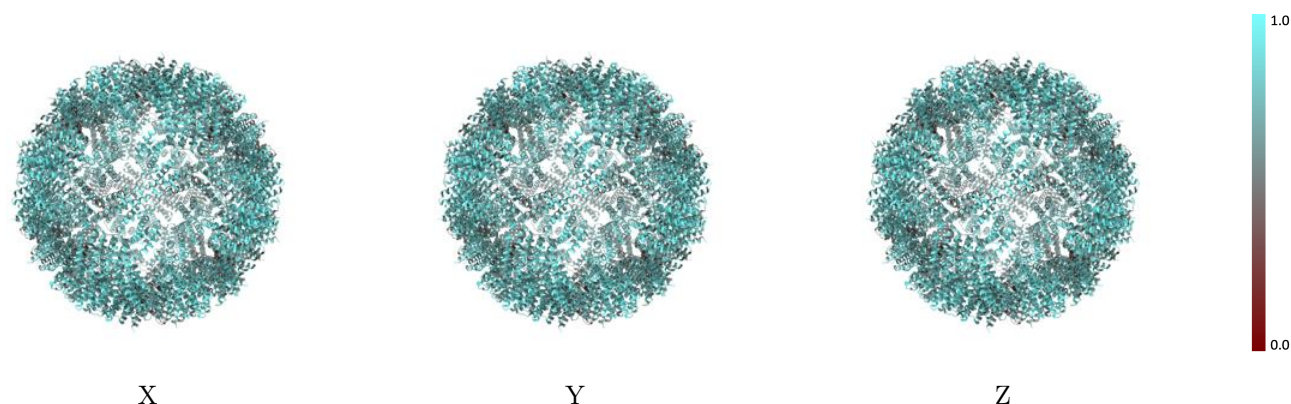
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



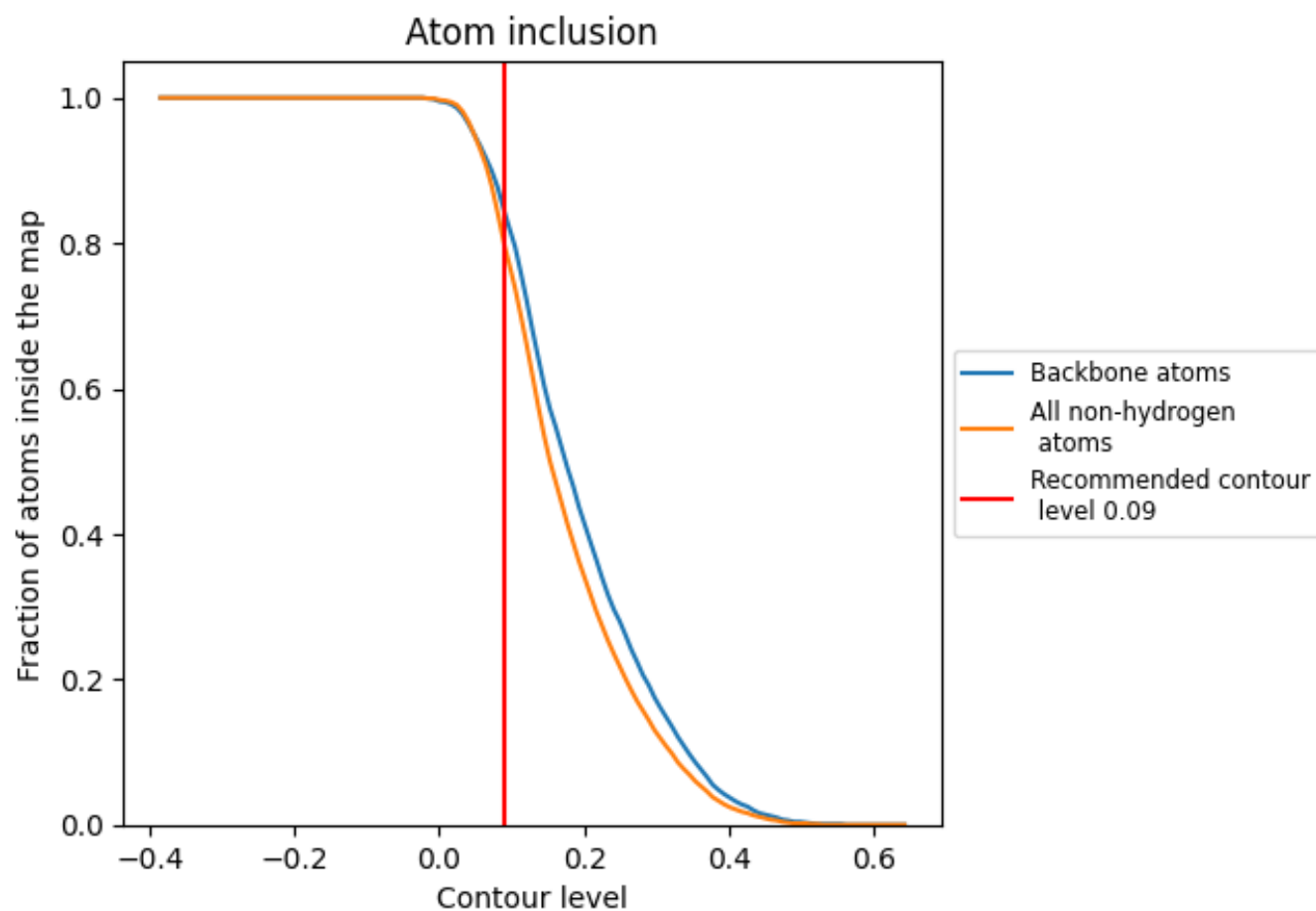
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.09) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7970   |  0.5170   |
| 0     |  0.7990   |  0.5180   |
| 1     |  0.7930   |  0.5140   |
| 2     |  0.7990   |  0.5170   |
| 3     |  0.7990   |  0.5190   |
| 4     |  0.7940   |  0.5130   |
| 5     |  0.7920   |  0.5180   |
| 6     |  0.7990   |  0.5180   |
| 7     |  0.7970   |  0.5160   |
| A     |  0.8000   |  0.5180   |
| B     |  0.7980   |  0.5200   |
| C     |  0.7950   |  0.5180   |
| D     |  0.7960   |  0.5190   |
| E     |  0.7970   |  0.5170   |
| F     |  0.7960  |  0.5180  |
| G     |  0.8000 |  0.5140 |
| H     |  0.7970 |  0.5170 |
| I     |  0.8000 |  0.5170 |
| J     |  0.7940 |  0.5140 |
| K     |  0.8000 |  0.5180 |
| L     |  0.8000 |  0.5170 |
| M     |  0.7940 |  0.5180 |
| N     |  0.7990 |  0.5190 |
| O     |  0.7960 |  0.5190 |
| P     |  0.8000 |  0.5160 |
| Q     |  0.7970 |  0.5170 |
| R     |  0.8010 |  0.5160 |
| S     |  0.7960 |  0.5180 |
| T     |  0.7940 |  0.5120 |
| U     |  0.8000 |  0.5160 |
| V     |  0.7940 |  0.5160 |
| W     |  0.7970 |  0.5130 |
| X     |  0.8000 |  0.5180 |
| Y     |  0.8010 |  0.5180 |
| Z     |  0.7970 |  0.5170 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.7950   |  0.5170   |
| b     |  0.7990   |  0.5180   |
| c     |  0.7980   |  0.5160   |
| d     |  0.7950   |  0.5170   |
| e     |  0.7960   |  0.5130   |
| f     |  0.8030   |  0.5170   |
| g     |  0.7930   |  0.5180   |
| h     |  0.7950   |  0.5140   |
| i     |  0.8020   |  0.5170   |
| j     |  0.7960   |  0.5160   |
| k     |  0.7990   |  0.5130   |
| l     |  0.7950   |  0.5180   |
| m     |  0.8000   |  0.5180   |
| n     |  0.7940   |  0.5190   |
| o     |  0.8000   |  0.5200   |
| p     |  0.7950   |  0.5180   |
| q     |  0.7970   |  0.5150   |
| r     |  0.7960  |  0.5170  |
| s     |  0.8000 |  0.5160 |
| t     |  0.7960 |  0.5100 |
| u     |  0.7920 |  0.5180 |
| v     |  0.8020 |  0.5140 |
| w     |  0.7950 |  0.5200 |
| x     |  0.7950 |  0.5160 |
| y     |  0.7950 |  0.5170 |
| z     |  0.8010 |  0.5170 |