



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 07:08 pm GMT

PDB ID : 6T34  
EMDB ID : EMD-10373  
Title : Atomic model for Turnip mosaic virus (TuMV)  
Authors : Valle, M.V.; Cuesta, R.  
Deposited on : 2019-10-10  
Resolution : 5.20 Å (reported)  
Based on initial model : 5ODV

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:

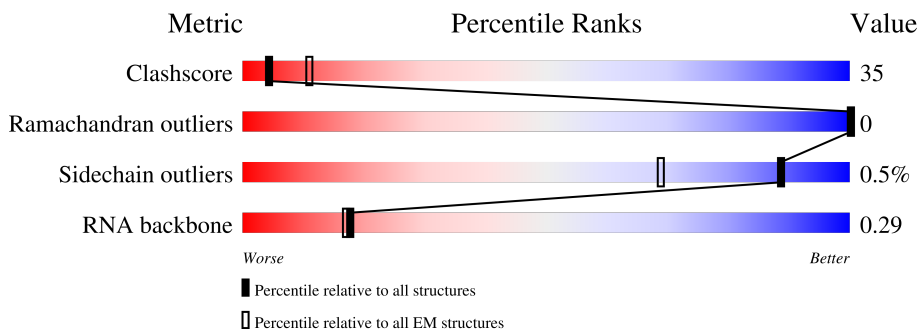
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 5.20 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.









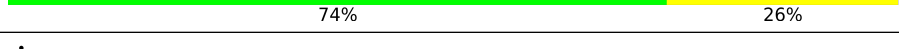
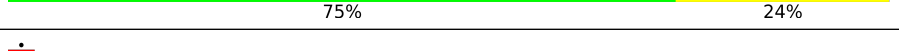
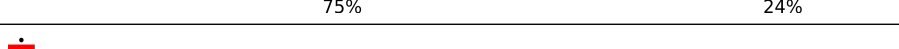
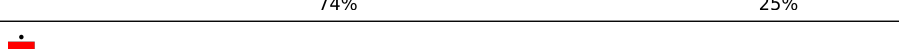
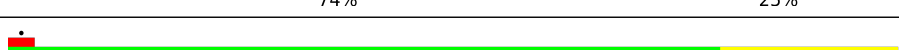

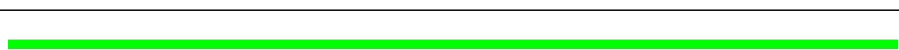
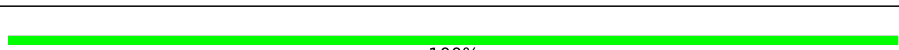
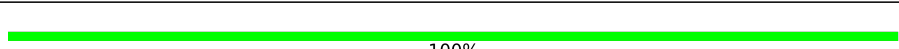

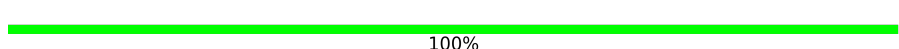
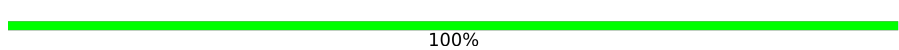
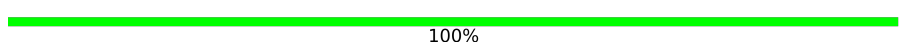
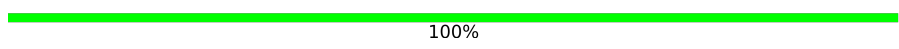
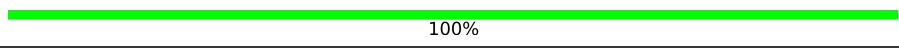
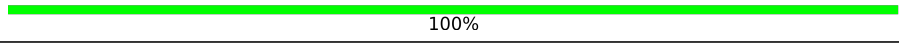
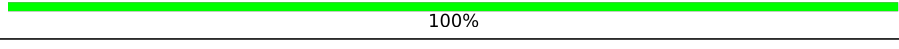
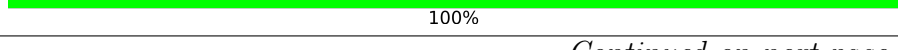

| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers    | 154315                   | 3826                     |
| RNA backbone          | 4643                     | 859                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 207    | 78% 22%          |
| 1   | B     | 207    | 72% 27%          |
| 1   | C     | 207    | 73% 26%          |
| 1   | D     | 207    | 73% 26%          |
| 1   | E     | 207    | 74% 26%          |
| 1   | F     | 207    | 73% 27%          |
| 1   | G     | 207    | 73% 27%          |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 1   | H     | 207    |  73% 27%   |
| 1   | I     | 207    |  71% 29%   |
| 1   | J     | 207    |  70% 29%   |
| 1   | K     | 207    |  71% 29%   |
| 1   | L     | 207    |  74% 25%   |
| 1   | M     | 207    |  74% 25%   |
| 1   | N     | 207    |  74% 26%   |
| 1   | O     | 207    |  75% 24%   |
| 1   | P     | 207    |  75% 24%   |
| 1   | Q     | 207    |  74% 25%   |
| 1   | R     | 207    |  74% 25%   |
| 1   | S     | 207    |  80% 20% |
| 2   | a     | 5      |  100%    |
| 2   | b     | 5      |  100%    |
| 2   | c     | 5      |  100%    |
| 2   | d     | 5      |  100%    |
| 2   | e     | 5      |  100%    |
| 2   | f     | 5      |  100%    |
| 2   | g     | 5      |  100%    |
| 2   | h     | 5      |  100%    |
| 2   | i     | 5      |  100%    |
| 2   | j     | 5      |  100%    |
| 2   | k     | 5      |  100%    |
| 2   | l     | 5      |  100%    |
| 2   | m     | 5      |  100%    |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 2   | n     | 5      |  100% |
| 2   | o     | 5      |  100% |
| 2   | p     | 5      |  100% |
| 2   | q     | 5      |  100% |
| 2   | r     | 5      |  100% |
| 2   | s     | 5      |  100% |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 65474 atoms, of which 31559 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 Coat protein.

| Mol | Chain | Residues | Atoms |      |      |     |     | AltConf | Trace |   |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
|     |       |          | Total | C    | H    | N   | O   |         |       | S |
| 1   | A     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | B     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | C     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | D     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | E     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | F     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | G     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | H     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | I     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | J     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | K     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | L     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | M     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | N     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | O     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | P     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |
| 1   | Q     | 207      | 3335  | 1056 | 1650 | 301 | 315 | 13      | 0     | 0 |

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| Mol | Chain | Residues | Atoms |      |      |     |     | AltConf | Trace |   |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| 1   | R     | 207      | Total | C    | H    | N   | O   | S       | 0     | 0 |
|     |       |          | 3335  | 1056 | 1650 | 301 | 315 | 13      |       |   |
| 1   | S     | 207      | Total | C    | H    | N   | O   | S       | 0     | 0 |
|     |       |          | 3335  | 1056 | 1650 | 301 | 315 | 13      |       |   |

- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3').

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |   |
|-----|-------|----------|-------|----|----|----|----|---------|-------|---|
| 2   | a     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | b     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | c     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | d     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | e     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | f     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | g     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | h     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | i     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | j     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | k     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | l     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | m     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | n     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | o     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | p     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | q     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |

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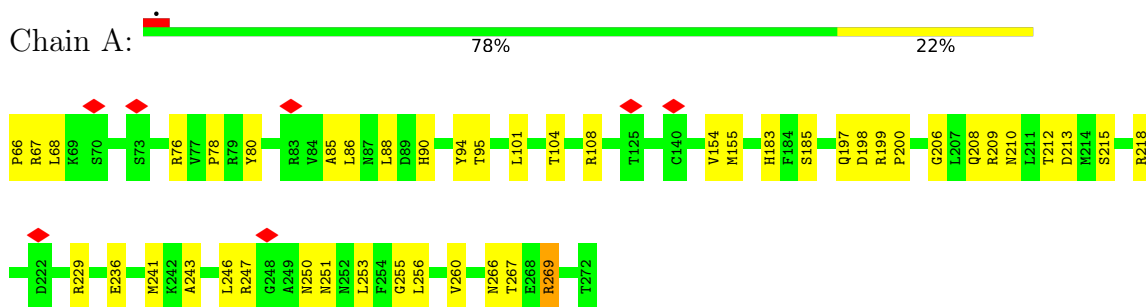
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| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |   |
|-----|-------|----------|-------|----|----|----|----|---------|-------|---|
|     |       |          | Total | C  | H  | N  | O  |         |       | P |
| 2   | r     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |
| 2   | s     | 5        | Total | C  | H  | N  | O  | P       | 0     | 0 |
|     |       |          | 111   | 45 | 11 | 10 | 40 | 5       |       |   |

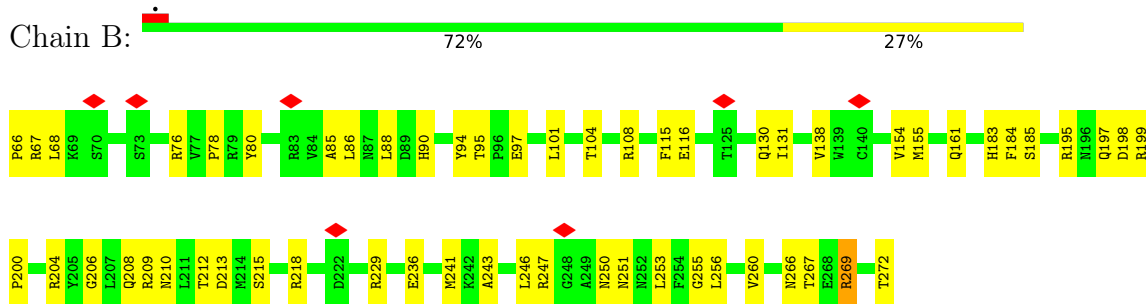
### 3 Residue-property plots [i](#)

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

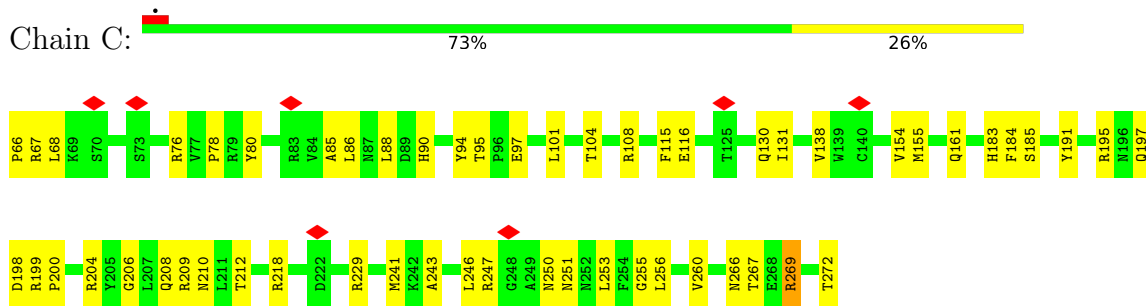
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



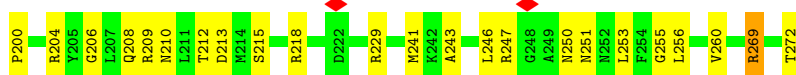
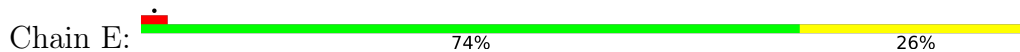
- Molecule 1: Coat protein



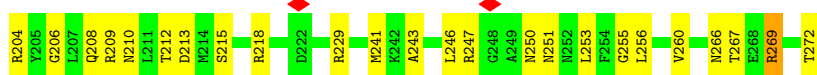




• Molecule 1: Coat protein



• Molecule 1: Coat protein

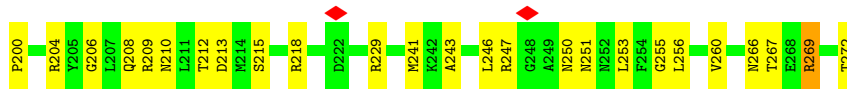


• Molecule 1: Coat protein



• Molecule 1: Coat protein





• Molecule 1: Coat protein



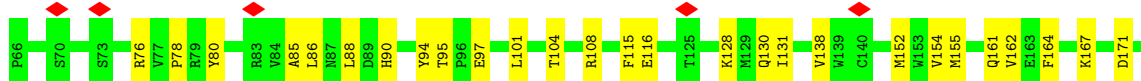
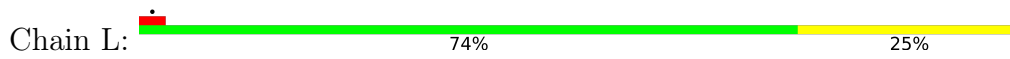
• Molecule 1: Coat protein



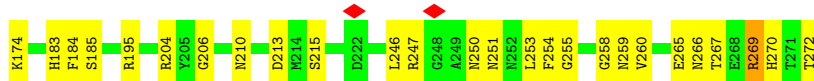
• Molecule 1: Coat protein

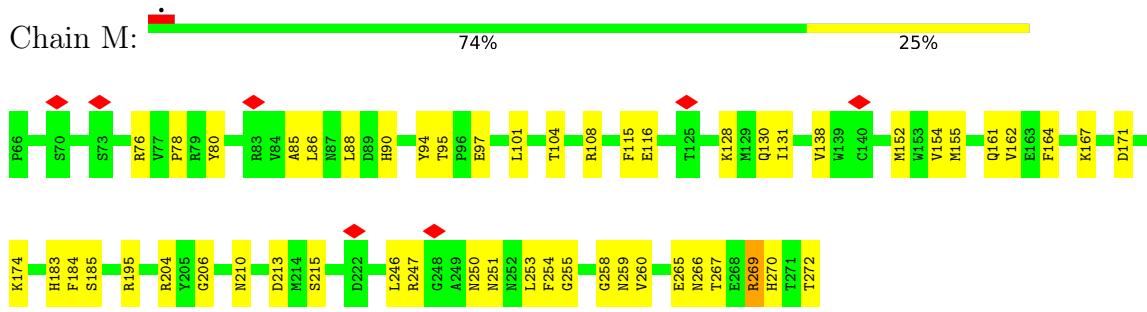


• Molecule 1: Coat protein

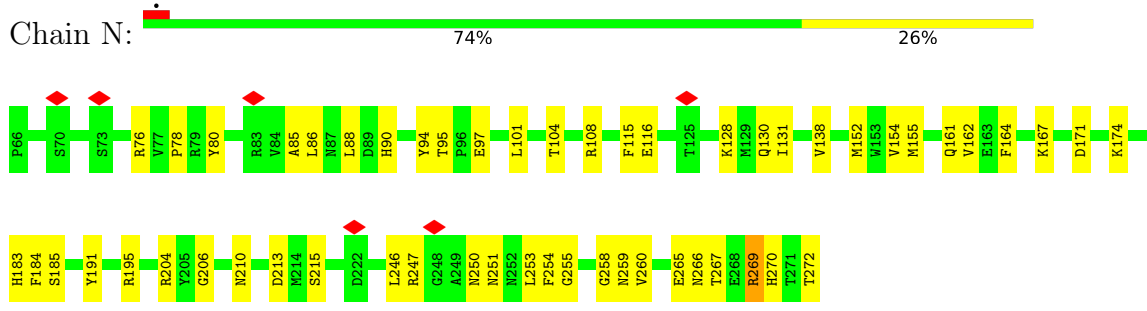


• Molecule 1: Coat protein

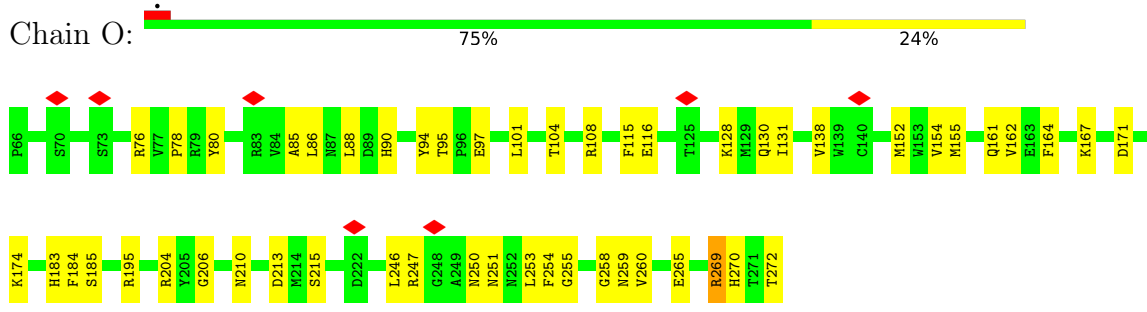




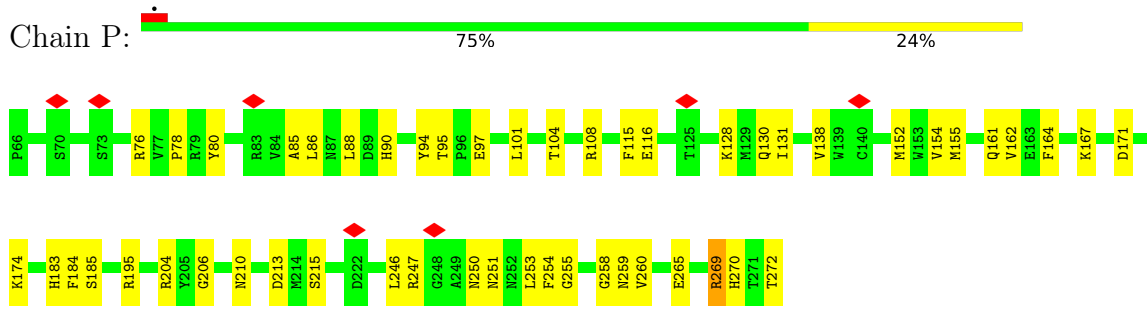
• Molecule 1: Coat protein



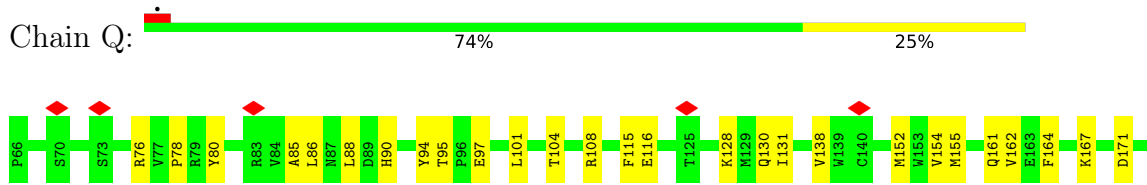
• Molecule 1: Coat protein

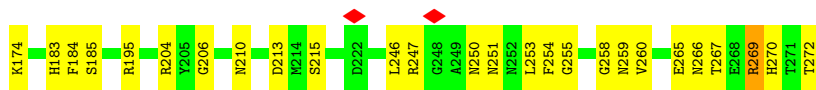


• Molecule 1: Coat protein

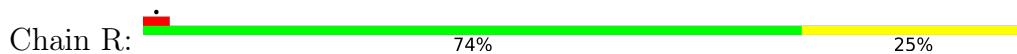


• Molecule 1: Coat protein

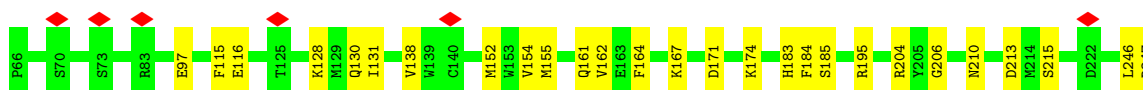
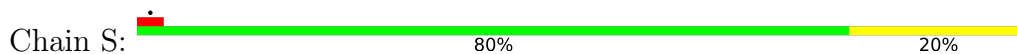




- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*UP\*U)-3')

Chain s:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

| Property                           | Value                                         | Source    |
|------------------------------------|-----------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                       | Depositor |
| Imposed symmetry                   | HELICAL, twist=-40.8°, rise=4 Å, axial sym=C1 | Depositor |
| Number of segments used            | 194432                                        | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                             | Depositor |
| CTF correction method              | PHASE FLIPPING ONLY                           | Depositor |
| Microscope                         | FEI TITAN KRIOS                               | Depositor |
| Voltage (kV)                       | 300                                           | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 40                                            | Depositor |
| Minimum defocus (nm)               | Not provided                                  |           |
| Maximum defocus (nm)               | Not provided                                  |           |
| Magnification                      | Not provided                                  |           |
| Image detector                     | GATAN K2 SUMMIT (4k x 4k)                     | Depositor |
| Maximum map value                  | 0.142                                         | Depositor |
| Minimum map value                  | -0.083                                        | Depositor |
| Average map value                  | 0.003                                         | Depositor |
| Map value standard deviation       | 0.013                                         | Depositor |
| Recommended contour level          | 0.03                                          | Depositor |
| Map size (Å)                       | 275.0, 275.0, 275.0                           | wwPDB     |
| Map dimensions                     | 250, 250, 250                                 | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                              | wwPDB     |
| Pixel spacing (Å)                  | 1.1, 1.1, 1.1                                 | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | B     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | C     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | D     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | E     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | F     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | G     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | H     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | I     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | J     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | K     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | L     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | M     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | N     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | O     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | P     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | Q     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | R     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 1   | S     | 0.49         | 0/1721  | 0.63        | 0/2326  |
| 2   | a     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | b     | 0.39         | 0/109   | 0.97        | 0/166   |
| 2   | c     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | d     | 0.40         | 0/109   | 0.95        | 0/166   |
| 2   | e     | 0.40         | 0/109   | 0.97        | 0/166   |
| 2   | f     | 0.40         | 0/109   | 0.96        | 0/166   |
| 2   | g     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | h     | 0.41         | 0/109   | 0.95        | 0/166   |
| 2   | i     | 0.39         | 0/109   | 0.97        | 0/166   |
| 2   | j     | 0.40         | 0/109   | 0.96        | 0/166   |
| 2   | k     | 0.40         | 0/109   | 0.96        | 0/166   |
| 2   | l     | 0.40         | 0/109   | 0.96        | 0/166   |
| 2   | m     | 0.40         | 0/109   | 0.96        | 0/166   |
| 2   | n     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | o     | 0.41         | 0/109   | 0.95        | 0/166   |



| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 2   | p     | 0.39         | 0/109   | 0.97        | 0/166   |
| 2   | q     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | r     | 0.39         | 0/109   | 0.96        | 0/166   |
| 2   | s     | 0.40         | 0/109   | 0.96        | 0/166   |
| All | All   | 0.49         | 0/34770 | 0.66        | 0/47348 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1685  | 1650     | 1652     | 159     | 0            |
| 1   | B     | 1685  | 1650     | 1648     | 230     | 0            |
| 1   | C     | 1685  | 1650     | 1648     | 223     | 0            |
| 1   | D     | 1685  | 1650     | 1648     | 223     | 0            |
| 1   | E     | 1685  | 1650     | 1648     | 226     | 0            |
| 1   | F     | 1685  | 1650     | 1648     | 227     | 0            |
| 1   | G     | 1685  | 1650     | 1648     | 226     | 0            |
| 1   | H     | 1685  | 1650     | 1648     | 224     | 0            |
| 1   | I     | 1685  | 1650     | 1646     | 250     | 0            |
| 1   | J     | 1685  | 1650     | 1647     | 261     | 0            |
| 1   | K     | 1685  | 1650     | 1646     | 251     | 0            |
| 1   | L     | 1685  | 1650     | 1646     | 222     | 0            |
| 1   | M     | 1685  | 1650     | 1646     | 224     | 0            |
| 1   | N     | 1685  | 1650     | 1646     | 227     | 0            |
| 1   | O     | 1685  | 1650     | 1646     | 226     | 0            |
| 1   | P     | 1685  | 1650     | 1646     | 222     | 0            |
| 1   | Q     | 1685  | 1650     | 1646     | 222     | 0            |
| 1   | R     | 1685  | 1650     | 1647     | 228     | 0            |
| 1   | S     | 1685  | 1650     | 1647     | 157     | 0            |
| 2   | a     | 100   | 11       | 51       | 0       | 0            |
| 2   | b     | 100   | 11       | 51       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | c     | 100   | 11       | 51       | 0       | 0            |
| 2   | d     | 100   | 11       | 51       | 0       | 0            |
| 2   | e     | 100   | 11       | 51       | 0       | 0            |
| 2   | f     | 100   | 11       | 51       | 0       | 0            |
| 2   | g     | 100   | 11       | 51       | 0       | 0            |
| 2   | h     | 100   | 11       | 51       | 0       | 0            |
| 2   | i     | 100   | 11       | 51       | 0       | 0            |
| 2   | j     | 100   | 11       | 51       | 0       | 0            |
| 2   | k     | 100   | 11       | 51       | 0       | 0            |
| 2   | l     | 100   | 11       | 51       | 0       | 0            |
| 2   | m     | 100   | 11       | 51       | 0       | 0            |
| 2   | n     | 100   | 11       | 51       | 0       | 0            |
| 2   | o     | 100   | 11       | 51       | 0       | 0            |
| 2   | p     | 100   | 11       | 51       | 0       | 0            |
| 2   | q     | 100   | 11       | 51       | 0       | 0            |
| 2   | r     | 100   | 11       | 51       | 0       | 0            |
| 2   | s     | 100   | 11       | 51       | 0       | 0            |
| All | All   | 33915 | 31559    | 32266    | 2188    | 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 35.

All (2188) 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:M:95:THR:CG2 | 1:N:195:ARG:HD3 | 1.29                     | 1.63              |
| 1:R:95:THR:CG2 | 1:S:195:ARG:HD3 | 1.29                     | 1.63              |
| 1:A:95:THR:CG2 | 1:B:195:ARG:HD3 | 1.29                     | 1.63              |
| 1:N:95:THR:CG2 | 1:O:195:ARG:HD3 | 1.29                     | 1.62              |
| 1:L:95:THR:CG2 | 1:M:195:ARG:HD3 | 1.29                     | 1.61              |
| 1:G:95:THR:CG2 | 1:H:195:ARG:HD3 | 1.29                     | 1.60              |
| 1:B:95:THR:CG2 | 1:C:195:ARG:HD3 | 1.29                     | 1.60              |
| 1:F:95:THR:CG2 | 1:G:195:ARG:HD3 | 1.29                     | 1.60              |
| 1:K:95:THR:CG2 | 1:L:195:ARG:HD3 | 1.29                     | 1.59              |
| 1:H:95:THR:CG2 | 1:I:195:ARG:HD3 | 1.29                     | 1.59              |
| 1:Q:95:THR:CG2 | 1:R:195:ARG:HD3 | 1.29                     | 1.59              |
| 1:C:95:THR:CG2 | 1:D:195:ARG:HD3 | 1.29                     | 1.58              |
| 1:O:95:THR:CG2 | 1:P:195:ARG:HD3 | 1.29                     | 1.58              |
| 1:J:95:THR:CG2 | 1:K:195:ARG:HD3 | 1.29                     | 1.57              |
| 1:E:95:THR:CG2 | 1:F:195:ARG:HD3 | 1.29                     | 1.57              |
| 1:D:95:THR:CG2 | 1:E:195:ARG:HD3 | 1.29                     | 1.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:95:THR:CG2  | 1:J:195:ARG:HD3 | 1.29                     | 1.55              |
| 1:P:95:THR:CG2  | 1:Q:195:ARG:HD3 | 1.29                     | 1.54              |
| 1:H:90:HIS:CE1  | 1:I:131:ILE:CD1 | 1.93                     | 1.51              |
| 1:G:90:HIS:CE1  | 1:H:131:ILE:CD1 | 1.93                     | 1.50              |
| 1:I:90:HIS:CE1  | 1:J:131:ILE:CD1 | 1.93                     | 1.50              |
| 1:Q:90:HIS:CE1  | 1:R:131:ILE:CD1 | 1.93                     | 1.50              |
| 1:R:90:HIS:CE1  | 1:S:131:ILE:CD1 | 1.93                     | 1.50              |
| 1:N:90:HIS:CE1  | 1:O:131:ILE:CD1 | 1.93                     | 1.50              |
| 1:B:90:HIS:CE1  | 1:C:131:ILE:CD1 | 1.93                     | 1.49              |
| 1:C:90:HIS:CE1  | 1:D:131:ILE:CD1 | 1.93                     | 1.49              |
| 1:K:90:HIS:CE1  | 1:L:131:ILE:CD1 | 1.93                     | 1.49              |
| 1:P:90:HIS:CE1  | 1:Q:131:ILE:CD1 | 1.93                     | 1.49              |
| 1:O:90:HIS:CE1  | 1:P:131:ILE:CD1 | 1.93                     | 1.48              |
| 1:E:90:HIS:CE1  | 1:F:131:ILE:CD1 | 1.93                     | 1.48              |
| 1:L:90:HIS:CE1  | 1:M:131:ILE:CD1 | 1.93                     | 1.48              |
| 1:J:90:HIS:CE1  | 1:K:131:ILE:CD1 | 1.93                     | 1.48              |
| 1:D:90:HIS:CE1  | 1:E:131:ILE:CD1 | 1.93                     | 1.47              |
| 1:A:90:HIS:CE1  | 1:B:131:ILE:CD1 | 1.93                     | 1.47              |
| 1:F:90:HIS:CE1  | 1:G:131:ILE:CD1 | 1.93                     | 1.47              |
| 1:M:90:HIS:CE1  | 1:N:131:ILE:CD1 | 1.93                     | 1.46              |
| 1:C:66:PRO:HB3  | 1:M:128:LYS:CE  | 1.50                     | 1.42              |
| 1:D:66:PRO:HB3  | 1:N:128:LYS:CE  | 1.50                     | 1.42              |
| 1:I:66:PRO:HB3  | 1:S:128:LYS:CE  | 1.50                     | 1.41              |
| 1:E:66:PRO:HB3  | 1:O:128:LYS:CE  | 1.50                     | 1.41              |
| 1:G:256:LEU:CD2 | 1:P:270:HIS:HB3 | 1.51                     | 1.41              |
| 1:B:66:PRO:HB3  | 1:L:128:LYS:CE  | 1.50                     | 1.41              |
| 1:F:256:LEU:CD2 | 1:O:270:HIS:HB3 | 1.51                     | 1.40              |
| 1:F:66:PRO:HB3  | 1:P:128:LYS:CE  | 1.50                     | 1.40              |
| 1:H:66:PRO:HB3  | 1:R:128:LYS:CE  | 1.50                     | 1.40              |
| 1:A:256:LEU:CD2 | 1:J:270:HIS:HB3 | 1.51                     | 1.40              |
| 1:H:256:LEU:CD2 | 1:Q:270:HIS:HB3 | 1.51                     | 1.40              |
| 1:J:256:LEU:CD2 | 1:S:270:HIS:HB3 | 1.51                     | 1.39              |
| 1:G:66:PRO:HB3  | 1:Q:128:LYS:CE  | 1.50                     | 1.39              |
| 1:F:90:HIS:HE1  | 1:G:131:ILE:CD1 | 1.32                     | 1.39              |
| 1:A:66:PRO:HB3  | 1:K:128:LYS:CE  | 1.50                     | 1.38              |
| 1:E:256:LEU:CD2 | 1:N:270:HIS:HB3 | 1.51                     | 1.38              |
| 1:I:256:LEU:CD2 | 1:R:270:HIS:HB3 | 1.51                     | 1.38              |
| 1:B:256:LEU:CD2 | 1:K:270:HIS:HB3 | 1.51                     | 1.37              |
| 1:F:256:LEU:CD2 | 1:O:270:HIS:CB  | 2.03                     | 1.37              |
| 1:O:90:HIS:HE1  | 1:P:131:ILE:CD1 | 1.32                     | 1.37              |
| 1:B:256:LEU:CD2 | 1:K:270:HIS:CB  | 2.03                     | 1.37              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:90:HIS:HE1   | 1:H:131:ILE:CD1  | 1.32                     | 1.37              |
| 1:L:90:HIS:HE1   | 1:M:131:ILE:CD1  | 1.32                     | 1.37              |
| 1:P:90:HIS:HE1   | 1:Q:131:ILE:CD1  | 1.32                     | 1.37              |
| 1:G:256:LEU:CD2  | 1:P:270:HIS:CB   | 2.03                     | 1.37              |
| 1:C:90:HIS:HE1   | 1:D:131:ILE:CD1  | 1.32                     | 1.37              |
| 1:C:256:LEU:CD2  | 1:L:270:HIS:CB   | 2.03                     | 1.37              |
| 1:A:256:LEU:CD2  | 1:J:270:HIS:CB   | 2.03                     | 1.36              |
| 1:D:256:LEU:CD2  | 1:M:270:HIS:HB3  | 1.51                     | 1.36              |
| 1:E:90:HIS:HE1   | 1:F:131:ILE:CD1  | 1.32                     | 1.36              |
| 1:H:256:LEU:CD2  | 1:Q:270:HIS:CB   | 2.03                     | 1.36              |
| 1:E:256:LEU:CD2  | 1:N:270:HIS:CB   | 2.03                     | 1.36              |
| 1:I:256:LEU:CD2  | 1:R:270:HIS:CB   | 2.03                     | 1.36              |
| 1:J:256:LEU:CD2  | 1:S:270:HIS:CB   | 2.03                     | 1.36              |
| 1:C:256:LEU:CD2  | 1:L:270:HIS:HB3  | 1.51                     | 1.35              |
| 1:F:256:LEU:HD21 | 1:O:270:HIS:CB   | 1.57                     | 1.35              |
| 1:D:256:LEU:HD21 | 1:M:270:HIS:CB   | 1.57                     | 1.34              |
| 1:A:90:HIS:CE1   | 1:B:131:ILE:HD11 | 1.59                     | 1.34              |
| 1:D:256:LEU:CD2  | 1:M:270:HIS:CB   | 2.03                     | 1.34              |
| 1:B:90:HIS:CE1   | 1:C:131:ILE:HD11 | 1.59                     | 1.34              |
| 1:K:90:HIS:CE1   | 1:L:131:ILE:HD11 | 1.59                     | 1.34              |
| 1:N:90:HIS:HE1   | 1:O:131:ILE:CD1  | 1.32                     | 1.34              |
| 1:J:90:HIS:CE1   | 1:K:131:ILE:HD11 | 1.59                     | 1.34              |
| 1:C:256:LEU:HD21 | 1:L:270:HIS:CB   | 1.57                     | 1.33              |
| 1:H:256:LEU:HD21 | 1:Q:270:HIS:CB   | 1.57                     | 1.33              |
| 1:I:90:HIS:HE1   | 1:J:131:ILE:CD1  | 1.31                     | 1.33              |
| 1:J:90:HIS:HE1   | 1:K:131:ILE:CD1  | 1.32                     | 1.33              |
| 1:B:90:HIS:HE1   | 1:C:131:ILE:CD1  | 1.32                     | 1.33              |
| 1:B:256:LEU:HD21 | 1:K:270:HIS:CB   | 1.57                     | 1.33              |
| 1:Q:90:HIS:HE1   | 1:R:131:ILE:CD1  | 1.32                     | 1.33              |
| 1:J:256:LEU:HD21 | 1:S:270:HIS:CB   | 1.57                     | 1.32              |
| 1:R:90:HIS:HE1   | 1:S:131:ILE:CD1  | 1.32                     | 1.32              |
| 1:A:256:LEU:HD21 | 1:J:270:HIS:CB   | 1.57                     | 1.32              |
| 1:K:90:HIS:HE1   | 1:L:131:ILE:CD1  | 1.32                     | 1.32              |
| 1:A:90:HIS:HE1   | 1:B:131:ILE:CD1  | 1.31                     | 1.31              |
| 1:G:256:LEU:HD21 | 1:P:270:HIS:CB   | 1.57                     | 1.31              |
| 1:H:90:HIS:HE1   | 1:I:131:ILE:CD1  | 1.32                     | 1.31              |
| 1:L:90:HIS:CE1   | 1:M:131:ILE:HD11 | 1.59                     | 1.31              |
| 1:Q:90:HIS:CE1   | 1:R:131:ILE:HD11 | 1.59                     | 1.31              |
| 1:D:90:HIS:HE1   | 1:E:131:ILE:CD1  | 1.32                     | 1.31              |
| 1:E:256:LEU:HD21 | 1:N:270:HIS:CB   | 1.57                     | 1.31              |
| 1:I:256:LEU:HD21 | 1:R:270:HIS:CB   | 1.56                     | 1.31              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:R:90:HIS:CE1 | 1:S:131:ILE:HD11 | 1.59                     | 1.30              |
| 1:H:90:HIS:CE1 | 1:I:131:ILE:HD11 | 1.59                     | 1.30              |
| 1:C:90:HIS:CE1 | 1:D:131:ILE:HD11 | 1.59                     | 1.30              |
| 1:D:90:HIS:CE1 | 1:E:131:ILE:HD11 | 1.59                     | 1.29              |
| 1:I:90:HIS:CE1 | 1:J:131:ILE:HD11 | 1.59                     | 1.29              |
| 1:N:90:HIS:CE1 | 1:O:131:ILE:HD11 | 1.59                     | 1.29              |
| 1:G:90:HIS:CE1 | 1:H:131:ILE:HD11 | 1.59                     | 1.29              |
| 1:E:90:HIS:CE1 | 1:F:131:ILE:HD11 | 1.59                     | 1.28              |
| 1:P:90:HIS:CE1 | 1:Q:131:ILE:HD11 | 1.59                     | 1.28              |
| 1:M:90:HIS:HE1 | 1:N:131:ILE:CD1  | 1.32                     | 1.28              |
| 1:M:90:HIS:CE1 | 1:N:131:ILE:HD11 | 1.59                     | 1.28              |
| 1:C:200:PRO:N  | 1:K:174:LYS:HG2  | 1.48                     | 1.27              |
| 1:D:200:PRO:N  | 1:L:174:LYS:HG2  | 1.48                     | 1.27              |
| 1:C:66:PRO:HB3 | 1:M:128:LYS:NZ   | 1.50                     | 1.27              |
| 1:A:200:PRO:N  | 1:I:174:LYS:HG2  | 1.48                     | 1.26              |
| 1:G:66:PRO:HB3 | 1:Q:128:LYS:NZ   | 1.50                     | 1.26              |
| 1:C:200:PRO:CD | 1:K:174:LYS:HG2  | 1.66                     | 1.26              |
| 1:F:66:PRO:HB3 | 1:P:128:LYS:NZ   | 1.50                     | 1.26              |
| 1:F:200:PRO:N  | 1:N:174:LYS:HG2  | 1.48                     | 1.26              |
| 1:G:200:PRO:N  | 1:O:174:LYS:HG2  | 1.48                     | 1.26              |
| 1:J:200:PRO:CD | 1:R:174:LYS:HG2  | 1.66                     | 1.26              |
| 1:K:200:PRO:CD | 1:S:174:LYS:HG2  | 1.66                     | 1.26              |
| 1:B:200:PRO:CD | 1:J:174:LYS:HG2  | 1.66                     | 1.26              |
| 1:D:66:PRO:HB3 | 1:N:128:LYS:NZ   | 1.50                     | 1.26              |
| 1:O:90:HIS:CE1 | 1:P:131:ILE:HD11 | 1.59                     | 1.26              |
| 1:E:200:PRO:N  | 1:M:174:LYS:HG2  | 1.48                     | 1.25              |
| 1:H:200:PRO:CD | 1:P:174:LYS:HG2  | 1.66                     | 1.25              |
| 1:I:66:PRO:HB3 | 1:S:128:LYS:NZ   | 1.50                     | 1.25              |
| 1:K:200:PRO:N  | 1:S:174:LYS:HG2  | 1.48                     | 1.25              |
| 1:E:200:PRO:CD | 1:M:174:LYS:HG2  | 1.66                     | 1.25              |
| 1:B:66:PRO:HB3 | 1:L:128:LYS:NZ   | 1.50                     | 1.25              |
| 1:I:200:PRO:CD | 1:Q:174:LYS:HG2  | 1.66                     | 1.25              |
| 1:J:200:PRO:N  | 1:R:174:LYS:HG2  | 1.48                     | 1.25              |
| 1:A:66:PRO:HB3 | 1:K:128:LYS:NZ   | 1.50                     | 1.25              |
| 1:A:200:PRO:CD | 1:I:174:LYS:HG2  | 1.66                     | 1.25              |
| 1:B:200:PRO:N  | 1:J:174:LYS:HG2  | 1.48                     | 1.25              |
| 1:D:95:THR:CG2 | 1:E:195:ARG:CD   | 2.15                     | 1.25              |
| 1:H:200:PRO:N  | 1:P:174:LYS:HG2  | 1.48                     | 1.25              |
| 1:I:95:THR:CG2 | 1:J:195:ARG:CD   | 2.15                     | 1.25              |
| 1:M:95:THR:CG2 | 1:N:195:ARG:CD   | 2.15                     | 1.25              |
| 1:K:95:THR:CG2 | 1:L:195:ARG:CD   | 2.15                     | 1.25              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:95:THR:CG2   | 1:S:195:ARG:CD   | 2.15                     | 1.25              |
| 1:B:95:THR:CG2   | 1:C:195:ARG:CD   | 2.15                     | 1.24              |
| 1:D:200:PRO:CD   | 1:L:174:LYS:HG2  | 1.66                     | 1.24              |
| 1:G:200:PRO:CD   | 1:O:174:LYS:HG2  | 1.66                     | 1.24              |
| 1:H:66:PRO:HB3   | 1:R:128:LYS:NZ   | 1.50                     | 1.24              |
| 1:F:200:PRO:CD   | 1:N:174:LYS:HG2  | 1.66                     | 1.24              |
| 1:E:66:PRO:HB3   | 1:O:128:LYS:NZ   | 1.50                     | 1.24              |
| 1:F:90:HIS:CE1   | 1:G:131:ILE:HD11 | 1.59                     | 1.24              |
| 1:A:95:THR:CG2   | 1:B:195:ARG:CD   | 2.15                     | 1.24              |
| 1:C:95:THR:CG2   | 1:D:195:ARG:CD   | 2.15                     | 1.24              |
| 1:F:95:THR:CG2   | 1:G:195:ARG:CD   | 2.15                     | 1.24              |
| 1:N:95:THR:CG2   | 1:O:195:ARG:CD   | 2.15                     | 1.24              |
| 1:P:95:THR:CG2   | 1:Q:195:ARG:CD   | 2.15                     | 1.24              |
| 1:L:95:THR:CG2   | 1:M:195:ARG:CD   | 2.15                     | 1.23              |
| 1:G:95:THR:CG2   | 1:H:195:ARG:CD   | 2.15                     | 1.23              |
| 1:I:200:PRO:N    | 1:Q:174:LYS:HG2  | 1.48                     | 1.23              |
| 1:J:95:THR:CG2   | 1:K:195:ARG:CD   | 2.15                     | 1.23              |
| 1:H:95:THR:CG2   | 1:I:195:ARG:CD   | 2.15                     | 1.23              |
| 1:Q:95:THR:CG2   | 1:R:195:ARG:CD   | 2.15                     | 1.23              |
| 1:E:95:THR:CG2   | 1:F:195:ARG:CD   | 2.15                     | 1.23              |
| 1:O:95:THR:CG2   | 1:P:195:ARG:CD   | 2.15                     | 1.23              |
| 1:J:253:LEU:HD11 | 1:S:265:GLU:OE2  | 1.42                     | 1.18              |
| 1:G:253:LEU:HD11 | 1:P:265:GLU:OE2  | 1.42                     | 1.18              |
| 1:A:253:LEU:HD11 | 1:J:265:GLU:OE2  | 1.42                     | 1.17              |
| 1:G:108:ARG:HD2  | 1:H:161:GLN:OE1  | 1.44                     | 1.17              |
| 1:H:253:LEU:HD11 | 1:Q:265:GLU:OE2  | 1.42                     | 1.17              |
| 1:D:253:LEU:HD11 | 1:M:265:GLU:OE2  | 1.42                     | 1.16              |
| 1:F:253:LEU:HD11 | 1:O:265:GLU:OE2  | 1.42                     | 1.16              |
| 1:I:253:LEU:HD11 | 1:R:265:GLU:OE2  | 1.42                     | 1.16              |
| 1:D:90:HIS:CE1   | 1:E:131:ILE:HD12 | 1.80                     | 1.16              |
| 1:I:90:HIS:CE1   | 1:J:131:ILE:HD12 | 1.80                     | 1.16              |
| 1:K:95:THR:HG22  | 1:L:195:ARG:HD3  | 1.18                     | 1.16              |
| 1:F:66:PRO:HB3   | 1:P:128:LYS:HE2  | 1.16                     | 1.16              |
| 1:A:108:ARG:HD2  | 1:B:161:GLN:OE1  | 1.44                     | 1.15              |
| 1:C:253:LEU:HD11 | 1:L:265:GLU:OE2  | 1.42                     | 1.15              |
| 1:E:253:LEU:HD11 | 1:N:265:GLU:OE2  | 1.42                     | 1.15              |
| 1:F:108:ARG:HD2  | 1:G:161:GLN:OE1  | 1.44                     | 1.15              |
| 1:P:90:HIS:CE1   | 1:Q:131:ILE:HD12 | 1.80                     | 1.15              |
| 1:B:253:LEU:HD11 | 1:K:265:GLU:OE2  | 1.42                     | 1.15              |
| 1:K:90:HIS:CE1   | 1:L:131:ILE:HD12 | 1.80                     | 1.15              |
| 1:E:66:PRO:HB3   | 1:O:128:LYS:HE2  | 1.16                     | 1.14              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:108:ARG:HD2 | 1:I:161:GLN:OE1  | 1.44                     | 1.14              |
| 1:I:95:THR:HG22 | 1:J:195:ARG:HD3  | 1.18                     | 1.14              |
| 1:Q:90:HIS:CE1  | 1:R:131:ILE:HD12 | 1.80                     | 1.14              |
| 1:B:95:THR:HG22 | 1:C:195:ARG:HD3  | 1.18                     | 1.14              |
| 1:C:90:HIS:CE1  | 1:D:131:ILE:HD12 | 1.80                     | 1.14              |
| 1:A:90:HIS:CE1  | 1:B:131:ILE:HD12 | 1.80                     | 1.14              |
| 1:E:78:PRO:HG3  | 1:F:183:HIS:HB3  | 1.30                     | 1.14              |
| 1:G:78:PRO:HG3  | 1:H:183:HIS:HB3  | 1.30                     | 1.14              |
| 1:N:78:PRO:HG3  | 1:O:183:HIS:HB3  | 1.30                     | 1.14              |
| 1:P:78:PRO:HG3  | 1:Q:183:HIS:HB3  | 1.30                     | 1.14              |
| 1:D:66:PRO:HB3  | 1:N:128:LYS:HE2  | 1.16                     | 1.14              |
| 1:G:66:PRO:HB3  | 1:Q:128:LYS:HE2  | 1.16                     | 1.13              |
| 1:H:90:HIS:CE1  | 1:I:131:ILE:HD12 | 1.80                     | 1.13              |
| 1:L:90:HIS:CE1  | 1:M:131:ILE:HD12 | 1.80                     | 1.13              |
| 1:C:66:PRO:HB3  | 1:M:128:LYS:HE2  | 1.16                     | 1.13              |
| 1:F:78:PRO:HG3  | 1:G:183:HIS:HB3  | 1.30                     | 1.12              |
| 1:M:86:LEU:HA   | 1:N:130:GLN:HE22 | 1.13                     | 1.12              |
| 1:O:108:ARG:HD2 | 1:P:161:GLN:OE1  | 1.44                     | 1.12              |
| 1:Q:95:THR:HG22 | 1:R:195:ARG:HD3  | 1.18                     | 1.12              |
| 1:O:78:PRO:HG3  | 1:P:183:HIS:HB3  | 1.30                     | 1.12              |
| 1:R:108:ARG:HD2 | 1:S:161:GLN:OE1  | 1.45                     | 1.12              |
| 1:D:78:PRO:HG3  | 1:E:183:HIS:HB3  | 1.30                     | 1.12              |
| 1:L:86:LEU:HA   | 1:M:130:GLN:HE22 | 1.13                     | 1.12              |
| 1:B:108:ARG:HD2 | 1:C:161:GLN:OE1  | 1.44                     | 1.12              |
| 1:H:78:PRO:HG3  | 1:I:183:HIS:HB3  | 1.30                     | 1.12              |
| 1:L:108:ARG:HD2 | 1:M:161:GLN:OE1  | 1.44                     | 1.12              |
| 1:N:108:ARG:HD2 | 1:O:161:GLN:OE1  | 1.44                     | 1.12              |
| 1:Q:78:PRO:HG3  | 1:R:183:HIS:HB3  | 1.30                     | 1.12              |
| 1:A:95:THR:HG22 | 1:B:195:ARG:HD3  | 1.18                     | 1.12              |
| 1:C:95:THR:HG22 | 1:D:195:ARG:HD3  | 1.18                     | 1.12              |
| 1:I:78:PRO:HG3  | 1:J:183:HIS:HB3  | 1.30                     | 1.11              |
| 1:K:108:ARG:HD2 | 1:L:161:GLN:OE1  | 1.44                     | 1.11              |
| 1:M:108:ARG:HD2 | 1:N:161:GLN:OE1  | 1.44                     | 1.11              |
| 1:O:90:HIS:CE1  | 1:P:131:ILE:HD12 | 1.80                     | 1.11              |
| 1:B:86:LEU:HA   | 1:C:130:GLN:HE22 | 1.13                     | 1.11              |
| 1:E:90:HIS:CE1  | 1:F:131:ILE:HD12 | 1.80                     | 1.11              |
| 1:I:108:ARG:HD2 | 1:J:161:GLN:OE1  | 1.44                     | 1.11              |
| 1:R:78:PRO:HG3  | 1:S:183:HIS:HB3  | 1.30                     | 1.11              |
| 1:M:78:PRO:HG3  | 1:N:183:HIS:HB3  | 1.30                     | 1.11              |
| 1:E:108:ARG:HD2 | 1:F:161:GLN:OE1  | 1.44                     | 1.11              |
| 1:L:90:HIS:NE2  | 1:M:131:ILE:HD12 | 1.66                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:90:HIS:CE1   | 1:O:131:ILE:HD12 | 1.80                     | 1.10              |
| 1:A:86:LEU:HA    | 1:B:130:GLN:HE22 | 1.13                     | 1.10              |
| 1:B:90:HIS:NE2   | 1:C:131:ILE:HD12 | 1.66                     | 1.10              |
| 1:L:78:PRO:HG3   | 1:M:183:HIS:HB3  | 1.30                     | 1.10              |
| 1:N:95:THR:HG22  | 1:O:195:ARG:HD3  | 1.18                     | 1.10              |
| 1:P:108:ARG:HD2  | 1:Q:161:GLN:OE1  | 1.44                     | 1.10              |
| 1:C:90:HIS:NE2   | 1:D:131:ILE:HD12 | 1.66                     | 1.10              |
| 1:G:256:LEU:HD23 | 1:P:270:HIS:HB2  | 1.34                     | 1.10              |
| 1:M:90:HIS:NE2   | 1:N:131:ILE:HD12 | 1.66                     | 1.10              |
| 1:O:95:THR:HG22  | 1:P:195:ARG:HD3  | 1.18                     | 1.10              |
| 1:J:95:THR:HG22  | 1:K:195:ARG:HD3  | 1.18                     | 1.10              |
| 1:B:256:LEU:HD23 | 1:K:270:HIS:CB   | 1.80                     | 1.10              |
| 1:C:256:LEU:HD23 | 1:L:270:HIS:CB   | 1.80                     | 1.10              |
| 1:H:95:THR:HG22  | 1:I:195:ARG:HD3  | 1.19                     | 1.10              |
| 1:I:66:PRO:HB3   | 1:S:128:LYS:HE2  | 1.16                     | 1.10              |
| 1:K:90:HIS:NE2   | 1:L:131:ILE:HD12 | 1.66                     | 1.10              |
| 1:R:95:THR:HG22  | 1:S:195:ARG:HD3  | 1.18                     | 1.10              |
| 1:A:66:PRO:HB3   | 1:K:128:LYS:HE2  | 1.16                     | 1.09              |
| 1:B:90:HIS:CE1   | 1:C:131:ILE:HD12 | 1.80                     | 1.09              |
| 1:B:256:LEU:HD23 | 1:K:270:HIS:HB2  | 1.34                     | 1.09              |
| 1:J:256:LEU:HD23 | 1:S:270:HIS:HB2  | 1.34                     | 1.09              |
| 1:P:90:HIS:NE2   | 1:Q:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:Q:108:ARG:HD2  | 1:R:161:GLN:OE1  | 1.44                     | 1.09              |
| 1:B:66:PRO:HB3   | 1:L:128:LYS:HE2  | 1.16                     | 1.09              |
| 1:C:78:PRO:HG3   | 1:D:183:HIS:HB3  | 1.30                     | 1.09              |
| 1:M:90:HIS:CE1   | 1:N:131:ILE:HD12 | 1.80                     | 1.09              |
| 1:M:95:THR:HG22  | 1:N:195:ARG:HD3  | 1.18                     | 1.09              |
| 1:N:86:LEU:HA    | 1:O:130:GLN:HE22 | 1.13                     | 1.09              |
| 1:N:90:HIS:NE2   | 1:O:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:A:90:HIS:NE2   | 1:B:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:F:256:LEU:HD23 | 1:O:270:HIS:HB2  | 1.33                     | 1.09              |
| 1:R:90:HIS:CE1   | 1:S:131:ILE:HD12 | 1.80                     | 1.09              |
| 1:B:78:PRO:HG3   | 1:C:183:HIS:HB3  | 1.30                     | 1.09              |
| 1:C:86:LEU:HA    | 1:D:130:GLN:HE22 | 1.13                     | 1.09              |
| 1:D:256:LEU:HD23 | 1:M:270:HIS:HB2  | 1.33                     | 1.09              |
| 1:E:86:LEU:HA    | 1:F:130:GLN:HE22 | 1.13                     | 1.09              |
| 1:E:90:HIS:NE2   | 1:F:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:H:90:HIS:NE2   | 1:I:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:I:90:HIS:NE2   | 1:J:131:ILE:HD12 | 1.66                     | 1.09              |
| 1:K:86:LEU:HA    | 1:L:130:GLN:HE22 | 1.13                     | 1.09              |
| 1:D:80:TYR:CD1   | 1:E:115:PHE:CD2  | 2.41                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:78:PRO:HG3   | 1:L:183:HIS:HB3  | 1.30                     | 1.09              |
| 1:M:80:TYR:CD1   | 1:N:115:PHE:CD2  | 2.41                     | 1.09              |
| 1:D:90:HIS:NE2   | 1:E:131:ILE:HD12 | 1.66                     | 1.08              |
| 1:E:200:PRO:HD3  | 1:M:174:LYS:CG   | 1.83                     | 1.08              |
| 1:F:90:HIS:NE2   | 1:G:131:ILE:HD12 | 1.66                     | 1.08              |
| 1:O:80:TYR:CD1   | 1:P:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:A:78:PRO:HG3   | 1:B:183:HIS:HB3  | 1.30                     | 1.08              |
| 1:E:80:TYR:CD1   | 1:F:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:F:80:TYR:CD1   | 1:G:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:J:78:PRO:HG3   | 1:K:183:HIS:HB3  | 1.30                     | 1.08              |
| 1:J:108:ARG:HD2  | 1:K:161:GLN:OE1  | 1.44                     | 1.08              |
| 1:F:86:LEU:HA    | 1:G:130:GLN:HE22 | 1.14                     | 1.08              |
| 1:G:200:PRO:HD3  | 1:O:174:LYS:CG   | 1.83                     | 1.08              |
| 1:H:200:PRO:HD3  | 1:P:174:LYS:CG   | 1.83                     | 1.08              |
| 1:J:90:HIS:NE2   | 1:K:131:ILE:HD12 | 1.66                     | 1.08              |
| 1:L:80:TYR:CD1   | 1:M:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:D:108:ARG:HD2  | 1:E:161:GLN:OE1  | 1.45                     | 1.08              |
| 1:E:95:THR:HG22  | 1:F:195:ARG:HD3  | 1.18                     | 1.08              |
| 1:G:80:TYR:CD1   | 1:H:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:H:66:PRO:HB3   | 1:R:128:LYS:HE2  | 1.16                     | 1.08              |
| 1:H:256:LEU:HD23 | 1:Q:270:HIS:HB2  | 1.33                     | 1.08              |
| 1:O:90:HIS:NE2   | 1:P:131:ILE:HD12 | 1.66                     | 1.08              |
| 1:R:90:HIS:NE2   | 1:S:131:ILE:HD12 | 1.66                     | 1.08              |
| 1:B:80:TYR:CD1   | 1:C:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:I:80:TYR:CD1   | 1:J:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:R:80:TYR:CD1   | 1:S:115:PHE:CD2  | 2.41                     | 1.08              |
| 1:R:86:LEU:HA    | 1:S:130:GLN:HE22 | 1.13                     | 1.08              |
| 1:A:80:TYR:CD1   | 1:B:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:E:256:LEU:HD23 | 1:N:270:HIS:CB   | 1.81                     | 1.07              |
| 1:F:200:PRO:HD3  | 1:N:174:LYS:CG   | 1.83                     | 1.07              |
| 1:G:90:HIS:NE2   | 1:H:131:ILE:HD12 | 1.66                     | 1.07              |
| 1:K:80:TYR:CD1   | 1:L:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:B:200:PRO:HD3  | 1:J:174:LYS:CG   | 1.83                     | 1.07              |
| 1:H:80:TYR:CD1   | 1:I:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:J:80:TYR:CD1   | 1:K:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:N:80:TYR:CD1   | 1:O:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:Q:80:TYR:CD1   | 1:R:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:Q:90:HIS:NE2   | 1:R:131:ILE:HD12 | 1.66                     | 1.07              |
| 1:G:95:THR:HG22  | 1:H:195:ARG:HD3  | 1.18                     | 1.07              |
| 1:J:256:LEU:HD23 | 1:S:270:HIS:CB   | 1.81                     | 1.07              |
| 1:B:236:GLU:OE2  | 1:S:267:THR:HB   | 1.54                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:TYR:CD1   | 1:D:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:D:95:THR:HG22  | 1:E:195:ARG:HD3  | 1.18                     | 1.07              |
| 1:I:200:PRO:HD3  | 1:Q:174:LYS:CG   | 1.83                     | 1.07              |
| 1:J:90:HIS:CE1   | 1:K:131:ILE:HD12 | 1.80                     | 1.07              |
| 1:P:80:TYR:CD1   | 1:Q:115:PHE:CD2  | 2.41                     | 1.07              |
| 1:A:200:PRO:HD3  | 1:I:174:LYS:CG   | 1.84                     | 1.06              |
| 1:C:200:PRO:HD3  | 1:K:174:LYS:CG   | 1.83                     | 1.06              |
| 1:E:256:LEU:HD23 | 1:N:270:HIS:HB2  | 1.34                     | 1.06              |
| 1:G:86:LEU:HA    | 1:H:130:GLN:HE22 | 1.13                     | 1.06              |
| 1:G:90:HIS:CE1   | 1:H:131:ILE:HD12 | 1.80                     | 1.06              |
| 1:L:95:THR:HG22  | 1:M:195:ARG:HD3  | 1.18                     | 1.06              |
| 1:A:256:LEU:HD23 | 1:J:270:HIS:HB2  | 1.33                     | 1.06              |
| 1:C:108:ARG:HD2  | 1:D:161:GLN:OE1  | 1.44                     | 1.06              |
| 1:D:86:LEU:HA    | 1:E:130:GLN:HE22 | 1.13                     | 1.06              |
| 1:F:95:THR:HG22  | 1:G:195:ARG:HD3  | 1.18                     | 1.06              |
| 1:J:200:PRO:HD3  | 1:R:174:LYS:CG   | 1.83                     | 1.06              |
| 1:H:86:LEU:HA    | 1:I:130:GLN:HE22 | 1.13                     | 1.06              |
| 1:K:200:PRO:HD3  | 1:S:174:LYS:CG   | 1.83                     | 1.06              |
| 1:P:95:THR:HG22  | 1:Q:195:ARG:HD3  | 1.18                     | 1.06              |
| 1:I:86:LEU:HA    | 1:J:130:GLN:HE22 | 1.13                     | 1.06              |
| 1:D:200:PRO:HD3  | 1:L:174:LYS:CG   | 1.84                     | 1.06              |
| 1:P:86:LEU:HA    | 1:Q:130:GLN:HE22 | 1.13                     | 1.05              |
| 1:A:236:GLU:OE2  | 1:R:267:THR:HB   | 1.54                     | 1.05              |
| 1:C:256:LEU:HD23 | 1:L:270:HIS:HB2  | 1.33                     | 1.05              |
| 1:D:95:THR:HG21  | 1:E:195:ARG:HD3  | 1.05                     | 1.05              |
| 1:E:95:THR:HG21  | 1:F:195:ARG:HD3  | 1.05                     | 1.05              |
| 1:I:95:THR:HG21  | 1:J:195:ARG:HD3  | 1.05                     | 1.05              |
| 1:O:86:LEU:HA    | 1:P:130:GLN:HE22 | 1.13                     | 1.05              |
| 1:D:256:LEU:HD23 | 1:M:270:HIS:CB   | 1.80                     | 1.05              |
| 1:J:86:LEU:HA    | 1:K:130:GLN:HE22 | 1.13                     | 1.05              |
| 1:F:256:LEU:HD23 | 1:O:270:HIS:CB   | 1.80                     | 1.04              |
| 1:H:241:MET:SD   | 1:P:254:PHE:CE1  | 2.51                     | 1.04              |
| 1:I:256:LEU:HD23 | 1:R:270:HIS:HB2  | 1.33                     | 1.04              |
| 1:J:95:THR:HG21  | 1:K:195:ARG:HD3  | 1.05                     | 1.04              |
| 1:B:241:MET:SD   | 1:J:254:PHE:CE1  | 2.51                     | 1.04              |
| 1:I:241:MET:SD   | 1:Q:254:PHE:CE1  | 2.51                     | 1.04              |
| 1:O:95:THR:HG21  | 1:P:195:ARG:HD3  | 1.05                     | 1.04              |
| 1:Q:86:LEU:HA    | 1:R:130:GLN:HE22 | 1.13                     | 1.04              |
| 1:A:241:MET:SD   | 1:I:254:PHE:CE1  | 2.51                     | 1.04              |
| 1:C:241:MET:SD   | 1:K:254:PHE:CE1  | 2.51                     | 1.04              |
| 1:J:241:MET:SD   | 1:R:254:PHE:CE1  | 2.50                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:95:THR:HG21  | 1:D:195:ARG:HD3  | 1.05                     | 1.04              |
| 1:P:95:THR:HG21  | 1:Q:195:ARG:HD3  | 1.05                     | 1.04              |
| 1:B:66:PRO:CB    | 1:L:128:LYS:NZ   | 2.21                     | 1.04              |
| 1:G:66:PRO:CB    | 1:Q:128:LYS:NZ   | 2.21                     | 1.04              |
| 1:F:90:HIS:CE1   | 1:G:131:ILE:HD12 | 1.80                     | 1.03              |
| 1:F:241:MET:SD   | 1:N:254:PHE:CE1  | 2.51                     | 1.03              |
| 1:K:95:THR:HG21  | 1:L:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:C:66:PRO:CB    | 1:M:128:LYS:NZ   | 2.21                     | 1.03              |
| 1:E:241:MET:SD   | 1:M:254:PHE:CE1  | 2.51                     | 1.03              |
| 1:F:66:PRO:CB    | 1:P:128:LYS:NZ   | 2.21                     | 1.03              |
| 1:G:241:MET:SD   | 1:O:254:PHE:CE1  | 2.51                     | 1.03              |
| 1:H:95:THR:HG21  | 1:I:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:K:241:MET:SD   | 1:S:254:PHE:CE1  | 2.51                     | 1.03              |
| 1:B:95:THR:HG21  | 1:C:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:N:95:THR:HG21  | 1:O:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:A:66:PRO:CB    | 1:K:128:LYS:NZ   | 2.21                     | 1.03              |
| 1:A:256:LEU:HD23 | 1:J:270:HIS:CB   | 1.80                     | 1.03              |
| 1:C:256:LEU:CD2  | 1:L:270:HIS:HB2  | 1.87                     | 1.03              |
| 1:F:95:THR:HG21  | 1:G:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:H:66:PRO:CB    | 1:R:128:LYS:NZ   | 2.21                     | 1.03              |
| 1:Q:95:THR:HG21  | 1:R:195:ARG:HD3  | 1.05                     | 1.03              |
| 1:K:200:PRO:HD3  | 1:S:174:LYS:HG2  | 1.37                     | 1.03              |
| 1:G:256:LEU:HD23 | 1:P:270:HIS:CB   | 1.80                     | 1.02              |
| 1:E:200:PRO:HD3  | 1:M:174:LYS:HG2  | 1.37                     | 1.02              |
| 1:F:200:PRO:HD3  | 1:N:174:LYS:HG2  | 1.37                     | 1.02              |
| 1:I:66:PRO:CB    | 1:S:128:LYS:NZ   | 2.21                     | 1.02              |
| 1:A:256:LEU:CD2  | 1:J:270:HIS:HB2  | 1.87                     | 1.02              |
| 1:D:241:MET:SD   | 1:L:254:PHE:CE1  | 2.51                     | 1.02              |
| 1:L:95:THR:HG21  | 1:M:195:ARG:HD3  | 1.05                     | 1.02              |
| 1:A:95:THR:HG21  | 1:B:195:ARG:HD3  | 1.05                     | 1.02              |
| 1:B:256:LEU:CD2  | 1:K:270:HIS:HB2  | 1.88                     | 1.02              |
| 1:E:66:PRO:CB    | 1:O:128:LYS:NZ   | 2.21                     | 1.02              |
| 1:D:66:PRO:CB    | 1:N:128:LYS:NZ   | 2.21                     | 1.02              |
| 1:D:253:LEU:CD1  | 1:M:265:GLU:OE2  | 2.08                     | 1.01              |
| 1:E:253:LEU:CD1  | 1:N:265:GLU:OE2  | 2.08                     | 1.01              |
| 1:M:95:THR:HG21  | 1:N:195:ARG:HD3  | 1.05                     | 1.01              |
| 1:A:253:LEU:CD1  | 1:J:265:GLU:OE2  | 2.09                     | 1.01              |
| 1:H:253:LEU:CD1  | 1:Q:265:GLU:OE2  | 2.09                     | 1.01              |
| 1:H:256:LEU:HD23 | 1:Q:270:HIS:CB   | 1.80                     | 1.01              |
| 1:R:95:THR:HG21  | 1:S:195:ARG:HD3  | 1.05                     | 1.01              |
| 1:C:253:LEU:CD1  | 1:L:265:GLU:OE2  | 2.09                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:253:LEU:CD1  | 1:S:265:GLU:OE2  | 2.09                     | 1.01              |
| 1:F:253:LEU:CD1  | 1:O:265:GLU:OE2  | 2.09                     | 1.01              |
| 1:G:95:THR:HG21  | 1:H:195:ARG:HD3  | 1.05                     | 1.00              |
| 1:G:253:LEU:CD1  | 1:P:265:GLU:OE2  | 2.09                     | 1.00              |
| 1:B:253:LEU:CD1  | 1:K:265:GLU:OE2  | 2.09                     | 1.00              |
| 1:C:67:ARG:HG2   | 1:M:162:VAL:HG11 | 1.44                     | 1.00              |
| 1:A:200:PRO:HD3  | 1:I:174:LYS:HG2  | 1.37                     | 0.99              |
| 1:D:200:PRO:HD3  | 1:L:174:LYS:HG2  | 1.37                     | 0.99              |
| 1:I:256:LEU:HD23 | 1:R:270:HIS:CB   | 1.81                     | 0.99              |
| 1:A:67:ARG:HG2   | 1:K:162:VAL:HG11 | 1.44                     | 0.99              |
| 1:G:200:PRO:HD3  | 1:O:174:LYS:HG2  | 1.37                     | 0.99              |
| 1:I:253:LEU:CD1  | 1:R:265:GLU:OE2  | 2.09                     | 0.99              |
| 1:I:67:ARG:HG2   | 1:S:162:VAL:HG11 | 1.44                     | 0.98              |
| 1:B:80:TYR:CE1   | 1:C:115:PHE:HD2  | 1.82                     | 0.98              |
| 1:A:80:TYR:CE1   | 1:B:115:PHE:HD2  | 1.82                     | 0.98              |
| 1:E:67:ARG:HG2   | 1:O:162:VAL:HG11 | 1.44                     | 0.98              |
| 1:H:80:TYR:CE1   | 1:I:115:PHE:HD2  | 1.82                     | 0.98              |
| 1:I:80:TYR:CE1   | 1:J:115:PHE:HD2  | 1.82                     | 0.98              |
| 1:B:95:THR:HG21  | 1:C:195:ARG:CD   | 1.89                     | 0.98              |
| 1:C:80:TYR:CE1   | 1:D:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:G:80:TYR:CE1   | 1:H:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:G:256:LEU:CD2  | 1:P:270:HIS:HB2  | 1.88                     | 0.97              |
| 1:L:95:THR:HG21  | 1:M:195:ARG:CD   | 1.89                     | 0.97              |
| 1:H:256:LEU:CD2  | 1:Q:270:HIS:HB2  | 1.87                     | 0.97              |
| 1:J:80:TYR:CE1   | 1:K:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:O:95:THR:HG22  | 1:P:195:ARG:CD   | 1.90                     | 0.97              |
| 1:R:80:TYR:CE1   | 1:S:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:B:67:ARG:HG2   | 1:L:162:VAL:HG11 | 1.44                     | 0.97              |
| 1:O:80:TYR:CE1   | 1:P:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:P:80:TYR:CE1   | 1:Q:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:G:66:PRO:CB    | 1:Q:128:LYS:CE   | 2.43                     | 0.97              |
| 1:N:80:TYR:CE1   | 1:O:115:PHE:HD2  | 1.82                     | 0.97              |
| 1:H:67:ARG:HG2   | 1:R:162:VAL:HG11 | 1.44                     | 0.97              |
| 1:C:66:PRO:CB    | 1:M:128:LYS:CE   | 2.43                     | 0.97              |
| 1:C:95:THR:HG21  | 1:D:195:ARG:CD   | 1.90                     | 0.97              |
| 1:H:200:PRO:HD3  | 1:P:174:LYS:HG2  | 1.37                     | 0.97              |
| 1:K:95:THR:HG21  | 1:L:195:ARG:CD   | 1.90                     | 0.97              |
| 1:M:80:TYR:CE1   | 1:N:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:G:67:ARG:HG2   | 1:Q:162:VAL:HG11 | 1.44                     | 0.96              |
| 1:E:66:PRO:CB    | 1:O:128:LYS:CE   | 2.43                     | 0.96              |
| 1:I:66:PRO:CB    | 1:S:128:LYS:CE   | 2.43                     | 0.96              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:66:PRO:CB   | 1:L:128:LYS:CE   | 2.43                     | 0.96              |
| 1:D:80:TYR:CE1  | 1:E:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:F:80:TYR:CE1  | 1:G:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:L:80:TYR:CE1  | 1:M:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:A:95:THR:HG21 | 1:B:195:ARG:CD   | 1.90                     | 0.96              |
| 1:Q:80:TYR:CE1  | 1:R:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:D:95:THR:HG22 | 1:E:195:ARG:CD   | 1.90                     | 0.96              |
| 1:J:95:THR:HG21 | 1:K:195:ARG:CD   | 1.89                     | 0.96              |
| 1:I:95:THR:HG22 | 1:J:195:ARG:CD   | 1.90                     | 0.96              |
| 1:I:200:PRO:HD3 | 1:Q:174:LYS:HG2  | 1.37                     | 0.96              |
| 1:K:80:TYR:CE1  | 1:L:115:PHE:HD2  | 1.82                     | 0.96              |
| 1:P:95:THR:HB   | 1:Q:195:ARG:HD2  | 1.47                     | 0.96              |
| 1:D:67:ARG:HG2  | 1:N:162:VAL:HG11 | 1.44                     | 0.96              |
| 1:H:66:PRO:CB   | 1:R:128:LYS:CE   | 2.43                     | 0.96              |
| 1:H:66:PRO:CB   | 1:R:128:LYS:HE2  | 1.96                     | 0.96              |
| 1:I:66:PRO:CB   | 1:S:128:LYS:HE2  | 1.96                     | 0.96              |
| 1:G:95:THR:HB   | 1:H:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:H:95:THR:HG22 | 1:I:195:ARG:CD   | 1.90                     | 0.95              |
| 1:J:95:THR:HG22 | 1:K:195:ARG:CD   | 1.90                     | 0.95              |
| 1:M:95:THR:HG21 | 1:N:195:ARG:CD   | 1.90                     | 0.95              |
| 1:D:66:PRO:CB   | 1:N:128:LYS:CE   | 2.43                     | 0.95              |
| 1:Q:95:THR:HB   | 1:R:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:C:200:PRO:HD3 | 1:K:174:LYS:HG2  | 1.37                     | 0.95              |
| 1:I:95:THR:HB   | 1:J:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:C:95:THR:HB   | 1:D:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:H:95:THR:HB   | 1:I:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:I:95:THR:HG21 | 1:J:195:ARG:CD   | 1.90                     | 0.95              |
| 1:B:66:PRO:CB   | 1:L:128:LYS:HE2  | 1.96                     | 0.95              |
| 1:D:95:THR:HG21 | 1:E:195:ARG:CD   | 1.90                     | 0.95              |
| 1:E:80:TYR:CE1  | 1:F:115:PHE:HD2  | 1.82                     | 0.95              |
| 1:F:66:PRO:CB   | 1:P:128:LYS:CE   | 2.43                     | 0.95              |
| 1:F:256:LEU:CD2 | 1:O:270:HIS:HB2  | 1.87                     | 0.95              |
| 1:F:80:TYR:CD1  | 1:G:115:PHE:HD2  | 1.84                     | 0.95              |
| 1:M:95:THR:HB   | 1:N:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:J:200:PRO:HD3 | 1:R:174:LYS:HG2  | 1.37                     | 0.95              |
| 1:C:66:PRO:CB   | 1:M:128:LYS:HE2  | 1.96                     | 0.95              |
| 1:F:67:ARG:HG2  | 1:P:162:VAL:HG11 | 1.44                     | 0.95              |
| 1:R:95:THR:HB   | 1:S:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:G:66:PRO:CB   | 1:Q:128:LYS:HE2  | 1.96                     | 0.95              |
| 1:O:95:THR:HB   | 1:P:195:ARG:HD2  | 1.47                     | 0.95              |
| 1:A:66:PRO:CB   | 1:K:128:LYS:HE2  | 1.96                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:95:THR:HG21  | 1:S:195:ARG:CD   | 1.90                     | 0.94              |
| 1:I:256:LEU:CD2  | 1:R:270:HIS:HB2  | 1.87                     | 0.94              |
| 1:E:66:PRO:CB    | 1:O:128:LYS:HE2  | 1.96                     | 0.94              |
| 1:L:80:TYR:CD1   | 1:M:115:PHE:HD2  | 1.84                     | 0.94              |
| 1:A:66:PRO:CB    | 1:K:128:LYS:CE   | 2.43                     | 0.94              |
| 1:D:66:PRO:CB    | 1:N:128:LYS:HE2  | 1.96                     | 0.94              |
| 1:F:95:THR:HB    | 1:G:195:ARG:HD2  | 1.47                     | 0.94              |
| 1:E:95:THR:HG21  | 1:F:195:ARG:CD   | 1.90                     | 0.94              |
| 1:G:95:THR:HG22  | 1:H:195:ARG:CD   | 1.90                     | 0.94              |
| 1:B:200:PRO:HD3  | 1:J:174:LYS:HG2  | 1.37                     | 0.94              |
| 1:E:95:THR:HB    | 1:F:195:ARG:HD2  | 1.47                     | 0.94              |
| 1:K:95:THR:HB    | 1:L:195:ARG:HD2  | 1.47                     | 0.94              |
| 1:L:95:THR:HB    | 1:M:195:ARG:HD2  | 1.47                     | 0.94              |
| 1:D:78:PRO:HG2   | 1:E:184:PHE:CE1  | 2.03                     | 0.94              |
| 1:F:66:PRO:CB    | 1:P:128:LYS:HE2  | 1.96                     | 0.94              |
| 1:H:197:GLN:HE21 | 1:Q:152:MET:HG2  | 1.32                     | 0.94              |
| 1:M:78:PRO:HG2   | 1:N:184:PHE:CE1  | 2.03                     | 0.94              |
| 1:N:95:THR:HG22  | 1:O:195:ARG:CD   | 1.90                     | 0.94              |
| 1:Q:78:PRO:HG2   | 1:R:184:PHE:CE1  | 2.03                     | 0.94              |
| 1:B:197:GLN:HE21 | 1:K:152:MET:HG2  | 1.33                     | 0.94              |
| 1:E:256:LEU:CD2  | 1:N:270:HIS:HB2  | 1.87                     | 0.93              |
| 1:J:78:PRO:HG2   | 1:K:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:L:90:HIS:HE2   | 1:M:131:ILE:HD12 | 1.33                     | 0.93              |
| 1:B:95:THR:HB    | 1:C:195:ARG:HD2  | 1.47                     | 0.93              |
| 1:C:95:THR:HG22  | 1:D:195:ARG:CD   | 1.90                     | 0.93              |
| 1:E:78:PRO:HG2   | 1:F:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:L:78:PRO:HG2   | 1:M:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:E:197:GLN:HE21 | 1:N:152:MET:HG2  | 1.33                     | 0.93              |
| 1:I:78:PRO:HG2   | 1:J:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:K:108:ARG:CD   | 1:L:161:GLN:OE1  | 2.16                     | 0.93              |
| 1:M:80:TYR:CD1   | 1:N:115:PHE:HD2  | 1.84                     | 0.93              |
| 1:R:78:PRO:HG2   | 1:S:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:G:78:PRO:HG2   | 1:H:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:H:95:THR:HG21  | 1:I:195:ARG:CD   | 1.89                     | 0.93              |
| 1:J:95:THR:HB    | 1:K:195:ARG:HD2  | 1.47                     | 0.93              |
| 1:J:197:GLN:HE21 | 1:S:152:MET:HG2  | 1.33                     | 0.93              |
| 1:N:95:THR:HB    | 1:O:195:ARG:HD2  | 1.47                     | 0.93              |
| 1:R:108:ARG:CD   | 1:S:161:GLN:OE1  | 2.17                     | 0.93              |
| 1:A:197:GLN:HE21 | 1:J:152:MET:HG2  | 1.33                     | 0.93              |
| 1:H:108:ARG:CD   | 1:I:161:GLN:OE1  | 2.17                     | 0.93              |
| 1:O:78:PRO:HG2   | 1:P:184:PHE:CE1  | 2.03                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:THR:HB    | 1:B:195:ARG:HD2  | 1.47                     | 0.93              |
| 1:B:78:PRO:HG2   | 1:C:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:J:108:ARG:CD   | 1:K:161:GLN:OE1  | 2.17                     | 0.93              |
| 1:P:78:PRO:HG2   | 1:Q:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:F:78:PRO:HG2   | 1:G:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:G:108:ARG:CD   | 1:H:161:GLN:OE1  | 2.17                     | 0.93              |
| 1:K:78:PRO:HG2   | 1:L:184:PHE:CE1  | 2.03                     | 0.93              |
| 1:N:80:TYR:CD1   | 1:O:115:PHE:HD2  | 1.84                     | 0.93              |
| 1:I:197:GLN:HE21 | 1:R:152:MET:HG2  | 1.33                     | 0.92              |
| 1:N:95:THR:HG21  | 1:O:195:ARG:CD   | 1.89                     | 0.92              |
| 1:Q:95:THR:HG21  | 1:R:195:ARG:CD   | 1.90                     | 0.92              |
| 1:A:78:PRO:HG2   | 1:B:184:PHE:CE1  | 2.03                     | 0.92              |
| 1:A:108:ARG:CD   | 1:B:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:D:95:THR:HB    | 1:E:195:ARG:HD2  | 1.47                     | 0.92              |
| 1:N:78:PRO:HG2   | 1:O:184:PHE:CE1  | 2.03                     | 0.92              |
| 1:D:197:GLN:HE21 | 1:M:152:MET:HG2  | 1.33                     | 0.92              |
| 1:F:95:THR:HG21  | 1:G:195:ARG:CD   | 1.90                     | 0.92              |
| 1:H:78:PRO:HG2   | 1:I:184:PHE:CE1  | 2.03                     | 0.92              |
| 1:N:108:ARG:CD   | 1:O:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:O:80:TYR:CD1   | 1:P:115:PHE:HD2  | 1.84                     | 0.92              |
| 1:P:95:THR:HG21  | 1:Q:195:ARG:CD   | 1.89                     | 0.92              |
| 1:B:88:LEU:HD11  | 1:C:130:GLN:CB   | 2.00                     | 0.92              |
| 1:C:78:PRO:HG2   | 1:D:184:PHE:CE1  | 2.03                     | 0.92              |
| 1:C:108:ARG:CD   | 1:D:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:Q:108:ARG:CD   | 1:R:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:M:88:LEU:HD11  | 1:N:130:GLN:CB   | 2.00                     | 0.92              |
| 1:C:88:LEU:HD11  | 1:D:130:GLN:CB   | 2.00                     | 0.92              |
| 1:E:80:TYR:CD1   | 1:F:115:PHE:HD2  | 1.84                     | 0.92              |
| 1:M:108:ARG:CD   | 1:N:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:B:108:ARG:CD   | 1:C:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:D:256:LEU:CD2  | 1:M:270:HIS:HB2  | 1.87                     | 0.92              |
| 1:F:197:GLN:HE21 | 1:O:152:MET:HG2  | 1.33                     | 0.92              |
| 1:P:108:ARG:CD   | 1:Q:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:B:95:THR:HG22  | 1:C:195:ARG:CD   | 1.90                     | 0.92              |
| 1:G:197:GLN:HE21 | 1:P:152:MET:HG2  | 1.33                     | 0.92              |
| 1:I:108:ARG:CD   | 1:J:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:O:95:THR:HG21  | 1:P:195:ARG:CD   | 1.90                     | 0.92              |
| 1:O:108:ARG:CD   | 1:P:161:GLN:OE1  | 2.17                     | 0.92              |
| 1:F:90:HIS:HE2   | 1:G:131:ILE:HD12 | 1.33                     | 0.92              |
| 1:J:256:LEU:CD2  | 1:S:270:HIS:HB2  | 1.87                     | 0.92              |
| 1:L:108:ARG:CD   | 1:M:161:GLN:OE1  | 2.17                     | 0.92              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:197:GLN:NE2  | 1:Q:152:MET:HG2 | 1.85                     | 0.92              |
| 1:D:197:GLN:NE2  | 1:M:152:MET:HG2 | 1.85                     | 0.91              |
| 1:F:108:ARG:CD   | 1:G:161:GLN:OE1 | 2.17                     | 0.91              |
| 1:L:88:LEU:HD11  | 1:M:130:GLN:CB  | 2.00                     | 0.91              |
| 1:A:95:THR:HG22  | 1:B:195:ARG:CD  | 1.90                     | 0.91              |
| 1:B:236:GLU:OE2  | 1:S:267:THR:CB  | 2.17                     | 0.91              |
| 1:E:197:GLN:NE2  | 1:N:152:MET:HG2 | 1.85                     | 0.91              |
| 1:I:88:LEU:HD11  | 1:J:130:GLN:CB  | 2.00                     | 0.91              |
| 1:I:197:GLN:NE2  | 1:R:152:MET:HG2 | 1.85                     | 0.91              |
| 1:J:88:LEU:HD11  | 1:K:130:GLN:CB  | 2.00                     | 0.91              |
| 1:N:88:LEU:HD11  | 1:O:130:GLN:CB  | 2.00                     | 0.91              |
| 1:C:197:GLN:HE21 | 1:L:152:MET:HG2 | 1.33                     | 0.91              |
| 1:E:108:ARG:CD   | 1:F:161:GLN:OE1 | 2.17                     | 0.91              |
| 1:F:66:PRO:CB    | 1:P:128:LYS:HZ1 | 1.82                     | 0.91              |
| 1:A:88:LEU:HD11  | 1:B:130:GLN:CB  | 2.00                     | 0.91              |
| 1:A:236:GLU:OE2  | 1:R:267:THR:CB  | 2.17                     | 0.91              |
| 1:D:108:ARG:CD   | 1:E:161:GLN:OE1 | 2.17                     | 0.91              |
| 1:K:80:TYR:CD1   | 1:L:115:PHE:HD2 | 1.84                     | 0.91              |
| 1:P:88:LEU:HD11  | 1:Q:130:GLN:CB  | 2.00                     | 0.91              |
| 1:D:88:LEU:HD11  | 1:E:130:GLN:CB  | 2.00                     | 0.91              |
| 1:H:88:LEU:HD11  | 1:I:130:GLN:CB  | 2.00                     | 0.91              |
| 1:M:86:LEU:HA    | 1:N:130:GLN:NE2 | 1.86                     | 0.91              |
| 1:B:86:LEU:HA    | 1:C:130:GLN:NE2 | 1.86                     | 0.91              |
| 1:D:80:TYR:CD1   | 1:E:115:PHE:HD2 | 1.84                     | 0.91              |
| 1:F:197:GLN:NE2  | 1:O:152:MET:HG2 | 1.85                     | 0.91              |
| 1:K:88:LEU:HD11  | 1:L:130:GLN:CB  | 2.00                     | 0.91              |
| 1:A:200:PRO:CD   | 1:I:174:LYS:CG  | 2.46                     | 0.91              |
| 1:C:197:GLN:NE2  | 1:L:152:MET:HG2 | 1.85                     | 0.91              |
| 1:G:88:LEU:HD11  | 1:H:130:GLN:CB  | 2.00                     | 0.91              |
| 1:G:95:THR:HG21  | 1:H:195:ARG:CD  | 1.89                     | 0.91              |
| 1:J:197:GLN:NE2  | 1:S:152:MET:HG2 | 1.85                     | 0.91              |
| 1:L:86:LEU:HA    | 1:M:130:GLN:NE2 | 1.86                     | 0.91              |
| 1:O:88:LEU:HD11  | 1:P:130:GLN:CB  | 2.00                     | 0.91              |
| 1:E:88:LEU:HD11  | 1:F:130:GLN:CB  | 2.00                     | 0.90              |
| 1:F:88:LEU:HD11  | 1:G:130:GLN:CB  | 2.00                     | 0.90              |
| 1:M:95:THR:HG22  | 1:N:195:ARG:CD  | 1.90                     | 0.90              |
| 1:R:95:THR:HG22  | 1:S:195:ARG:CD  | 1.90                     | 0.90              |
| 1:C:86:LEU:HA    | 1:D:130:GLN:NE2 | 1.86                     | 0.90              |
| 1:E:86:LEU:HA    | 1:F:130:GLN:NE2 | 1.86                     | 0.90              |
| 1:F:95:THR:HG22  | 1:G:195:ARG:CD  | 1.90                     | 0.90              |
| 1:G:197:GLN:NE2  | 1:P:152:MET:HG2 | 1.85                     | 0.90              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Q:88:LEU:HD11 | 1:R:130:GLN:CB   | 2.00                     | 0.90              |
| 1:G:66:PRO:CB   | 1:Q:128:LYS:HZ1  | 1.82                     | 0.90              |
| 1:P:80:TYR:CD1  | 1:Q:115:PHE:HD2  | 1.84                     | 0.90              |
| 1:B:197:GLN:NE2 | 1:K:152:MET:HG2  | 1.85                     | 0.90              |
| 1:F:86:LEU:HA   | 1:G:130:GLN:NE2  | 1.86                     | 0.90              |
| 1:R:88:LEU:HD11 | 1:S:130:GLN:CB   | 2.00                     | 0.90              |
| 1:H:200:PRO:HB3 | 1:P:174:LYS:HA   | 1.54                     | 0.90              |
| 1:I:86:LEU:HA   | 1:J:130:GLN:NE2  | 1.86                     | 0.90              |
| 1:I:199:ARG:C   | 1:Q:174:LYS:HG2  | 1.90                     | 0.90              |
| 1:J:86:LEU:HA   | 1:K:130:GLN:NE2  | 1.86                     | 0.90              |
| 1:A:90:HIS:HE2  | 1:B:131:ILE:HD12 | 1.33                     | 0.90              |
| 1:C:94:TYR:OH   | 1:D:155:MET:HB2  | 1.72                     | 0.90              |
| 1:D:200:PRO:CD  | 1:L:174:LYS:CG   | 2.46                     | 0.90              |
| 1:A:197:GLN:NE2 | 1:J:152:MET:HG2  | 1.85                     | 0.90              |
| 1:A:200:PRO:HB3 | 1:I:174:LYS:HA   | 1.54                     | 0.90              |
| 1:K:200:PRO:HB3 | 1:S:174:LYS:HA   | 1.54                     | 0.90              |
| 1:P:86:LEU:HA   | 1:Q:130:GLN:NE2  | 1.86                     | 0.90              |
| 1:A:94:TYR:OH   | 1:B:155:MET:HB2  | 1.72                     | 0.90              |
| 1:J:200:PRO:HB3 | 1:R:174:LYS:HA   | 1.54                     | 0.90              |
| 1:N:86:LEU:HA   | 1:O:130:GLN:NE2  | 1.86                     | 0.90              |
| 1:O:94:TYR:OH   | 1:P:155:MET:HB2  | 1.72                     | 0.90              |
| 1:R:94:TYR:OH   | 1:S:155:MET:HB2  | 1.72                     | 0.90              |
| 1:B:200:PRO:HB3 | 1:J:174:LYS:HA   | 1.54                     | 0.89              |
| 1:C:80:TYR:CD1  | 1:D:115:PHE:HD2  | 1.84                     | 0.89              |
| 1:I:200:PRO:HB3 | 1:Q:174:LYS:HA   | 1.54                     | 0.89              |
| 1:B:88:LEU:CD1  | 1:C:130:GLN:CB   | 2.51                     | 0.89              |
| 1:G:94:TYR:OH   | 1:H:155:MET:HB2  | 1.72                     | 0.89              |
| 1:J:94:TYR:OH   | 1:K:155:MET:HB2  | 1.72                     | 0.89              |
| 1:N:94:TYR:OH   | 1:O:155:MET:HB2  | 1.72                     | 0.89              |
| 1:Q:95:THR:HG22 | 1:R:195:ARG:CD   | 1.90                     | 0.89              |
| 1:A:86:LEU:HA   | 1:B:130:GLN:NE2  | 1.86                     | 0.89              |
| 1:D:88:LEU:CD1  | 1:E:130:GLN:CB   | 2.51                     | 0.89              |
| 1:F:94:TYR:OH   | 1:G:155:MET:HB2  | 1.72                     | 0.89              |
| 1:L:94:TYR:OH   | 1:M:155:MET:HB2  | 1.72                     | 0.89              |
| 1:O:78:PRO:CG   | 1:P:183:HIS:HB3  | 2.03                     | 0.89              |
| 1:A:88:LEU:CD1  | 1:B:130:GLN:CB   | 2.51                     | 0.89              |
| 1:C:88:LEU:CD1  | 1:D:130:GLN:CB   | 2.51                     | 0.89              |
| 1:G:200:PRO:HB3 | 1:O:174:LYS:HA   | 1.54                     | 0.89              |
| 1:H:78:PRO:CG   | 1:I:183:HIS:HB3  | 2.03                     | 0.89              |
| 1:K:90:HIS:HE1  | 1:L:131:ILE:HD13 | 1.38                     | 0.89              |
| 1:O:86:LEU:HA   | 1:P:130:GLN:NE2  | 1.86                     | 0.89              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:86:LEU:HA   | 1:E:130:GLN:NE2  | 1.86                     | 0.89              |
| 1:E:78:PRO:CG   | 1:F:183:HIS:HB3  | 2.03                     | 0.89              |
| 1:E:88:LEU:CD1  | 1:F:130:GLN:CB   | 2.51                     | 0.89              |
| 1:I:94:TYR:OH   | 1:J:155:MET:HB2  | 1.72                     | 0.89              |
| 1:O:88:LEU:CD1  | 1:P:130:GLN:CB   | 2.51                     | 0.89              |
| 1:L:90:HIS:HE1  | 1:M:131:ILE:HD13 | 1.38                     | 0.89              |
| 1:N:88:LEU:CD1  | 1:O:130:GLN:CB   | 2.51                     | 0.89              |
| 1:D:94:TYR:OH   | 1:E:155:MET:HB2  | 1.72                     | 0.89              |
| 1:P:78:PRO:CG   | 1:Q:183:HIS:HB3  | 2.03                     | 0.89              |
| 1:Q:86:LEU:HA   | 1:R:130:GLN:NE2  | 1.86                     | 0.89              |
| 1:A:90:HIS:HE1  | 1:B:131:ILE:HD13 | 1.38                     | 0.89              |
| 1:K:86:LEU:HA   | 1:L:130:GLN:NE2  | 1.86                     | 0.89              |
| 1:R:88:LEU:CD1  | 1:S:130:GLN:CB   | 2.51                     | 0.89              |
| 1:E:200:PRO:HB3 | 1:M:174:LYS:HA   | 1.54                     | 0.89              |
| 1:F:200:PRO:HB3 | 1:N:174:LYS:HA   | 1.54                     | 0.89              |
| 1:M:88:LEU:CD1  | 1:N:130:GLN:CB   | 2.51                     | 0.89              |
| 1:B:199:ARG:C   | 1:J:174:LYS:HG2  | 1.90                     | 0.89              |
| 1:D:199:ARG:C   | 1:L:174:LYS:HG2  | 1.89                     | 0.89              |
| 1:G:86:LEU:HA   | 1:H:130:GLN:NE2  | 1.86                     | 0.89              |
| 1:I:78:PRO:CG   | 1:J:183:HIS:HB3  | 2.03                     | 0.89              |
| 1:I:88:LEU:CD1  | 1:J:130:GLN:CB   | 2.51                     | 0.89              |
| 1:J:90:HIS:HE1  | 1:K:131:ILE:HD13 | 1.38                     | 0.89              |
| 1:P:94:TYR:OH   | 1:Q:155:MET:HB2  | 1.72                     | 0.89              |
| 1:R:90:HIS:HE1  | 1:S:131:ILE:HD11 | 1.06                     | 0.89              |
| 1:A:78:PRO:CG   | 1:B:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:C:199:ARG:C   | 1:K:174:LYS:HG2  | 1.89                     | 0.88              |
| 1:D:78:PRO:CG   | 1:E:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:D:200:PRO:HB3 | 1:L:174:LYS:HA   | 1.54                     | 0.88              |
| 1:H:94:TYR:OH   | 1:I:155:MET:HB2  | 1.72                     | 0.88              |
| 1:K:94:TYR:OH   | 1:L:155:MET:HB2  | 1.72                     | 0.88              |
| 1:R:78:PRO:CG   | 1:S:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:B:90:HIS:HE1  | 1:C:131:ILE:HD13 | 1.38                     | 0.88              |
| 1:F:78:PRO:CG   | 1:G:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:F:88:LEU:CD1  | 1:G:130:GLN:CB   | 2.51                     | 0.88              |
| 1:H:88:LEU:CD1  | 1:I:130:GLN:CB   | 2.51                     | 0.88              |
| 1:K:88:LEU:CD1  | 1:L:130:GLN:CB   | 2.51                     | 0.88              |
| 1:L:88:LEU:CD1  | 1:M:130:GLN:CB   | 2.51                     | 0.88              |
| 1:N:78:PRO:CG   | 1:O:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:Q:94:TYR:OH   | 1:R:155:MET:HB2  | 1.72                     | 0.88              |
| 1:G:78:PRO:CG   | 1:H:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:H:86:LEU:HA   | 1:I:130:GLN:NE2  | 1.86                     | 0.88              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:90:HIS:HE1  | 1:P:131:ILE:HD11 | 1.05                     | 0.88              |
| 1:P:88:LEU:CD1  | 1:Q:130:GLN:CB   | 2.51                     | 0.88              |
| 1:C:200:PRO:HB3 | 1:K:174:LYS:HA   | 1.54                     | 0.88              |
| 1:L:78:PRO:CG   | 1:M:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:M:90:HIS:HE1  | 1:N:131:ILE:HD13 | 1.38                     | 0.88              |
| 1:A:199:ARG:C   | 1:I:174:LYS:HG2  | 1.90                     | 0.88              |
| 1:E:94:TYR:OH   | 1:F:155:MET:HB2  | 1.72                     | 0.88              |
| 1:B:78:PRO:CG   | 1:C:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:J:88:LEU:CD1  | 1:K:130:GLN:CB   | 2.51                     | 0.88              |
| 1:R:86:LEU:HA   | 1:S:130:GLN:NE2  | 1.86                     | 0.88              |
| 1:A:90:HIS:HE1  | 1:B:131:ILE:HD11 | 1.05                     | 0.88              |
| 1:K:78:PRO:CG   | 1:L:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:B:94:TYR:OH   | 1:C:155:MET:HB2  | 1.72                     | 0.88              |
| 1:G:88:LEU:CD1  | 1:H:130:GLN:CB   | 2.51                     | 0.88              |
| 1:I:200:PRO:CD  | 1:Q:174:LYS:CG   | 2.46                     | 0.88              |
| 1:M:78:PRO:CG   | 1:N:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:Q:78:PRO:CG   | 1:R:183:HIS:HB3  | 2.03                     | 0.88              |
| 1:F:199:ARG:C   | 1:N:174:LYS:HG2  | 1.90                     | 0.88              |
| 1:M:94:TYR:OH   | 1:N:155:MET:HB2  | 1.72                     | 0.88              |
| 1:I:80:TYR:CD1  | 1:J:115:PHE:HD2  | 1.84                     | 0.87              |
| 1:E:90:HIS:HE1  | 1:F:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:J:78:PRO:HG3  | 1:K:183:HIS:CB   | 2.04                     | 0.87              |
| 1:C:78:PRO:HG3  | 1:D:183:HIS:CB   | 2.04                     | 0.87              |
| 1:E:200:PRO:CD  | 1:M:174:LYS:CG   | 2.46                     | 0.87              |
| 1:I:90:HIS:HE1  | 1:J:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:P:95:THR:HG22 | 1:Q:195:ARG:CD   | 1.90                     | 0.87              |
| 1:Q:88:LEU:CD1  | 1:R:130:GLN:CB   | 2.51                     | 0.87              |
| 1:A:80:TYR:CD1  | 1:B:115:PHE:HD2  | 1.84                     | 0.87              |
| 1:L:95:THR:HG22 | 1:M:195:ARG:CD   | 1.90                     | 0.87              |
| 1:R:80:TYR:CD1  | 1:S:115:PHE:HD2  | 1.84                     | 0.87              |
| 1:R:90:HIS:HE1  | 1:S:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:F:66:PRO:CA   | 1:P:128:LYS:HZ1  | 1.88                     | 0.87              |
| 1:K:78:PRO:HG3  | 1:L:183:HIS:CB   | 2.04                     | 0.87              |
| 1:N:90:HIS:HE1  | 1:O:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:C:90:HIS:HE1  | 1:D:131:ILE:HD11 | 1.05                     | 0.87              |
| 1:F:90:HIS:HE1  | 1:G:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:J:78:PRO:CG   | 1:K:183:HIS:HB3  | 2.03                     | 0.87              |
| 1:B:78:PRO:HG3  | 1:C:183:HIS:CB   | 2.04                     | 0.87              |
| 1:Q:80:TYR:CD1  | 1:R:115:PHE:HD2  | 1.84                     | 0.87              |
| 1:D:90:HIS:HE1  | 1:E:131:ILE:HD13 | 1.38                     | 0.87              |
| 1:F:78:PRO:HG3  | 1:G:183:HIS:CB   | 2.04                     | 0.87              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:78:PRO:HG3  | 1:E:183:HIS:CB   | 2.04                     | 0.87              |
| 1:E:66:PRO:HB3  | 1:O:128:LYS:HZ3  | 1.40                     | 0.87              |
| 1:G:66:PRO:CA   | 1:Q:128:LYS:HZ1  | 1.88                     | 0.87              |
| 1:H:80:TYR:CD1  | 1:I:115:PHE:HD2  | 1.84                     | 0.87              |
| 1:M:78:PRO:HG3  | 1:N:183:HIS:CB   | 2.04                     | 0.87              |
| 1:B:90:HIS:NE2  | 1:C:131:ILE:CD1  | 2.32                     | 0.86              |
| 1:P:78:PRO:HG3  | 1:Q:183:HIS:CB   | 2.04                     | 0.86              |
| 1:C:78:PRO:CG   | 1:D:183:HIS:HB3  | 2.03                     | 0.86              |
| 1:G:90:HIS:HE1  | 1:H:131:ILE:HD13 | 1.38                     | 0.86              |
| 1:H:90:HIS:HE1  | 1:I:131:ILE:HD13 | 1.38                     | 0.86              |
| 1:H:200:PRO:CD  | 1:P:174:LYS:CG   | 2.46                     | 0.86              |
| 1:E:78:PRO:HG3  | 1:F:183:HIS:CB   | 2.04                     | 0.86              |
| 1:E:95:THR:HG22 | 1:F:195:ARG:CD   | 1.90                     | 0.86              |
| 1:Q:90:HIS:HE1  | 1:R:131:ILE:HD13 | 1.38                     | 0.86              |
| 1:Q:78:PRO:HG3  | 1:R:183:HIS:CB   | 2.04                     | 0.86              |
| 1:I:78:PRO:HG3  | 1:J:183:HIS:CB   | 2.04                     | 0.86              |
| 1:O:78:PRO:HG3  | 1:P:183:HIS:CB   | 2.04                     | 0.86              |
| 1:P:88:LEU:HG   | 1:Q:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:R:78:PRO:HG3  | 1:S:183:HIS:CB   | 2.04                     | 0.86              |
| 1:G:78:PRO:HG3  | 1:H:183:HIS:CB   | 2.04                     | 0.86              |
| 1:G:88:LEU:HG   | 1:H:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:L:88:LEU:HG   | 1:M:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:O:90:HIS:HE1  | 1:P:131:ILE:HD13 | 1.38                     | 0.86              |
| 1:C:88:LEU:HG   | 1:D:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:P:90:HIS:HE1  | 1:Q:131:ILE:HD13 | 1.38                     | 0.86              |
| 1:A:78:PRO:HG3  | 1:B:183:HIS:CB   | 2.04                     | 0.86              |
| 1:B:88:LEU:HG   | 1:C:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:F:90:HIS:NE2  | 1:G:131:ILE:CD1  | 2.33                     | 0.86              |
| 1:L:78:PRO:HG3  | 1:M:183:HIS:CB   | 2.04                     | 0.86              |
| 1:N:78:PRO:HG3  | 1:O:183:HIS:CB   | 2.04                     | 0.86              |
| 1:I:88:LEU:HG   | 1:J:130:GLN:HB3  | 1.58                     | 0.86              |
| 1:J:80:TYR:CD1  | 1:K:115:PHE:HD2  | 1.84                     | 0.86              |
| 1:Q:88:LEU:HG   | 1:R:130:GLN:HB3  | 1.57                     | 0.85              |
| 1:J:88:LEU:HG   | 1:K:130:GLN:HB3  | 1.58                     | 0.85              |
| 1:H:199:ARG:C   | 1:P:174:LYS:HG2  | 1.89                     | 0.85              |
| 1:Q:90:HIS:NE2  | 1:R:131:ILE:CD1  | 2.33                     | 0.85              |
| 1:F:88:LEU:HG   | 1:G:130:GLN:HB3  | 1.58                     | 0.85              |
| 1:J:253:LEU:CG  | 1:S:265:GLU:OE2  | 2.25                     | 0.85              |
| 1:K:95:THR:HG22 | 1:L:195:ARG:CD   | 1.90                     | 0.85              |
| 1:B:80:TYR:CD1  | 1:C:115:PHE:HD2  | 1.84                     | 0.85              |
| 1:R:88:LEU:HG   | 1:S:130:GLN:HB3  | 1.58                     | 0.85              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:253:LEU:CG  | 1:J:265:GLU:OE2  | 2.25                     | 0.85              |
| 1:C:90:HIS:HE1  | 1:D:131:ILE:HD13 | 1.38                     | 0.85              |
| 1:I:253:LEU:CG  | 1:R:265:GLU:OE2  | 2.25                     | 0.85              |
| 1:J:90:HIS:NE2  | 1:K:131:ILE:CD1  | 2.33                     | 0.85              |
| 1:K:88:LEU:HG   | 1:L:130:GLN:HB3  | 1.58                     | 0.85              |
| 1:H:253:LEU:CG  | 1:Q:265:GLU:OE2  | 2.25                     | 0.85              |
| 1:M:88:LEU:HG   | 1:N:130:GLN:HB3  | 1.58                     | 0.85              |
| 1:E:199:ARG:C   | 1:M:174:LYS:HG2  | 1.89                     | 0.85              |
| 1:H:78:PRO:HG3  | 1:I:183:HIS:CB   | 2.04                     | 0.85              |
| 1:J:199:ARG:C   | 1:R:174:LYS:HG2  | 1.89                     | 0.85              |
| 1:P:86:LEU:CA   | 1:Q:130:GLN:HE22 | 1.90                     | 0.85              |
| 1:Q:86:LEU:CA   | 1:R:130:GLN:HE22 | 1.90                     | 0.85              |
| 1:R:86:LEU:CA   | 1:S:130:GLN:HE22 | 1.90                     | 0.85              |
| 1:A:88:LEU:HG   | 1:B:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:E:86:LEU:CA   | 1:F:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:G:80:TYR:CD1  | 1:H:115:PHE:HD2  | 1.84                     | 0.84              |
| 1:G:253:LEU:CG  | 1:P:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:H:88:LEU:HG   | 1:I:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:A:68:LEU:HD21 | 1:K:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:F:86:LEU:CA   | 1:G:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:F:90:HIS:HE1  | 1:G:131:ILE:HD11 | 1.05                     | 0.84              |
| 1:O:88:LEU:HG   | 1:P:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:B:253:LEU:CG  | 1:K:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:C:253:LEU:CG  | 1:L:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:G:86:LEU:CA   | 1:H:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:I:68:LEU:HD21 | 1:S:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:N:90:HIS:HE1  | 1:O:131:ILE:HD11 | 1.06                     | 0.84              |
| 1:D:253:LEU:CG  | 1:M:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:E:88:LEU:HG   | 1:F:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:E:253:LEU:CG  | 1:N:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:F:200:PRO:CD  | 1:N:174:LYS:CG   | 2.46                     | 0.84              |
| 1:F:253:LEU:CG  | 1:O:265:GLU:OE2  | 2.25                     | 0.84              |
| 1:G:68:LEU:HD21 | 1:Q:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:C:68:LEU:HD21 | 1:M:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:D:68:LEU:HD21 | 1:N:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:D:88:LEU:HG   | 1:E:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:E:68:LEU:HD21 | 1:O:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:F:68:LEU:HD21 | 1:P:164:PHE:CE1  | 2.13                     | 0.84              |
| 1:I:86:LEU:CA   | 1:J:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:A:86:LEU:CA   | 1:B:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:L:86:LEU:CA   | 1:M:130:GLN:HE22 | 1.90                     | 0.84              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:88:LEU:HG   | 1:O:130:GLN:HB3  | 1.58                     | 0.84              |
| 1:O:86:LEU:CA   | 1:P:130:GLN:HE22 | 1.90                     | 0.84              |
| 1:I:90:HIS:HE1  | 1:J:131:ILE:HD11 | 1.05                     | 0.83              |
| 1:M:86:LEU:CA   | 1:N:130:GLN:HE22 | 1.90                     | 0.83              |
| 1:H:68:LEU:HD21 | 1:R:164:PHE:CE1  | 2.13                     | 0.83              |
| 1:P:88:LEU:CD1  | 1:Q:130:GLN:HB3  | 2.09                     | 0.83              |
| 1:N:86:LEU:CA   | 1:O:130:GLN:HE22 | 1.90                     | 0.83              |
| 1:B:68:LEU:HD21 | 1:L:164:PHE:CE1  | 2.13                     | 0.83              |
| 1:H:86:LEU:CA   | 1:I:130:GLN:HE22 | 1.90                     | 0.83              |
| 1:B:200:PRO:HD3 | 1:J:174:LYS:HG3  | 1.61                     | 0.83              |
| 1:E:90:HIS:NE2  | 1:F:131:ILE:CD1  | 2.33                     | 0.83              |
| 1:Q:88:LEU:CD1  | 1:R:130:GLN:HB3  | 2.09                     | 0.83              |
| 1:D:90:HIS:NE2  | 1:E:131:ILE:CD1  | 2.33                     | 0.83              |
| 1:O:88:LEU:CD1  | 1:P:130:GLN:HB3  | 2.09                     | 0.83              |
| 1:A:200:PRO:HD3 | 1:I:174:LYS:HG3  | 1.61                     | 0.83              |
| 1:R:88:LEU:CD1  | 1:S:130:GLN:HB3  | 2.09                     | 0.83              |
| 1:C:200:PRO:HD3 | 1:K:174:LYS:HG3  | 1.61                     | 0.83              |
| 1:H:88:LEU:CD1  | 1:I:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:J:88:LEU:CD1  | 1:K:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:B:86:LEU:CA   | 1:C:130:GLN:HE22 | 1.90                     | 0.82              |
| 1:I:88:LEU:CD1  | 1:J:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:C:88:LEU:CD1  | 1:D:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:E:88:LEU:CD1  | 1:F:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:C:90:HIS:NE2  | 1:D:131:ILE:CD1  | 2.33                     | 0.82              |
| 1:F:88:LEU:CD1  | 1:G:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:K:88:LEU:CD1  | 1:L:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:K:90:HIS:HE1  | 1:L:131:ILE:HD11 | 1.05                     | 0.82              |
| 1:A:88:LEU:CD1  | 1:B:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:D:200:PRO:HD3 | 1:L:174:LYS:HG3  | 1.61                     | 0.82              |
| 1:C:86:LEU:CA   | 1:D:130:GLN:HE22 | 1.90                     | 0.82              |
| 1:D:88:LEU:CD1  | 1:E:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:R:90:HIS:NE2  | 1:S:131:ILE:CD1  | 2.33                     | 0.82              |
| 1:K:86:LEU:CA   | 1:L:130:GLN:HE22 | 1.90                     | 0.82              |
| 1:G:88:LEU:CD1  | 1:H:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:M:88:LEU:CD1  | 1:N:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:N:88:LEU:CD1  | 1:O:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:Q:78:PRO:HG2  | 1:R:184:PHE:HE1  | 1.45                     | 0.82              |
| 1:D:66:PRO:CB   | 1:N:128:LYS:HZ1  | 1.89                     | 0.82              |
| 1:D:86:LEU:CA   | 1:E:130:GLN:HE22 | 1.90                     | 0.82              |
| 1:L:88:LEU:CD1  | 1:M:130:GLN:HB3  | 2.09                     | 0.82              |
| 1:I:200:PRO:HD3 | 1:Q:174:LYS:HG3  | 1.61                     | 0.81              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:200:PRO:HD3 | 1:P:174:LYS:HG3  | 1.61                     | 0.81              |
| 1:E:200:PRO:HD3 | 1:M:174:LYS:HG3  | 1.61                     | 0.81              |
| 1:K:200:PRO:HD3 | 1:S:174:LYS:HG3  | 1.61                     | 0.81              |
| 1:A:66:PRO:HB3  | 1:K:128:LYS:HZ3  | 1.46                     | 0.81              |
| 1:G:200:PRO:CD  | 1:O:174:LYS:CG   | 2.46                     | 0.81              |
| 1:F:200:PRO:HD3 | 1:N:174:LYS:HG3  | 1.61                     | 0.81              |
| 1:G:78:PRO:HG2  | 1:H:184:PHE:HE1  | 1.45                     | 0.81              |
| 1:G:200:PRO:HD3 | 1:O:174:LYS:HG3  | 1.61                     | 0.81              |
| 1:J:86:LEU:CA   | 1:K:130:GLN:HE22 | 1.90                     | 0.81              |
| 1:J:200:PRO:HD3 | 1:R:174:LYS:HG3  | 1.60                     | 0.81              |
| 1:J:78:PRO:HG2  | 1:K:184:PHE:HE1  | 1.46                     | 0.81              |
| 1:B:88:LEU:CD1  | 1:C:130:GLN:HB3  | 2.09                     | 0.81              |
| 1:B:200:PRO:CD  | 1:J:174:LYS:CG   | 2.46                     | 0.80              |
| 1:J:200:PRO:CD  | 1:R:174:LYS:CG   | 2.46                     | 0.80              |
| 1:F:78:PRO:HG2  | 1:G:184:PHE:HE1  | 1.45                     | 0.80              |
| 1:I:66:PRO:CB   | 1:S:128:LYS:HZ1  | 1.92                     | 0.80              |
| 1:Q:90:HIS:HE1  | 1:R:131:ILE:HD11 | 1.05                     | 0.80              |
| 1:R:78:PRO:HG2  | 1:S:184:PHE:HE1  | 1.46                     | 0.80              |
| 1:K:199:ARG:C   | 1:S:174:LYS:HG2  | 1.90                     | 0.80              |
| 1:P:78:PRO:HG2  | 1:Q:184:PHE:HE1  | 1.46                     | 0.80              |
| 1:I:78:PRO:HG2  | 1:J:184:PHE:HE1  | 1.45                     | 0.80              |
| 1:C:66:PRO:CA   | 1:M:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:D:66:PRO:CA   | 1:N:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:E:66:PRO:CA   | 1:O:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:E:90:HIS:HE1  | 1:F:131:ILE:HD11 | 1.05                     | 0.79              |
| 1:B:66:PRO:CA   | 1:L:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:F:66:PRO:CA   | 1:P:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:C:66:PRO:HB3  | 1:M:128:LYS:HZ3  | 1.47                     | 0.79              |
| 1:H:269:ARG:NH2 | 1:I:272:THR:HG22 | 1.98                     | 0.79              |
| 1:G:269:ARG:NH2 | 1:H:272:THR:HG22 | 1.98                     | 0.79              |
| 1:I:269:ARG:NH2 | 1:J:272:THR:HG22 | 1.98                     | 0.79              |
| 1:G:199:ARG:C   | 1:O:174:LYS:HG2  | 1.89                     | 0.79              |
| 1:P:90:HIS:NE2  | 1:Q:131:ILE:CD1  | 2.33                     | 0.79              |
| 1:E:256:LEU:CD2 | 1:N:270:HIS:C    | 2.52                     | 0.79              |
| 1:H:66:PRO:CA   | 1:R:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:I:66:PRO:CA   | 1:S:128:LYS:NZ   | 2.45                     | 0.79              |
| 1:K:78:PRO:HG2  | 1:L:184:PHE:HE1  | 1.45                     | 0.79              |
| 1:B:269:ARG:NH2 | 1:C:272:THR:HG22 | 1.98                     | 0.79              |
| 1:C:78:PRO:HG2  | 1:D:184:PHE:HE1  | 1.45                     | 0.79              |
| 1:J:269:ARG:NH2 | 1:K:272:THR:HG22 | 1.98                     | 0.79              |
| 1:A:78:PRO:HG2  | 1:B:184:PHE:HE1  | 1.45                     | 0.79              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:269:ARG:NH2 | 1:D:272:THR:HG22 | 1.98                     | 0.79              |
| 1:D:66:PRO:CA   | 1:N:128:LYS:HZ1  | 1.95                     | 0.79              |
| 1:D:269:ARG:NH2 | 1:E:272:THR:HG22 | 1.98                     | 0.79              |
| 1:H:78:PRO:HG2  | 1:I:184:PHE:HE1  | 1.45                     | 0.79              |
| 1:N:78:PRO:HG2  | 1:O:184:PHE:HE1  | 1.45                     | 0.79              |
| 1:G:66:PRO:CA   | 1:Q:128:LYS:NZ   | 2.45                     | 0.78              |
| 1:Q:269:ARG:NH2 | 1:R:272:THR:HG22 | 1.98                     | 0.78              |
| 1:R:269:ARG:NH2 | 1:S:272:THR:HG22 | 1.98                     | 0.78              |
| 1:B:78:PRO:HG2  | 1:C:184:PHE:HE1  | 1.45                     | 0.78              |
| 1:B:256:LEU:CD2 | 1:K:270:HIS:C    | 2.52                     | 0.78              |
| 1:G:88:LEU:HD11 | 1:H:130:GLN:HB2  | 1.65                     | 0.78              |
| 1:F:88:LEU:HD11 | 1:G:130:GLN:HB2  | 1.66                     | 0.78              |
| 1:G:256:LEU:CD2 | 1:P:270:HIS:C    | 2.52                     | 0.78              |
| 1:I:90:HIS:NE2  | 1:J:131:ILE:CD1  | 2.33                     | 0.78              |
| 1:A:66:PRO:CA   | 1:K:128:LYS:NZ   | 2.45                     | 0.78              |
| 1:B:66:PRO:HB3  | 1:L:128:LYS:HZ3  | 1.48                     | 0.78              |
| 1:E:269:ARG:NH2 | 1:F:272:THR:HG22 | 1.98                     | 0.78              |
| 1:H:256:LEU:CD2 | 1:Q:270:HIS:C    | 2.52                     | 0.78              |
| 1:I:256:LEU:CD2 | 1:R:270:HIS:C    | 2.52                     | 0.78              |
| 1:A:269:ARG:NH2 | 1:B:272:THR:HG22 | 1.98                     | 0.78              |
| 1:C:256:LEU:CD2 | 1:L:270:HIS:C    | 2.52                     | 0.78              |
| 1:F:269:ARG:NH2 | 1:G:272:THR:HG22 | 1.98                     | 0.78              |
| 1:F:256:LEU:CD2 | 1:O:270:HIS:C    | 2.52                     | 0.78              |
| 1:H:88:LEU:HD11 | 1:I:130:GLN:HB2  | 1.65                     | 0.78              |
| 1:D:256:LEU:CD2 | 1:M:270:HIS:C    | 2.52                     | 0.78              |
| 1:E:88:LEU:HD11 | 1:F:130:GLN:HB2  | 1.66                     | 0.78              |
| 1:A:256:LEU:CD2 | 1:J:270:HIS:C    | 2.52                     | 0.78              |
| 1:M:78:PRO:HG2  | 1:N:184:PHE:HE1  | 1.46                     | 0.78              |
| 1:M:90:HIS:HE1  | 1:N:131:ILE:HD11 | 1.05                     | 0.78              |
| 1:P:269:ARG:NH2 | 1:Q:272:THR:HG22 | 1.98                     | 0.78              |
| 1:O:88:LEU:HD11 | 1:P:130:GLN:HB2  | 1.65                     | 0.78              |
| 1:C:200:PRO:CD  | 1:K:174:LYS:CG   | 2.46                     | 0.78              |
| 1:K:269:ARG:NH2 | 1:L:272:THR:HG22 | 1.98                     | 0.78              |
| 1:J:256:LEU:CD2 | 1:S:270:HIS:C    | 2.52                     | 0.77              |
| 1:K:200:PRO:CD  | 1:S:174:LYS:CG   | 2.46                     | 0.77              |
| 1:N:95:THR:CB   | 1:O:195:ARG:CD   | 2.63                     | 0.77              |
| 1:D:88:LEU:HD11 | 1:E:130:GLN:HB2  | 1.65                     | 0.77              |
| 1:M:269:ARG:NH2 | 1:N:272:THR:HG22 | 1.98                     | 0.77              |
| 1:N:88:LEU:HD11 | 1:O:130:GLN:HB2  | 1.65                     | 0.77              |
| 1:D:95:THR:CB   | 1:E:195:ARG:CD   | 2.63                     | 0.77              |
| 1:L:269:ARG:NH2 | 1:M:272:THR:HG22 | 1.98                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:95:THR:CB    | 1:P:195:ARG:CD   | 2.63                     | 0.77              |
| 1:A:256:LEU:HD21 | 1:J:270:HIS:HB3  | 0.78                     | 0.77              |
| 1:C:68:LEU:HD21  | 1:M:164:PHE:HE1  | 1.48                     | 0.77              |
| 1:E:95:THR:CB    | 1:F:195:ARG:CD   | 2.63                     | 0.77              |
| 1:L:78:PRO:HG2   | 1:M:184:PHE:HE1  | 1.45                     | 0.77              |
| 1:O:269:ARG:NH2  | 1:P:272:THR:HG22 | 1.98                     | 0.77              |
| 1:R:95:THR:CB    | 1:S:195:ARG:CD   | 2.63                     | 0.77              |
| 1:C:95:THR:CB    | 1:D:195:ARG:CD   | 2.63                     | 0.77              |
| 1:I:88:LEU:HD11  | 1:J:130:GLN:HB2  | 1.65                     | 0.77              |
| 1:P:88:LEU:HD11  | 1:Q:130:GLN:HB2  | 1.66                     | 0.77              |
| 1:Q:88:LEU:HD11  | 1:R:130:GLN:HB2  | 1.65                     | 0.77              |
| 1:F:95:THR:CB    | 1:G:195:ARG:CD   | 2.63                     | 0.77              |
| 1:I:68:LEU:HD21  | 1:S:164:PHE:HE1  | 1.48                     | 0.77              |
| 1:M:95:THR:CB    | 1:N:195:ARG:CD   | 2.63                     | 0.77              |
| 1:B:95:THR:CB    | 1:C:195:ARG:CD   | 2.63                     | 0.77              |
| 1:D:78:PRO:HG2   | 1:E:184:PHE:HE1  | 1.45                     | 0.77              |
| 1:J:95:THR:CB    | 1:K:195:ARG:CD   | 2.63                     | 0.77              |
| 1:I:95:THR:CB    | 1:J:195:ARG:CD   | 2.63                     | 0.77              |
| 1:O:90:HIS:NE2   | 1:P:131:ILE:CD1  | 2.33                     | 0.77              |
| 1:P:95:THR:CB    | 1:Q:195:ARG:CD   | 2.63                     | 0.77              |
| 1:Q:95:THR:CB    | 1:R:195:ARG:CD   | 2.63                     | 0.77              |
| 1:D:68:LEU:HD21  | 1:N:164:PHE:HE1  | 1.48                     | 0.77              |
| 1:N:269:ARG:NH2  | 1:O:272:THR:HG22 | 1.98                     | 0.77              |
| 1:H:68:LEU:HD21  | 1:R:164:PHE:HE1  | 1.48                     | 0.77              |
| 1:E:78:PRO:HG2   | 1:F:184:PHE:HE1  | 1.45                     | 0.76              |
| 1:E:80:TYR:CE1   | 1:F:115:PHE:CD2  | 2.70                     | 0.76              |
| 1:F:256:LEU:HD21 | 1:O:270:HIS:HB3  | 0.78                     | 0.76              |
| 1:G:95:THR:CB    | 1:H:195:ARG:CD   | 2.63                     | 0.76              |
| 1:I:88:LEU:CG    | 1:J:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:K:88:LEU:HD11  | 1:L:130:GLN:HB2  | 1.65                     | 0.76              |
| 1:O:88:LEU:CG    | 1:P:130:GLN:HB3  | 2.15                     | 0.76              |
| 1:B:256:LEU:HD21 | 1:K:270:HIS:HB3  | 0.78                     | 0.76              |
| 1:E:256:LEU:HD21 | 1:N:270:HIS:HB3  | 0.78                     | 0.76              |
| 1:H:95:THR:CB    | 1:I:195:ARG:CD   | 2.63                     | 0.76              |
| 1:K:95:THR:CB    | 1:L:195:ARG:CD   | 2.63                     | 0.76              |
| 1:L:95:THR:CB    | 1:M:195:ARG:CD   | 2.63                     | 0.76              |
| 1:M:88:LEU:HD11  | 1:N:130:GLN:HB2  | 1.65                     | 0.76              |
| 1:Q:88:LEU:CG    | 1:R:130:GLN:HB3  | 2.15                     | 0.76              |
| 1:A:88:LEU:CG    | 1:B:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:A:95:THR:CB    | 1:B:195:ARG:CD   | 2.63                     | 0.76              |
| 1:C:80:TYR:OH    | 1:D:116:GLU:OE2  | 2.03                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:88:LEU:CG    | 1:F:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:G:88:LEU:CG    | 1:H:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:G:256:LEU:HD21 | 1:P:270:HIS:HB3  | 0.78                     | 0.76              |
| 1:M:88:LEU:CG    | 1:N:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:O:78:PRO:HG2   | 1:P:184:PHE:HE1  | 1.45                     | 0.76              |
| 1:R:88:LEU:HD11  | 1:S:130:GLN:HB2  | 1.65                     | 0.76              |
| 1:I:66:PRO:CA    | 1:S:128:LYS:HZ1  | 1.98                     | 0.76              |
| 1:C:88:LEU:HD11  | 1:D:130:GLN:HB2  | 1.65                     | 0.76              |
| 1:D:88:LEU:CG    | 1:E:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:R:88:LEU:CG    | 1:S:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:A:88:LEU:HD11  | 1:B:130:GLN:HB2  | 1.66                     | 0.76              |
| 1:B:80:TYR:OH    | 1:C:116:GLU:OE2  | 2.03                     | 0.76              |
| 1:D:80:TYR:OH    | 1:E:116:GLU:OE2  | 2.04                     | 0.76              |
| 1:F:68:LEU:HD21  | 1:P:164:PHE:HE1  | 1.48                     | 0.76              |
| 1:G:80:TYR:OH    | 1:H:116:GLU:OE2  | 2.03                     | 0.76              |
| 1:B:68:LEU:HD21  | 1:L:164:PHE:HE1  | 1.48                     | 0.76              |
| 1:E:66:PRO:CA    | 1:O:128:LYS:HZ3  | 1.99                     | 0.76              |
| 1:H:256:LEU:HD21 | 1:Q:270:HIS:HB3  | 0.78                     | 0.76              |
| 1:M:80:TYR:OH    | 1:N:116:GLU:OE2  | 2.03                     | 0.76              |
| 1:P:88:LEU:CG    | 1:Q:130:GLN:HB3  | 2.15                     | 0.76              |
| 1:B:90:HIS:HE1   | 1:C:131:ILE:HD11 | 1.05                     | 0.76              |
| 1:J:88:LEU:CG    | 1:K:130:GLN:HB3  | 2.15                     | 0.76              |
| 1:L:80:TYR:OH    | 1:M:116:GLU:OE2  | 2.03                     | 0.76              |
| 1:L:88:LEU:CG    | 1:M:130:GLN:HB3  | 2.16                     | 0.76              |
| 1:N:90:HIS:NE2   | 1:O:131:ILE:CD1  | 2.33                     | 0.76              |
| 1:F:88:LEU:CG    | 1:G:130:GLN:HB3  | 2.16                     | 0.75              |
| 1:N:88:LEU:CG    | 1:O:130:GLN:HB3  | 2.15                     | 0.75              |
| 1:P:80:TYR:OH    | 1:Q:116:GLU:OE2  | 2.03                     | 0.75              |
| 1:Q:80:TYR:OH    | 1:R:116:GLU:OE2  | 2.03                     | 0.75              |
| 1:B:88:LEU:CG    | 1:C:130:GLN:HB3  | 2.16                     | 0.75              |
| 1:E:66:PRO:CB    | 1:O:128:LYS:HZ3  | 1.94                     | 0.75              |
| 1:H:88:LEU:CG    | 1:I:130:GLN:HB3  | 2.16                     | 0.75              |
| 1:I:80:TYR:OH    | 1:J:116:GLU:OE2  | 2.04                     | 0.75              |
| 1:L:88:LEU:HD11  | 1:M:130:GLN:HB2  | 1.65                     | 0.75              |
| 1:M:90:HIS:NE2   | 1:N:131:ILE:CD1  | 2.33                     | 0.75              |
| 1:A:90:HIS:NE2   | 1:B:131:ILE:CD1  | 2.33                     | 0.75              |
| 1:J:88:LEU:HD11  | 1:K:130:GLN:HB2  | 1.66                     | 0.75              |
| 1:N:80:TYR:CE1   | 1:O:115:PHE:CD2  | 2.70                     | 0.75              |
| 1:N:80:TYR:OH    | 1:O:116:GLU:OE2  | 2.03                     | 0.75              |
| 1:E:80:TYR:OH    | 1:F:116:GLU:OE2  | 2.04                     | 0.75              |
| 1:G:68:LEU:HD21  | 1:Q:164:PHE:HE1  | 1.48                     | 0.75              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:256:LEU:HD21 | 1:R:270:HIS:HB3 | 0.78                     | 0.75              |
| 1:A:68:LEU:HD21  | 1:K:164:PHE:HE1 | 1.48                     | 0.75              |
| 1:A:80:TYR:OH    | 1:B:116:GLU:OE2 | 2.03                     | 0.75              |
| 1:O:80:TYR:OH    | 1:P:116:GLU:OE2 | 2.03                     | 0.75              |
| 1:O:95:THR:HB    | 1:P:195:ARG:CD  | 2.17                     | 0.75              |
| 1:R:80:TYR:OH    | 1:S:116:GLU:OE2 | 2.03                     | 0.75              |
| 1:B:88:LEU:HD11  | 1:C:130:GLN:HB2 | 1.65                     | 0.75              |
| 1:K:80:TYR:OH    | 1:L:116:GLU:OE2 | 2.03                     | 0.75              |
| 1:N:95:THR:HB    | 1:O:195:ARG:CD  | 2.17                     | 0.75              |
| 1:B:95:THR:HB    | 1:C:195:ARG:CD  | 2.17                     | 0.75              |
| 1:C:88:LEU:CG    | 1:D:130:GLN:HB3 | 2.16                     | 0.75              |
| 1:C:256:LEU:HD21 | 1:L:270:HIS:HB3 | 0.78                     | 0.75              |
| 1:L:90:HIS:NE2   | 1:M:131:ILE:CD1 | 2.33                     | 0.75              |
| 1:E:68:LEU:HD21  | 1:O:164:PHE:HE1 | 1.48                     | 0.75              |
| 1:H:66:PRO:HB3   | 1:R:128:LYS:HZ3 | 1.50                     | 0.75              |
| 1:H:66:PRO:CB    | 1:R:128:LYS:HZ1 | 1.97                     | 0.75              |
| 1:H:95:THR:HB    | 1:I:195:ARG:CD  | 2.17                     | 0.74              |
| 1:K:88:LEU:CG    | 1:L:130:GLN:HB3 | 2.16                     | 0.74              |
| 1:A:95:THR:HB    | 1:B:195:ARG:CD  | 2.18                     | 0.74              |
| 1:G:95:THR:HB    | 1:H:195:ARG:CD  | 2.17                     | 0.74              |
| 1:I:95:THR:HB    | 1:J:195:ARG:CD  | 2.17                     | 0.74              |
| 1:M:95:THR:HB    | 1:N:195:ARG:CD  | 2.17                     | 0.74              |
| 1:F:80:TYR:OH    | 1:G:116:GLU:OE2 | 2.03                     | 0.74              |
| 1:C:95:THR:HB    | 1:D:195:ARG:CD  | 2.17                     | 0.74              |
| 1:P:95:THR:HB    | 1:Q:195:ARG:CD  | 2.17                     | 0.74              |
| 1:R:95:THR:HB    | 1:S:195:ARG:CD  | 2.17                     | 0.74              |
| 1:J:256:LEU:HD21 | 1:S:270:HIS:HB3 | 0.78                     | 0.74              |
| 1:L:95:THR:HB    | 1:M:195:ARG:CD  | 2.17                     | 0.74              |
| 1:D:256:LEU:HD21 | 1:M:270:HIS:HB3 | 0.78                     | 0.74              |
| 1:D:95:THR:HB    | 1:E:195:ARG:CD  | 2.17                     | 0.74              |
| 1:H:80:TYR:OH    | 1:I:116:GLU:OE2 | 2.03                     | 0.74              |
| 1:J:80:TYR:OH    | 1:K:116:GLU:OE2 | 2.03                     | 0.74              |
| 1:F:80:TYR:CE1   | 1:G:115:PHE:CD2 | 2.70                     | 0.74              |
| 1:H:90:HIS:NE2   | 1:I:131:ILE:CD1 | 2.33                     | 0.73              |
| 1:P:88:LEU:CD1   | 1:Q:130:GLN:HB2 | 2.18                     | 0.73              |
| 1:B:88:LEU:CD1   | 1:C:130:GLN:HB2 | 2.18                     | 0.73              |
| 1:L:88:LEU:CD1   | 1:M:130:GLN:HB2 | 2.18                     | 0.73              |
| 1:C:88:LEU:CD1   | 1:D:130:GLN:HB2 | 2.18                     | 0.73              |
| 1:B:66:PRO:CB    | 1:L:128:LYS:HZ1 | 2.00                     | 0.73              |
| 1:M:88:LEU:CD1   | 1:N:130:GLN:HB2 | 2.18                     | 0.73              |
| 1:F:88:LEU:CD1   | 1:G:130:GLN:HB2 | 2.18                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:200:PRO:N    | 1:O:174:LYS:CG   | 2.42                     | 0.73              |
| 1:H:88:LEU:CD1   | 1:I:130:GLN:HB2  | 2.18                     | 0.73              |
| 1:D:88:LEU:CD1   | 1:E:130:GLN:HB2  | 2.18                     | 0.73              |
| 1:K:90:HIS:NE2   | 1:L:131:ILE:CD1  | 2.33                     | 0.73              |
| 1:A:88:LEU:CD1   | 1:B:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:Q:88:LEU:CD1   | 1:R:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:O:88:LEU:CD1   | 1:P:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:G:88:LEU:CD1   | 1:H:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:H:66:PRO:CA    | 1:R:128:LYS:HZ1  | 2.03                     | 0.72              |
| 1:M:95:THR:CB    | 1:N:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:B:80:TYR:CE1   | 1:C:115:PHE:CD2  | 2.70                     | 0.72              |
| 1:L:95:THR:CB    | 1:M:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:N:95:THR:CB    | 1:O:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:O:80:TYR:CE1   | 1:P:115:PHE:CD2  | 2.70                     | 0.72              |
| 1:B:95:THR:CB    | 1:C:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:I:66:PRO:HB3   | 1:S:128:LYS:HZ3  | 1.54                     | 0.72              |
| 1:N:88:LEU:CD1   | 1:O:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:R:95:THR:CB    | 1:S:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:A:95:THR:CB    | 1:B:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:G:95:THR:CB    | 1:H:195:ARG:HD2  | 2.20                     | 0.72              |
| 1:I:88:LEU:CD1   | 1:J:130:GLN:HB2  | 2.18                     | 0.72              |
| 1:C:88:LEU:CD2   | 1:D:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:K:88:LEU:CD2   | 1:L:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:R:88:LEU:CD1   | 1:S:130:GLN:HB2  | 2.18                     | 0.71              |
| 1:C:80:TYR:CE1   | 1:D:115:PHE:CD2  | 2.70                     | 0.71              |
| 1:H:95:THR:CB    | 1:I:195:ARG:HD2  | 2.20                     | 0.71              |
| 1:N:88:LEU:CD2   | 1:O:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:O:88:LEU:CD2   | 1:P:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:E:88:LEU:CD1   | 1:F:130:GLN:HB2  | 2.18                     | 0.71              |
| 1:F:88:LEU:CD2   | 1:G:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:H:88:LEU:CD2   | 1:I:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:M:88:LEU:CD2   | 1:N:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:O:95:THR:CB    | 1:P:195:ARG:HD2  | 2.20                     | 0.71              |
| 1:R:101:LEU:HD21 | 1:S:138:VAL:HG12 | 1.72                     | 0.71              |
| 1:B:88:LEU:CD2   | 1:C:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:D:88:LEU:CD2   | 1:E:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:G:88:LEU:CD2   | 1:H:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:J:88:LEU:CD2   | 1:K:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:P:88:LEU:CD2   | 1:Q:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:E:88:LEU:CD2   | 1:F:130:GLN:HE21 | 2.04                     | 0.71              |
| 1:J:101:LEU:HD21 | 1:K:138:VAL:HG12 | 1.73                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:80:TYR:CE1   | 1:L:115:PHE:CD2  | 2.70                     | 0.71              |
| 1:J:90:HIS:HE1   | 1:K:131:ILE:HD11 | 1.05                     | 0.70              |
| 1:N:101:LEU:HD21 | 1:O:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:A:88:LEU:CD2   | 1:B:130:GLN:HE21 | 2.04                     | 0.70              |
| 1:A:256:LEU:HD22 | 1:J:270:HIS:C    | 2.12                     | 0.70              |
| 1:B:256:LEU:HD22 | 1:K:270:HIS:C    | 2.12                     | 0.70              |
| 1:J:256:LEU:HD22 | 1:S:270:HIS:C    | 2.12                     | 0.70              |
| 1:R:88:LEU:CD2   | 1:S:130:GLN:HE21 | 2.04                     | 0.70              |
| 1:B:101:LEU:HD21 | 1:C:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:D:256:LEU:HD22 | 1:M:270:HIS:C    | 2.11                     | 0.70              |
| 1:F:256:LEU:HD22 | 1:O:270:HIS:C    | 2.11                     | 0.70              |
| 1:H:101:LEU:HD21 | 1:I:138:VAL:HG12 | 1.73                     | 0.70              |
| 1:L:88:LEU:CD2   | 1:M:130:GLN:HE21 | 2.04                     | 0.70              |
| 1:M:101:LEU:HD21 | 1:N:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:Q:95:THR:HB    | 1:R:195:ARG:CD   | 2.17                     | 0.70              |
| 1:E:101:LEU:HD21 | 1:F:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:H:256:LEU:HD22 | 1:Q:270:HIS:C    | 2.12                     | 0.70              |
| 1:J:88:LEU:CD1   | 1:K:130:GLN:HB2  | 2.18                     | 0.70              |
| 1:D:66:PRO:HB3   | 1:N:128:LYS:HZ3  | 1.56                     | 0.70              |
| 1:G:256:LEU:HD22 | 1:P:270:HIS:C    | 2.12                     | 0.70              |
| 1:I:88:LEU:CD2   | 1:J:130:GLN:HE21 | 2.04                     | 0.70              |
| 1:I:256:LEU:HD22 | 1:R:270:HIS:C    | 2.12                     | 0.70              |
| 1:C:66:PRO:CB    | 1:M:128:LYS:HZ1  | 2.01                     | 0.70              |
| 1:K:101:LEU:HD21 | 1:L:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:A:66:PRO:CB    | 1:K:128:LYS:HZ1  | 2.03                     | 0.70              |
| 1:O:101:LEU:HD21 | 1:P:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:A:66:PRO:CB    | 1:K:128:LYS:HZ3  | 2.02                     | 0.70              |
| 1:G:80:TYR:CE1   | 1:H:115:PHE:CD2  | 2.70                     | 0.70              |
| 1:K:88:LEU:CD1   | 1:L:130:GLN:HB2  | 2.18                     | 0.70              |
| 1:C:256:LEU:HD22 | 1:L:270:HIS:C    | 2.12                     | 0.70              |
| 1:D:101:LEU:HD21 | 1:E:138:VAL:HG12 | 1.73                     | 0.70              |
| 1:F:101:LEU:HD21 | 1:G:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:P:101:LEU:HD21 | 1:Q:138:VAL:HG12 | 1.72                     | 0.70              |
| 1:Q:88:LEU:CD2   | 1:R:130:GLN:HE21 | 2.04                     | 0.70              |
| 1:A:101:LEU:HD21 | 1:B:138:VAL:HG12 | 1.73                     | 0.69              |
| 1:I:101:LEU:HD21 | 1:J:138:VAL:HG12 | 1.73                     | 0.69              |
| 1:K:95:THR:HB    | 1:L:195:ARG:CD   | 2.17                     | 0.69              |
| 1:L:80:TYR:CE1   | 1:M:115:PHE:CD2  | 2.70                     | 0.69              |
| 1:E:95:THR:HB    | 1:F:195:ARG:CD   | 2.17                     | 0.69              |
| 1:G:90:HIS:NE2   | 1:H:131:ILE:CD1  | 2.33                     | 0.69              |
| 1:B:101:LEU:CD2  | 1:C:138:VAL:HG12 | 2.23                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:95:THR:HB    | 1:G:195:ARG:CD   | 2.17                     | 0.69              |
| 1:R:101:LEU:CD2  | 1:S:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:L:101:LEU:HD21 | 1:M:138:VAL:HG12 | 1.73                     | 0.69              |
| 1:D:90:HIS:HE1   | 1:E:131:ILE:HD11 | 1.05                     | 0.69              |
| 1:G:101:LEU:HD21 | 1:H:138:VAL:HG12 | 1.72                     | 0.69              |
| 1:K:101:LEU:CD2  | 1:L:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:A:101:LEU:CD2  | 1:B:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:D:80:TYR:CE1   | 1:E:115:PHE:CD2  | 2.70                     | 0.69              |
| 1:H:101:LEU:CD2  | 1:I:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:P:95:THR:CB    | 1:Q:195:ARG:HD2  | 2.20                     | 0.69              |
| 1:C:101:LEU:HD21 | 1:D:138:VAL:HG12 | 1.73                     | 0.69              |
| 1:D:67:ARG:HG2   | 1:N:162:VAL:CG1  | 2.22                     | 0.69              |
| 1:E:256:LEU:HD22 | 1:N:270:HIS:C    | 2.11                     | 0.69              |
| 1:I:101:LEU:CD2  | 1:J:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:J:243:ALA:HB1  | 1:S:260:VAL:HG21 | 1.75                     | 0.69              |
| 1:P:101:LEU:CD2  | 1:Q:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:Q:101:LEU:HD21 | 1:R:138:VAL:HG12 | 1.73                     | 0.69              |
| 1:Q:101:LEU:CD2  | 1:R:138:VAL:HG12 | 2.23                     | 0.69              |
| 1:B:66:PRO:CA    | 1:L:128:LYS:HZ1  | 2.05                     | 0.69              |
| 1:A:243:ALA:HB1  | 1:J:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:I:243:ALA:HB1  | 1:R:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:N:101:LEU:CD2  | 1:O:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:A:67:ARG:HG2   | 1:K:162:VAL:CG1  | 2.23                     | 0.68              |
| 1:B:243:ALA:HB1  | 1:K:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:C:66:PRO:CA    | 1:M:128:LYS:HZ1  | 2.07                     | 0.68              |
| 1:C:243:ALA:HB1  | 1:L:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:Q:95:THR:CB    | 1:R:195:ARG:HD2  | 2.20                     | 0.68              |
| 1:J:101:LEU:CD2  | 1:K:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:O:101:LEU:CD2  | 1:P:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:G:101:LEU:CD2  | 1:H:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:I:95:THR:CB    | 1:J:195:ARG:HD2  | 2.20                     | 0.68              |
| 1:L:101:LEU:CD2  | 1:M:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:M:101:LEU:CD2  | 1:N:138:VAL:HG12 | 2.23                     | 0.68              |
| 1:H:243:ALA:HB1  | 1:Q:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:P:80:TYR:CE1   | 1:Q:115:PHE:CD2  | 2.70                     | 0.68              |
| 1:D:243:ALA:HB1  | 1:M:260:VAL:HG21 | 1.75                     | 0.68              |
| 1:E:66:PRO:HA    | 1:O:128:LYS:HZ3  | 1.58                     | 0.68              |
| 1:I:67:ARG:HG2   | 1:S:162:VAL:CG1  | 2.22                     | 0.68              |
| 1:P:90:HIS:HE1   | 1:Q:131:ILE:HD11 | 1.05                     | 0.68              |
| 1:B:67:ARG:HG2   | 1:L:162:VAL:CG1  | 2.23                     | 0.68              |
| 1:C:67:ARG:HG2   | 1:M:162:VAL:CG1  | 2.22                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:95:THR:HB    | 1:K:195:ARG:CD   | 2.17                     | 0.68              |
| 1:B:66:PRO:CB    | 1:L:128:LYS:HZ3  | 2.04                     | 0.67              |
| 1:D:101:LEU:CD2  | 1:E:138:VAL:HG12 | 2.23                     | 0.67              |
| 1:K:199:ARG:C    | 1:S:174:LYS:CG   | 2.51                     | 0.67              |
| 1:C:101:LEU:CD2  | 1:D:138:VAL:HG12 | 2.23                     | 0.67              |
| 1:F:101:LEU:CD2  | 1:G:138:VAL:HG12 | 2.23                     | 0.67              |
| 1:E:101:LEU:CD2  | 1:F:138:VAL:HG12 | 2.23                     | 0.67              |
| 1:Q:206:GLY:O    | 1:Q:210:ASN:N    | 2.28                     | 0.67              |
| 1:R:206:GLY:O    | 1:R:210:ASN:N    | 2.28                     | 0.67              |
| 1:P:206:GLY:O    | 1:P:210:ASN:N    | 2.28                     | 0.67              |
| 1:G:206:GLY:O    | 1:G:210:ASN:N    | 2.28                     | 0.67              |
| 1:F:95:THR:CB    | 1:G:195:ARG:HD2  | 2.20                     | 0.67              |
| 1:F:206:GLY:O    | 1:F:210:ASN:N    | 2.28                     | 0.67              |
| 1:H:206:GLY:O    | 1:H:210:ASN:N    | 2.28                     | 0.67              |
| 1:I:206:GLY:O    | 1:I:210:ASN:N    | 2.28                     | 0.67              |
| 1:E:95:THR:CB    | 1:F:195:ARG:HD2  | 2.20                     | 0.67              |
| 1:G:243:ALA:HB1  | 1:P:260:VAL:HG21 | 1.75                     | 0.67              |
| 1:M:80:TYR:CE1   | 1:N:115:PHE:CD2  | 2.70                     | 0.67              |
| 1:C:66:PRO:CB    | 1:M:128:LYS:HZ3  | 2.03                     | 0.67              |
| 1:F:243:ALA:HB1  | 1:O:260:VAL:HG21 | 1.75                     | 0.67              |
| 1:J:206:GLY:O    | 1:J:210:ASN:N    | 2.28                     | 0.67              |
| 1:A:206:GLY:O    | 1:A:210:ASN:N    | 2.28                     | 0.67              |
| 1:E:206:GLY:O    | 1:E:210:ASN:N    | 2.28                     | 0.67              |
| 1:B:269:ARG:HH22 | 1:C:272:THR:HG22 | 1.59                     | 0.66              |
| 1:H:67:ARG:HG2   | 1:R:162:VAL:CG1  | 2.23                     | 0.66              |
| 1:D:198:ASP:CB   | 1:L:174:LYS:NZ   | 2.30                     | 0.66              |
| 1:E:243:ALA:HB1  | 1:N:260:VAL:HG21 | 1.75                     | 0.66              |
| 1:J:95:THR:CB    | 1:K:195:ARG:HD2  | 2.20                     | 0.66              |
| 1:S:206:GLY:O    | 1:S:210:ASN:N    | 2.28                     | 0.66              |
| 1:K:206:GLY:O    | 1:K:210:ASN:N    | 2.28                     | 0.66              |
| 1:F:200:PRO:N    | 1:N:174:LYS:CG   | 2.43                     | 0.66              |
| 1:N:269:ARG:HH22 | 1:O:272:THR:HG22 | 1.60                     | 0.66              |
| 1:A:269:ARG:HH22 | 1:B:272:THR:HG22 | 1.59                     | 0.66              |
| 1:O:269:ARG:HH22 | 1:P:272:THR:HG22 | 1.60                     | 0.66              |
| 1:A:66:PRO:CA    | 1:K:128:LYS:HZ3  | 2.07                     | 0.66              |
| 1:C:269:ARG:HH22 | 1:D:272:THR:HG22 | 1.60                     | 0.66              |
| 1:O:206:GLY:O    | 1:O:210:ASN:N    | 2.28                     | 0.66              |
| 1:B:206:GLY:O    | 1:B:210:ASN:N    | 2.28                     | 0.66              |
| 1:D:208:GLN:HE21 | 1:L:258:GLY:HA3  | 1.61                     | 0.66              |
| 1:C:66:PRO:CA    | 1:M:128:LYS:HZ3  | 2.08                     | 0.66              |
| 1:C:206:GLY:O    | 1:C:210:ASN:N    | 2.28                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:95:THR:CB    | 1:E:195:ARG:HD2  | 2.20                     | 0.66              |
| 1:G:269:ARG:HH22 | 1:H:272:THR:HG22 | 1.59                     | 0.66              |
| 1:N:206:GLY:O    | 1:N:210:ASN:N    | 2.28                     | 0.66              |
| 1:C:208:GLN:HE21 | 1:K:258:GLY:HA3  | 1.61                     | 0.66              |
| 1:D:206:GLY:O    | 1:D:210:ASN:N    | 2.28                     | 0.66              |
| 1:L:206:GLY:O    | 1:L:210:ASN:N    | 2.28                     | 0.66              |
| 1:I:269:ARG:HH22 | 1:J:272:THR:HG22 | 1.59                     | 0.66              |
| 1:M:206:GLY:O    | 1:M:210:ASN:N    | 2.28                     | 0.66              |
| 1:J:200:PRO:N    | 1:R:174:LYS:CG   | 2.43                     | 0.65              |
| 1:J:269:ARG:HH22 | 1:K:272:THR:HG22 | 1.59                     | 0.65              |
| 1:M:269:ARG:HH22 | 1:N:272:THR:HG22 | 1.59                     | 0.65              |
| 1:O:90:HIS:CE1   | 1:P:131:ILE:HD13 | 2.20                     | 0.65              |
| 1:Q:269:ARG:HH22 | 1:R:272:THR:HG22 | 1.59                     | 0.65              |
| 1:G:67:ARG:HG2   | 1:Q:162:VAL:CG1  | 2.22                     | 0.65              |
| 1:H:80:TYR:CE1   | 1:I:115:PHE:CD2  | 2.71                     | 0.65              |
| 1:F:269:ARG:HH22 | 1:G:272:THR:HG22 | 1.59                     | 0.65              |
| 1:C:95:THR:CB    | 1:D:195:ARG:HD2  | 2.20                     | 0.65              |
| 1:H:269:ARG:HH22 | 1:I:272:THR:HG22 | 1.60                     | 0.65              |
| 1:P:269:ARG:HH22 | 1:Q:272:THR:HG22 | 1.60                     | 0.65              |
| 1:Q:80:TYR:CE1   | 1:R:115:PHE:CD2  | 2.70                     | 0.65              |
| 1:E:208:GLN:HE21 | 1:M:258:GLY:HA3  | 1.61                     | 0.65              |
| 1:F:208:GLN:HE21 | 1:N:258:GLY:HA3  | 1.61                     | 0.65              |
| 1:I:208:GLN:HE21 | 1:Q:258:GLY:HA3  | 1.61                     | 0.65              |
| 1:I:241:MET:CE   | 1:Q:254:PHE:CE1  | 2.80                     | 0.65              |
| 1:G:241:MET:CE   | 1:O:254:PHE:CE1  | 2.80                     | 0.65              |
| 1:K:95:THR:CB    | 1:L:195:ARG:HD2  | 2.20                     | 0.65              |
| 1:R:269:ARG:HH22 | 1:S:272:THR:HG22 | 1.59                     | 0.65              |
| 1:H:208:GLN:HE21 | 1:P:258:GLY:HA3  | 1.61                     | 0.65              |
| 1:B:208:GLN:HE21 | 1:J:258:GLY:HA3  | 1.60                     | 0.65              |
| 1:K:269:ARG:HH22 | 1:L:272:THR:HG22 | 1.59                     | 0.65              |
| 1:D:241:MET:CE   | 1:L:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:K:208:GLN:HE21 | 1:S:258:GLY:HA3  | 1.61                     | 0.64              |
| 1:A:241:MET:CE   | 1:I:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:B:66:PRO:CA    | 1:L:128:LYS:HZ3  | 2.09                     | 0.64              |
| 1:J:208:GLN:HE21 | 1:R:258:GLY:HA3  | 1.61                     | 0.64              |
| 1:C:241:MET:CE   | 1:K:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:D:269:ARG:HH22 | 1:E:272:THR:HG22 | 1.59                     | 0.64              |
| 1:F:67:ARG:HG2   | 1:P:162:VAL:CG1  | 2.22                     | 0.64              |
| 1:B:241:MET:CE   | 1:J:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:E:66:PRO:CB    | 1:O:128:LYS:HZ1  | 2.11                     | 0.64              |
| 1:H:241:MET:CE   | 1:P:254:PHE:CE1  | 2.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:241:MET:CE   | 1:R:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:K:241:MET:CE   | 1:S:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:J:198:ASP:CB   | 1:R:174:LYS:NZ   | 2.31                     | 0.64              |
| 1:G:208:GLN:HE21 | 1:O:258:GLY:HA3  | 1.61                     | 0.64              |
| 1:I:198:ASP:CB   | 1:Q:174:LYS:NZ   | 2.30                     | 0.64              |
| 1:E:241:MET:CE   | 1:M:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:F:241:MET:CE   | 1:N:254:PHE:CE1  | 2.80                     | 0.64              |
| 1:A:208:GLN:HE21 | 1:I:258:GLY:HA3  | 1.61                     | 0.64              |
| 1:B:212:THR:HG21 | 1:J:253:LEU:O    | 1.98                     | 0.64              |
| 1:A:212:THR:HG21 | 1:I:253:LEU:O    | 1.98                     | 0.63              |
| 1:E:269:ARG:HH22 | 1:F:272:THR:HG22 | 1.59                     | 0.63              |
| 1:A:66:PRO:CA    | 1:K:128:LYS:HZ1  | 2.08                     | 0.63              |
| 1:L:269:ARG:HH22 | 1:M:272:THR:HG22 | 1.59                     | 0.63              |
| 1:H:212:THR:HG21 | 1:P:253:LEU:O    | 1.99                     | 0.63              |
| 1:K:212:THR:CG2  | 1:S:253:LEU:O    | 2.47                     | 0.63              |
| 1:C:212:THR:HG21 | 1:K:253:LEU:O    | 1.98                     | 0.63              |
| 1:F:212:THR:CG2  | 1:N:253:LEU:O    | 2.47                     | 0.63              |
| 1:I:212:THR:HG21 | 1:Q:253:LEU:O    | 1.98                     | 0.63              |
| 1:A:200:PRO:CB   | 1:I:174:LYS:HA   | 2.28                     | 0.63              |
| 1:E:212:THR:HG21 | 1:M:253:LEU:O    | 1.99                     | 0.63              |
| 1:G:212:THR:HG21 | 1:O:253:LEU:O    | 1.99                     | 0.63              |
| 1:J:212:THR:CG2  | 1:R:253:LEU:O    | 2.47                     | 0.63              |
| 1:F:212:THR:HG21 | 1:N:253:LEU:O    | 1.99                     | 0.63              |
| 1:G:212:THR:CG2  | 1:O:253:LEU:O    | 2.47                     | 0.63              |
| 1:A:212:THR:CG2  | 1:I:253:LEU:O    | 2.47                     | 0.63              |
| 1:C:212:THR:CG2  | 1:K:253:LEU:O    | 2.47                     | 0.63              |
| 1:E:212:THR:CG2  | 1:M:253:LEU:O    | 2.47                     | 0.63              |
| 1:I:80:TYR:CE1   | 1:J:115:PHE:CD2  | 2.70                     | 0.63              |
| 1:B:212:THR:CG2  | 1:J:253:LEU:O    | 2.47                     | 0.62              |
| 1:D:212:THR:CG2  | 1:L:253:LEU:O    | 2.47                     | 0.62              |
| 1:E:67:ARG:HG2   | 1:O:162:VAL:CG1  | 2.22                     | 0.62              |
| 1:I:212:THR:CG2  | 1:Q:253:LEU:O    | 2.47                     | 0.62              |
| 1:H:200:PRO:CB   | 1:P:174:LYS:HA   | 2.28                     | 0.62              |
| 1:J:200:PRO:CB   | 1:R:174:LYS:HA   | 2.28                     | 0.62              |
| 1:K:200:PRO:CB   | 1:S:174:LYS:HA   | 2.28                     | 0.62              |
| 1:D:212:THR:HG21 | 1:L:253:LEU:O    | 1.98                     | 0.62              |
| 1:J:212:THR:HG21 | 1:R:253:LEU:O    | 1.98                     | 0.62              |
| 1:B:200:PRO:CB   | 1:J:174:LYS:HA   | 2.28                     | 0.62              |
| 1:K:212:THR:HG21 | 1:S:253:LEU:O    | 1.99                     | 0.62              |
| 1:G:200:PRO:CB   | 1:O:174:LYS:HA   | 2.28                     | 0.62              |
| 1:Q:90:HIS:CE1   | 1:R:131:ILE:HD13 | 2.20                     | 0.62              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:198:ASP:CB  | 1:K:174:LYS:NZ   | 2.30                     | 0.62              |
| 1:D:78:PRO:HG3  | 1:E:183:HIS:CG   | 2.35                     | 0.62              |
| 1:H:212:THR:CG2 | 1:P:253:LEU:O    | 2.47                     | 0.62              |
| 1:J:78:PRO:HG3  | 1:K:183:HIS:CG   | 2.35                     | 0.62              |
| 1:N:78:PRO:HG3  | 1:O:183:HIS:CG   | 2.35                     | 0.62              |
| 1:O:78:PRO:HG3  | 1:P:183:HIS:CG   | 2.35                     | 0.62              |
| 1:C:78:PRO:HG3  | 1:D:183:HIS:CG   | 2.35                     | 0.62              |
| 1:K:78:PRO:HG3  | 1:L:183:HIS:CG   | 2.35                     | 0.62              |
| 1:P:78:PRO:HG3  | 1:Q:183:HIS:CG   | 2.35                     | 0.62              |
| 1:Q:78:PRO:HG3  | 1:R:183:HIS:CG   | 2.35                     | 0.62              |
| 1:H:66:PRO:CA   | 1:R:128:LYS:HZ3  | 2.13                     | 0.62              |
| 1:H:198:ASP:CB  | 1:P:174:LYS:NZ   | 2.30                     | 0.62              |
| 1:I:78:PRO:HG3  | 1:J:183:HIS:CG   | 2.35                     | 0.62              |
| 1:A:80:TYR:CE1  | 1:B:115:PHE:CD2  | 2.70                     | 0.61              |
| 1:A:199:ARG:C   | 1:I:174:LYS:CG   | 2.51                     | 0.61              |
| 1:A:200:PRO:N   | 1:I:174:LYS:CG   | 2.43                     | 0.61              |
| 1:E:78:PRO:HG3  | 1:F:183:HIS:CG   | 2.35                     | 0.61              |
| 1:G:90:HIS:CE1  | 1:H:131:ILE:HD13 | 2.20                     | 0.61              |
| 1:B:66:PRO:HA   | 1:L:128:LYS:HZ3  | 1.65                     | 0.61              |
| 1:R:78:PRO:HG3  | 1:S:183:HIS:CG   | 2.35                     | 0.61              |
| 1:B:78:PRO:HG3  | 1:C:183:HIS:CG   | 2.35                     | 0.61              |
| 1:M:78:PRO:HG3  | 1:N:183:HIS:CG   | 2.35                     | 0.61              |
| 1:O:88:LEU:HD21 | 1:P:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:A:66:PRO:HA   | 1:K:128:LYS:HZ3  | 1.64                     | 0.61              |
| 1:H:78:PRO:HG3  | 1:I:183:HIS:CG   | 2.35                     | 0.61              |
| 1:H:88:LEU:HD21 | 1:I:130:GLN:HE21 | 1.66                     | 0.61              |
| 1:I:200:PRO:CB  | 1:Q:174:LYS:HA   | 2.28                     | 0.61              |
| 1:C:66:PRO:HA   | 1:M:128:LYS:HZ3  | 1.65                     | 0.61              |
| 1:P:88:LEU:HD21 | 1:Q:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:F:66:PRO:HB3  | 1:P:128:LYS:HZ3  | 1.63                     | 0.61              |
| 1:I:88:LEU:HD21 | 1:J:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:F:199:ARG:C   | 1:N:174:LYS:CG   | 2.51                     | 0.61              |
| 1:L:78:PRO:HG3  | 1:M:183:HIS:CG   | 2.35                     | 0.61              |
| 1:A:78:PRO:HG3  | 1:B:183:HIS:CG   | 2.35                     | 0.61              |
| 1:E:256:LEU:CD2 | 1:N:270:HIS:CA   | 2.79                     | 0.61              |
| 1:F:78:PRO:HG3  | 1:G:183:HIS:CG   | 2.35                     | 0.61              |
| 1:G:78:PRO:HG3  | 1:H:183:HIS:CG   | 2.35                     | 0.61              |
| 1:A:88:LEU:HD21 | 1:B:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:E:88:LEU:HD21 | 1:F:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:G:88:LEU:HD21 | 1:H:130:GLN:HE21 | 1.65                     | 0.61              |
| 1:G:198:ASP:CB  | 1:O:174:LYS:NZ   | 2.30                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:200:PRO:CB   | 1:L:174:LYS:HA   | 2.28                     | 0.60              |
| 1:M:88:LEU:HD21  | 1:N:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:B:76:ARG:HE    | 1:C:97:GLU:CD    | 2.05                     | 0.60              |
| 1:K:88:LEU:HD21  | 1:L:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:L:88:LEU:HD21  | 1:M:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:E:199:ARG:C    | 1:M:174:LYS:CG   | 2.51                     | 0.60              |
| 1:K:76:ARG:HE    | 1:L:97:GLU:CD    | 2.05                     | 0.60              |
| 1:I:76:ARG:HE    | 1:J:97:GLU:CD    | 2.05                     | 0.60              |
| 1:R:76:ARG:HE    | 1:S:97:GLU:CD    | 2.05                     | 0.60              |
| 1:R:88:LEU:HD21  | 1:S:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:A:76:ARG:HE    | 1:B:97:GLU:CD    | 2.05                     | 0.60              |
| 1:E:200:PRO:N    | 1:M:174:LYS:CG   | 2.43                     | 0.60              |
| 1:E:200:PRO:CB   | 1:M:174:LYS:HA   | 2.28                     | 0.60              |
| 1:L:76:ARG:HE    | 1:M:97:GLU:CD    | 2.05                     | 0.60              |
| 1:E:210:ASN:HD22 | 1:M:255:GLY:HA3  | 1.67                     | 0.60              |
| 1:F:200:PRO:CB   | 1:N:174:LYS:HA   | 2.28                     | 0.60              |
| 1:G:199:ARG:C    | 1:O:174:LYS:CG   | 2.51                     | 0.60              |
| 1:H:210:ASN:HD22 | 1:P:255:GLY:HA3  | 1.67                     | 0.60              |
| 1:I:256:LEU:CD2  | 1:R:270:HIS:CA   | 2.79                     | 0.60              |
| 1:P:76:ARG:HE    | 1:Q:97:GLU:CD    | 2.05                     | 0.60              |
| 1:Q:76:ARG:HE    | 1:R:97:GLU:CD    | 2.05                     | 0.60              |
| 1:D:88:LEU:HD21  | 1:E:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:G:76:ARG:HE    | 1:H:97:GLU:CD    | 2.05                     | 0.60              |
| 1:G:90:HIS:HE1   | 1:H:131:ILE:HD11 | 1.05                     | 0.60              |
| 1:J:76:ARG:HE    | 1:K:97:GLU:CD    | 2.05                     | 0.60              |
| 1:K:198:ASP:CB   | 1:S:174:LYS:NZ   | 2.31                     | 0.60              |
| 1:N:88:LEU:HD21  | 1:O:130:GLN:HE21 | 1.66                     | 0.60              |
| 1:C:76:ARG:HE    | 1:D:97:GLU:CD    | 2.05                     | 0.60              |
| 1:F:88:LEU:HD21  | 1:G:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:H:76:ARG:HE    | 1:I:97:GLU:CD    | 2.05                     | 0.60              |
| 1:J:256:LEU:CD2  | 1:S:270:HIS:CA   | 2.79                     | 0.60              |
| 1:Q:88:LEU:HD21  | 1:R:130:GLN:HE21 | 1.65                     | 0.60              |
| 1:A:210:ASN:HD22 | 1:I:255:GLY:HA3  | 1.67                     | 0.60              |
| 1:F:210:ASN:HD22 | 1:N:255:GLY:HA3  | 1.67                     | 0.60              |
| 1:H:256:LEU:CD2  | 1:Q:270:HIS:CA   | 2.79                     | 0.60              |
| 1:O:76:ARG:HE    | 1:P:97:GLU:CD    | 2.05                     | 0.60              |
| 1:R:80:TYR:CE1   | 1:S:115:PHE:CD2  | 2.70                     | 0.60              |
| 1:D:76:ARG:HE    | 1:E:97:GLU:CD    | 2.05                     | 0.59              |
| 1:J:210:ASN:HD22 | 1:R:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:K:210:ASN:HD22 | 1:S:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:F:66:PRO:N     | 1:P:128:LYS:HZ1  | 2.00                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:88:LEU:HD21  | 1:C:130:GLN:HE21 | 1.65                     | 0.59              |
| 1:D:210:ASN:HD22 | 1:L:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:E:253:LEU:HG   | 1:N:265:GLU:OE2  | 2.02                     | 0.59              |
| 1:A:256:LEU:CD2  | 1:J:270:HIS:CA   | 2.79                     | 0.59              |
| 1:B:256:LEU:CD2  | 1:K:270:HIS:CA   | 2.79                     | 0.59              |
| 1:I:210:ASN:HD22 | 1:Q:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:C:88:LEU:HD21  | 1:D:130:GLN:HE21 | 1.65                     | 0.59              |
| 1:C:200:PRO:CB   | 1:K:174:LYS:HA   | 2.29                     | 0.59              |
| 1:E:76:ARG:HE    | 1:F:97:GLU:CD    | 2.05                     | 0.59              |
| 1:F:76:ARG:HE    | 1:G:97:GLU:CD    | 2.05                     | 0.59              |
| 1:G:66:PRO:HB3   | 1:Q:128:LYS:HZ3  | 1.63                     | 0.59              |
| 1:G:253:LEU:HG   | 1:P:265:GLU:OE2  | 2.03                     | 0.59              |
| 1:J:80:TYR:CE1   | 1:K:115:PHE:CD2  | 2.71                     | 0.59              |
| 1:B:210:ASN:HD22 | 1:J:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:F:198:ASP:CB   | 1:N:174:LYS:NZ   | 2.30                     | 0.59              |
| 1:G:66:PRO:N     | 1:Q:128:LYS:HZ1  | 2.00                     | 0.59              |
| 1:N:76:ARG:HE    | 1:O:97:GLU:CD    | 2.05                     | 0.59              |
| 1:A:198:ASP:CB   | 1:I:174:LYS:NZ   | 2.30                     | 0.59              |
| 1:G:210:ASN:HD22 | 1:O:255:GLY:HA3  | 1.67                     | 0.59              |
| 1:G:256:LEU:CD2  | 1:P:270:HIS:CA   | 2.79                     | 0.59              |
| 1:C:210:ASN:HD22 | 1:K:255:GLY:HA3  | 1.67                     | 0.58              |
| 1:H:66:PRO:CB    | 1:R:128:LYS:HZ3  | 2.07                     | 0.58              |
| 1:I:200:PRO:N    | 1:Q:174:LYS:CG   | 2.43                     | 0.58              |
| 1:J:88:LEU:HD21  | 1:K:130:GLN:HE21 | 1.65                     | 0.58              |
| 1:D:253:LEU:HG   | 1:M:265:GLU:OE2  | 2.03                     | 0.58              |
| 1:J:253:LEU:HG   | 1:S:265:GLU:OE2  | 2.02                     | 0.58              |
| 1:M:76:ARG:HE    | 1:N:97:GLU:CD    | 2.05                     | 0.58              |
| 1:E:66:PRO:CA    | 1:O:128:LYS:HZ1  | 2.16                     | 0.58              |
| 1:E:88:LEU:HD11  | 1:F:130:GLN:CG   | 2.33                     | 0.58              |
| 1:F:253:LEU:HG   | 1:O:265:GLU:OE2  | 2.02                     | 0.58              |
| 1:L:88:LEU:HD11  | 1:M:130:GLN:CG   | 2.33                     | 0.58              |
| 1:M:88:LEU:HD11  | 1:N:130:GLN:CG   | 2.33                     | 0.58              |
| 1:D:88:LEU:HD11  | 1:E:130:GLN:CG   | 2.33                     | 0.58              |
| 1:B:199:ARG:C    | 1:J:174:LYS:CG   | 2.51                     | 0.58              |
| 1:H:199:ARG:C    | 1:P:174:LYS:CG   | 2.51                     | 0.58              |
| 1:I:88:LEU:HD11  | 1:J:130:GLN:CG   | 2.33                     | 0.58              |
| 1:H:66:PRO:HA    | 1:R:128:LYS:HZ3  | 1.67                     | 0.58              |
| 1:B:253:LEU:HG   | 1:K:265:GLU:OE2  | 2.03                     | 0.58              |
| 1:D:250:ASN:OD1  | 1:D:251:ASN:N    | 2.37                     | 0.58              |
| 1:F:256:LEU:CD2  | 1:O:270:HIS:CA   | 2.79                     | 0.58              |
| 1:Q:88:LEU:HD11  | 1:R:130:GLN:CG   | 2.33                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:250:ASN:OD1 | 1:C:251:ASN:N    | 2.37                     | 0.58              |
| 1:F:88:LEU:HD11 | 1:G:130:GLN:CG   | 2.33                     | 0.58              |
| 1:K:88:LEU:HD11 | 1:L:130:GLN:CG   | 2.33                     | 0.58              |
| 1:M:250:ASN:OD1 | 1:M:251:ASN:N    | 2.37                     | 0.58              |
| 1:E:250:ASN:OD1 | 1:E:251:ASN:N    | 2.37                     | 0.58              |
| 1:K:250:ASN:OD1 | 1:K:251:ASN:N    | 2.37                     | 0.58              |
| 1:L:250:ASN:OD1 | 1:L:251:ASN:N    | 2.37                     | 0.58              |
| 1:N:250:ASN:OD1 | 1:N:251:ASN:N    | 2.37                     | 0.58              |
| 1:A:88:LEU:HD11 | 1:B:130:GLN:CG   | 2.33                     | 0.57              |
| 1:B:88:LEU:HD11 | 1:C:130:GLN:CG   | 2.33                     | 0.57              |
| 1:D:66:PRO:N    | 1:N:128:LYS:HZ1  | 2.02                     | 0.57              |
| 1:D:199:ARG:C   | 1:L:174:LYS:CG   | 2.51                     | 0.57              |
| 1:D:256:LEU:CD2 | 1:M:270:HIS:CA   | 2.79                     | 0.57              |
| 1:A:253:LEU:HG  | 1:J:265:GLU:OE2  | 2.02                     | 0.57              |
| 1:G:88:LEU:HD11 | 1:H:130:GLN:CG   | 2.33                     | 0.57              |
| 1:I:253:LEU:HG  | 1:R:265:GLU:OE2  | 2.02                     | 0.57              |
| 1:O:88:LEU:HD11 | 1:P:130:GLN:CG   | 2.33                     | 0.57              |
| 1:D:90:HIS:CE1  | 1:E:131:ILE:HD13 | 2.20                     | 0.57              |
| 1:P:88:LEU:HD11 | 1:Q:130:GLN:CG   | 2.33                     | 0.57              |
| 1:H:88:LEU:HD11 | 1:I:130:GLN:CG   | 2.33                     | 0.57              |
| 1:I:199:ARG:C   | 1:Q:174:LYS:CG   | 2.51                     | 0.57              |
| 1:N:86:LEU:O    | 1:O:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:S:250:ASN:OD1 | 1:S:251:ASN:N    | 2.37                     | 0.57              |
| 1:C:88:LEU:HD11 | 1:D:130:GLN:CG   | 2.33                     | 0.57              |
| 1:D:86:LEU:O    | 1:E:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:F:250:ASN:OD1 | 1:F:251:ASN:N    | 2.37                     | 0.57              |
| 1:H:86:LEU:O    | 1:I:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:H:250:ASN:OD1 | 1:H:251:ASN:N    | 2.37                     | 0.57              |
| 1:N:88:LEU:HD11 | 1:O:130:GLN:CG   | 2.33                     | 0.57              |
| 1:O:86:LEU:O    | 1:P:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:P:86:LEU:O    | 1:Q:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:B:250:ASN:OD1 | 1:B:251:ASN:N    | 2.37                     | 0.57              |
| 1:E:86:LEU:O    | 1:F:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:H:66:PRO:HA   | 1:R:128:LYS:NZ   | 2.20                     | 0.57              |
| 1:C:256:LEU:CD2 | 1:L:270:HIS:CA   | 2.79                     | 0.57              |
| 1:G:66:PRO:HA   | 1:Q:128:LYS:NZ   | 2.20                     | 0.57              |
| 1:L:86:LEU:O    | 1:M:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:M:86:LEU:O    | 1:N:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:Q:86:LEU:O    | 1:R:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:R:250:ASN:OD1 | 1:R:251:ASN:N    | 2.37                     | 0.57              |
| 1:E:198:ASP:CB  | 1:M:174:LYS:NZ   | 2.30                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:86:LEU:O     | 1:G:130:GLN:NE2  | 2.38                     | 0.57              |
| 1:I:250:ASN:OD1  | 1:I:251:ASN:N    | 2.37                     | 0.57              |
| 1:J:250:ASN:OD1  | 1:J:251:ASN:N    | 2.37                     | 0.57              |
| 1:R:88:LEU:HD11  | 1:S:130:GLN:CG   | 2.33                     | 0.57              |
| 1:G:86:LEU:O     | 1:H:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:I:66:PRO:N     | 1:S:128:LYS:HZ1  | 2.03                     | 0.56              |
| 1:I:66:PRO:HA    | 1:S:128:LYS:NZ   | 2.20                     | 0.56              |
| 1:A:86:LEU:O     | 1:B:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:G:250:ASN:OD1  | 1:G:251:ASN:N    | 2.37                     | 0.56              |
| 1:H:253:LEU:HG   | 1:Q:265:GLU:OE2  | 2.03                     | 0.56              |
| 1:Q:250:ASN:OD1  | 1:Q:251:ASN:N    | 2.37                     | 0.56              |
| 1:C:253:LEU:HG   | 1:L:265:GLU:OE2  | 2.02                     | 0.56              |
| 1:H:90:HIS:HE1   | 1:I:131:ILE:HD11 | 1.05                     | 0.56              |
| 1:J:88:LEU:HD11  | 1:K:130:GLN:CG   | 2.33                     | 0.56              |
| 1:F:66:PRO:HA    | 1:P:128:LYS:NZ   | 2.20                     | 0.56              |
| 1:I:86:LEU:O     | 1:J:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:K:86:LEU:O     | 1:L:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:R:86:LEU:O     | 1:S:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:C:86:LEU:O     | 1:D:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:P:250:ASN:OD1  | 1:P:251:ASN:N    | 2.37                     | 0.56              |
| 1:A:250:ASN:OD1  | 1:A:251:ASN:N    | 2.37                     | 0.56              |
| 1:O:250:ASN:OD1  | 1:O:251:ASN:N    | 2.37                     | 0.56              |
| 1:I:88:LEU:HD11  | 1:J:130:GLN:HG3  | 1.88                     | 0.56              |
| 1:A:88:LEU:HD11  | 1:B:130:GLN:HG3  | 1.88                     | 0.56              |
| 1:B:86:LEU:O     | 1:C:130:GLN:NE2  | 2.38                     | 0.56              |
| 1:I:66:PRO:HA    | 1:S:128:LYS:HZ3  | 1.71                     | 0.56              |
| 1:H:88:LEU:HD11  | 1:I:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:J:86:LEU:O     | 1:K:130:GLN:NE2  | 2.38                     | 0.55              |
| 1:R:88:LEU:HD11  | 1:S:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:D:200:PRO:N    | 1:L:174:LYS:CG   | 2.43                     | 0.55              |
| 1:J:88:LEU:HD11  | 1:K:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:B:88:LEU:HD11  | 1:C:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:B:256:LEU:HD23 | 1:K:270:HIS:C    | 2.27                     | 0.55              |
| 1:E:66:PRO:HA    | 1:O:128:LYS:NZ   | 2.20                     | 0.55              |
| 1:K:88:LEU:HD11  | 1:L:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:P:88:LEU:HD11  | 1:Q:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:A:256:LEU:HD23 | 1:J:270:HIS:C    | 2.27                     | 0.55              |
| 1:F:88:LEU:HD11  | 1:G:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:G:88:LEU:HD11  | 1:H:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:J:199:ARG:C    | 1:R:174:LYS:CG   | 2.51                     | 0.55              |
| 1:O:88:LEU:HD11  | 1:P:130:GLN:HG3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:88:LEU:HD11  | 1:R:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:C:88:LEU:HD11  | 1:D:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:I:256:LEU:CD2  | 1:R:270:HIS:O    | 2.55                     | 0.55              |
| 1:B:256:LEU:CD2  | 1:K:270:HIS:O    | 2.55                     | 0.55              |
| 1:L:88:LEU:HD11  | 1:M:130:GLN:HG3  | 1.89                     | 0.55              |
| 1:D:88:LEU:HD11  | 1:E:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:J:256:LEU:HD23 | 1:S:270:HIS:C    | 2.27                     | 0.55              |
| 1:L:90:HIS:HE1   | 1:M:131:ILE:HD11 | 1.05                     | 0.55              |
| 1:M:88:LEU:HD11  | 1:N:130:GLN:HG3  | 1.88                     | 0.55              |
| 1:B:90:HIS:CE1   | 1:C:131:ILE:HD13 | 2.20                     | 0.54              |
| 1:E:256:LEU:CD2  | 1:N:270:HIS:O    | 2.55                     | 0.54              |
| 1:H:253:LEU:HD21 | 1:Q:265:GLU:OE2  | 2.07                     | 0.54              |
| 1:H:256:LEU:HD23 | 1:Q:270:HIS:CA   | 2.37                     | 0.54              |
| 1:I:256:LEU:HD23 | 1:R:270:HIS:CA   | 2.37                     | 0.54              |
| 1:F:94:TYR:CE1   | 1:G:155:MET:HE2  | 2.42                     | 0.54              |
| 1:A:253:LEU:HD21 | 1:J:265:GLU:OE2  | 2.07                     | 0.54              |
| 1:D:256:LEU:CD2  | 1:M:270:HIS:O    | 2.55                     | 0.54              |
| 1:G:253:LEU:HD21 | 1:P:265:GLU:OE2  | 2.07                     | 0.54              |
| 1:N:88:LEU:HD11  | 1:O:130:GLN:HG3  | 1.89                     | 0.54              |
| 1:A:256:LEU:CD2  | 1:J:270:HIS:O    | 2.55                     | 0.54              |
| 1:D:66:PRO:HA    | 1:N:128:LYS:NZ   | 2.20                     | 0.54              |
| 1:E:88:LEU:HD11  | 1:F:130:GLN:HG3  | 1.89                     | 0.54              |
| 1:G:256:LEU:CD2  | 1:P:270:HIS:O    | 2.55                     | 0.54              |
| 1:G:256:LEU:HD23 | 1:P:270:HIS:C    | 2.27                     | 0.54              |
| 1:H:66:PRO:N     | 1:R:128:LYS:HZ1  | 2.06                     | 0.54              |
| 1:J:253:LEU:HD21 | 1:S:265:GLU:OE2  | 2.07                     | 0.54              |
| 1:D:253:LEU:HD21 | 1:M:265:GLU:OE2  | 2.07                     | 0.54              |
| 1:H:256:LEU:HD23 | 1:Q:270:HIS:C    | 2.27                     | 0.54              |
| 1:I:256:LEU:HD23 | 1:R:270:HIS:C    | 2.27                     | 0.54              |
| 1:L:94:TYR:CE1   | 1:M:155:MET:HE2  | 2.42                     | 0.54              |
| 1:B:256:LEU:HD23 | 1:K:270:HIS:CA   | 2.37                     | 0.54              |
| 1:D:66:PRO:CA    | 1:N:128:LYS:HZ3  | 2.21                     | 0.54              |
| 1:D:78:PRO:HG2   | 1:E:184:PHE:CD1  | 2.43                     | 0.54              |
| 1:I:94:TYR:CE1   | 1:J:155:MET:HE2  | 2.43                     | 0.54              |
| 1:B:66:PRO:HA    | 1:L:128:LYS:NZ   | 2.20                     | 0.54              |
| 1:C:256:LEU:CD2  | 1:L:270:HIS:O    | 2.55                     | 0.54              |
| 1:E:256:LEU:HD23 | 1:N:270:HIS:C    | 2.27                     | 0.54              |
| 1:H:256:LEU:CD2  | 1:Q:270:HIS:O    | 2.55                     | 0.54              |
| 1:J:256:LEU:HD23 | 1:S:270:HIS:CA   | 2.37                     | 0.54              |
| 1:A:66:PRO:HA    | 1:K:128:LYS:NZ   | 2.20                     | 0.54              |
| 1:C:66:PRO:HA    | 1:M:128:LYS:NZ   | 2.20                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:256:LEU:HD23 | 1:O:270:HIS:C    | 2.27                     | 0.54              |
| 1:I:243:ALA:CB   | 1:R:260:VAL:HG21 | 2.38                     | 0.54              |
| 1:J:256:LEU:CD2  | 1:S:270:HIS:O    | 2.55                     | 0.54              |
| 1:M:90:HIS:CE1   | 1:N:131:ILE:HD13 | 2.20                     | 0.54              |
| 1:O:78:PRO:HG2   | 1:P:184:PHE:CD1  | 2.43                     | 0.54              |
| 1:A:243:ALA:CB   | 1:J:260:VAL:HG21 | 2.38                     | 0.53              |
| 1:E:253:LEU:HD21 | 1:N:265:GLU:OE2  | 2.07                     | 0.53              |
| 1:F:243:ALA:CB   | 1:O:260:VAL:HG21 | 2.38                     | 0.53              |
| 1:F:253:LEU:HD21 | 1:O:265:GLU:OE2  | 2.07                     | 0.53              |
| 1:G:78:PRO:CG    | 1:H:184:PHE:HE1  | 2.20                     | 0.53              |
| 1:C:253:LEU:HD21 | 1:L:265:GLU:OE2  | 2.07                     | 0.53              |
| 1:E:78:PRO:HG2   | 1:F:184:PHE:CD1  | 2.43                     | 0.53              |
| 1:E:243:ALA:CB   | 1:N:260:VAL:HG21 | 2.38                     | 0.53              |
| 1:I:253:LEU:HD21 | 1:R:265:GLU:OE2  | 2.07                     | 0.53              |
| 1:B:198:ASP:CB   | 1:J:174:LYS:NZ   | 2.31                     | 0.53              |
| 1:F:256:LEU:HD23 | 1:O:270:HIS:CA   | 2.37                     | 0.53              |
| 1:I:66:PRO:CA    | 1:S:128:LYS:HZ3  | 2.18                     | 0.53              |
| 1:D:256:LEU:HD23 | 1:M:270:HIS:CA   | 2.37                     | 0.53              |
| 1:I:94:TYR:CE1   | 1:J:155:MET:CE   | 2.92                     | 0.53              |
| 1:L:94:TYR:CE1   | 1:M:155:MET:CE   | 2.92                     | 0.53              |
| 1:Q:94:TYR:CE1   | 1:R:155:MET:CE   | 2.92                     | 0.53              |
| 1:B:66:PRO:N     | 1:L:128:LYS:HZ1  | 2.07                     | 0.53              |
| 1:B:94:TYR:CE1   | 1:C:155:MET:CE   | 2.92                     | 0.53              |
| 1:F:256:LEU:CD2  | 1:O:270:HIS:O    | 2.55                     | 0.53              |
| 1:A:94:TYR:CE1   | 1:B:155:MET:CE   | 2.92                     | 0.53              |
| 1:J:94:TYR:CE1   | 1:K:155:MET:CE   | 2.92                     | 0.53              |
| 1:F:253:LEU:CD2  | 1:O:265:GLU:OE2  | 2.57                     | 0.53              |
| 1:G:94:TYR:CE1   | 1:H:155:MET:CE   | 2.92                     | 0.53              |
| 1:H:94:TYR:CE1   | 1:I:155:MET:CE   | 2.92                     | 0.53              |
| 1:L:78:PRO:HG2   | 1:M:184:PHE:CD1  | 2.43                     | 0.53              |
| 1:P:94:TYR:CE1   | 1:Q:155:MET:CE   | 2.92                     | 0.53              |
| 1:A:253:LEU:CD2  | 1:J:265:GLU:OE2  | 2.57                     | 0.53              |
| 1:B:253:LEU:CD2  | 1:K:265:GLU:OE2  | 2.57                     | 0.53              |
| 1:C:94:TYR:CE1   | 1:D:155:MET:CE   | 2.92                     | 0.53              |
| 1:C:199:ARG:C    | 1:K:174:LYS:CG   | 2.51                     | 0.53              |
| 1:E:241:MET:SD   | 1:M:254:PHE:CD1  | 3.02                     | 0.53              |
| 1:E:253:LEU:CD2  | 1:N:265:GLU:OE2  | 2.57                     | 0.53              |
| 1:G:256:LEU:HD23 | 1:P:270:HIS:CA   | 2.37                     | 0.53              |
| 1:J:78:PRO:CG    | 1:K:184:PHE:HE1  | 2.21                     | 0.53              |
| 1:K:94:TYR:CE1   | 1:L:155:MET:CE   | 2.92                     | 0.53              |
| 1:B:108:ARG:NH1  | 1:C:161:GLN:CG   | 2.71                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:243:ALA:CB   | 1:K:260:VAL:HG21 | 2.38                     | 0.53              |
| 1:F:241:MET:SD   | 1:N:254:PHE:CD1  | 3.02                     | 0.53              |
| 1:I:253:LEU:CD2  | 1:R:265:GLU:OE2  | 2.57                     | 0.53              |
| 1:M:94:TYR:CE1   | 1:N:155:MET:CE   | 2.92                     | 0.53              |
| 1:R:94:TYR:CE1   | 1:S:155:MET:CE   | 2.92                     | 0.53              |
| 1:A:90:HIS:CE1   | 1:B:131:ILE:HD13 | 2.20                     | 0.52              |
| 1:C:243:ALA:CB   | 1:L:260:VAL:HG21 | 2.38                     | 0.52              |
| 1:G:243:ALA:CB   | 1:P:260:VAL:HG21 | 2.38                     | 0.52              |
| 1:J:253:LEU:CD2  | 1:S:265:GLU:OE2  | 2.57                     | 0.52              |
| 1:K:200:PRO:N    | 1:S:174:LYS:CG   | 2.43                     | 0.52              |
| 1:Q:95:THR:HG22  | 1:R:195:ARG:NE   | 2.25                     | 0.52              |
| 1:A:78:PRO:HG2   | 1:B:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:C:256:LEU:HD23 | 1:L:270:HIS:CA   | 2.37                     | 0.52              |
| 1:N:94:TYR:CE1   | 1:O:155:MET:CE   | 2.92                     | 0.52              |
| 1:O:94:TYR:CE1   | 1:P:155:MET:CE   | 2.92                     | 0.52              |
| 1:R:78:PRO:HG2   | 1:S:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:B:253:LEU:HD21 | 1:K:265:GLU:OE2  | 2.07                     | 0.52              |
| 1:C:66:PRO:N     | 1:M:128:LYS:HZ1  | 2.08                     | 0.52              |
| 1:C:90:HIS:CE1   | 1:D:131:ILE:HD13 | 2.20                     | 0.52              |
| 1:D:241:MET:SD   | 1:L:254:PHE:CD1  | 3.02                     | 0.52              |
| 1:D:253:LEU:CD2  | 1:M:265:GLU:OE2  | 2.57                     | 0.52              |
| 1:F:94:TYR:CE1   | 1:G:155:MET:CE   | 2.92                     | 0.52              |
| 1:F:95:THR:HG22  | 1:G:195:ARG:NE   | 2.25                     | 0.52              |
| 1:G:95:THR:HG22  | 1:H:195:ARG:NE   | 2.25                     | 0.52              |
| 1:G:241:MET:SD   | 1:O:254:PHE:CD1  | 3.01                     | 0.52              |
| 1:J:95:THR:HG22  | 1:K:195:ARG:NE   | 2.25                     | 0.52              |
| 1:J:243:ALA:CB   | 1:S:260:VAL:HG21 | 2.38                     | 0.52              |
| 1:P:78:PRO:HG2   | 1:Q:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:M:95:THR:HG22  | 1:N:195:ARG:NE   | 2.25                     | 0.52              |
| 1:Q:108:ARG:NH1  | 1:R:161:GLN:CG   | 2.71                     | 0.52              |
| 1:E:94:TYR:CE1   | 1:F:155:MET:CE   | 2.92                     | 0.52              |
| 1:H:243:ALA:CB   | 1:Q:260:VAL:HG21 | 2.38                     | 0.52              |
| 1:H:253:LEU:CD2  | 1:Q:265:GLU:OE2  | 2.57                     | 0.52              |
| 1:K:241:MET:SD   | 1:S:254:PHE:CD1  | 3.02                     | 0.52              |
| 1:N:95:THR:HG22  | 1:O:195:ARG:NE   | 2.25                     | 0.52              |
| 1:Q:78:PRO:CG    | 1:R:184:PHE:HE1  | 2.20                     | 0.52              |
| 1:R:80:TYR:HD1   | 1:S:115:PHE:CD2  | 2.22                     | 0.52              |
| 1:R:95:THR:HG22  | 1:S:195:ARG:NE   | 2.25                     | 0.52              |
| 1:B:78:PRO:HG2   | 1:C:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:C:200:PRO:N    | 1:K:174:LYS:CG   | 2.43                     | 0.52              |
| 1:C:253:LEU:CD2  | 1:L:265:GLU:OE2  | 2.57                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:253:LEU:CD2  | 1:P:265:GLU:OE2  | 2.57                     | 0.52              |
| 1:J:241:MET:SD   | 1:R:254:PHE:CD1  | 3.02                     | 0.52              |
| 1:K:94:TYR:CE1   | 1:L:155:MET:HE2  | 2.45                     | 0.52              |
| 1:D:94:TYR:CE1   | 1:E:155:MET:CE   | 2.92                     | 0.52              |
| 1:E:80:TYR:HD1   | 1:F:115:PHE:CD2  | 2.22                     | 0.52              |
| 1:H:78:PRO:HG2   | 1:I:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:N:104:THR:HG21 | 1:O:204:ARG:HH12 | 1.75                     | 0.52              |
| 1:C:95:THR:HG22  | 1:D:195:ARG:NE   | 2.25                     | 0.52              |
| 1:D:66:PRO:HA    | 1:N:128:LYS:HZ3  | 1.73                     | 0.52              |
| 1:E:256:LEU:HD23 | 1:N:270:HIS:CA   | 2.37                     | 0.52              |
| 1:F:78:PRO:HG2   | 1:G:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:F:78:PRO:CG    | 1:G:184:PHE:HE1  | 2.20                     | 0.52              |
| 1:H:241:MET:SD   | 1:P:254:PHE:CD1  | 3.02                     | 0.52              |
| 1:I:78:PRO:HG2   | 1:J:184:PHE:CD1  | 2.43                     | 0.52              |
| 1:M:78:PRO:CG    | 1:N:184:PHE:HE1  | 2.21                     | 0.52              |
| 1:M:104:THR:HG21 | 1:N:204:ARG:HH12 | 1.75                     | 0.52              |
| 1:P:108:ARG:NH1  | 1:Q:161:GLN:CG   | 2.72                     | 0.52              |
| 1:Q:94:TYR:CE1   | 1:R:155:MET:HE2  | 2.45                     | 0.52              |
| 1:A:104:THR:HG21 | 1:B:204:ARG:HH12 | 1.75                     | 0.52              |
| 1:B:78:PRO:CG    | 1:C:184:PHE:HE1  | 2.20                     | 0.52              |
| 1:D:95:THR:HG22  | 1:E:195:ARG:NE   | 2.25                     | 0.52              |
| 1:L:108:ARG:NH1  | 1:M:161:GLN:CG   | 2.71                     | 0.52              |
| 1:M:108:ARG:NH1  | 1:N:161:GLN:CG   | 2.71                     | 0.52              |
| 1:D:243:ALA:CB   | 1:M:260:VAL:HG21 | 2.38                     | 0.52              |
| 1:I:95:THR:HG22  | 1:J:195:ARG:NE   | 2.25                     | 0.52              |
| 1:O:108:ARG:NH1  | 1:P:161:GLN:CG   | 2.71                     | 0.52              |
| 1:R:94:TYR:CE1   | 1:S:155:MET:HE2  | 2.45                     | 0.52              |
| 1:A:95:THR:HG22  | 1:B:195:ARG:NE   | 2.25                     | 0.51              |
| 1:H:94:TYR:CE1   | 1:I:155:MET:HE2  | 2.45                     | 0.51              |
| 1:H:95:THR:HG22  | 1:I:195:ARG:NE   | 2.25                     | 0.51              |
| 1:I:241:MET:SD   | 1:Q:254:PHE:CD1  | 3.02                     | 0.51              |
| 1:K:78:PRO:HG2   | 1:L:184:PHE:CD1  | 2.43                     | 0.51              |
| 1:K:90:HIS:CE1   | 1:L:131:ILE:HD13 | 2.20                     | 0.51              |
| 1:K:95:THR:HG22  | 1:L:195:ARG:NE   | 2.25                     | 0.51              |
| 1:L:104:THR:HG21 | 1:M:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:M:78:PRO:HG2   | 1:N:184:PHE:CD1  | 2.43                     | 0.51              |
| 1:Q:78:PRO:HG2   | 1:R:184:PHE:CD1  | 2.43                     | 0.51              |
| 1:C:256:LEU:HD23 | 1:L:270:HIS:C    | 2.27                     | 0.51              |
| 1:D:104:THR:HG21 | 1:E:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:N:108:ARG:NH1  | 1:O:161:GLN:CG   | 2.72                     | 0.51              |
| 1:B:95:THR:HG22  | 1:C:195:ARG:NE   | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:104:THR:HG21 | 1:C:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:C:241:MET:SD   | 1:K:254:PHE:CD1  | 3.02                     | 0.51              |
| 1:G:104:THR:HG21 | 1:H:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:A:66:PRO:N     | 1:K:128:LYS:HZ1  | 2.08                     | 0.51              |
| 1:A:108:ARG:NH1  | 1:B:161:GLN:CG   | 2.72                     | 0.51              |
| 1:A:256:LEU:HD23 | 1:J:270:HIS:CA   | 2.37                     | 0.51              |
| 1:J:90:HIS:CE1   | 1:K:131:ILE:HD13 | 2.20                     | 0.51              |
| 1:K:104:THR:HG21 | 1:L:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:K:108:ARG:NH1  | 1:L:161:GLN:CG   | 2.71                     | 0.51              |
| 1:O:95:THR:HG22  | 1:P:195:ARG:NE   | 2.25                     | 0.51              |
| 1:O:104:THR:HG21 | 1:P:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:F:104:THR:HG21 | 1:G:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:E:90:HIS:CE1   | 1:F:131:ILE:HD13 | 2.20                     | 0.51              |
| 1:G:94:TYR:CE1   | 1:H:155:MET:HE2  | 2.45                     | 0.51              |
| 1:J:78:PRO:HG2   | 1:K:184:PHE:CD1  | 2.43                     | 0.51              |
| 1:L:95:THR:HG22  | 1:M:195:ARG:NE   | 2.25                     | 0.51              |
| 1:R:104:THR:HG21 | 1:S:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:D:66:PRO:CB    | 1:N:128:LYS:HZ3  | 2.16                     | 0.51              |
| 1:H:104:THR:HG21 | 1:I:204:ARG:HH12 | 1.75                     | 0.51              |
| 1:G:78:PRO:HG2   | 1:H:184:PHE:CD1  | 2.43                     | 0.51              |
| 1:A:256:LEU:HD23 | 1:J:270:HIS:O    | 2.11                     | 0.51              |
| 1:Q:78:PRO:CG    | 1:R:183:HIS:CB   | 2.80                     | 0.51              |
| 1:C:78:PRO:HG2   | 1:D:184:PHE:CD1  | 2.43                     | 0.50              |
| 1:C:104:THR:HG21 | 1:D:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:E:95:THR:HG22  | 1:F:195:ARG:NE   | 2.25                     | 0.50              |
| 1:I:104:THR:HG21 | 1:J:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:I:256:LEU:HD23 | 1:R:270:HIS:O    | 2.11                     | 0.50              |
| 1:C:94:TYR:CE1   | 1:D:155:MET:HE2  | 2.47                     | 0.50              |
| 1:C:256:LEU:HD23 | 1:L:270:HIS:O    | 2.11                     | 0.50              |
| 1:K:241:MET:SD   | 1:S:254:PHE:CZ   | 3.04                     | 0.50              |
| 1:A:80:TYR:HD1   | 1:B:115:PHE:CD2  | 2.22                     | 0.50              |
| 1:B:241:MET:SD   | 1:J:254:PHE:CD1  | 3.02                     | 0.50              |
| 1:H:256:LEU:HD23 | 1:Q:270:HIS:O    | 2.11                     | 0.50              |
| 1:A:241:MET:SD   | 1:I:254:PHE:CD1  | 3.02                     | 0.50              |
| 1:D:256:LEU:HD23 | 1:M:270:HIS:C    | 2.27                     | 0.50              |
| 1:I:78:PRO:CG    | 1:J:184:PHE:HE1  | 2.20                     | 0.50              |
| 1:L:213:ASP:OD2  | 1:L:215:SER:OG   | 2.29                     | 0.50              |
| 1:P:104:THR:HG21 | 1:Q:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:E:104:THR:HG21 | 1:F:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:B:241:MET:SD   | 1:J:254:PHE:CZ   | 3.05                     | 0.50              |
| 1:C:198:ASP:HB3  | 1:K:174:LYS:NZ   | 2.25                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:256:LEU:HD23 | 1:S:270:HIS:O    | 2.11                     | 0.50              |
| 1:K:80:TYR:HD1   | 1:L:115:PHE:CD2  | 2.22                     | 0.50              |
| 1:I:67:ARG:CG    | 1:S:162:VAL:HG11 | 2.31                     | 0.50              |
| 1:Q:104:THR:HG21 | 1:R:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:B:210:ASN:ND2  | 1:J:255:GLY:HA3  | 2.27                     | 0.50              |
| 1:D:241:MET:SD   | 1:L:254:PHE:CZ   | 3.04                     | 0.50              |
| 1:F:241:MET:SD   | 1:N:254:PHE:CZ   | 3.04                     | 0.50              |
| 1:H:200:PRO:N    | 1:P:174:LYS:CG   | 2.43                     | 0.50              |
| 1:J:104:THR:HG21 | 1:K:204:ARG:HH12 | 1.75                     | 0.50              |
| 1:C:210:ASN:ND2  | 1:K:255:GLY:HA3  | 2.27                     | 0.50              |
| 1:D:213:ASP:OD2  | 1:D:215:SER:OG   | 2.29                     | 0.50              |
| 1:E:210:ASN:ND2  | 1:M:255:GLY:HA3  | 2.27                     | 0.50              |
| 1:L:78:PRO:CG    | 1:M:184:PHE:HE1  | 2.20                     | 0.50              |
| 1:M:213:ASP:OD2  | 1:M:215:SER:OG   | 2.29                     | 0.50              |
| 1:G:66:PRO:CD    | 1:Q:128:LYS:HZ1  | 2.25                     | 0.49              |
| 1:I:66:PRO:CD    | 1:S:128:LYS:HZ1  | 2.25                     | 0.49              |
| 1:J:108:ARG:NH1  | 1:K:161:GLN:CG   | 2.72                     | 0.49              |
| 1:P:94:TYR:CE1   | 1:Q:155:MET:HE2  | 2.47                     | 0.49              |
| 1:P:95:THR:HG22  | 1:Q:195:ARG:NE   | 2.24                     | 0.49              |
| 1:F:210:ASN:ND2  | 1:N:255:GLY:HA3  | 2.27                     | 0.49              |
| 1:G:241:MET:SD   | 1:O:254:PHE:CZ   | 3.04                     | 0.49              |
| 1:G:256:LEU:HD23 | 1:P:270:HIS:O    | 2.11                     | 0.49              |
| 1:O:78:PRO:CG    | 1:P:183:HIS:CB   | 2.80                     | 0.49              |
| 1:D:198:ASP:HB3  | 1:L:174:LYS:NZ   | 2.25                     | 0.49              |
| 1:E:78:PRO:CG    | 1:F:184:PHE:HE1  | 2.20                     | 0.49              |
| 1:P:78:PRO:CG    | 1:Q:184:PHE:HE1  | 2.21                     | 0.49              |
| 1:B:154:VAL:HG22 | 1:B:155:MET:O    | 2.13                     | 0.49              |
| 1:B:213:ASP:OD2  | 1:B:215:SER:OG   | 2.29                     | 0.49              |
| 1:E:154:VAL:HG22 | 1:E:155:MET:O    | 2.13                     | 0.49              |
| 1:G:108:ARG:NH1  | 1:H:161:GLN:CG   | 2.71                     | 0.49              |
| 1:J:94:TYR:CE1   | 1:K:155:MET:HE2  | 2.48                     | 0.49              |
| 1:S:154:VAL:HG22 | 1:S:155:MET:O    | 2.13                     | 0.49              |
| 1:A:154:VAL:HG22 | 1:A:155:MET:O    | 2.13                     | 0.49              |
| 1:B:256:LEU:HD23 | 1:K:270:HIS:O    | 2.11                     | 0.49              |
| 1:D:210:ASN:ND2  | 1:L:255:GLY:HA3  | 2.27                     | 0.49              |
| 1:D:256:LEU:HD23 | 1:M:270:HIS:O    | 2.11                     | 0.49              |
| 1:H:108:ARG:NH1  | 1:I:161:GLN:CG   | 2.72                     | 0.49              |
| 1:K:213:ASP:OD2  | 1:K:215:SER:OG   | 2.29                     | 0.49              |
| 1:N:78:PRO:HG2   | 1:O:184:PHE:CD1  | 2.43                     | 0.49              |
| 1:C:154:VAL:HG22 | 1:C:155:MET:O    | 2.13                     | 0.49              |
| 1:D:154:VAL:HG22 | 1:D:155:MET:O    | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:256:LEU:HD23 | 1:N:270:HIS:O    | 2.11                     | 0.49              |
| 1:B:198:ASP:HB3  | 1:J:174:LYS:NZ   | 2.26                     | 0.49              |
| 1:E:213:ASP:OD2  | 1:E:215:SER:OG   | 2.29                     | 0.49              |
| 1:F:256:LEU:HD23 | 1:O:270:HIS:O    | 2.12                     | 0.49              |
| 1:N:94:TYR:CE1   | 1:O:155:MET:HE2  | 2.47                     | 0.49              |
| 1:P:260:VAL:O    | 1:P:260:VAL:HG23 | 2.13                     | 0.49              |
| 1:S:213:ASP:OD2  | 1:S:215:SER:OG   | 2.29                     | 0.49              |
| 1:B:67:ARG:CG    | 1:L:162:VAL:HG11 | 2.31                     | 0.49              |
| 1:B:260:VAL:O    | 1:B:260:VAL:HG23 | 2.13                     | 0.49              |
| 1:D:66:PRO:CD    | 1:N:128:LYS:HZ1  | 2.25                     | 0.49              |
| 1:F:154:VAL:HG22 | 1:F:155:MET:O    | 2.13                     | 0.49              |
| 1:F:260:VAL:HG23 | 1:F:260:VAL:O    | 2.13                     | 0.49              |
| 1:I:154:VAL:HG22 | 1:I:155:MET:O    | 2.13                     | 0.49              |
| 1:L:260:VAL:HG23 | 1:L:260:VAL:O    | 2.13                     | 0.49              |
| 1:P:154:VAL:HG22 | 1:P:155:MET:O    | 2.13                     | 0.49              |
| 1:R:154:VAL:HG22 | 1:R:155:MET:O    | 2.13                     | 0.49              |
| 1:A:213:ASP:OD2  | 1:A:215:SER:OG   | 2.29                     | 0.49              |
| 1:B:200:PRO:N    | 1:J:174:LYS:CG   | 2.43                     | 0.49              |
| 1:H:80:TYR:HD1   | 1:I:115:PHE:CD2  | 2.22                     | 0.49              |
| 1:J:210:ASN:ND2  | 1:R:255:GLY:HA3  | 2.27                     | 0.49              |
| 1:Q:154:VAL:HG22 | 1:Q:155:MET:O    | 2.13                     | 0.49              |
| 1:A:260:VAL:HG23 | 1:A:260:VAL:O    | 2.13                     | 0.49              |
| 1:H:154:VAL:HG22 | 1:H:155:MET:O    | 2.13                     | 0.49              |
| 1:O:86:LEU:CA    | 1:P:130:GLN:NE2  | 2.64                     | 0.49              |
| 1:S:260:VAL:HG23 | 1:S:260:VAL:O    | 2.13                     | 0.49              |
| 1:F:66:PRO:CD    | 1:P:128:LYS:HZ1  | 2.25                     | 0.48              |
| 1:G:154:VAL:HG22 | 1:G:155:MET:O    | 2.13                     | 0.48              |
| 1:G:210:ASN:ND2  | 1:O:255:GLY:HA3  | 2.27                     | 0.48              |
| 1:H:260:VAL:HG23 | 1:H:260:VAL:O    | 2.13                     | 0.48              |
| 1:I:260:VAL:HG23 | 1:I:260:VAL:O    | 2.13                     | 0.48              |
| 1:D:78:PRO:CG    | 1:E:183:HIS:CB   | 2.79                     | 0.48              |
| 1:G:266:ASN:O    | 1:G:267:THR:OG1  | 2.28                     | 0.48              |
| 1:J:198:ASP:HB3  | 1:R:174:LYS:NZ   | 2.25                     | 0.48              |
| 1:N:260:VAL:HG23 | 1:N:260:VAL:O    | 2.13                     | 0.48              |
| 1:D:80:TYR:HD1   | 1:E:115:PHE:CD2  | 2.22                     | 0.48              |
| 1:H:210:ASN:ND2  | 1:P:255:GLY:HA3  | 2.27                     | 0.48              |
| 1:B:94:TYR:CE1   | 1:C:155:MET:HE2  | 2.49                     | 0.48              |
| 1:D:260:VAL:HG23 | 1:D:260:VAL:O    | 2.13                     | 0.48              |
| 1:H:78:PRO:CG    | 1:I:184:PHE:HE1  | 2.20                     | 0.48              |
| 1:I:90:HIS:CE1   | 1:J:131:ILE:HD13 | 2.20                     | 0.48              |
| 1:K:260:VAL:HG23 | 1:K:260:VAL:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:154:VAL:HG22 | 1:N:155:MET:O    | 2.13                     | 0.48              |
| 1:A:78:PRO:CG    | 1:B:184:PHE:HE1  | 2.20                     | 0.48              |
| 1:C:78:PRO:CG    | 1:D:184:PHE:HE1  | 2.20                     | 0.48              |
| 1:C:260:VAL:HG23 | 1:C:260:VAL:O    | 2.13                     | 0.48              |
| 1:H:66:PRO:CD    | 1:R:128:LYS:HZ1  | 2.26                     | 0.48              |
| 1:H:241:MET:SD   | 1:P:254:PHE:CZ   | 3.04                     | 0.48              |
| 1:K:210:ASN:ND2  | 1:S:255:GLY:HA3  | 2.27                     | 0.48              |
| 1:M:154:VAL:HG22 | 1:M:155:MET:O    | 2.13                     | 0.48              |
| 1:N:80:TYR:HD1   | 1:O:115:PHE:CD2  | 2.22                     | 0.48              |
| 1:Q:260:VAL:HG23 | 1:Q:260:VAL:O    | 2.13                     | 0.48              |
| 1:I:210:ASN:ND2  | 1:Q:255:GLY:HA3  | 2.27                     | 0.48              |
| 1:J:260:VAL:O    | 1:J:260:VAL:HG23 | 2.13                     | 0.48              |
| 1:O:154:VAL:HG22 | 1:O:155:MET:O    | 2.13                     | 0.48              |
| 1:A:210:ASN:ND2  | 1:I:255:GLY:HA3  | 2.27                     | 0.48              |
| 1:I:108:ARG:NH1  | 1:J:161:GLN:CG   | 2.71                     | 0.48              |
| 1:M:260:VAL:O    | 1:M:260:VAL:HG23 | 2.13                     | 0.48              |
| 1:E:198:ASP:HB3  | 1:M:174:LYS:NZ   | 2.25                     | 0.48              |
| 1:E:241:MET:SD   | 1:M:254:PHE:CZ   | 3.04                     | 0.48              |
| 1:F:80:TYR:HD1   | 1:G:115:PHE:CD2  | 2.22                     | 0.48              |
| 1:J:213:ASP:OD2  | 1:J:215:SER:OG   | 2.29                     | 0.48              |
| 1:L:154:VAL:HG22 | 1:L:155:MET:O    | 2.13                     | 0.48              |
| 1:N:213:ASP:OD2  | 1:N:215:SER:OG   | 2.29                     | 0.48              |
| 1:N:266:ASN:O    | 1:N:267:THR:OG1  | 2.28                     | 0.48              |
| 1:B:66:PRO:CD    | 1:L:128:LYS:HZ1  | 2.27                     | 0.48              |
| 1:C:241:MET:SD   | 1:K:254:PHE:CZ   | 3.04                     | 0.48              |
| 1:E:260:VAL:O    | 1:E:260:VAL:HG23 | 2.13                     | 0.48              |
| 1:J:154:VAL:HG22 | 1:J:155:MET:O    | 2.13                     | 0.48              |
| 1:C:108:ARG:NH1  | 1:D:161:GLN:CG   | 2.71                     | 0.48              |
| 1:G:260:VAL:HG23 | 1:G:260:VAL:O    | 2.13                     | 0.48              |
| 1:K:154:VAL:HG22 | 1:K:155:MET:O    | 2.13                     | 0.48              |
| 1:A:66:PRO:CD    | 1:K:128:LYS:HZ1  | 2.27                     | 0.47              |
| 1:F:108:ARG:NH1  | 1:G:161:GLN:CG   | 2.72                     | 0.47              |
| 1:I:213:ASP:OD2  | 1:I:215:SER:OG   | 2.29                     | 0.47              |
| 1:K:88:LEU:HD12  | 1:L:130:GLN:CB   | 2.43                     | 0.47              |
| 1:M:94:TYR:CE1   | 1:N:155:MET:HE2  | 2.49                     | 0.47              |
| 1:N:78:PRO:CG    | 1:O:184:PHE:HE1  | 2.20                     | 0.47              |
| 1:O:260:VAL:HG23 | 1:O:260:VAL:O    | 2.13                     | 0.47              |
| 1:R:260:VAL:HG23 | 1:R:260:VAL:O    | 2.13                     | 0.47              |
| 1:A:198:ASP:HB3  | 1:I:174:LYS:NZ   | 2.25                     | 0.47              |
| 1:P:88:LEU:HD12  | 1:Q:130:GLN:CB   | 2.43                     | 0.47              |
| 1:I:241:MET:SD   | 1:Q:254:PHE:CZ   | 3.04                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:M:88:LEU:HD12 | 1:N:130:GLN:CB   | 2.43                     | 0.47              |
| 1:D:241:MET:HE2 | 1:L:254:PHE:HE1  | 1.79                     | 0.47              |
| 1:F:213:ASP:OD2 | 1:F:215:SER:OG   | 2.29                     | 0.47              |
| 1:J:80:TYR:HD1  | 1:K:115:PHE:CD2  | 2.22                     | 0.47              |
| 1:A:241:MET:SD  | 1:I:254:PHE:CZ   | 3.04                     | 0.47              |
| 1:D:78:PRO:CG   | 1:E:184:PHE:HE1  | 2.20                     | 0.47              |
| 1:D:94:TYR:CE1  | 1:E:155:MET:HE2  | 2.49                     | 0.47              |
| 1:E:86:LEU:CA   | 1:F:130:GLN:NE2  | 2.64                     | 0.47              |
| 1:H:266:ASN:O   | 1:H:267:THR:OG1  | 2.28                     | 0.47              |
| 1:I:198:ASP:HB3 | 1:Q:174:LYS:NZ   | 2.25                     | 0.47              |
| 1:J:241:MET:SD  | 1:R:254:PHE:CZ   | 3.04                     | 0.47              |
| 1:K:78:PRO:CG   | 1:L:184:PHE:HE1  | 2.20                     | 0.47              |
| 1:R:90:HIS:CE1  | 1:S:131:ILE:HD13 | 2.19                     | 0.47              |
| 1:O:213:ASP:OD2 | 1:O:215:SER:OG   | 2.29                     | 0.47              |
| 1:B:78:PRO:CG   | 1:C:183:HIS:CB   | 2.80                     | 0.47              |
| 1:C:66:PRO:CD   | 1:M:128:LYS:HZ1  | 2.27                     | 0.47              |
| 1:C:67:ARG:CG   | 1:M:162:VAL:HG11 | 2.31                     | 0.47              |
| 1:H:88:LEU:HD12 | 1:I:130:GLN:CB   | 2.43                     | 0.47              |
| 1:H:90:HIS:CE1  | 1:I:131:ILE:HD13 | 2.20                     | 0.47              |
| 1:O:78:PRO:CG   | 1:P:184:PHE:HE1  | 2.20                     | 0.47              |
| 1:Q:213:ASP:OD2 | 1:Q:215:SER:OG   | 2.29                     | 0.47              |
| 1:E:199:ARG:HG3 | 1:M:174:LYS:NZ   | 2.30                     | 0.46              |
| 1:H:213:ASP:OD2 | 1:H:215:SER:OG   | 2.29                     | 0.46              |
| 1:O:88:LEU:HD12 | 1:P:130:GLN:CB   | 2.43                     | 0.46              |
| 1:P:213:ASP:OD2 | 1:P:215:SER:OG   | 2.29                     | 0.46              |
| 1:R:213:ASP:OD2 | 1:R:215:SER:OG   | 2.29                     | 0.46              |
| 1:N:90:HIS:CE1  | 1:O:131:ILE:HD13 | 2.20                     | 0.46              |
| 1:J:86:LEU:CA   | 1:K:130:GLN:NE2  | 2.64                     | 0.46              |
| 1:M:266:ASN:O   | 1:M:267:THR:OG1  | 2.28                     | 0.46              |
| 1:G:78:PRO:CG   | 1:H:183:HIS:CB   | 2.80                     | 0.46              |
| 1:M:78:PRO:CG   | 1:N:183:HIS:CB   | 2.80                     | 0.46              |
| 1:C:108:ARG:NH1 | 1:D:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:E:108:ARG:NH1 | 1:F:161:GLN:CG   | 2.71                     | 0.46              |
| 1:B:108:ARG:NH1 | 1:C:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:C:80:TYR:CD1  | 1:D:115:PHE:CE2  | 3.02                     | 0.46              |
| 1:K:85:ALA:O    | 1:L:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:K:198:ASP:HB3 | 1:S:174:LYS:NZ   | 2.26                     | 0.46              |
| 1:Q:266:ASN:O   | 1:Q:267:THR:OG1  | 2.28                     | 0.46              |
| 1:C:85:ALA:O    | 1:D:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:G:85:ALA:O    | 1:H:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:G:88:LEU:HD12 | 1:H:130:GLN:CB   | 2.43                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:199:ARG:HG3 | 1:O:174:LYS:NZ   | 2.31                     | 0.46              |
| 1:I:78:PRO:CG   | 1:J:183:HIS:CB   | 2.80                     | 0.46              |
| 1:O:108:ARG:NH1 | 1:P:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:D:108:ARG:NH1 | 1:E:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:G:108:ARG:NH1 | 1:H:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:H:108:ARG:NH1 | 1:I:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:J:108:ARG:NH1 | 1:K:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:Q:85:ALA:O    | 1:R:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:R:80:TYR:CD1  | 1:S:115:PHE:CE2  | 3.02                     | 0.46              |
| 1:A:85:ALA:O    | 1:B:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:D:241:MET:HE2 | 1:L:254:PHE:CE1  | 2.50                     | 0.46              |
| 1:E:85:ALA:O    | 1:F:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:F:198:ASP:HB3 | 1:N:174:LYS:NZ   | 2.25                     | 0.46              |
| 1:I:85:ALA:O    | 1:J:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:I:108:ARG:NH1 | 1:J:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:N:85:ALA:O    | 1:O:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:N:108:ARG:NH1 | 1:O:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:P:90:HIS:CE1  | 1:Q:131:ILE:HD13 | 2.20                     | 0.46              |
| 1:R:86:LEU:CA   | 1:S:130:GLN:NE2  | 2.64                     | 0.46              |
| 1:R:108:ARG:NH1 | 1:S:161:GLN:HG3  | 2.31                     | 0.46              |
| 1:F:85:ALA:O    | 1:G:130:GLN:NE2  | 2.49                     | 0.46              |
| 1:G:213:ASP:OD2 | 1:G:215:SER:OG   | 2.29                     | 0.46              |
| 1:E:66:PRO:N    | 1:O:128:LYS:HZ1  | 2.13                     | 0.45              |
| 1:H:197:GLN:NE2 | 1:Q:152:MET:CG   | 2.71                     | 0.45              |
| 1:L:108:ARG:NH1 | 1:M:161:GLN:HG3  | 2.31                     | 0.45              |
| 1:M:85:ALA:O    | 1:N:130:GLN:NE2  | 2.49                     | 0.45              |
| 1:P:85:ALA:O    | 1:Q:130:GLN:NE2  | 2.49                     | 0.45              |
| 1:Q:80:TYR:HD1  | 1:R:115:PHE:CD2  | 2.22                     | 0.45              |
| 1:A:108:ARG:NH1 | 1:B:161:GLN:HG3  | 2.31                     | 0.45              |
| 1:C:199:ARG:HG3 | 1:K:174:LYS:NZ   | 2.30                     | 0.45              |
| 1:D:85:ALA:O    | 1:E:130:GLN:NE2  | 2.49                     | 0.45              |
| 1:F:78:PRO:CG   | 1:G:183:HIS:CB   | 2.80                     | 0.45              |
| 1:G:241:MET:CE  | 1:O:254:PHE:CD1  | 3.00                     | 0.45              |
| 1:I:86:LEU:CA   | 1:J:130:GLN:NE2  | 2.64                     | 0.45              |
| 1:R:85:ALA:O    | 1:S:130:GLN:NE2  | 2.49                     | 0.45              |
| 1:D:67:ARG:CG   | 1:N:162:VAL:HG11 | 2.31                     | 0.45              |
| 1:D:86:LEU:CA   | 1:E:130:GLN:NE2  | 2.64                     | 0.45              |
| 1:D:199:ARG:HG3 | 1:L:174:LYS:NZ   | 2.31                     | 0.45              |
| 1:H:198:ASP:HB3 | 1:P:174:LYS:NZ   | 2.25                     | 0.45              |
| 1:J:85:ALA:O    | 1:K:130:GLN:NE2  | 2.49                     | 0.45              |
| 1:K:108:ARG:NH1 | 1:L:161:GLN:HG3  | 2.31                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:199:ARG:HG3 | 1:S:174:LYS:NZ  | 2.30                     | 0.45              |
| 1:O:85:ALA:O    | 1:P:130:GLN:NE2 | 2.49                     | 0.45              |
| 1:A:80:TYR:CD1  | 1:B:115:PHE:CE2 | 3.02                     | 0.45              |
| 1:A:199:ARG:HG3 | 1:I:174:LYS:NZ  | 2.31                     | 0.45              |
| 1:F:66:PRO:HA   | 1:P:128:LYS:HZ3 | 1.79                     | 0.45              |
| 1:L:85:ALA:O    | 1:M:130:GLN:NE2 | 2.49                     | 0.45              |
| 1:O:94:TYR:CE1  | 1:P:155:MET:HE2 | 2.50                     | 0.45              |
| 1:R:78:PRO:CG   | 1:S:184:PHE:HE1 | 2.20                     | 0.45              |
| 1:E:108:ARG:NH1 | 1:F:161:GLN:HG3 | 2.31                     | 0.45              |
| 1:G:66:PRO:HA   | 1:Q:128:LYS:HZ3 | 1.79                     | 0.45              |
| 1:J:199:ARG:HG3 | 1:R:174:LYS:NZ  | 2.30                     | 0.45              |
| 1:P:108:ARG:NH1 | 1:Q:161:GLN:HG3 | 2.31                     | 0.45              |
| 1:A:241:MET:HE2 | 1:I:254:PHE:HE1 | 1.82                     | 0.45              |
| 1:B:241:MET:CE  | 1:J:254:PHE:CD1 | 3.00                     | 0.45              |
| 1:C:241:MET:CE  | 1:K:254:PHE:CD1 | 3.00                     | 0.45              |
| 1:D:229:ARG:O   | 1:M:171:ASP:OD1 | 2.35                     | 0.45              |
| 1:E:241:MET:HE2 | 1:M:254:PHE:HE1 | 1.81                     | 0.45              |
| 1:F:199:ARG:HG3 | 1:N:174:LYS:NZ  | 2.30                     | 0.45              |
| 1:H:85:ALA:O    | 1:I:130:GLN:NE2 | 2.49                     | 0.45              |
| 1:H:241:MET:HE2 | 1:P:254:PHE:HE1 | 1.82                     | 0.45              |
| 1:D:88:LEU:HD12 | 1:E:130:GLN:HB2 | 1.98                     | 0.45              |
| 1:D:266:ASN:O   | 1:D:267:THR:OG1 | 2.28                     | 0.45              |
| 1:E:229:ARG:O   | 1:N:171:ASP:OD1 | 2.35                     | 0.45              |
| 1:G:198:ASP:HB3 | 1:O:174:LYS:NZ  | 2.25                     | 0.45              |
| 1:L:80:TYR:CD1  | 1:M:115:PHE:CE2 | 3.02                     | 0.45              |
| 1:N:86:LEU:CA   | 1:O:130:GLN:NE2 | 2.64                     | 0.45              |
| 1:Q:108:ARG:NH1 | 1:R:161:GLN:HG3 | 2.31                     | 0.45              |
| 1:H:241:MET:CE  | 1:P:254:PHE:CD1 | 3.00                     | 0.45              |
| 1:I:241:MET:CE  | 1:Q:254:PHE:CD1 | 3.00                     | 0.45              |
| 1:O:80:TYR:HD1  | 1:P:115:PHE:CD2 | 2.23                     | 0.45              |
| 1:P:94:TYR:HH   | 1:Q:155:MET:HB2 | 1.79                     | 0.45              |
| 1:B:85:ALA:O    | 1:C:130:GLN:NE2 | 2.49                     | 0.45              |
| 1:E:241:MET:CE  | 1:M:254:PHE:CD1 | 3.00                     | 0.45              |
| 1:H:199:ARG:HG3 | 1:P:174:LYS:NZ  | 2.30                     | 0.45              |
| 1:I:199:ARG:HG3 | 1:Q:174:LYS:NZ  | 2.30                     | 0.45              |
| 1:C:229:ARG:O   | 1:L:171:ASP:OD1 | 2.35                     | 0.45              |
| 1:I:266:ASN:O   | 1:I:267:THR:OG1 | 2.28                     | 0.45              |
| 1:J:80:TYR:CD1  | 1:K:115:PHE:CE2 | 3.02                     | 0.45              |
| 1:R:266:ASN:O   | 1:R:267:THR:OG1 | 2.28                     | 0.45              |
| 1:B:88:LEU:HD12 | 1:C:130:GLN:CB  | 2.43                     | 0.44              |
| 1:F:241:MET:CE  | 1:N:254:PHE:CD1 | 3.00                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:197:GLN:NE2 | 1:P:152:MET:CG   | 2.71                     | 0.44              |
| 1:M:86:LEU:CA   | 1:N:130:GLN:NE2  | 2.64                     | 0.44              |
| 1:Q:86:LEU:CA   | 1:R:130:GLN:NE2  | 2.64                     | 0.44              |
| 1:E:241:MET:HE2 | 1:M:254:PHE:CE1  | 2.52                     | 0.44              |
| 1:F:229:ARG:O   | 1:O:171:ASP:OD1  | 2.35                     | 0.44              |
| 1:K:199:ARG:HG2 | 1:S:174:LYS:HE3  | 1.81                     | 0.44              |
| 1:A:241:MET:CE  | 1:I:254:PHE:CD1  | 3.00                     | 0.44              |
| 1:E:94:TYR:CE1  | 1:F:155:MET:HE2  | 2.51                     | 0.44              |
| 1:F:90:HIS:CE1  | 1:G:131:ILE:HD13 | 2.20                     | 0.44              |
| 1:G:229:ARG:O   | 1:P:171:ASP:OD1  | 2.35                     | 0.44              |
| 1:M:80:TYR:HD1  | 1:N:115:PHE:CD2  | 2.23                     | 0.44              |
| 1:M:108:ARG:NH1 | 1:N:161:GLN:HG3  | 2.31                     | 0.44              |
| 1:N:88:LEU:HD12 | 1:O:130:GLN:HB2  | 1.98                     | 0.44              |
| 1:B:199:ARG:HG3 | 1:J:174:LYS:NZ   | 2.30                     | 0.44              |
| 1:D:80:TYR:CD1  | 1:E:115:PHE:CE2  | 3.02                     | 0.44              |
| 1:D:241:MET:CE  | 1:L:254:PHE:CD1  | 3.00                     | 0.44              |
| 1:E:67:ARG:CG   | 1:O:162:VAL:HG11 | 2.31                     | 0.44              |
| 1:E:88:LEU:HD12 | 1:F:130:GLN:HB2  | 1.98                     | 0.44              |
| 1:F:108:ARG:NH1 | 1:G:161:GLN:HG3  | 2.31                     | 0.44              |
| 1:J:199:ARG:HG2 | 1:R:174:LYS:HE3  | 1.81                     | 0.44              |
| 1:J:241:MET:CE  | 1:R:254:PHE:CD1  | 3.00                     | 0.44              |
| 1:K:78:PRO:CG   | 1:L:183:HIS:CB   | 2.80                     | 0.44              |
| 1:K:241:MET:CE  | 1:S:254:PHE:CD1  | 3.00                     | 0.44              |
| 1:L:266:ASN:O   | 1:L:267:THR:OG1  | 2.28                     | 0.44              |
| 1:A:229:ARG:O   | 1:J:171:ASP:OD1  | 2.35                     | 0.44              |
| 1:I:229:ARG:O   | 1:R:171:ASP:OD1  | 2.35                     | 0.44              |
| 1:J:88:LEU:HD12 | 1:K:130:GLN:CB   | 2.43                     | 0.44              |
| 1:R:88:LEU:HD12 | 1:S:130:GLN:CB   | 2.43                     | 0.44              |
| 1:D:88:LEU:HD12 | 1:E:130:GLN:CB   | 2.43                     | 0.44              |
| 1:G:241:MET:HE2 | 1:O:254:PHE:HE1  | 1.83                     | 0.44              |
| 1:H:78:PRO:CG   | 1:I:183:HIS:CB   | 2.80                     | 0.44              |
| 1:P:86:LEU:CA   | 1:Q:130:GLN:NE2  | 2.64                     | 0.44              |
| 1:A:241:MET:HE2 | 1:I:254:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:78:PRO:CG   | 1:D:183:HIS:CB   | 2.80                     | 0.44              |
| 1:E:66:PRO:CD   | 1:O:128:LYS:HZ1  | 2.31                     | 0.44              |
| 1:L:78:PRO:CG   | 1:M:183:HIS:CB   | 2.80                     | 0.44              |
| 1:M:88:LEU:HD12 | 1:N:130:GLN:HB2  | 1.98                     | 0.44              |
| 1:A:94:TYR:CE1  | 1:B:155:MET:HE2  | 2.52                     | 0.44              |
| 1:G:67:ARG:CG   | 1:Q:162:VAL:HG11 | 2.31                     | 0.44              |
| 1:J:229:ARG:O   | 1:S:171:ASP:OD1  | 2.35                     | 0.44              |
| 1:O:88:LEU:HD12 | 1:P:130:GLN:HB2  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:108:ARG:NH1  | 1:S:161:GLN:CG   | 2.72                     | 0.44              |
| 1:A:94:TYR:CE1   | 1:B:155:MET:HE3  | 2.52                     | 0.44              |
| 1:A:266:ASN:O    | 1:A:267:THR:OG1  | 2.28                     | 0.44              |
| 1:C:88:LEU:HD12  | 1:D:130:GLN:HB2  | 1.98                     | 0.44              |
| 1:E:94:TYR:CE1   | 1:F:155:MET:HE3  | 2.53                     | 0.44              |
| 1:B:229:ARG:O    | 1:K:171:ASP:OD1  | 2.35                     | 0.43              |
| 1:B:256:LEU:HD22 | 1:K:270:HIS:O    | 2.18                     | 0.43              |
| 1:E:78:PRO:CG    | 1:F:183:HIS:CB   | 2.80                     | 0.43              |
| 1:G:80:TYR:CD1   | 1:H:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:H:86:LEU:CA    | 1:I:130:GLN:NE2  | 2.64                     | 0.43              |
| 1:H:229:ARG:O    | 1:Q:171:ASP:OD1  | 2.35                     | 0.43              |
| 1:I:256:LEU:HD22 | 1:R:270:HIS:O    | 2.18                     | 0.43              |
| 1:C:80:TYR:HD1   | 1:D:115:PHE:CD2  | 2.22                     | 0.43              |
| 1:S:266:ASN:O    | 1:S:267:THR:OG1  | 2.28                     | 0.43              |
| 1:J:256:LEU:HD22 | 1:S:270:HIS:O    | 2.18                     | 0.43              |
| 1:A:256:LEU:HD22 | 1:J:270:HIS:O    | 2.17                     | 0.43              |
| 1:F:67:ARG:CG    | 1:P:162:VAL:HG11 | 2.31                     | 0.43              |
| 1:F:88:LEU:HD12  | 1:G:130:GLN:CB   | 2.43                     | 0.43              |
| 1:F:197:GLN:NE2  | 1:O:152:MET:CG   | 2.71                     | 0.43              |
| 1:P:78:PRO:CG    | 1:Q:183:HIS:CB   | 2.80                     | 0.43              |
| 1:Q:80:TYR:CD1   | 1:R:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:A:197:GLN:NE2  | 1:J:152:MET:CG   | 2.71                     | 0.43              |
| 1:B:80:TYR:CD1   | 1:C:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:C:86:LEU:CA    | 1:D:130:GLN:NE2  | 2.64                     | 0.43              |
| 1:A:94:TYR:CZ    | 1:B:155:MET:HE3  | 2.54                     | 0.43              |
| 1:D:256:LEU:HD22 | 1:M:270:HIS:O    | 2.18                     | 0.43              |
| 1:E:256:LEU:HD22 | 1:N:270:HIS:O    | 2.18                     | 0.43              |
| 1:G:241:MET:HE2  | 1:O:254:PHE:CE1  | 2.54                     | 0.43              |
| 1:P:80:TYR:CD1   | 1:Q:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:B:197:GLN:NE2  | 1:K:152:MET:CG   | 2.71                     | 0.43              |
| 1:C:256:LEU:HD22 | 1:L:270:HIS:O    | 2.18                     | 0.43              |
| 1:C:266:ASN:O    | 1:C:267:THR:OG1  | 2.28                     | 0.43              |
| 1:D:108:ARG:NH1  | 1:E:161:GLN:CG   | 2.72                     | 0.43              |
| 1:F:80:TYR:CD1   | 1:G:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:H:80:TYR:CD1   | 1:I:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:M:80:TYR:CD1   | 1:N:115:PHE:CE2  | 3.02                     | 0.43              |
| 1:R:78:PRO:CG    | 1:S:183:HIS:CB   | 2.80                     | 0.43              |
| 1:E:218:ARG:HH21 | 1:N:167:LYS:HD3  | 1.84                     | 0.43              |
| 1:J:78:PRO:CG    | 1:K:183:HIS:CB   | 2.80                     | 0.43              |
| 1:J:218:ARG:HH21 | 1:S:167:LYS:HD3  | 1.84                     | 0.43              |
| 1:L:88:LEU:HD12  | 1:M:130:GLN:CB   | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:ARG:HH21 | 1:K:167:LYS:HD3  | 1.84                     | 0.42              |
| 1:B:266:ASN:O    | 1:B:267:THR:OG1  | 2.28                     | 0.42              |
| 1:K:266:ASN:O    | 1:K:267:THR:OG1  | 2.28                     | 0.42              |
| 1:O:80:TYR:CD1   | 1:P:115:PHE:CE2  | 3.02                     | 0.42              |
| 1:F:218:ARG:HH21 | 1:O:167:LYS:HD3  | 1.84                     | 0.42              |
| 1:P:88:LEU:HD12  | 1:Q:130:GLN:HB2  | 1.98                     | 0.42              |
| 1:C:197:GLN:NE2  | 1:L:152:MET:CG   | 2.71                     | 0.42              |
| 1:C:218:ARG:HH21 | 1:L:167:LYS:HD3  | 1.84                     | 0.42              |
| 1:C:241:MET:HE2  | 1:K:254:PHE:HE1  | 1.85                     | 0.42              |
| 1:E:80:TYR:CD1   | 1:F:115:PHE:CE2  | 3.02                     | 0.42              |
| 1:I:80:TYR:CD1   | 1:J:115:PHE:CE2  | 3.02                     | 0.42              |
| 1:K:209:ARG:NH2  | 1:S:259:ASN:ND2  | 2.68                     | 0.42              |
| 1:K:241:MET:HE2  | 1:S:254:PHE:HE1  | 1.84                     | 0.42              |
| 1:B:209:ARG:NH2  | 1:J:259:ASN:ND2  | 2.68                     | 0.42              |
| 1:C:209:ARG:NH2  | 1:K:259:ASN:ND2  | 2.68                     | 0.42              |
| 1:H:218:ARG:HH21 | 1:Q:167:LYS:HD3  | 1.84                     | 0.42              |
| 1:J:266:ASN:O    | 1:J:267:THR:OG1  | 2.28                     | 0.42              |
| 1:L:88:LEU:HD12  | 1:M:130:GLN:HB2  | 1.98                     | 0.42              |
| 1:M:246:LEU:HD23 | 1:M:247:ARG:N    | 2.35                     | 0.42              |
| 1:N:88:LEU:HD12  | 1:O:130:GLN:CB   | 2.43                     | 0.42              |
| 1:O:94:TYR:CE1   | 1:P:155:MET:HE3  | 2.55                     | 0.42              |
| 1:B:88:LEU:HD12  | 1:C:130:GLN:HB2  | 1.98                     | 0.42              |
| 1:D:209:ARG:NH2  | 1:L:259:ASN:ND2  | 2.68                     | 0.42              |
| 1:I:80:TYR:HD1   | 1:J:115:PHE:CD2  | 2.22                     | 0.42              |
| 1:L:183:HIS:O    | 1:L:185:SER:N    | 2.53                     | 0.42              |
| 1:M:94:TYR:O     | 1:N:191:TYR:OH   | 2.27                     | 0.42              |
| 1:A:183:HIS:O    | 1:A:185:SER:N    | 2.53                     | 0.42              |
| 1:F:246:LEU:HD23 | 1:F:247:ARG:N    | 2.35                     | 0.42              |
| 1:G:246:LEU:HD23 | 1:G:247:ARG:N    | 2.35                     | 0.42              |
| 1:H:67:ARG:CG    | 1:R:162:VAL:HG11 | 2.31                     | 0.42              |
| 1:Q:183:HIS:O    | 1:Q:185:SER:N    | 2.53                     | 0.42              |
| 1:R:183:HIS:O    | 1:R:185:SER:N    | 2.53                     | 0.42              |
| 1:S:183:HIS:O    | 1:S:185:SER:N    | 2.53                     | 0.42              |
| 1:A:78:PRO:CG    | 1:B:183:HIS:CB   | 2.80                     | 0.42              |
| 1:E:94:TYR:CZ    | 1:F:155:MET:HE3  | 2.55                     | 0.42              |
| 1:F:241:MET:HE2  | 1:N:254:PHE:HE1  | 1.84                     | 0.42              |
| 1:F:256:LEU:HD22 | 1:O:270:HIS:O    | 2.18                     | 0.42              |
| 1:F:266:ASN:O    | 1:F:267:THR:OG1  | 2.28                     | 0.42              |
| 1:J:183:HIS:O    | 1:J:185:SER:N    | 2.53                     | 0.42              |
| 1:J:209:ARG:NH2  | 1:R:259:ASN:ND2  | 2.68                     | 0.42              |
| 1:K:183:HIS:O    | 1:K:185:SER:N    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:Q:246:LEU:HD23 | 1:Q:247:ARG:N   | 2.35                     | 0.42              |
| 1:C:246:LEU:HD23 | 1:C:247:ARG:N   | 2.35                     | 0.42              |
| 1:D:183:HIS:O    | 1:D:185:SER:N   | 2.53                     | 0.42              |
| 1:F:241:MET:HE2  | 1:N:254:PHE:CE1 | 2.55                     | 0.42              |
| 1:H:209:ARG:NH2  | 1:P:259:ASN:ND2 | 2.68                     | 0.42              |
| 1:H:256:LEU:HD22 | 1:Q:270:HIS:O   | 2.18                     | 0.42              |
| 1:K:80:TYR:CD1   | 1:L:115:PHE:CE2 | 3.02                     | 0.42              |
| 1:M:183:HIS:O    | 1:M:185:SER:N   | 2.53                     | 0.42              |
| 1:A:209:ARG:NH2  | 1:I:259:ASN:ND2 | 2.68                     | 0.42              |
| 1:D:94:TYR:CE1   | 1:E:155:MET:HE3 | 2.55                     | 0.42              |
| 1:I:183:HIS:O    | 1:I:185:SER:N   | 2.53                     | 0.42              |
| 1:Q:88:LEU:HD12  | 1:R:130:GLN:HB2 | 1.98                     | 0.42              |
| 1:B:80:TYR:HD1   | 1:C:115:PHE:CD2 | 2.22                     | 0.42              |
| 1:B:241:MET:HE2  | 1:J:254:PHE:CE1 | 2.55                     | 0.42              |
| 1:B:241:MET:HE2  | 1:J:254:PHE:HE1 | 1.84                     | 0.42              |
| 1:C:183:HIS:O    | 1:C:185:SER:N   | 2.53                     | 0.42              |
| 1:E:209:ARG:NH2  | 1:M:259:ASN:ND2 | 2.68                     | 0.42              |
| 1:N:80:TYR:CD1   | 1:O:115:PHE:CE2 | 3.02                     | 0.42              |
| 1:N:246:LEU:HD23 | 1:N:247:ARG:N   | 2.35                     | 0.42              |
| 1:P:246:LEU:HD23 | 1:P:247:ARG:N   | 2.35                     | 0.42              |
| 1:Q:88:LEU:HD12  | 1:R:130:GLN:CB  | 2.43                     | 0.42              |
| 1:D:197:GLN:NE2  | 1:M:152:MET:CG  | 2.71                     | 0.41              |
| 1:F:86:LEU:CA    | 1:G:130:GLN:NE2 | 2.64                     | 0.41              |
| 1:G:218:ARG:HH21 | 1:P:167:LYS:HD3 | 1.84                     | 0.41              |
| 1:J:88:LEU:HD12  | 1:K:130:GLN:HB2 | 1.98                     | 0.41              |
| 1:J:241:MET:HE2  | 1:R:254:PHE:HE1 | 1.85                     | 0.41              |
| 1:J:246:LEU:HD23 | 1:J:247:ARG:N   | 2.35                     | 0.41              |
| 1:E:183:HIS:O    | 1:E:185:SER:N   | 2.53                     | 0.41              |
| 1:G:209:ARG:NH2  | 1:O:259:ASN:ND2 | 2.67                     | 0.41              |
| 1:I:218:ARG:HH21 | 1:R:167:LYS:HD3 | 1.84                     | 0.41              |
| 1:B:246:LEU:HD23 | 1:B:247:ARG:N   | 2.35                     | 0.41              |
| 1:I:246:LEU:HD23 | 1:I:247:ARG:N   | 2.35                     | 0.41              |
| 1:L:246:LEU:HD23 | 1:L:247:ARG:N   | 2.35                     | 0.41              |
| 1:A:218:ARG:HH21 | 1:J:167:LYS:HD3 | 1.84                     | 0.41              |
| 1:D:246:LEU:HD23 | 1:D:247:ARG:N   | 2.35                     | 0.41              |
| 1:F:183:HIS:O    | 1:F:185:SER:N   | 2.53                     | 0.41              |
| 1:H:246:LEU:HD23 | 1:H:247:ARG:N   | 2.35                     | 0.41              |
| 1:P:183:HIS:O    | 1:P:185:SER:N   | 2.53                     | 0.41              |
| 1:R:88:LEU:HD12  | 1:S:130:GLN:HB2 | 1.98                     | 0.41              |
| 1:A:88:LEU:HD12  | 1:B:130:GLN:HB2 | 1.98                     | 0.41              |
| 1:E:246:LEU:HD23 | 1:E:247:ARG:N   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:88:LEU:HD21  | 1:G:130:GLN:NE2  | 2.35                     | 0.41              |
| 1:F:88:LEU:HD12  | 1:G:130:GLN:HB2  | 1.98                     | 0.41              |
| 1:F:255:GLY:O    | 1:O:270:HIS:HB2  | 2.21                     | 0.41              |
| 1:N:183:HIS:O    | 1:N:185:SER:N    | 2.53                     | 0.41              |
| 1:A:88:LEU:CG    | 1:B:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:B:86:LEU:CA    | 1:C:130:GLN:NE2  | 2.64                     | 0.41              |
| 1:B:183:HIS:O    | 1:B:185:SER:N    | 2.53                     | 0.41              |
| 1:D:218:ARG:HH21 | 1:M:167:LYS:HD3  | 1.84                     | 0.41              |
| 1:E:199:ARG:HG2  | 1:M:174:LYS:HE3  | 1.81                     | 0.41              |
| 1:F:209:ARG:NH2  | 1:N:259:ASN:ND2  | 2.68                     | 0.41              |
| 1:G:86:LEU:CA    | 1:H:130:GLN:NE2  | 2.64                     | 0.41              |
| 1:H:183:HIS:O    | 1:H:185:SER:N    | 2.53                     | 0.41              |
| 1:I:209:ARG:NH2  | 1:Q:259:ASN:ND2  | 2.68                     | 0.41              |
| 1:K:88:LEU:CG    | 1:L:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:L:88:LEU:CG    | 1:M:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:G:88:LEU:HD12  | 1:H:130:GLN:HB2  | 1.98                     | 0.41              |
| 1:G:255:GLY:O    | 1:P:270:HIS:HB2  | 2.21                     | 0.41              |
| 1:K:241:MET:HE2  | 1:S:254:PHE:CE1  | 2.55                     | 0.41              |
| 1:O:88:LEU:CG    | 1:P:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:R:246:LEU:HD23 | 1:R:247:ARG:N    | 2.35                     | 0.41              |
| 1:A:67:ARG:CG    | 1:K:162:VAL:HG11 | 2.31                     | 0.41              |
| 1:D:88:LEU:CG    | 1:E:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:G:66:PRO:CB    | 1:Q:128:LYS:HZ3  | 2.24                     | 0.41              |
| 1:H:78:PRO:HB3   | 1:I:183:HIS:ND1  | 2.36                     | 0.41              |
| 1:I:88:LEU:HD12  | 1:J:130:GLN:HB2  | 1.98                     | 0.41              |
| 1:J:255:GLY:O    | 1:S:270:HIS:HB2  | 2.21                     | 0.41              |
| 1:N:88:LEU:CG    | 1:O:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:R:88:LEU:CG    | 1:S:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:A:88:LEU:HD21  | 1:B:130:GLN:NE2  | 2.35                     | 0.41              |
| 1:A:246:LEU:HD23 | 1:A:247:ARG:N    | 2.35                     | 0.41              |
| 1:E:197:GLN:NE2  | 1:N:152:MET:CG   | 2.71                     | 0.41              |
| 1:F:199:ARG:HG2  | 1:N:174:LYS:HE3  | 1.81                     | 0.41              |
| 1:G:78:PRO:HB3   | 1:H:183:HIS:ND1  | 2.36                     | 0.41              |
| 1:G:88:LEU:CG    | 1:H:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:G:256:LEU:HD22 | 1:P:270:HIS:O    | 2.18                     | 0.41              |
| 1:H:88:LEU:CG    | 1:I:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:H:88:LEU:HD12  | 1:I:130:GLN:HB2  | 1.98                     | 0.41              |
| 1:I:78:PRO:HB3   | 1:J:183:HIS:ND1  | 2.36                     | 0.41              |
| 1:I:255:GLY:O    | 1:R:270:HIS:HB2  | 2.21                     | 0.41              |
| 1:K:246:LEU:HD23 | 1:K:247:ARG:N    | 2.35                     | 0.41              |
| 1:R:78:PRO:HB3   | 1:S:183:HIS:ND1  | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:246:LEU:HD23 | 1:S:247:ARG:N    | 2.35                     | 0.41              |
| 1:B:88:LEU:HD21  | 1:C:130:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:78:PRO:HB3   | 1:F:183:HIS:ND1  | 2.36                     | 0.41              |
| 1:E:88:LEU:CG    | 1:F:130:GLN:HE21 | 2.34                     | 0.41              |
| 1:G:183:HIS:O    | 1:G:185:SER:N    | 2.53                     | 0.41              |
| 1:I:88:LEU:HD12  | 1:J:130:GLN:CB   | 2.43                     | 0.41              |
| 1:O:183:HIS:O    | 1:O:185:SER:N    | 2.53                     | 0.41              |
| 1:O:246:LEU:HD23 | 1:O:247:ARG:N    | 2.35                     | 0.41              |
| 1:Q:78:PRO:HB3   | 1:R:183:HIS:ND1  | 2.36                     | 0.41              |
| 1:B:94:TYR:O     | 1:C:191:TYR:OH   | 2.28                     | 0.40              |
| 1:F:78:PRO:HB3   | 1:G:183:HIS:ND1  | 2.36                     | 0.40              |
| 1:I:108:ARG:CG   | 1:J:161:GLN:OE1  | 2.69                     | 0.40              |
| 1:K:88:LEU:HD12  | 1:L:130:GLN:HB2  | 1.98                     | 0.40              |
| 1:N:78:PRO:CG    | 1:O:183:HIS:CB   | 2.80                     | 0.40              |
| 1:R:88:LEU:HD21  | 1:S:130:GLN:NE2  | 2.35                     | 0.40              |
| 1:A:68:LEU:CD2   | 1:K:164:PHE:HE1  | 2.28                     | 0.40              |
| 1:B:88:LEU:CG    | 1:C:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:C:88:LEU:CG    | 1:D:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:F:88:LEU:CG    | 1:G:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:G:80:TYR:HD1   | 1:H:115:PHE:CD2  | 2.22                     | 0.40              |
| 1:M:88:LEU:HD21  | 1:N:130:GLN:NE2  | 2.35                     | 0.40              |
| 1:M:94:TYR:CE1   | 1:N:155:MET:HE3  | 2.56                     | 0.40              |
| 1:O:78:PRO:HB3   | 1:P:183:HIS:ND1  | 2.36                     | 0.40              |
| 1:O:94:TYR:CZ    | 1:P:155:MET:HE3  | 2.56                     | 0.40              |
| 1:Q:88:LEU:CG    | 1:R:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:A:255:GLY:O    | 1:J:270:HIS:HB2  | 2.21                     | 0.40              |
| 1:B:108:ARG:CG   | 1:C:161:GLN:OE1  | 2.70                     | 0.40              |
| 1:D:199:ARG:HG2  | 1:L:174:LYS:HE3  | 1.81                     | 0.40              |
| 1:H:255:GLY:O    | 1:Q:270:HIS:HB2  | 2.21                     | 0.40              |
| 1:I:88:LEU:CG    | 1:J:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:B:255:GLY:O    | 1:K:270:HIS:HB2  | 2.21                     | 0.40              |
| 1:I:88:LEU:HG    | 1:J:130:GLN:HE21 | 1.87                     | 0.40              |
| 1:J:78:PRO:HB3   | 1:K:183:HIS:ND1  | 2.36                     | 0.40              |
| 1:J:88:LEU:CG    | 1:K:130:GLN:HE21 | 2.34                     | 0.40              |
| 1:P:78:PRO:HB3   | 1:Q:183:HIS:ND1  | 2.36                     | 0.40              |
| 1:C:255:GLY:O    | 1:L:270:HIS:HB2  | 2.20                     | 0.40              |
| 1:E:255:GLY:O    | 1:N:270:HIS:HB2  | 2.21                     | 0.40              |
| 1:L:86:LEU:CA    | 1:M:130:GLN:NE2  | 2.64                     | 0.40              |
| 1:N:78:PRO:HB3   | 1:O:183:HIS:ND1  | 2.36                     | 0.40              |
| 1:Q:88:LEU:HD21  | 1:R:130:GLN:NE2  | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | B     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | C     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | D     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | E     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | F     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | G     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | H     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | I     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | J     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | K     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | L     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | M     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | N     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | O     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | P     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | Q     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | R     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| 1   | S     | 205/207 (99%)   | 170 (83%)  | 35 (17%)  | 0        | 100         | 100 |
| All | All   | 3895/3933 (99%) | 3230 (83%) | 665 (17%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |    |
|-----|-------|------------------|-------------|----------|-------------|----|
| 1   | A     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | B     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | C     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | D     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | E     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | F     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | G     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | H     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | I     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | J     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | K     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | L     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | M     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | N     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | O     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | P     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | Q     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | R     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| 1   | S     | 183/183 (100%)   | 182 (100%)  | 1 (0%)   | 88          | 93 |
| All | All   | 3477/3477 (100%) | 3458 (100%) | 19 (0%)  | 89          | 93 |

All (19) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 269 | ARG  |
| 1   | B     | 269 | ARG  |
| 1   | C     | 269 | ARG  |
| 1   | D     | 269 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 269 | ARG  |
| 1   | F     | 269 | ARG  |
| 1   | G     | 269 | ARG  |
| 1   | H     | 269 | ARG  |
| 1   | I     | 269 | ARG  |
| 1   | J     | 269 | ARG  |
| 1   | K     | 269 | ARG  |
| 1   | L     | 269 | ARG  |
| 1   | M     | 269 | ARG  |
| 1   | N     | 269 | ARG  |
| 1   | O     | 269 | ARG  |
| 1   | P     | 269 | ARG  |
| 1   | Q     | 269 | ARG  |
| 1   | R     | 269 | ARG  |
| 1   | S     | 269 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | ASN  |
| 1   | A     | 90  | HIS  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 208 | GLN  |
| 1   | A     | 210 | ASN  |
| 1   | B     | 87  | ASN  |
| 1   | B     | 90  | HIS  |
| 1   | B     | 130 | GLN  |
| 1   | B     | 197 | GLN  |
| 1   | B     | 208 | GLN  |
| 1   | B     | 210 | ASN  |
| 1   | C     | 87  | ASN  |
| 1   | C     | 90  | HIS  |
| 1   | C     | 130 | GLN  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 208 | GLN  |
| 1   | C     | 210 | ASN  |
| 1   | D     | 87  | ASN  |
| 1   | D     | 90  | HIS  |
| 1   | D     | 130 | GLN  |
| 1   | D     | 197 | GLN  |
| 1   | D     | 208 | GLN  |
| 1   | D     | 210 | ASN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | E            | 87         | ASN         |
| 1          | E            | 90         | HIS         |
| 1          | E            | 130        | GLN         |
| 1          | E            | 197        | GLN         |
| 1          | E            | 208        | GLN         |
| 1          | E            | 210        | ASN         |
| 1          | F            | 87         | ASN         |
| 1          | F            | 90         | HIS         |
| 1          | F            | 130        | GLN         |
| 1          | F            | 197        | GLN         |
| 1          | F            | 208        | GLN         |
| 1          | F            | 210        | ASN         |
| 1          | G            | 87         | ASN         |
| 1          | G            | 90         | HIS         |
| 1          | G            | 130        | GLN         |
| 1          | G            | 197        | GLN         |
| 1          | G            | 208        | GLN         |
| 1          | G            | 210        | ASN         |
| 1          | H            | 87         | ASN         |
| 1          | H            | 90         | HIS         |
| 1          | H            | 130        | GLN         |
| 1          | H            | 197        | GLN         |
| 1          | H            | 208        | GLN         |
| 1          | H            | 210        | ASN         |
| 1          | I            | 87         | ASN         |
| 1          | I            | 90         | HIS         |
| 1          | I            | 130        | GLN         |
| 1          | I            | 197        | GLN         |
| 1          | I            | 208        | GLN         |
| 1          | I            | 210        | ASN         |
| 1          | J            | 87         | ASN         |
| 1          | J            | 90         | HIS         |
| 1          | J            | 130        | GLN         |
| 1          | J            | 197        | GLN         |
| 1          | J            | 208        | GLN         |
| 1          | J            | 210        | ASN         |
| 1          | K            | 87         | ASN         |
| 1          | K            | 90         | HIS         |
| 1          | K            | 130        | GLN         |
| 1          | K            | 208        | GLN         |
| 1          | K            | 210        | ASN         |
| 1          | L            | 87         | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 90  | HIS  |
| 1   | L     | 130 | GLN  |
| 1   | M     | 87  | ASN  |
| 1   | M     | 90  | HIS  |
| 1   | M     | 130 | GLN  |
| 1   | N     | 87  | ASN  |
| 1   | N     | 90  | HIS  |
| 1   | N     | 130 | GLN  |
| 1   | O     | 87  | ASN  |
| 1   | O     | 90  | HIS  |
| 1   | O     | 130 | GLN  |
| 1   | P     | 87  | ASN  |
| 1   | P     | 90  | HIS  |
| 1   | P     | 130 | GLN  |
| 1   | Q     | 87  | ASN  |
| 1   | Q     | 90  | HIS  |
| 1   | Q     | 130 | GLN  |
| 1   | R     | 87  | ASN  |
| 1   | R     | 90  | HIS  |
| 1   | R     | 130 | GLN  |
| 1   | S     | 130 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 2   | a     | 4/5 (80%) | 0                 | 0               |
| 2   | b     | 4/5 (80%) | 0                 | 0               |
| 2   | c     | 4/5 (80%) | 0                 | 0               |
| 2   | d     | 4/5 (80%) | 0                 | 0               |
| 2   | e     | 4/5 (80%) | 0                 | 0               |
| 2   | f     | 4/5 (80%) | 0                 | 0               |
| 2   | g     | 4/5 (80%) | 0                 | 0               |
| 2   | h     | 4/5 (80%) | 0                 | 0               |
| 2   | i     | 4/5 (80%) | 0                 | 0               |
| 2   | j     | 4/5 (80%) | 0                 | 0               |
| 2   | k     | 4/5 (80%) | 0                 | 0               |
| 2   | l     | 4/5 (80%) | 0                 | 0               |
| 2   | m     | 4/5 (80%) | 0                 | 0               |
| 2   | n     | 4/5 (80%) | 0                 | 0               |
| 2   | o     | 4/5 (80%) | 0                 | 0               |
| 2   | p     | 4/5 (80%) | 0                 | 0               |

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| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | q     | 4/5 (80%)   | 0                 | 0               |
| 2   | r     | 4/5 (80%)   | 0                 | 0               |
| 2   | s     | 4/5 (80%)   | 0                 | 0               |
| All | All   | 76/95 (80%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

#### 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 monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

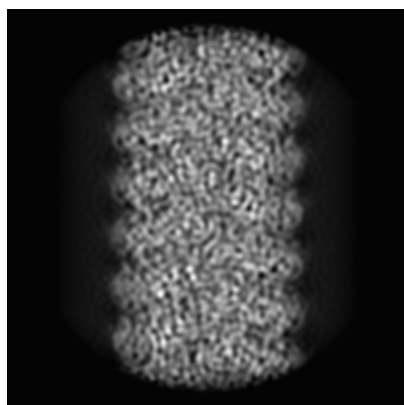
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10373. These allow visual inspection of the internal detail of the map and identification of artifacts.

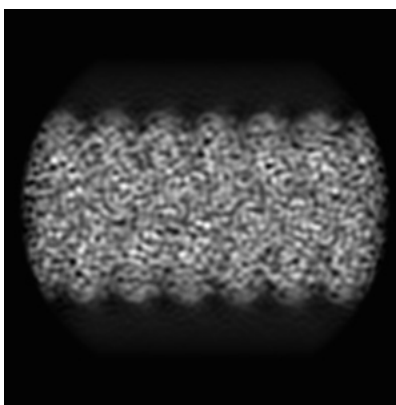
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

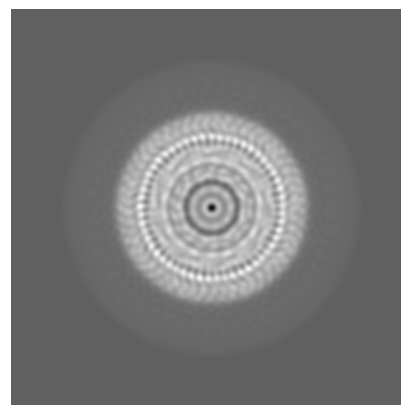
#### 6.1.1 Primary map



X



Y

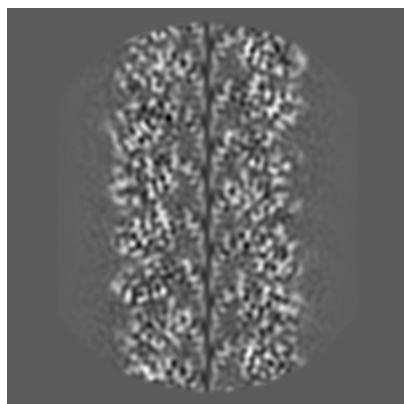


Z

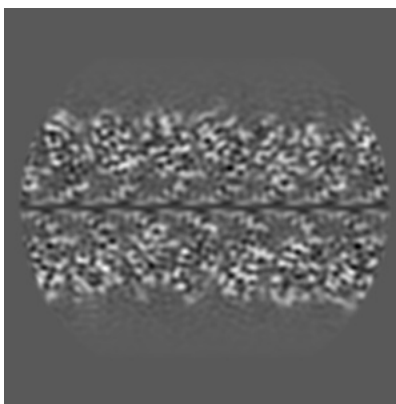
The images above show the map projected in three orthogonal directions.

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

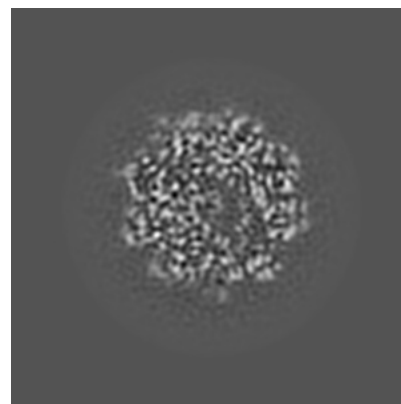
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

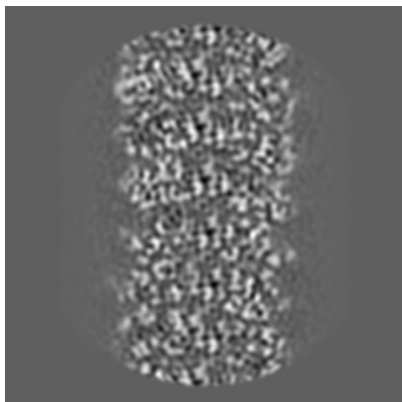


Z Index: 125

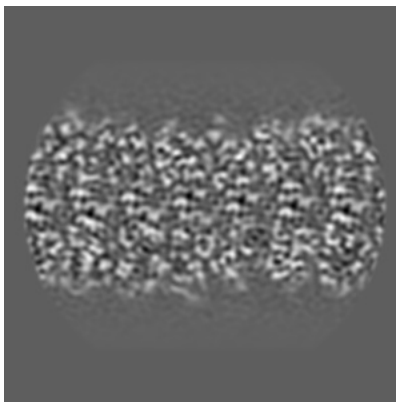
The images above show central slices of the map in three orthogonal directions.

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

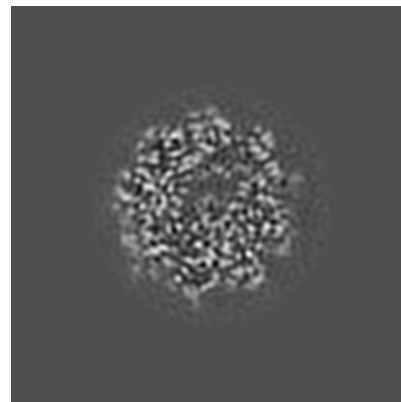
### 6.3.1 Primary map



X Index: 149



Y Index: 101

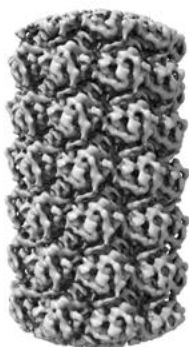


Z Index: 212

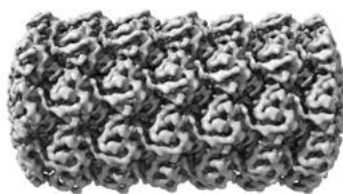
The images above show the largest variance slices of the map in three orthogonal directions.

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

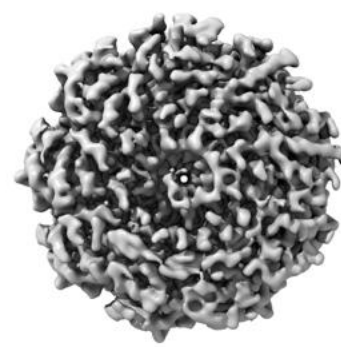
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

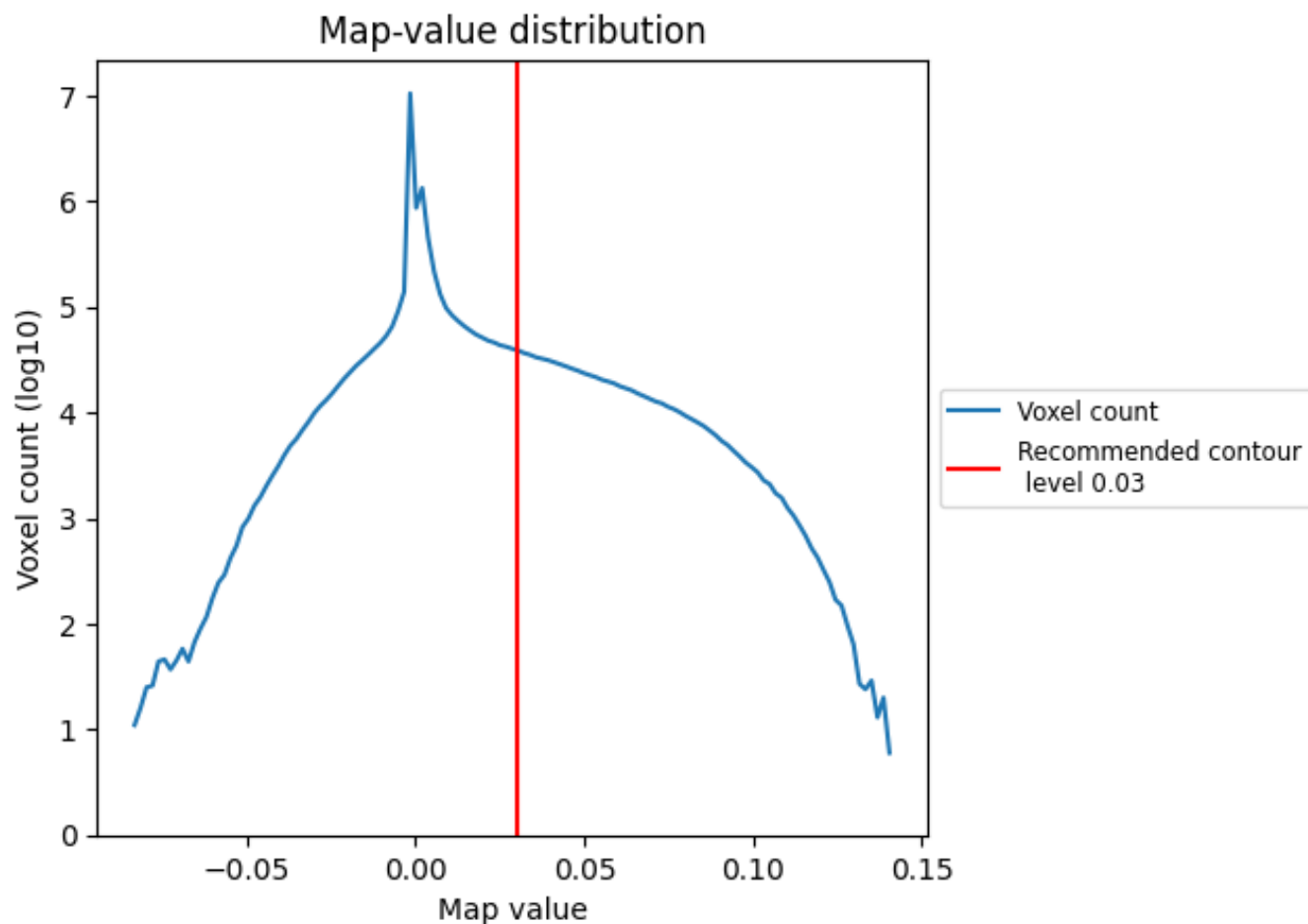
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

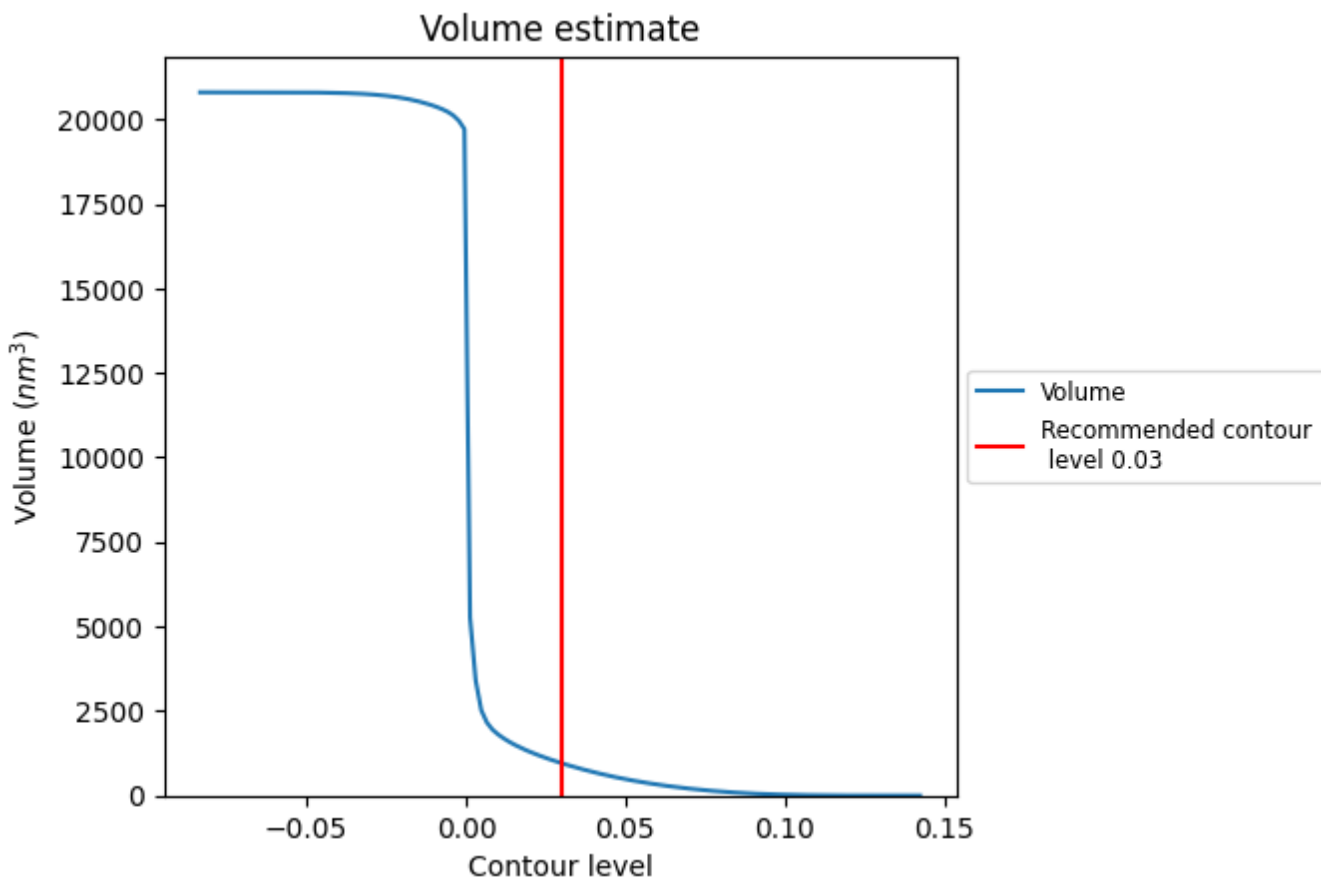
This section contains the results of statistical analysis of the map.

### 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.

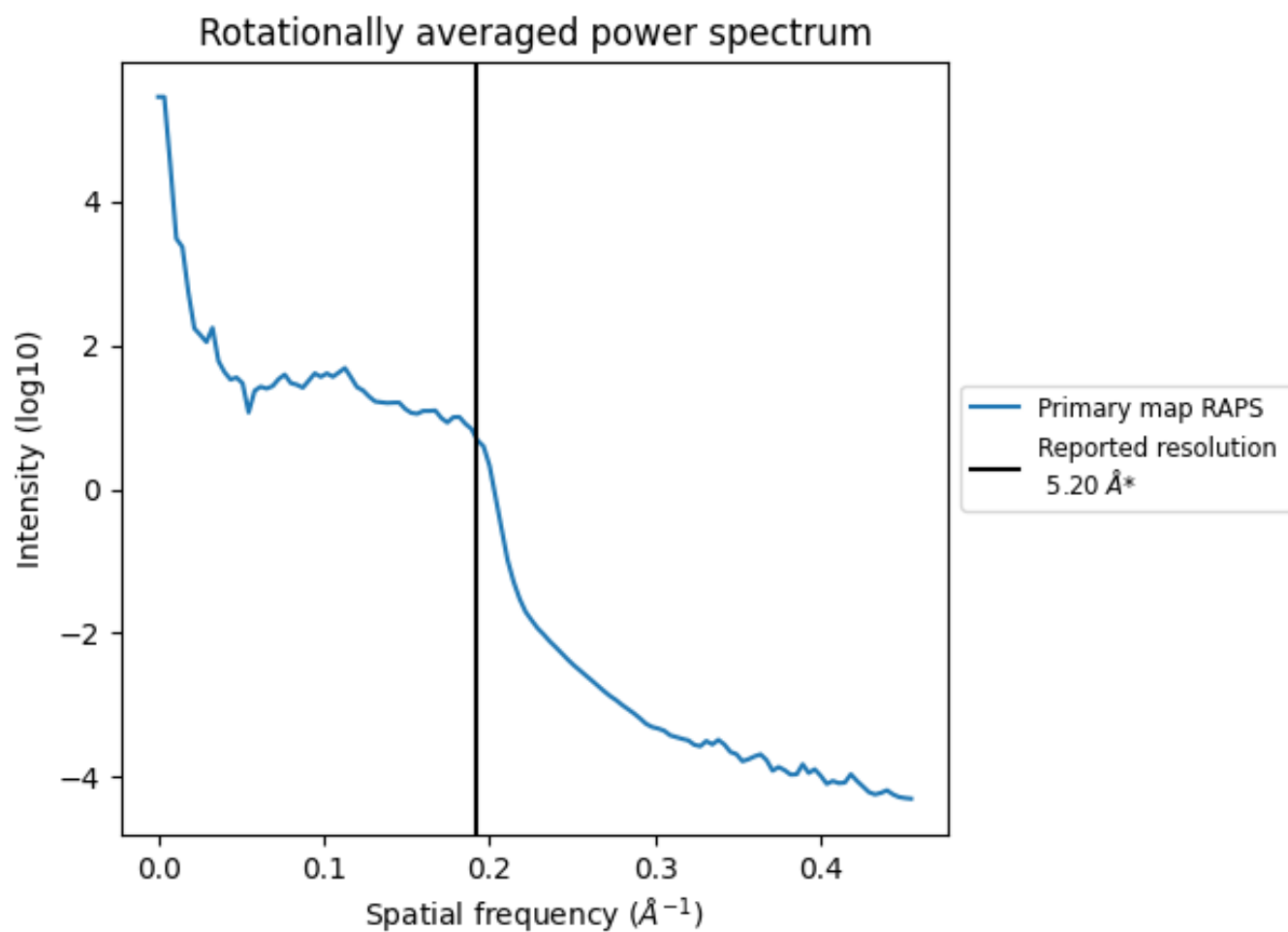
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 957 nm<sup>3</sup>; this corresponds to an approximate mass of 865 kDa.

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

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.192 Å<sup>-1</sup>

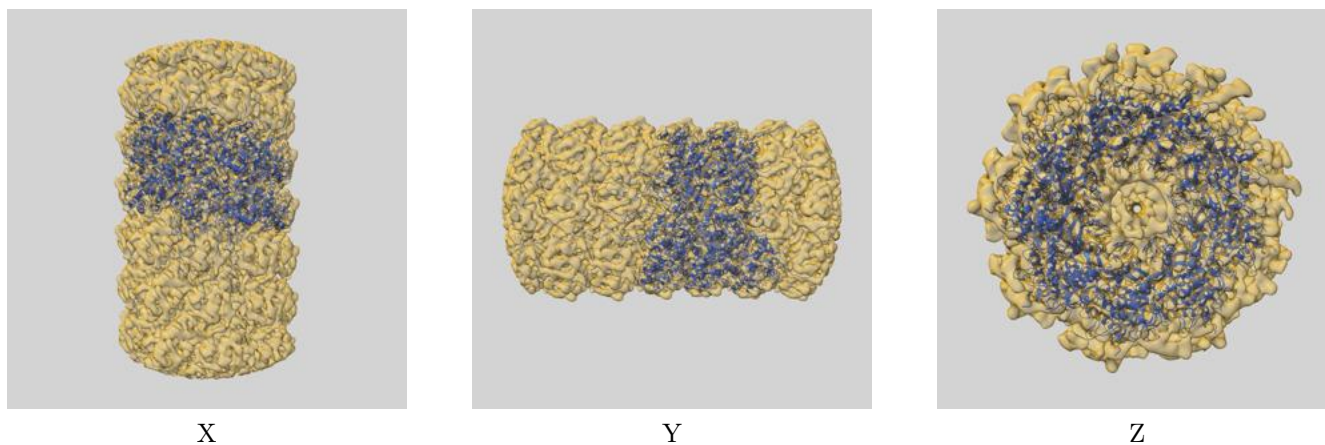
## 8 Fourier-Shell correlation

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

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

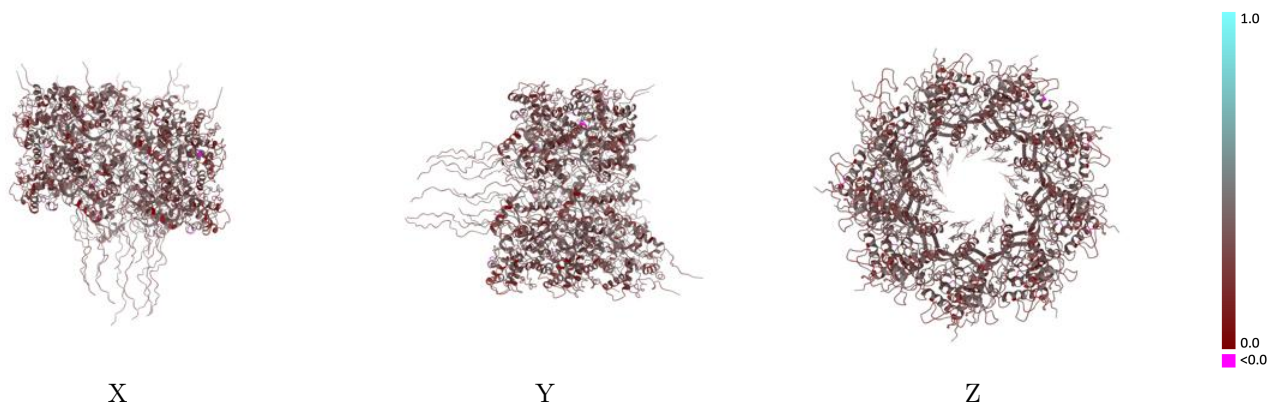
This section contains information regarding the fit between EMDB map EMD-10373 and PDB model 6T34. Per-residue inclusion information can be found in section 3 on page 8.

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



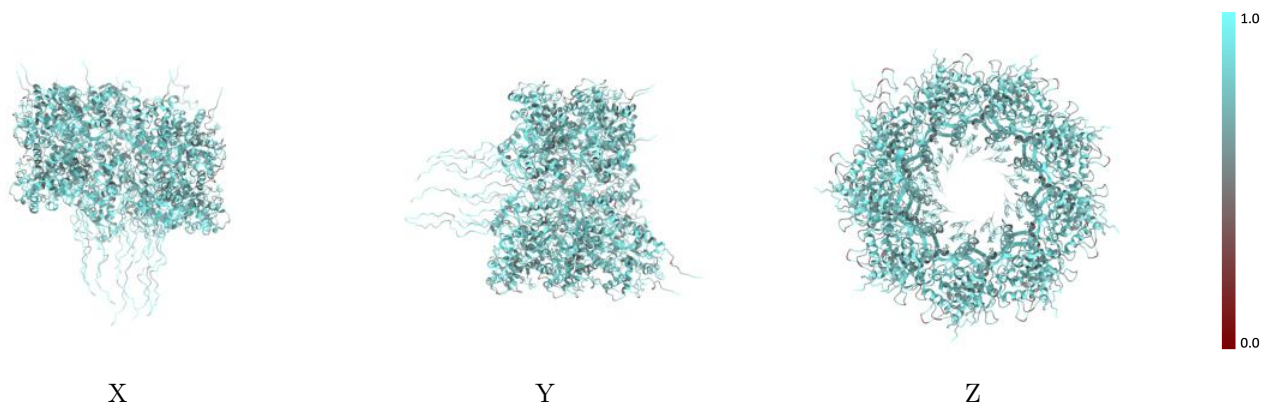
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



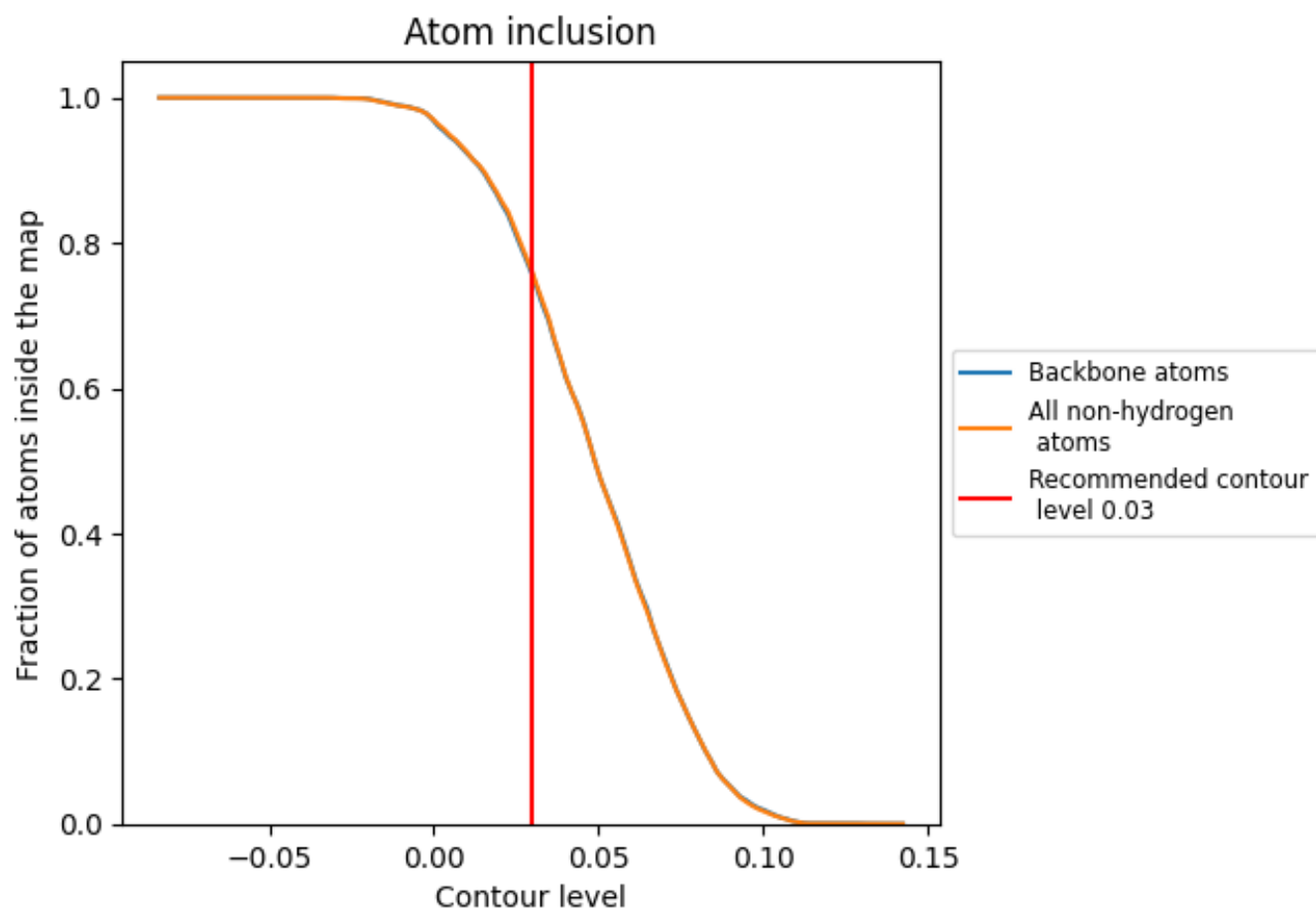
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% 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 (0.03) and Q-score for the entire model and for each chain.








| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7583   |  0.3290   |
| A     |  0.7585   |  0.3260   |
| B     |  0.7598   |  0.3270   |
| C     |  0.7622   |  0.3270   |
| D     |  0.7573   |  0.3260   |
| E     |  0.7591   |  0.3240   |
| F     |  0.7622   |  0.3260   |
| G     |  0.7604   |  0.3230   |
| H     |  0.7616   |  0.3270   |
| I     |  0.7610   |  0.3270   |
| J     |  0.7585   |  0.3250   |
| K     |  0.7622   |  0.3260   |
| L     |  0.7616   |  0.3280   |
| M     |  0.7616   |  0.3250   |
| N     |  0.7646  |  0.3260  |
| O     |  0.7598 |  0.3270 |
| P     |  0.7616 |  0.3260 |
| Q     |  0.7610 |  0.3280 |
| R     |  0.7604 |  0.3260 |
| S     |  0.7591 |  0.3260 |
| a     |  0.9200 |  0.3840 |
| b     |  0.9200 |  0.3880 |
| c     |  0.9200 |  0.3870 |
| d     |  0.9300 |  0.3820 |
| e     |  0.9400 |  0.3850 |
| f     |  0.9300 |  0.3810 |
| g     |  0.9300 |  0.3760 |
| h     |  0.9300 |  0.3880 |
| i     |  0.9200 |  0.3870 |
| j     |  0.9200 |  0.3870 |
| k     |  0.9300 |  0.3900 |
| l     |  0.9300 |  0.3890 |
| m     |  0.9400 |  0.3870 |
| n     |  0.9400 |  0.3830 |
| o     |  0.9300 |  0.3800 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| p     |  0.9300 |  0.3810 |
| q     |  0.9300 |  0.3790 |
| r     |  0.9200 |  0.3830 |
| s     |  0.9300 |  0.3860 |