



## Full wwPDB EM Validation Report ⓘ

Oct 27, 2025 – 09:54 am GMT

PDB ID : 9H5M / pdb\_00009h5m  
EMDB ID : EMD-51889  
Title : Cryo-EM structure of Gasdermin-E  
Authors : Yildiz, O.; Garcia-Saez, A.J.; Shalaby, R.  
Deposited on : 2024-10-22  
Resolution : 3.60 Å(reported)  
Based on initial model : .

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.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

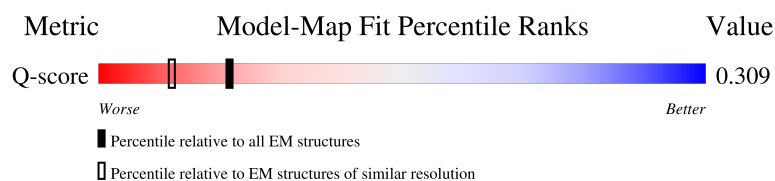
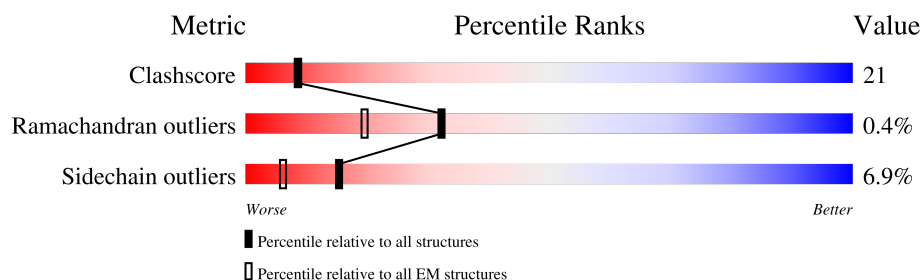
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









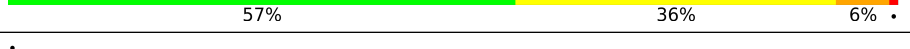
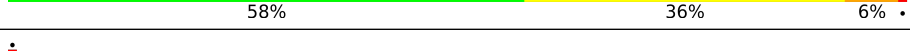
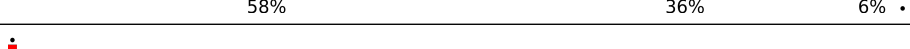
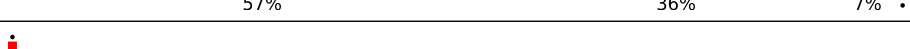
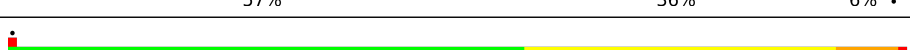

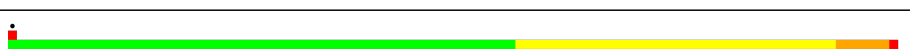

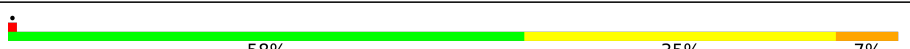





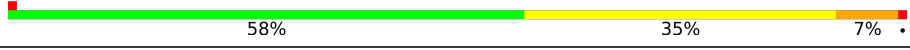
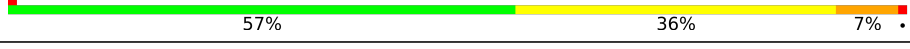



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 210492                      | 15764                       | -  |
| Ramachandran outliers | 207382                      | 16835                       | -  |
| Sidechain outliers    | 206894                      | 16415                       | -  |
| Q-score               | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 245    |                  |
| 1   | B     | 245    |                  |
| 1   | C     | 245    |                  |
| 1   | D     | 245    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | E     | 245    |    |
| 1   | F     | 245    |    |
| 1   | G     | 245    |    |
| 1   | H     | 245    |    |
| 1   | I     | 245    |    |
| 1   | J     | 245    |    |
| 1   | K     | 245    |    |
| 1   | L     | 245    |    |
| 1   | M     | 245    |    |
| 1   | N     | 245    |    |
| 1   | O     | 245    |    |
| 1   | P     | 245    |  |
| 1   | Q     | 245    |  |
| 1   | R     | 245    |  |
| 1   | S     | 245    |  |
| 1   | T     | 245    |  |
| 1   | U     | 245    |  |
| 1   | V     | 245    |  |
| 1   | W     | 245    |  |
| 1   | X     | 245    |  |
| 1   | Y     | 245    |  |
| 1   | Z     | 245    |  |
| 1   | a     | 245    |  |
| 1   | b     | 245    |  |
| 1   | c     | 245    |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | d     | 245    | <div><div></div><div>58%</div><div>35%</div><div>7%</div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Gasdermin-E, N-terminal.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | A     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | B     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | C     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | D     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | E     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | F     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | G     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | H     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | I     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | J     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | K     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | L     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | M     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | N     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | O     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | P     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | Q     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | R     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | S     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | T     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | U     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | V     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | W     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | X     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | Y     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | Z     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | a     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | b     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | c     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |
| 1   | d     | 245      | Total<br>1918 | C<br>1210 | N<br>329 | O<br>371 | S<br>8 | 0       | 0     |

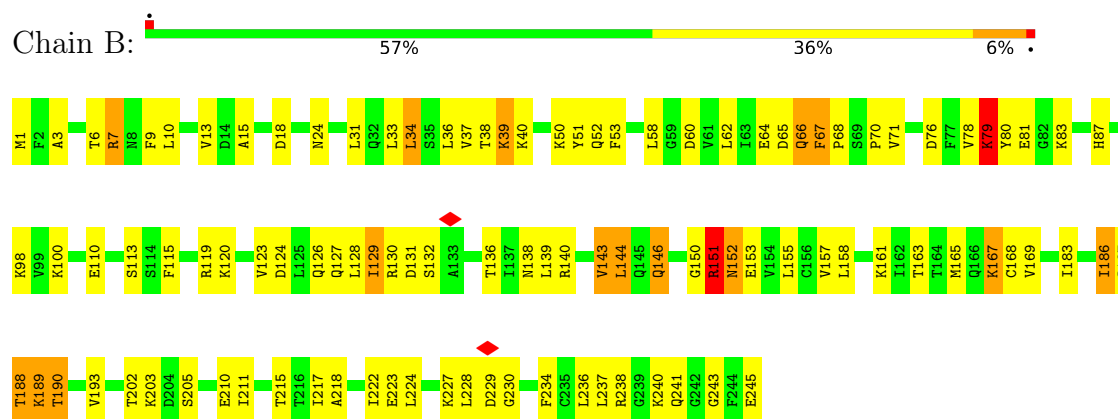
### 3 Residue-property plots

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

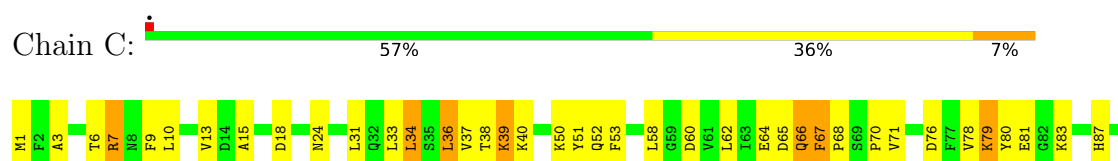
#### • Molecule 1: Gasdermin-E, N-terminal

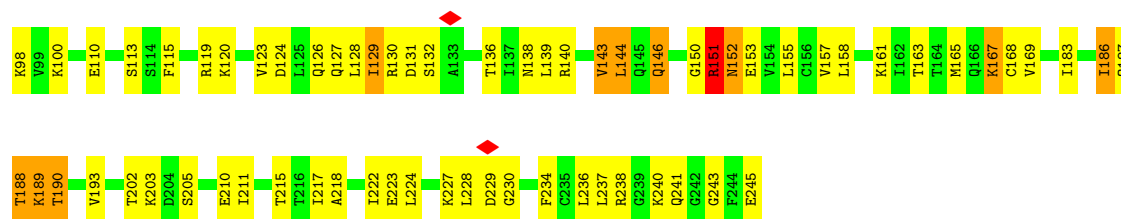


#### • Molecule 1: Gasdermin-E, N-terminal



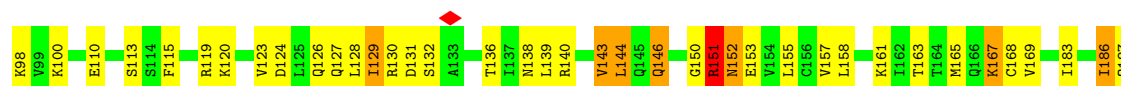
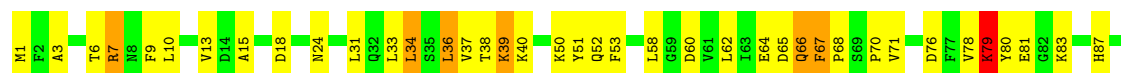
#### • Molecule 1: Gasdermin-E, N-terminal





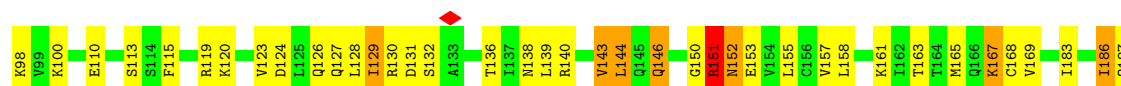
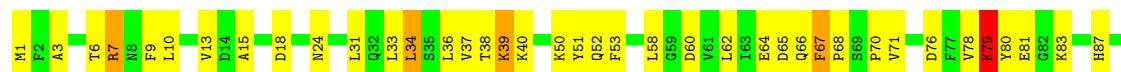
• Molecule 1: Gasdermin-E, N-terminal

Chain D: 57% 36% 7%



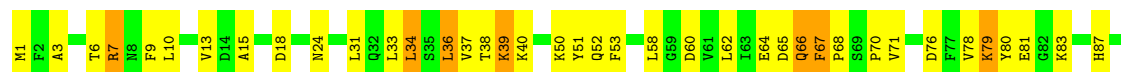
• Molecule 1: Gasdermin-E, N-terminal

Chain E: 58% 36% 6%

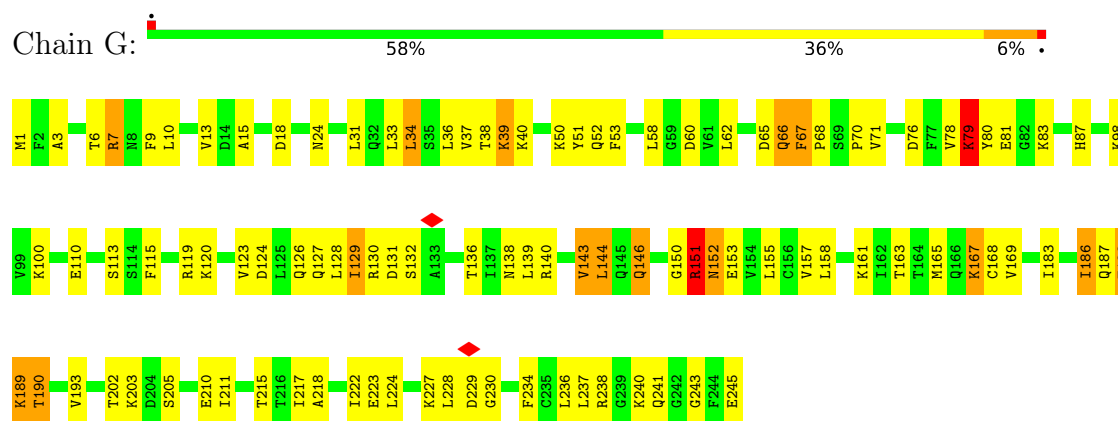


• Molecule 1: Gasdermin-E, N-terminal

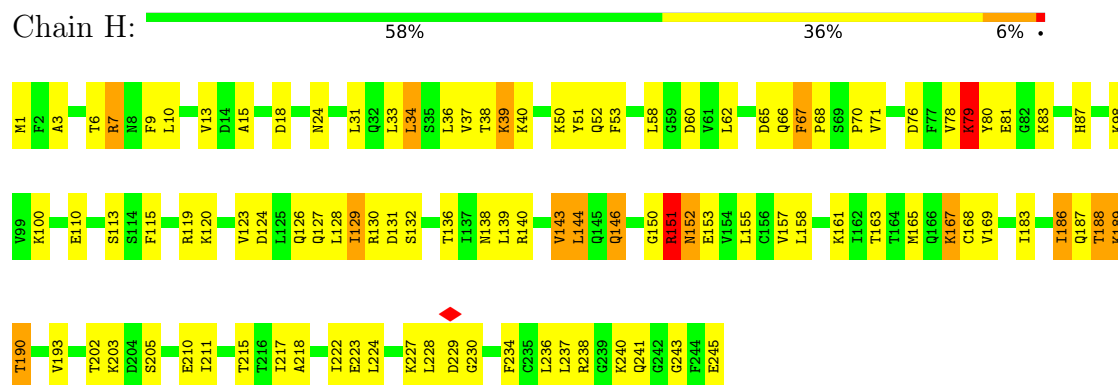
Chain F: 58% 36% 7%



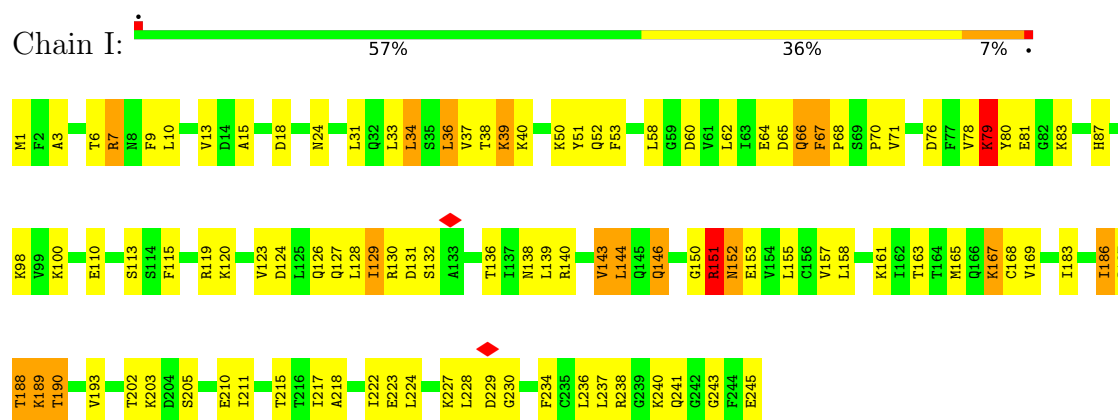
## ● Molecule 1: Gasdermin-E, N-terminal



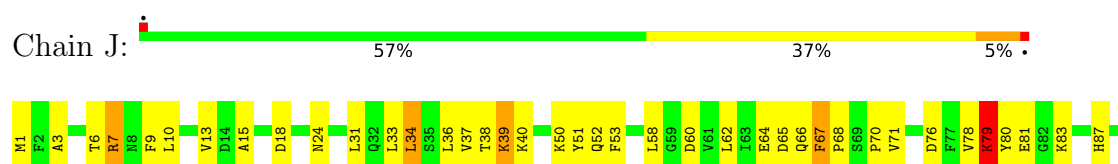
## ● Molecule 1: Gasdermin-E, N-terminal

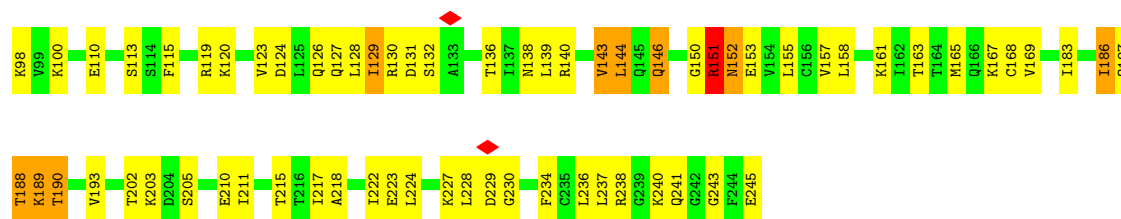


## ● Molecule 1: Gasdermin-E, N-terminal



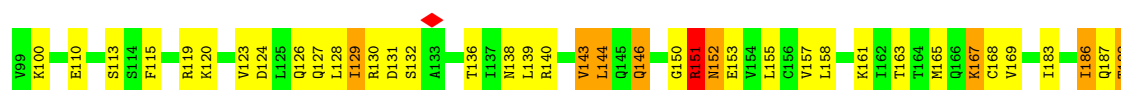
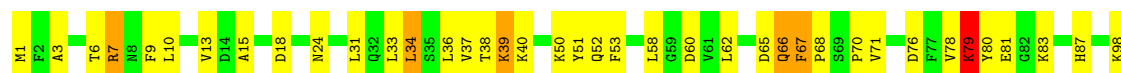
## ● Molecule 1: Gasdermin-E, N-terminal





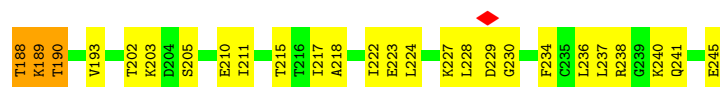
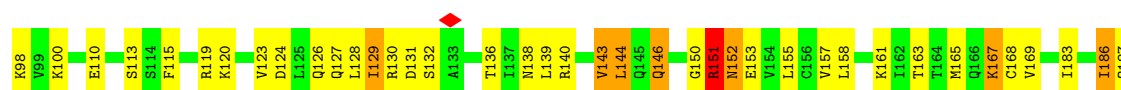
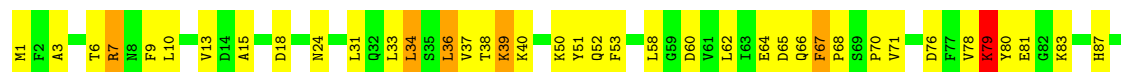
• Molecule 1: Gasdermin-E, N-terminal

Chain K: 57% 36% 6%



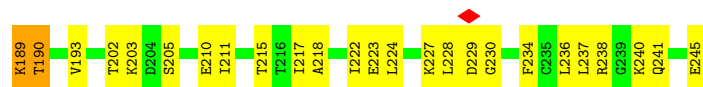
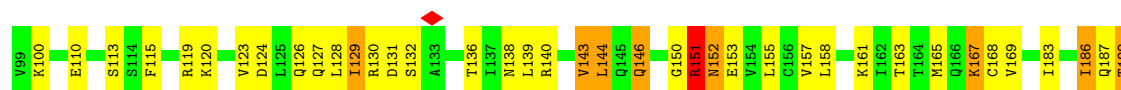
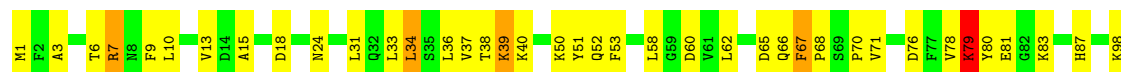
• Molecule 1: Gasdermin-E, N-terminal

Chain L: 58% 36% 6%

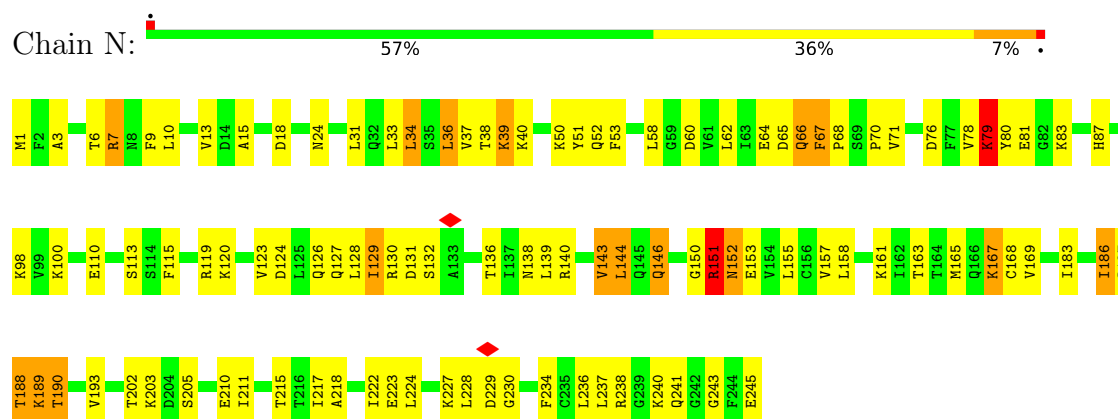


• Molecule 1: Gasdermin-E, N-terminal

Chain M: 58% 36% 6%



• Molecule 1: Gasdermin-E, N-terminal



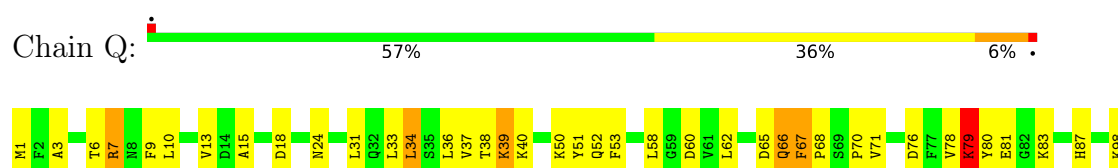
• Molecule 1: Gasdermin-E, N-terminal

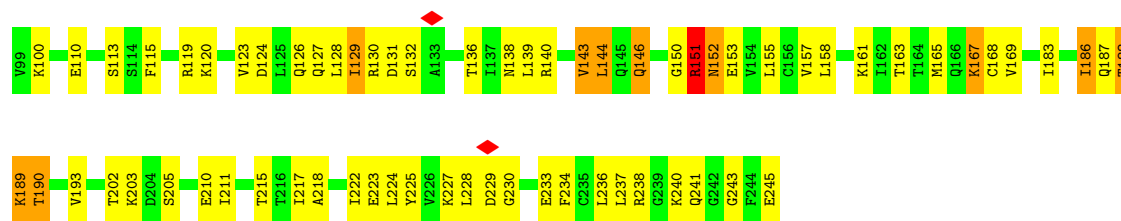


• Molecule 1: Gasdermin-E, N-terminal



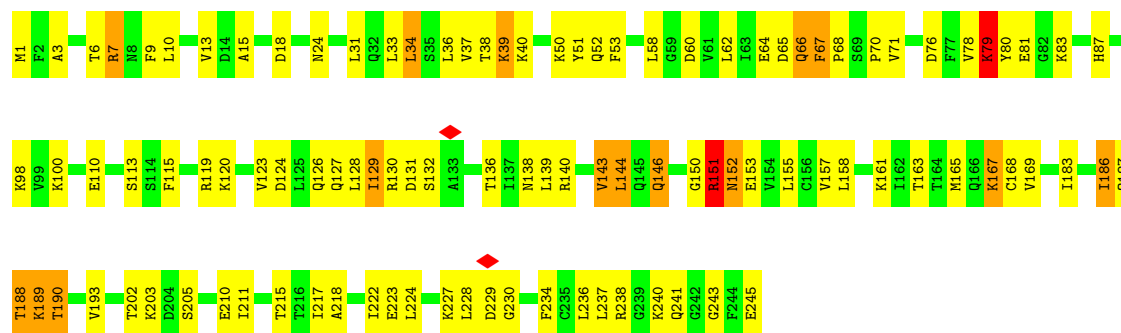
• Molecule 1: Gasdermin-E, N-terminal





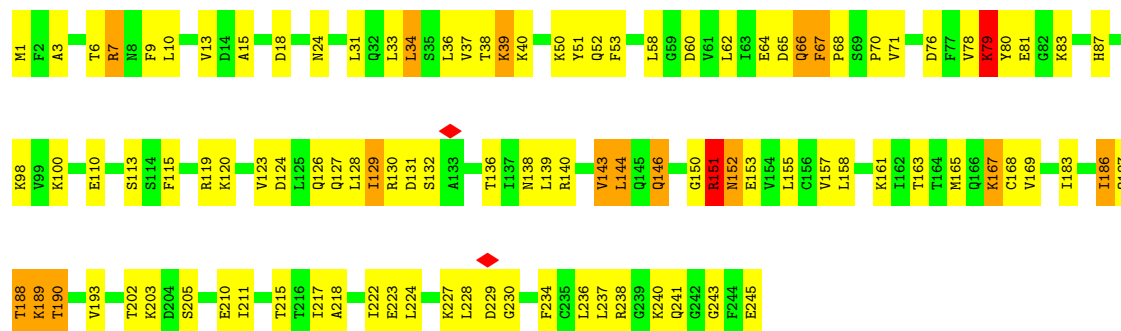
• Molecule 1: Gasdermin-E, N-terminal

Chain R: 57% 36% 6%



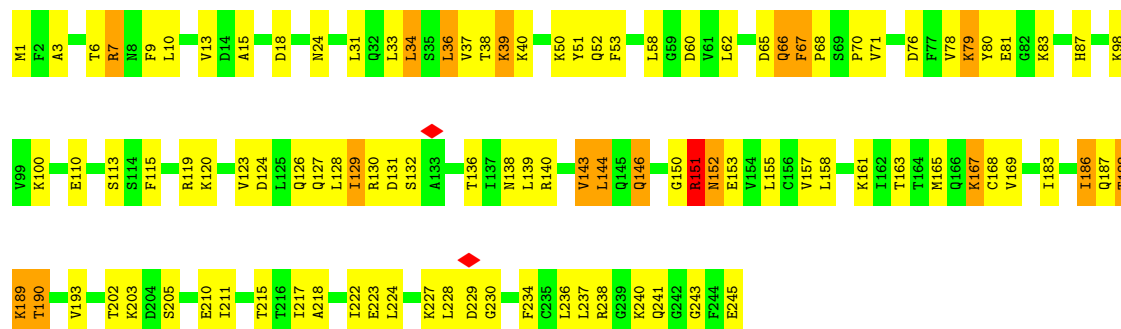
• Molecule 1: Gasdermin-E, N-terminal

Chain S: 57% 36% 6%



• Molecule 1: Gasdermin-E, N-terminal

Chain T: 58% 35% 7%



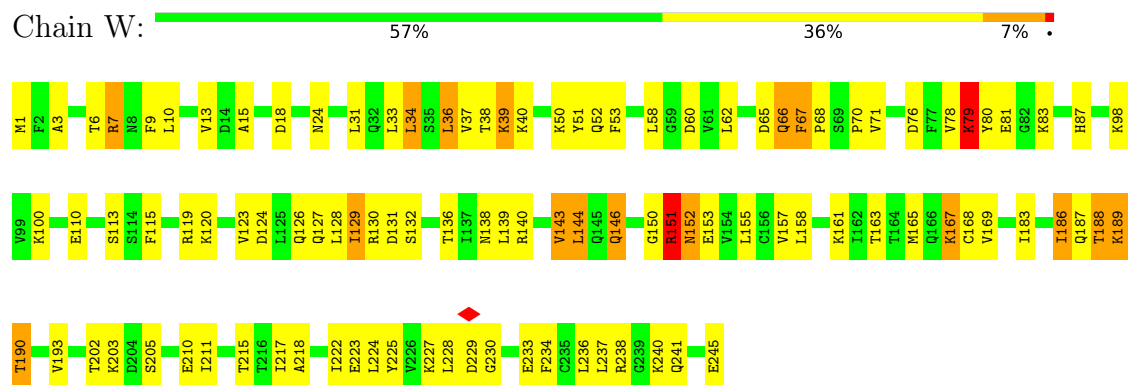
- Molecule 1: Gasdermin-E, N-terminal



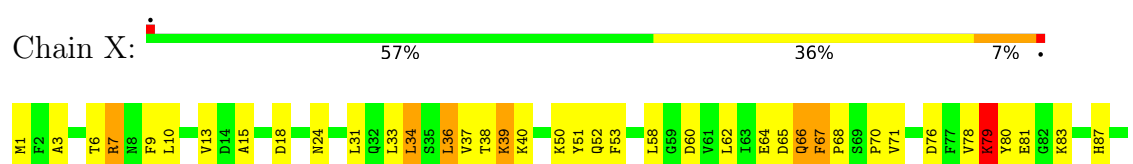
- Molecule 1: Gasdermin-E, N-terminal

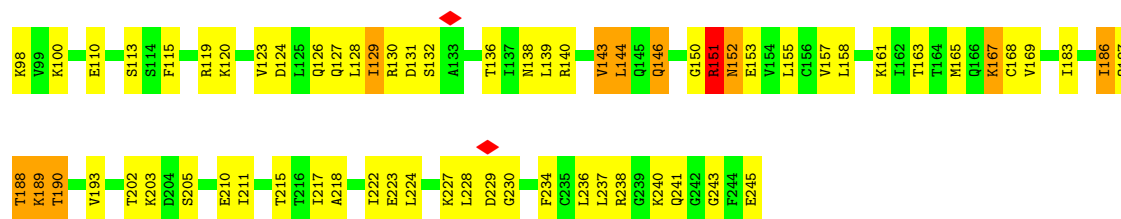


- Molecule 1: Gasdermin-E, N-terminal



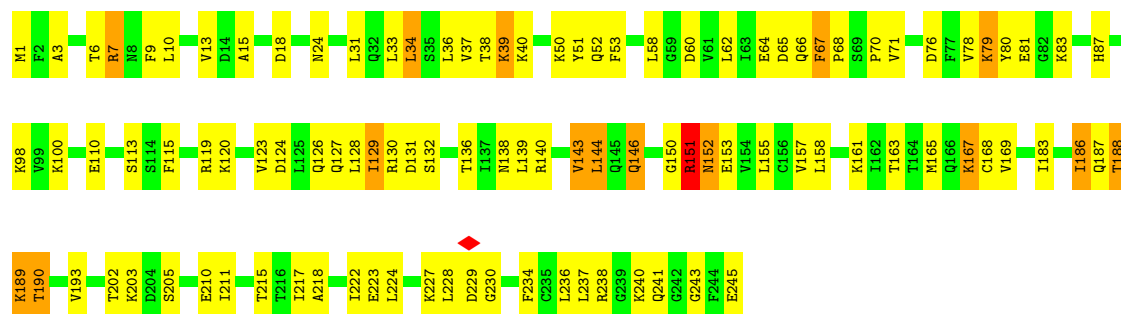
- Molecule 1: Gasdermin-E, N-terminal





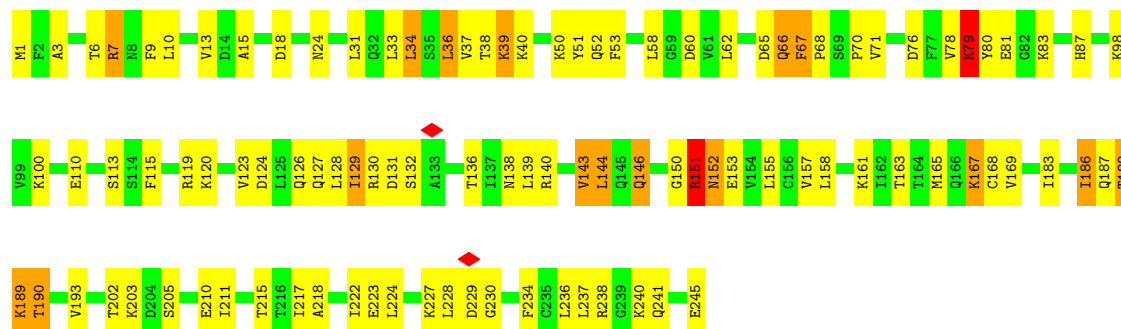
• Molecule 1: Gasdermin-E, N-terminal

Chain Y: 57% 36% 6%



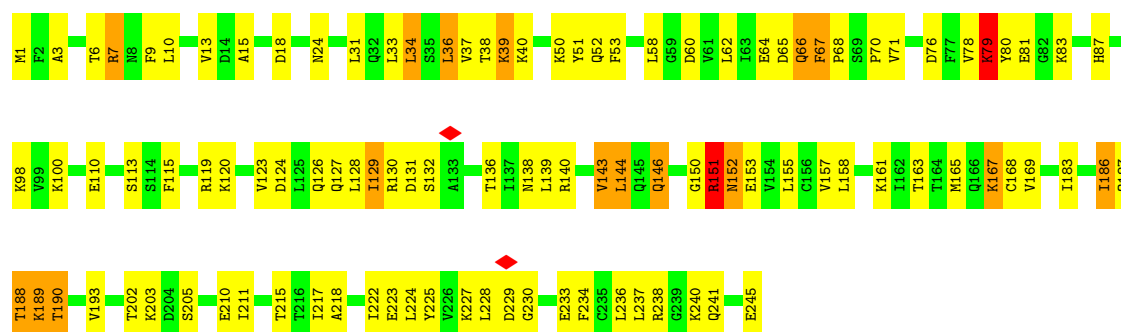
• Molecule 1: Gasdermin-E, N-terminal

Chain Z: 58% 35% 7%

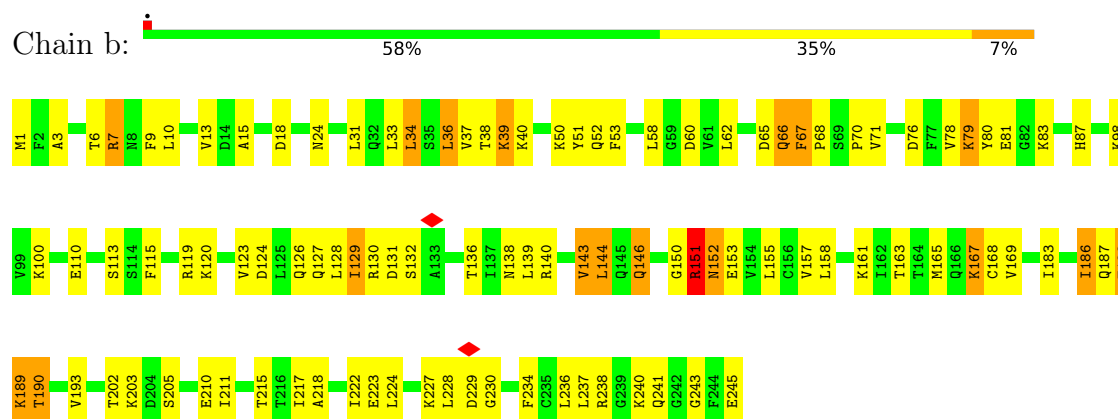


• Molecule 1: Gasdermin-E, N-terminal

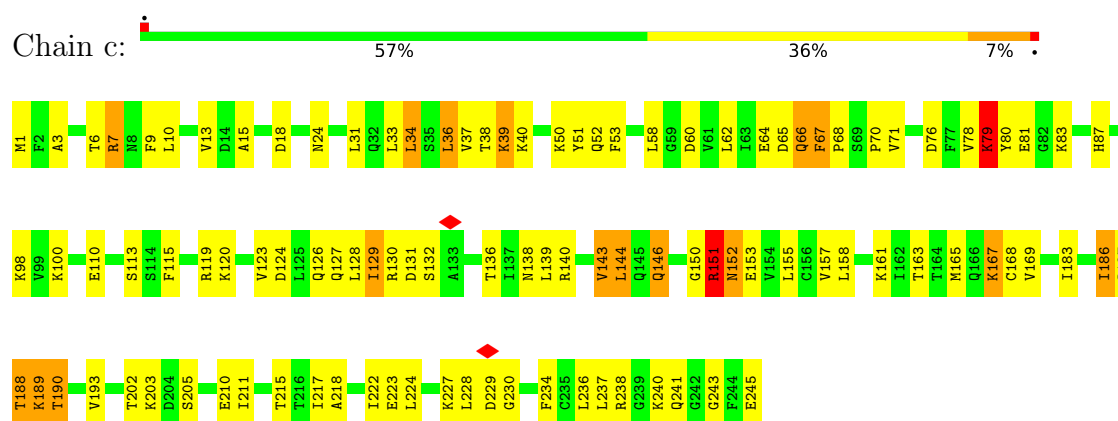
Chain a: 57% 36% 7%



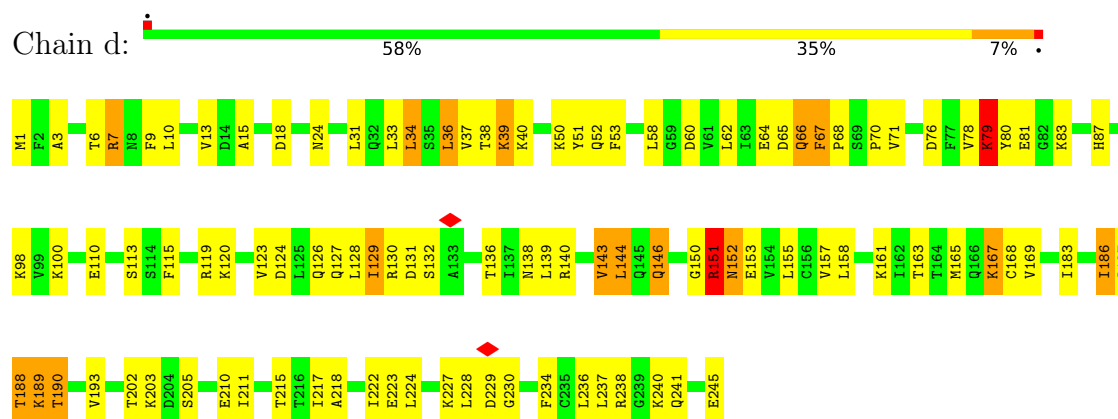
- Molecule 1: Gasdermin-E, N-terminal



- Molecule 1: Gasdermin-E, N-terminal



- Molecule 1: Gasdermin-E, N-terminal



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, C30          | Depositor |
| Number of particles used             | 88579               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | TFS KRIOS           | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                  | Depositor |
| Minimum defocus (nm)                 | 1600                | Depositor |
| Maximum defocus (nm)                 | 2400                | Depositor |
| Magnification                        | 105000              | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.486               | Depositor |
| Minimum map value                    | -0.269              | Depositor |
| Average map value                    | 0.001               | Depositor |
| Map value standard deviation         | 0.015               | Depositor |
| Recommended contour level            | 0.04                | Depositor |
| Map size ( $\text{\AA}$ )            | 418.5, 418.5, 418.5 | wwPDB     |
| Map dimensions                       | 500, 500, 500       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.837, 0.837, 0.837 | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | B     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | C     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | D     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | E     | 0.52         | 1/1943 (0.1%)   | 0.92        | 12/2620 (0.5%)   |
| 1   | F     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | G     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | H     | 0.52         | 1/1943 (0.1%)   | 0.92        | 12/2620 (0.5%)   |
| 1   | I     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | J     | 0.52         | 1/1943 (0.1%)   | 0.92        | 12/2620 (0.5%)   |
| 1   | K     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | L     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | M     | 0.52         | 1/1943 (0.1%)   | 0.92        | 12/2620 (0.5%)   |
| 1   | N     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | O     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | P     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | Q     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | R     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | S     | 0.52         | 1/1943 (0.1%)   | 0.92        | 13/2620 (0.5%)   |
| 1   | T     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | U     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | V     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | W     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | X     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | Y     | 0.52         | 1/1943 (0.1%)   | 0.92        | 12/2620 (0.5%)   |
| 1   | Z     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | a     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | b     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | c     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| 1   | d     | 0.52         | 1/1943 (0.1%)   | 0.92        | 14/2620 (0.5%)   |
| All | All   | 0.52         | 30/58290 (0.1%) | 0.92        | 401/78600 (0.5%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 2                   |
| 1   | F     | 0                   | 2                   |
| 1   | G     | 0                   | 2                   |
| 1   | H     | 0                   | 2                   |
| 1   | I     | 0                   | 2                   |
| 1   | J     | 0                   | 2                   |
| 1   | K     | 0                   | 2                   |
| 1   | L     | 0                   | 2                   |
| 1   | M     | 0                   | 2                   |
| 1   | N     | 0                   | 2                   |
| 1   | O     | 0                   | 2                   |
| 1   | P     | 0                   | 2                   |
| 1   | Q     | 0                   | 2                   |
| 1   | R     | 0                   | 2                   |
| 1   | S     | 0                   | 2                   |
| 1   | T     | 0                   | 2                   |
| 1   | U     | 0                   | 2                   |
| 1   | V     | 0                   | 2                   |
| 1   | W     | 0                   | 2                   |
| 1   | X     | 0                   | 2                   |
| 1   | Y     | 0                   | 2                   |
| 1   | Z     | 0                   | 2                   |
| 1   | a     | 0                   | 2                   |
| 1   | b     | 0                   | 2                   |
| 1   | c     | 0                   | 2                   |
| 1   | d     | 0                   | 2                   |
| All | All   | 0                   | 60                  |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | X     | 68  | PRO  | N-CD  | 11.94 | 1.64        | 1.47     |
| 1   | W     | 68  | PRO  | N-CD  | 11.93 | 1.64        | 1.47     |
| 1   | K     | 68  | PRO  | N-CD  | 11.90 | 1.64        | 1.47     |
| 1   | Z     | 68  | PRO  | N-CD  | 11.90 | 1.64        | 1.47     |
| 1   | H     | 68  | PRO  | N-CD  | 11.90 | 1.64        | 1.47     |
| 1   | L     | 68  | PRO  | N-CD  | 11.89 | 1.64        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 68  | PRO  | N-CD  | 11.88 | 1.64        | 1.47     |
| 1   | U     | 68  | PRO  | N-CD  | 11.88 | 1.64        | 1.47     |
| 1   | C     | 68  | PRO  | N-CD  | 11.87 | 1.64        | 1.47     |
| 1   | Q     | 68  | PRO  | N-CD  | 11.86 | 1.64        | 1.47     |
| 1   | a     | 68  | PRO  | N-CD  | 11.86 | 1.64        | 1.47     |
| 1   | Y     | 68  | PRO  | N-CD  | 11.86 | 1.64        | 1.47     |
| 1   | I     | 68  | PRO  | N-CD  | 11.86 | 1.64        | 1.47     |
| 1   | S     | 68  | PRO  | N-CD  | 11.84 | 1.64        | 1.47     |
| 1   | M     | 68  | PRO  | N-CD  | 11.83 | 1.64        | 1.47     |
| 1   | E     | 68  | PRO  | N-CD  | 11.81 | 1.64        | 1.47     |
| 1   | R     | 68  | PRO  | N-CD  | 11.81 | 1.64        | 1.47     |
| 1   | G     | 68  | PRO  | N-CD  | 11.81 | 1.64        | 1.47     |
| 1   | J     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | A     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | N     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | P     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | b     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | d     | 68  | PRO  | N-CD  | 11.80 | 1.64        | 1.47     |
| 1   | D     | 68  | PRO  | N-CD  | 11.79 | 1.64        | 1.47     |
| 1   | B     | 68  | PRO  | N-CD  | 11.79 | 1.64        | 1.47     |
| 1   | O     | 68  | PRO  | N-CD  | 11.78 | 1.64        | 1.47     |
| 1   | T     | 68  | PRO  | N-CD  | 11.77 | 1.64        | 1.47     |
| 1   | c     | 68  | PRO  | N-CD  | 11.73 | 1.64        | 1.47     |
| 1   | V     | 68  | PRO  | N-CD  | 11.70 | 1.64        | 1.47     |

All (401) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | R     | 68  | PRO  | N-CA-CB | 7.77 | 109.51      | 103.30   |
| 1   | S     | 68  | PRO  | N-CA-CB | 7.74 | 109.49      | 103.30   |
| 1   | N     | 68  | PRO  | N-CA-CB | 7.74 | 109.49      | 103.30   |
| 1   | Z     | 68  | PRO  | N-CA-CB | 7.71 | 109.47      | 103.30   |
| 1   | E     | 68  | PRO  | N-CA-CB | 7.71 | 109.46      | 103.30   |
| 1   | Q     | 68  | PRO  | N-CA-CB | 7.70 | 109.46      | 103.30   |
| 1   | W     | 68  | PRO  | N-CA-CB | 7.70 | 109.46      | 103.30   |
| 1   | b     | 68  | PRO  | N-CA-CB | 7.69 | 109.45      | 103.30   |
| 1   | P     | 68  | PRO  | N-CA-CB | 7.68 | 109.45      | 103.30   |
| 1   | U     | 68  | PRO  | N-CA-CB | 7.67 | 109.44      | 103.30   |
| 1   | M     | 68  | PRO  | N-CA-CB | 7.66 | 109.43      | 103.30   |
| 1   | X     | 68  | PRO  | N-CA-CB | 7.66 | 109.43      | 103.30   |
| 1   | I     | 68  | PRO  | N-CA-CB | 7.66 | 109.43      | 103.30   |
| 1   | D     | 68  | PRO  | N-CA-CB | 7.65 | 109.42      | 103.30   |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | A     | 68  | PRO  | N-CA-CB | 7.65 | 109.42      | 103.30   |
| 1   | H     | 68  | PRO  | N-CA-CB | 7.65 | 109.42      | 103.30   |
| 1   | F     | 68  | PRO  | N-CA-CB | 7.65 | 109.42      | 103.30   |
| 1   | a     | 68  | PRO  | N-CA-CB | 7.64 | 109.41      | 103.30   |
| 1   | C     | 68  | PRO  | N-CA-CB | 7.63 | 109.41      | 103.30   |
| 1   | c     | 68  | PRO  | N-CA-CB | 7.63 | 109.40      | 103.30   |
| 1   | G     | 68  | PRO  | N-CA-CB | 7.62 | 109.40      | 103.30   |
| 1   | O     | 68  | PRO  | N-CA-CB | 7.61 | 109.39      | 103.30   |
| 1   | J     | 68  | PRO  | N-CA-CB | 7.60 | 109.38      | 103.30   |
| 1   | V     | 68  | PRO  | N-CA-CB | 7.60 | 109.38      | 103.30   |
| 1   | T     | 68  | PRO  | N-CA-CB | 7.60 | 109.38      | 103.30   |
| 1   | Y     | 68  | PRO  | N-CA-CB | 7.59 | 109.37      | 103.30   |
| 1   | K     | 68  | PRO  | N-CA-CB | 7.58 | 109.36      | 103.30   |
| 1   | L     | 68  | PRO  | N-CA-CB | 7.57 | 109.36      | 103.30   |
| 1   | B     | 68  | PRO  | N-CA-CB | 7.57 | 109.35      | 103.30   |
| 1   | d     | 68  | PRO  | N-CA-CB | 7.54 | 109.33      | 103.30   |
| 1   | M     | 188 | THR  | N-CA-C  | 7.09 | 120.00      | 110.35   |
| 1   | R     | 188 | THR  | N-CA-C  | 7.05 | 119.94      | 110.35   |
| 1   | G     | 188 | THR  | N-CA-C  | 7.04 | 119.93      | 110.35   |
| 1   | J     | 188 | THR  | N-CA-C  | 7.04 | 119.93      | 110.35   |
| 1   | N     | 188 | THR  | N-CA-C  | 7.04 | 119.92      | 110.35   |
| 1   | O     | 188 | THR  | N-CA-C  | 7.04 | 119.92      | 110.35   |
| 1   | K     | 188 | THR  | N-CA-C  | 7.03 | 119.92      | 110.35   |
| 1   | B     | 188 | THR  | N-CA-C  | 7.03 | 119.91      | 110.35   |
| 1   | F     | 188 | THR  | N-CA-C  | 7.03 | 119.91      | 110.35   |
| 1   | A     | 188 | THR  | N-CA-C  | 7.02 | 119.90      | 110.35   |
| 1   | E     | 188 | THR  | N-CA-C  | 7.02 | 119.90      | 110.35   |
| 1   | S     | 188 | THR  | N-CA-C  | 7.02 | 119.90      | 110.35   |
| 1   | C     | 188 | THR  | N-CA-C  | 7.01 | 119.89      | 110.35   |
| 1   | c     | 188 | THR  | N-CA-C  | 7.01 | 119.88      | 110.35   |
| 1   | W     | 188 | THR  | N-CA-C  | 7.01 | 119.88      | 110.35   |
| 1   | b     | 188 | THR  | N-CA-C  | 7.00 | 119.87      | 110.35   |
| 1   | L     | 188 | THR  | N-CA-C  | 7.00 | 119.87      | 110.35   |
| 1   | Q     | 188 | THR  | N-CA-C  | 7.00 | 119.87      | 110.35   |
| 1   | T     | 188 | THR  | N-CA-C  | 7.00 | 119.87      | 110.35   |
| 1   | P     | 188 | THR  | N-CA-C  | 7.00 | 119.86      | 110.35   |
| 1   | V     | 188 | THR  | N-CA-C  | 7.00 | 119.87      | 110.35   |
| 1   | X     | 188 | THR  | N-CA-C  | 7.00 | 119.86      | 110.35   |
| 1   | D     | 188 | THR  | N-CA-C  | 6.99 | 119.86      | 110.35   |
| 1   | d     | 188 | THR  | N-CA-C  | 6.99 | 119.86      | 110.35   |
| 1   | Y     | 188 | THR  | N-CA-C  | 6.98 | 119.84      | 110.35   |
| 1   | I     | 188 | THR  | N-CA-C  | 6.97 | 119.83      | 110.35   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | H     | 188 | THR  | N-CA-C | 6.96 | 119.81      | 110.35   |
| 1   | Z     | 188 | THR  | N-CA-C | 6.96 | 119.81      | 110.35   |
| 1   | a     | 188 | THR  | N-CA-C | 6.96 | 119.81      | 110.35   |
| 1   | U     | 188 | THR  | N-CA-C | 6.95 | 119.80      | 110.35   |
| 1   | Q     | 70  | PRO  | N-CA-C | 6.94 | 122.42      | 111.38   |
| 1   | a     | 70  | PRO  | N-CA-C | 6.94 | 122.42      | 111.38   |
| 1   | N     | 70  | PRO  | N-CA-C | 6.93 | 122.40      | 111.38   |
| 1   | J     | 70  | PRO  | N-CA-C | 6.92 | 122.39      | 111.38   |
| 1   | R     | 70  | PRO  | N-CA-C | 6.92 | 122.39      | 111.38   |
| 1   | c     | 70  | PRO  | N-CA-C | 6.92 | 122.39      | 111.38   |
| 1   | G     | 70  | PRO  | N-CA-C | 6.92 | 122.38      | 111.38   |
| 1   | V     | 70  | PRO  | N-CA-C | 6.92 | 122.38      | 111.38   |
| 1   | Y     | 70  | PRO  | N-CA-C | 6.92 | 122.38      | 111.38   |
| 1   | F     | 70  | PRO  | N-CA-C | 6.91 | 122.37      | 111.38   |
| 1   | E     | 70  | PRO  | N-CA-C | 6.91 | 122.37      | 111.38   |
| 1   | T     | 70  | PRO  | N-CA-C | 6.91 | 122.37      | 111.38   |
| 1   | W     | 70  | PRO  | N-CA-C | 6.91 | 122.37      | 111.38   |
| 1   | L     | 70  | PRO  | N-CA-C | 6.91 | 122.36      | 111.38   |
| 1   | X     | 70  | PRO  | N-CA-C | 6.90 | 122.36      | 111.38   |
| 1   | O     | 70  | PRO  | N-CA-C | 6.90 | 122.36      | 111.38   |
| 1   | A     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | Z     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | d     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | S     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | B     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | D     | 70  | PRO  | N-CA-C | 6.90 | 122.35      | 111.38   |
| 1   | C     | 70  | PRO  | N-CA-C | 6.89 | 122.34      | 111.38   |
| 1   | I     | 70  | PRO  | N-CA-C | 6.89 | 122.34      | 111.38   |
| 1   | P     | 70  | PRO  | N-CA-C | 6.89 | 122.33      | 111.38   |
| 1   | U     | 70  | PRO  | N-CA-C | 6.88 | 122.33      | 111.38   |
| 1   | K     | 70  | PRO  | N-CA-C | 6.88 | 122.32      | 111.38   |
| 1   | b     | 70  | PRO  | N-CA-C | 6.88 | 122.32      | 111.38   |
| 1   | H     | 70  | PRO  | N-CA-C | 6.88 | 122.31      | 111.38   |
| 1   | M     | 70  | PRO  | N-CA-C | 6.88 | 122.31      | 111.38   |
| 1   | C     | 67  | PHE  | N-CA-C | 6.40 | 122.46      | 109.60   |
| 1   | U     | 67  | PHE  | N-CA-C | 6.39 | 122.45      | 109.60   |
| 1   | W     | 67  | PHE  | N-CA-C | 6.39 | 122.44      | 109.60   |
| 1   | L     | 67  | PHE  | N-CA-C | 6.39 | 122.44      | 109.60   |
| 1   | J     | 67  | PHE  | N-CA-C | 6.38 | 122.42      | 109.60   |
| 1   | S     | 67  | PHE  | N-CA-C | 6.38 | 122.42      | 109.60   |
| 1   | V     | 67  | PHE  | N-CA-C | 6.38 | 122.42      | 109.60   |
| 1   | X     | 67  | PHE  | N-CA-C | 6.38 | 122.42      | 109.60   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | Y     | 67  | PHE  | N-CA-C | 6.38 | 122.42      | 109.60   |
| 1   | Z     | 67  | PHE  | N-CA-C | 6.37 | 122.41      | 109.60   |
| 1   | A     | 67  | PHE  | N-CA-C | 6.37 | 122.41      | 109.60   |
| 1   | O     | 67  | PHE  | N-CA-C | 6.37 | 122.40      | 109.60   |
| 1   | E     | 67  | PHE  | N-CA-C | 6.36 | 122.39      | 109.60   |
| 1   | P     | 67  | PHE  | N-CA-C | 6.36 | 122.39      | 109.60   |
| 1   | F     | 67  | PHE  | N-CA-C | 6.36 | 122.38      | 109.60   |
| 1   | H     | 67  | PHE  | N-CA-C | 6.36 | 122.38      | 109.60   |
| 1   | B     | 67  | PHE  | N-CA-C | 6.36 | 122.38      | 109.60   |
| 1   | D     | 67  | PHE  | N-CA-C | 6.36 | 122.37      | 109.60   |
| 1   | K     | 67  | PHE  | N-CA-C | 6.36 | 122.38      | 109.60   |
| 1   | a     | 67  | PHE  | N-CA-C | 6.36 | 122.37      | 109.60   |
| 1   | M     | 67  | PHE  | N-CA-C | 6.35 | 122.37      | 109.60   |
| 1   | Q     | 67  | PHE  | N-CA-C | 6.35 | 122.36      | 109.60   |
| 1   | T     | 67  | PHE  | N-CA-C | 6.35 | 122.37      | 109.60   |
| 1   | N     | 67  | PHE  | N-CA-C | 6.35 | 122.36      | 109.60   |
| 1   | b     | 67  | PHE  | N-CA-C | 6.35 | 122.36      | 109.60   |
| 1   | G     | 67  | PHE  | N-CA-C | 6.35 | 122.36      | 109.60   |
| 1   | c     | 67  | PHE  | N-CA-C | 6.34 | 122.35      | 109.60   |
| 1   | R     | 67  | PHE  | N-CA-C | 6.34 | 122.34      | 109.60   |
| 1   | d     | 67  | PHE  | N-CA-C | 6.34 | 122.34      | 109.60   |
| 1   | I     | 67  | PHE  | N-CA-C | 6.34 | 122.34      | 109.60   |
| 1   | Q     | 152 | ASN  | N-CA-C | 6.21 | 124.03      | 110.80   |
| 1   | E     | 152 | ASN  | N-CA-C | 6.21 | 124.03      | 110.80   |
| 1   | Y     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | N     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | c     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | d     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | O     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | X     | 152 | ASN  | N-CA-C | 6.20 | 124.01      | 110.80   |
| 1   | V     | 152 | ASN  | N-CA-C | 6.20 | 124.00      | 110.80   |
| 1   | M     | 152 | ASN  | N-CA-C | 6.20 | 124.00      | 110.80   |
| 1   | W     | 152 | ASN  | N-CA-C | 6.20 | 124.00      | 110.80   |
| 1   | a     | 152 | ASN  | N-CA-C | 6.20 | 124.00      | 110.80   |
| 1   | F     | 152 | ASN  | N-CA-C | 6.19 | 123.99      | 110.80   |
| 1   | P     | 152 | ASN  | N-CA-C | 6.19 | 123.99      | 110.80   |
| 1   | H     | 152 | ASN  | N-CA-C | 6.19 | 123.98      | 110.80   |
| 1   | R     | 152 | ASN  | N-CA-C | 6.18 | 123.97      | 110.80   |
| 1   | J     | 152 | ASN  | N-CA-C | 6.18 | 123.97      | 110.80   |
| 1   | Z     | 152 | ASN  | N-CA-C | 6.18 | 123.97      | 110.80   |
| 1   | b     | 152 | ASN  | N-CA-C | 6.18 | 123.96      | 110.80   |
| 1   | B     | 152 | ASN  | N-CA-C | 6.18 | 123.96      | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 152 | ASN  | N-CA-C  | 6.18  | 123.96      | 110.80   |
| 1   | S     | 152 | ASN  | N-CA-C  | 6.18  | 123.96      | 110.80   |
| 1   | G     | 152 | ASN  | N-CA-C  | 6.18  | 123.95      | 110.80   |
| 1   | A     | 152 | ASN  | N-CA-C  | 6.17  | 123.95      | 110.80   |
| 1   | C     | 152 | ASN  | N-CA-C  | 6.17  | 123.95      | 110.80   |
| 1   | L     | 152 | ASN  | N-CA-C  | 6.17  | 123.94      | 110.80   |
| 1   | T     | 152 | ASN  | N-CA-C  | 6.17  | 123.94      | 110.80   |
| 1   | U     | 152 | ASN  | N-CA-C  | 6.17  | 123.93      | 110.80   |
| 1   | K     | 152 | ASN  | N-CA-C  | 6.17  | 123.93      | 110.80   |
| 1   | B     | 189 | LYS  | N-CA-C  | 6.16  | 118.49      | 108.63   |
| 1   | Q     | 189 | LYS  | N-CA-C  | 6.16  | 118.49      | 108.63   |
| 1   | A     | 189 | LYS  | N-CA-C  | 6.16  | 118.48      | 108.63   |
| 1   | D     | 152 | ASN  | N-CA-C  | 6.14  | 123.89      | 110.80   |
| 1   | R     | 189 | LYS  | N-CA-C  | 6.14  | 118.46      | 108.63   |
| 1   | G     | 189 | LYS  | N-CA-C  | 6.14  | 118.45      | 108.63   |
| 1   | c     | 189 | LYS  | N-CA-C  | 6.14  | 118.45      | 108.63   |
| 1   | C     | 189 | LYS  | N-CA-C  | 6.12  | 118.43      | 108.63   |
| 1   | I     | 189 | LYS  | N-CA-C  | 6.12  | 118.42      | 108.63   |
| 1   | M     | 34  | LEU  | CB-CA-C | -6.12 | 102.05      | 111.66   |
| 1   | d     | 189 | LYS  | N-CA-C  | 6.12  | 118.42      | 108.63   |
| 1   | V     | 189 | LYS  | N-CA-C  | 6.12  | 118.41      | 108.63   |
| 1   | d     | 34  | LEU  | CB-CA-C | -6.12 | 102.06      | 111.66   |
| 1   | U     | 189 | LYS  | N-CA-C  | 6.11  | 118.41      | 108.63   |
| 1   | Z     | 189 | LYS  | N-CA-C  | 6.11  | 118.41      | 108.63   |
| 1   | F     | 189 | LYS  | N-CA-C  | 6.11  | 118.41      | 108.63   |
| 1   | M     | 189 | LYS  | N-CA-C  | 6.11  | 118.41      | 108.63   |
| 1   | T     | 189 | LYS  | N-CA-C  | 6.11  | 118.41      | 108.63   |
| 1   | N     | 34  | LEU  | CB-CA-C | -6.11 | 102.07      | 111.66   |
| 1   | H     | 189 | LYS  | N-CA-C  | 6.11  | 118.40      | 108.63   |
| 1   | b     | 189 | LYS  | N-CA-C  | 6.11  | 118.40      | 108.63   |
| 1   | P     | 189 | LYS  | N-CA-C  | 6.11  | 118.40      | 108.63   |
| 1   | W     | 189 | LYS  | N-CA-C  | 6.11  | 118.40      | 108.63   |
| 1   | Z     | 34  | LEU  | CB-CA-C | -6.11 | 102.08      | 111.66   |
| 1   | X     | 189 | LYS  | N-CA-C  | 6.10  | 118.40      | 108.63   |
| 1   | b     | 34  | LEU  | CB-CA-C | -6.10 | 102.08      | 111.66   |
| 1   | D     | 189 | LYS  | N-CA-C  | 6.10  | 118.39      | 108.63   |
| 1   | L     | 34  | LEU  | CB-CA-C | -6.10 | 102.08      | 111.66   |
| 1   | N     | 189 | LYS  | N-CA-C  | 6.10  | 118.39      | 108.63   |
| 1   | a     | 189 | LYS  | N-CA-C  | 6.10  | 118.39      | 108.63   |
| 1   | J     | 34  | LEU  | CB-CA-C | -6.10 | 102.08      | 111.66   |
| 1   | O     | 34  | LEU  | CB-CA-C | -6.09 | 102.09      | 111.66   |
| 1   | K     | 189 | LYS  | N-CA-C  | 6.09  | 118.38      | 108.63   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | V     | 34  | LEU  | CB-CA-C | -6.09 | 102.10      | 111.66   |
| 1   | X     | 34  | LEU  | CB-CA-C | -6.09 | 102.09      | 111.66   |
| 1   | c     | 34  | LEU  | CB-CA-C | -6.09 | 102.09      | 111.66   |
| 1   | K     | 34  | LEU  | CB-CA-C | -6.09 | 102.10      | 111.66   |
| 1   | Y     | 189 | LYS  | N-CA-C  | 6.09  | 118.38      | 108.63   |
| 1   | O     | 189 | LYS  | N-CA-C  | 6.09  | 118.37      | 108.63   |
| 1   | H     | 34  | LEU  | CB-CA-C | -6.09 | 102.10      | 111.66   |
| 1   | W     | 34  | LEU  | CB-CA-C | -6.09 | 102.10      | 111.66   |
| 1   | B     | 34  | LEU  | CB-CA-C | -6.08 | 102.11      | 111.66   |
| 1   | G     | 34  | LEU  | CB-CA-C | -6.08 | 102.11      | 111.66   |
| 1   | E     | 189 | LYS  | N-CA-C  | 6.08  | 118.36      | 108.63   |
| 1   | J     | 189 | LYS  | N-CA-C  | 6.08  | 118.36      | 108.63   |
| 1   | T     | 34  | LEU  | CB-CA-C | -6.08 | 102.12      | 111.66   |
| 1   | Y     | 34  | LEU  | CB-CA-C | -6.07 | 102.12      | 111.66   |
| 1   | D     | 34  | LEU  | CB-CA-C | -6.07 | 102.13      | 111.66   |
| 1   | L     | 189 | LYS  | N-CA-C  | 6.07  | 118.35      | 108.63   |
| 1   | F     | 34  | LEU  | CB-CA-C | -6.07 | 102.13      | 111.66   |
| 1   | I     | 34  | LEU  | CB-CA-C | -6.07 | 102.13      | 111.66   |
| 1   | R     | 34  | LEU  | CB-CA-C | -6.07 | 102.13      | 111.66   |
| 1   | S     | 189 | LYS  | N-CA-C  | 6.07  | 118.34      | 108.63   |
| 1   | C     | 34  | LEU  | CB-CA-C | -6.07 | 102.13      | 111.66   |
| 1   | E     | 34  | LEU  | CB-CA-C | -6.05 | 102.15      | 111.66   |
| 1   | Q     | 34  | LEU  | CB-CA-C | -6.05 | 102.15      | 111.66   |
| 1   | S     | 34  | LEU  | CB-CA-C | -6.05 | 102.16      | 111.66   |
| 1   | a     | 34  | LEU  | CB-CA-C | -6.05 | 102.17      | 111.66   |
| 1   | P     | 34  | LEU  | CB-CA-C | -6.04 | 102.17      | 111.66   |
| 1   | A     | 34  | LEU  | CB-CA-C | -6.04 | 102.18      | 111.66   |
| 1   | U     | 34  | LEU  | CB-CA-C | -6.02 | 102.21      | 111.66   |
| 1   | X     | 68  | PRO  | CA-N-CD | -5.96 | 103.65      | 112.00   |
| 1   | R     | 68  | PRO  | CA-N-CD | -5.96 | 103.65      | 112.00   |
| 1   | E     | 68  | PRO  | CA-N-CD | -5.96 | 103.66      | 112.00   |
| 1   | S     | 68  | PRO  | CA-N-CD | -5.96 | 103.66      | 112.00   |
| 1   | M     | 68  | PRO  | CA-N-CD | -5.96 | 103.66      | 112.00   |
| 1   | N     | 68  | PRO  | CA-N-CD | -5.95 | 103.67      | 112.00   |
| 1   | W     | 68  | PRO  | CA-N-CD | -5.95 | 103.67      | 112.00   |
| 1   | Z     | 68  | PRO  | CA-N-CD | -5.95 | 103.68      | 112.00   |
| 1   | K     | 68  | PRO  | CA-N-CD | -5.94 | 103.68      | 112.00   |
| 1   | Q     | 68  | PRO  | CA-N-CD | -5.94 | 103.68      | 112.00   |
| 1   | U     | 68  | PRO  | CA-N-CD | -5.94 | 103.69      | 112.00   |
| 1   | Y     | 68  | PRO  | CA-N-CD | -5.94 | 103.69      | 112.00   |
| 1   | G     | 68  | PRO  | CA-N-CD | -5.93 | 103.69      | 112.00   |
| 1   | a     | 68  | PRO  | CA-N-CD | -5.93 | 103.70      | 112.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 68  | PRO  | CA-N-CD | -5.93 | 103.70      | 112.00   |
| 1   | B     | 68  | PRO  | CA-N-CD | -5.93 | 103.70      | 112.00   |
| 1   | T     | 68  | PRO  | CA-N-CD | -5.92 | 103.71      | 112.00   |
| 1   | D     | 68  | PRO  | CA-N-CD | -5.92 | 103.72      | 112.00   |
| 1   | H     | 68  | PRO  | CA-N-CD | -5.92 | 103.72      | 112.00   |
| 1   | I     | 68  | PRO  | CA-N-CD | -5.92 | 103.72      | 112.00   |
| 1   | C     | 68  | PRO  | CA-N-CD | -5.92 | 103.72      | 112.00   |
| 1   | A     | 68  | PRO  | CA-N-CD | -5.91 | 103.73      | 112.00   |
| 1   | F     | 68  | PRO  | CA-N-CD | -5.91 | 103.73      | 112.00   |
| 1   | V     | 68  | PRO  | CA-N-CD | -5.90 | 103.74      | 112.00   |
| 1   | Q     | 79  | LYS  | N-CA-C  | -5.90 | 104.85      | 111.28   |
| 1   | c     | 68  | PRO  | CA-N-CD | -5.89 | 103.75      | 112.00   |
| 1   | W     | 79  | LYS  | N-CA-C  | -5.89 | 104.86      | 111.28   |
| 1   | b     | 68  | PRO  | CA-N-CD | -5.89 | 103.76      | 112.00   |
| 1   | J     | 68  | PRO  | CA-N-CD | -5.89 | 103.76      | 112.00   |
| 1   | P     | 100 | LYS  | N-CA-C  | 5.89  | 118.11      | 108.52   |
| 1   | R     | 100 | LYS  | N-CA-C  | 5.88  | 118.11      | 108.52   |
| 1   | W     | 100 | LYS  | N-CA-C  | 5.88  | 118.11      | 108.52   |
| 1   | I     | 100 | LYS  | N-CA-C  | 5.88  | 118.11      | 108.52   |
| 1   | E     | 100 | LYS  | N-CA-C  | 5.88  | 118.11      | 108.52   |
| 1   | O     | 68  | PRO  | CA-N-CD | -5.88 | 103.77      | 112.00   |
| 1   | D     | 100 | LYS  | N-CA-C  | 5.88  | 118.10      | 108.52   |
| 1   | S     | 100 | LYS  | N-CA-C  | 5.88  | 118.10      | 108.52   |
| 1   | c     | 100 | LYS  | N-CA-C  | 5.87  | 118.09      | 108.52   |
| 1   | H     | 100 | LYS  | N-CA-C  | 5.87  | 118.09      | 108.52   |
| 1   | S     | 79  | LYS  | N-CA-C  | -5.87 | 104.88      | 111.28   |
| 1   | L     | 68  | PRO  | CA-N-CD | -5.87 | 103.79      | 112.00   |
| 1   | a     | 100 | LYS  | N-CA-C  | 5.87  | 118.08      | 108.52   |
| 1   | F     | 100 | LYS  | N-CA-C  | 5.86  | 118.08      | 108.52   |
| 1   | b     | 79  | LYS  | N-CA-C  | -5.86 | 104.89      | 111.28   |
| 1   | B     | 79  | LYS  | N-CA-C  | -5.86 | 104.89      | 111.28   |
| 1   | L     | 79  | LYS  | N-CA-C  | -5.86 | 104.90      | 111.28   |
| 1   | I     | 79  | LYS  | N-CA-C  | -5.85 | 104.90      | 111.28   |
| 1   | d     | 100 | LYS  | N-CA-C  | 5.85  | 118.06      | 108.52   |
| 1   | c     | 79  | LYS  | N-CA-C  | -5.85 | 104.91      | 111.28   |
| 1   | K     | 79  | LYS  | N-CA-C  | -5.85 | 104.91      | 111.28   |
| 1   | A     | 79  | LYS  | N-CA-C  | -5.84 | 104.91      | 111.28   |
| 1   | C     | 100 | LYS  | N-CA-C  | 5.84  | 118.04      | 108.52   |
| 1   | G     | 100 | LYS  | N-CA-C  | 5.84  | 118.03      | 108.52   |
| 1   | R     | 79  | LYS  | N-CA-C  | -5.84 | 104.92      | 111.28   |
| 1   | U     | 100 | LYS  | N-CA-C  | 5.84  | 118.03      | 108.52   |
| 1   | K     | 100 | LYS  | N-CA-C  | 5.83  | 118.03      | 108.52   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 79  | LYS  | N-CA-C  | -5.83 | 104.92      | 111.28   |
| 1   | E     | 79  | LYS  | N-CA-C  | -5.83 | 104.92      | 111.28   |
| 1   | b     | 100 | LYS  | N-CA-C  | 5.83  | 118.03      | 108.52   |
| 1   | V     | 79  | LYS  | N-CA-C  | -5.83 | 104.93      | 111.28   |
| 1   | J     | 100 | LYS  | N-CA-C  | 5.83  | 118.02      | 108.52   |
| 1   | O     | 79  | LYS  | N-CA-C  | -5.83 | 104.93      | 111.28   |
| 1   | P     | 79  | LYS  | N-CA-C  | -5.83 | 104.93      | 111.28   |
| 1   | Z     | 100 | LYS  | N-CA-C  | 5.82  | 118.01      | 108.52   |
| 1   | M     | 100 | LYS  | N-CA-C  | 5.82  | 118.01      | 108.52   |
| 1   | T     | 100 | LYS  | N-CA-C  | 5.82  | 118.01      | 108.52   |
| 1   | d     | 79  | LYS  | N-CA-C  | -5.82 | 104.94      | 111.28   |
| 1   | O     | 100 | LYS  | N-CA-C  | 5.82  | 118.00      | 108.52   |
| 1   | H     | 79  | LYS  | N-CA-C  | -5.82 | 104.94      | 111.28   |
| 1   | N     | 100 | LYS  | N-CA-C  | 5.81  | 118.00      | 108.52   |
| 1   | d     | 68  | PRO  | CA-N-CD | -5.81 | 103.86      | 112.00   |
| 1   | A     | 100 | LYS  | N-CA-C  | 5.81  | 118.00      | 108.52   |
| 1   | G     | 79  | LYS  | N-CA-C  | -5.81 | 104.94      | 111.28   |
| 1   | L     | 100 | LYS  | N-CA-C  | 5.81  | 118.00      | 108.52   |
| 1   | D     | 79  | LYS  | N-CA-C  | -5.81 | 104.95      | 111.28   |
| 1   | J     | 79  | LYS  | N-CA-C  | -5.81 | 104.95      | 111.28   |
| 1   | X     | 100 | LYS  | N-CA-C  | 5.81  | 117.99      | 108.52   |
| 1   | B     | 100 | LYS  | N-CA-C  | 5.81  | 117.99      | 108.52   |
| 1   | Y     | 100 | LYS  | N-CA-C  | 5.81  | 117.98      | 108.52   |
| 1   | C     | 79  | LYS  | N-CA-C  | -5.80 | 104.95      | 111.28   |
| 1   | X     | 79  | LYS  | N-CA-C  | -5.80 | 104.95      | 111.28   |
| 1   | N     | 79  | LYS  | N-CA-C  | -5.80 | 104.96      | 111.28   |
| 1   | M     | 79  | LYS  | N-CA-C  | -5.80 | 104.96      | 111.28   |
| 1   | F     | 79  | LYS  | N-CA-C  | -5.80 | 104.96      | 111.28   |
| 1   | T     | 79  | LYS  | N-CA-C  | -5.80 | 104.96      | 111.28   |
| 1   | Q     | 100 | LYS  | N-CA-C  | 5.80  | 117.97      | 108.52   |
| 1   | Z     | 79  | LYS  | N-CA-C  | -5.79 | 104.96      | 111.28   |
| 1   | V     | 100 | LYS  | N-CA-C  | 5.79  | 117.96      | 108.52   |
| 1   | U     | 79  | LYS  | N-CA-C  | -5.79 | 104.97      | 111.28   |
| 1   | Y     | 79  | LYS  | N-CA-C  | -5.79 | 104.97      | 111.28   |
| 1   | Y     | 144 | LEU  | CB-CA-C | 5.76  | 115.53      | 109.83   |
| 1   | G     | 144 | LEU  | CB-CA-C | 5.74  | 115.52      | 109.83   |
| 1   | b     | 144 | LEU  | CB-CA-C | 5.71  | 115.49      | 109.83   |
| 1   | A     | 144 | LEU  | CB-CA-C | 5.68  | 115.45      | 109.83   |
| 1   | F     | 144 | LEU  | CB-CA-C | 5.68  | 115.45      | 109.83   |
| 1   | Z     | 144 | LEU  | CB-CA-C | 5.67  | 115.45      | 109.83   |
| 1   | V     | 144 | LEU  | CB-CA-C | 5.67  | 115.45      | 109.83   |
| 1   | L     | 144 | LEU  | CB-CA-C | 5.66  | 115.44      | 109.83   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | R     | 144 | LEU  | CB-CA-C | 5.66  | 115.44      | 109.83   |
| 1   | I     | 144 | LEU  | CB-CA-C | 5.66  | 115.43      | 109.83   |
| 1   | M     | 144 | LEU  | CB-CA-C | 5.66  | 115.43      | 109.83   |
| 1   | D     | 144 | LEU  | CB-CA-C | 5.65  | 115.42      | 109.83   |
| 1   | N     | 144 | LEU  | CB-CA-C | 5.65  | 115.42      | 109.83   |
| 1   | Q     | 144 | LEU  | CB-CA-C | 5.65  | 115.42      | 109.83   |
| 1   | X     | 144 | LEU  | CB-CA-C | 5.64  | 115.42      | 109.83   |
| 1   | H     | 144 | LEU  | CB-CA-C | 5.64  | 115.42      | 109.83   |
| 1   | P     | 144 | LEU  | CB-CA-C | 5.64  | 115.42      | 109.83   |
| 1   | O     | 144 | LEU  | CB-CA-C | 5.64  | 115.41      | 109.83   |
| 1   | U     | 144 | LEU  | CB-CA-C | 5.63  | 115.40      | 109.83   |
| 1   | a     | 144 | LEU  | CB-CA-C | 5.63  | 115.40      | 109.83   |
| 1   | S     | 144 | LEU  | CB-CA-C | 5.62  | 115.40      | 109.83   |
| 1   | W     | 144 | LEU  | CB-CA-C | 5.62  | 115.40      | 109.83   |
| 1   | E     | 144 | LEU  | CB-CA-C | 5.62  | 115.39      | 109.83   |
| 1   | B     | 144 | LEU  | CB-CA-C | 5.62  | 115.39      | 109.83   |
| 1   | K     | 144 | LEU  | CB-CA-C | 5.61  | 115.39      | 109.83   |
| 1   | d     | 144 | LEU  | CB-CA-C | 5.60  | 115.38      | 109.83   |
| 1   | J     | 144 | LEU  | CB-CA-C | 5.60  | 115.37      | 109.83   |
| 1   | c     | 144 | LEU  | CB-CA-C | 5.59  | 115.37      | 109.83   |
| 1   | T     | 144 | LEU  | CB-CA-C | 5.59  | 115.36      | 109.83   |
| 1   | C     | 144 | LEU  | CB-CA-C | 5.58  | 115.35      | 109.83   |
| 1   | P     | 223 | GLU  | N-CA-CB | -5.26 | 102.45      | 110.45   |
| 1   | Z     | 223 | GLU  | N-CA-CB | -5.24 | 102.48      | 110.45   |
| 1   | c     | 223 | GLU  | N-CA-CB | -5.23 | 102.50      | 110.45   |
| 1   | F     | 223 | GLU  | N-CA-CB | -5.22 | 102.52      | 110.45   |
| 1   | G     | 223 | GLU  | N-CA-CB | -5.22 | 102.52      | 110.45   |
| 1   | B     | 223 | GLU  | N-CA-CB | -5.22 | 102.52      | 110.45   |
| 1   | D     | 223 | GLU  | N-CA-CB | -5.21 | 102.52      | 110.45   |
| 1   | Y     | 223 | GLU  | N-CA-CB | -5.21 | 102.53      | 110.45   |
| 1   | a     | 223 | GLU  | N-CA-CB | -5.21 | 102.53      | 110.45   |
| 1   | S     | 223 | GLU  | N-CA-CB | -5.21 | 102.54      | 110.45   |
| 1   | R     | 223 | GLU  | N-CA-CB | -5.21 | 102.54      | 110.45   |
| 1   | V     | 223 | GLU  | N-CA-CB | -5.20 | 102.55      | 110.45   |
| 1   | U     | 223 | GLU  | N-CA-CB | -5.19 | 102.56      | 110.45   |
| 1   | A     | 223 | GLU  | N-CA-CB | -5.19 | 102.56      | 110.45   |
| 1   | M     | 223 | GLU  | N-CA-CB | -5.19 | 102.56      | 110.45   |
| 1   | I     | 223 | GLU  | N-CA-CB | -5.19 | 102.56      | 110.45   |
| 1   | N     | 223 | GLU  | N-CA-CB | -5.19 | 102.56      | 110.45   |
| 1   | K     | 223 | GLU  | N-CA-CB | -5.18 | 102.57      | 110.45   |
| 1   | H     | 223 | GLU  | N-CA-CB | -5.18 | 102.58      | 110.45   |
| 1   | O     | 223 | GLU  | N-CA-CB | -5.18 | 102.58      | 110.45   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | T     | 223 | GLU  | N-CA-CB | -5.18 | 102.58      | 110.45   |
| 1   | d     | 223 | GLU  | N-CA-CB | -5.18 | 102.58      | 110.45   |
| 1   | J     | 223 | GLU  | N-CA-CB | -5.17 | 102.59      | 110.45   |
| 1   | C     | 223 | GLU  | N-CA-CB | -5.17 | 102.59      | 110.45   |
| 1   | Q     | 223 | GLU  | N-CA-CB | -5.16 | 102.60      | 110.45   |
| 1   | L     | 223 | GLU  | N-CA-CB | -5.16 | 102.61      | 110.45   |
| 1   | b     | 223 | GLU  | N-CA-CB | -5.15 | 102.62      | 110.45   |
| 1   | E     | 223 | GLU  | N-CA-CB | -5.15 | 102.62      | 110.45   |
| 1   | W     | 223 | GLU  | N-CA-CB | -5.14 | 102.64      | 110.45   |
| 1   | X     | 223 | GLU  | N-CA-CB | -5.12 | 102.66      | 110.45   |
| 1   | C     | 66  | GLN  | N-CA-C  | 5.05  | 117.62      | 110.50   |
| 1   | a     | 66  | GLN  | N-CA-C  | 5.05  | 117.62      | 110.50   |
| 1   | D     | 36  | LEU  | N-CA-CB | -5.04 | 102.06      | 110.23   |
| 1   | W     | 66  | GLN  | N-CA-C  | 5.04  | 117.61      | 110.50   |
| 1   | a     | 36  | LEU  | N-CA-CB | -5.04 | 102.07      | 110.23   |
| 1   | b     | 36  | LEU  | N-CA-CB | -5.04 | 102.07      | 110.23   |
| 1   | V     | 66  | GLN  | N-CA-C  | 5.04  | 117.60      | 110.50   |
| 1   | N     | 36  | LEU  | N-CA-CB | -5.03 | 102.08      | 110.23   |
| 1   | U     | 36  | LEU  | N-CA-CB | -5.03 | 102.08      | 110.23   |
| 1   | F     | 36  | LEU  | N-CA-CB | -5.03 | 102.09      | 110.23   |
| 1   | c     | 66  | GLN  | N-CA-C  | 5.03  | 117.59      | 110.50   |
| 1   | Q     | 66  | GLN  | N-CA-C  | 5.03  | 117.59      | 110.50   |
| 1   | B     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | Z     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | I     | 36  | LEU  | N-CA-CB | -5.02 | 102.09      | 110.23   |
| 1   | I     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | U     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | X     | 36  | LEU  | N-CA-CB | -5.02 | 102.09      | 110.23   |
| 1   | G     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | N     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | b     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | D     | 66  | GLN  | N-CA-C  | 5.02  | 117.58      | 110.50   |
| 1   | F     | 66  | GLN  | N-CA-C  | 5.02  | 117.57      | 110.50   |
| 1   | C     | 36  | LEU  | N-CA-CB | -5.02 | 102.10      | 110.23   |
| 1   | O     | 66  | GLN  | N-CA-C  | 5.01  | 117.57      | 110.50   |
| 1   | R     | 66  | GLN  | N-CA-C  | 5.01  | 117.57      | 110.50   |
| 1   | T     | 36  | LEU  | N-CA-CB | -5.01 | 102.11      | 110.23   |
| 1   | A     | 66  | GLN  | N-CA-C  | 5.01  | 117.56      | 110.50   |
| 1   | T     | 66  | GLN  | N-CA-C  | 5.01  | 117.57      | 110.50   |
| 1   | d     | 66  | GLN  | N-CA-C  | 5.01  | 117.56      | 110.50   |
| 1   | P     | 36  | LEU  | N-CA-CB | -5.01 | 102.12      | 110.23   |
| 1   | P     | 66  | GLN  | N-CA-C  | 5.01  | 117.56      | 110.50   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | S     | 66  | GLN  | N-CA-C  | 5.01  | 117.56      | 110.50   |
| 1   | V     | 36  | LEU  | N-CA-CB | -5.01 | 102.11      | 110.23   |
| 1   | d     | 36  | LEU  | N-CA-CB | -5.01 | 102.12      | 110.23   |
| 1   | X     | 66  | GLN  | N-CA-C  | 5.01  | 117.56      | 110.50   |
| 1   | W     | 36  | LEU  | N-CA-CB | -5.01 | 102.12      | 110.23   |
| 1   | K     | 66  | GLN  | N-CA-C  | 5.00  | 117.56      | 110.50   |
| 1   | Z     | 36  | LEU  | N-CA-CB | -5.00 | 102.12      | 110.23   |
| 1   | c     | 36  | LEU  | N-CA-CB | -5.00 | 102.13      | 110.23   |
| 1   | L     | 36  | LEU  | N-CA-CB | -5.00 | 102.13      | 110.23   |

There are no chirality outliers.

All (60) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 151 | ARG  | Sidechain |
| 1   | A     | 7   | ARG  | Sidechain |
| 1   | B     | 151 | ARG  | Sidechain |
| 1   | B     | 7   | ARG  | Sidechain |
| 1   | C     | 151 | ARG  | Sidechain |
| 1   | C     | 7   | ARG  | Sidechain |
| 1   | D     | 151 | ARG  | Sidechain |
| 1   | D     | 7   | ARG  | Sidechain |
| 1   | E     | 151 | ARG  | Sidechain |
| 1   | E     | 7   | ARG  | Sidechain |
| 1   | F     | 151 | ARG  | Sidechain |
| 1   | F     | 7   | ARG  | Sidechain |
| 1   | G     | 151 | ARG  | Sidechain |
| 1   | G     | 7   | ARG  | Sidechain |
| 1   | H     | 151 | ARG  | Sidechain |
| 1   | H     | 7   | ARG  | Sidechain |
| 1   | I     | 151 | ARG  | Sidechain |
| 1   | I     | 7   | ARG  | Sidechain |
| 1   | J     | 151 | ARG  | Sidechain |
| 1   | J     | 7   | ARG  | Sidechain |
| 1   | K     | 151 | ARG  | Sidechain |
| 1   | K     | 7   | ARG  | Sidechain |
| 1   | L     | 151 | ARG  | Sidechain |
| 1   | L     | 7   | ARG  | Sidechain |
| 1   | M     | 151 | ARG  | Sidechain |
| 1   | M     | 7   | ARG  | Sidechain |
| 1   | N     | 151 | ARG  | Sidechain |
| 1   | N     | 7   | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | O     | 151 | ARG  | Sidechain |
| 1   | O     | 7   | ARG  | Sidechain |
| 1   | P     | 151 | ARG  | Sidechain |
| 1   | P     | 7   | ARG  | Sidechain |
| 1   | Q     | 151 | ARG  | Sidechain |
| 1   | Q     | 7   | ARG  | Sidechain |
| 1   | R     | 151 | ARG  | Sidechain |
| 1   | R     | 7   | ARG  | Sidechain |
| 1   | S     | 151 | ARG  | Sidechain |
| 1   | S     | 7   | ARG  | Sidechain |
| 1   | T     | 151 | ARG  | Sidechain |
| 1   | T     | 7   | ARG  | Sidechain |
| 1   | U     | 151 | ARG  | Sidechain |
| 1   | U     | 7   | ARG  | Sidechain |
| 1   | V     | 151 | ARG  | Sidechain |
| 1   | V     | 7   | ARG  | Sidechain |
| 1   | W     | 151 | ARG  | Sidechain |
| 1   | W     | 7   | ARG  | Sidechain |
| 1   | X     | 151 | ARG  | Sidechain |
| 1   | X     | 7   | ARG  | Sidechain |
| 1   | Y     | 151 | ARG  | Sidechain |
| 1   | Y     | 7   | ARG  | Sidechain |
| 1   | Z     | 151 | ARG  | Sidechain |
| 1   | Z     | 7   | ARG  | Sidechain |
| 1   | a     | 151 | ARG  | Sidechain |
| 1   | a     | 7   | ARG  | Sidechain |
| 1   | b     | 151 | ARG  | Sidechain |
| 1   | b     | 7   | ARG  | Sidechain |
| 1   | c     | 151 | ARG  | Sidechain |
| 1   | c     | 7   | ARG  | Sidechain |
| 1   | d     | 151 | ARG  | Sidechain |
| 1   | d     | 7   | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1918  | 0        | 1955     | 84      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1918  | 0        | 1955     | 89      | 0            |
| 1   | C     | 1918  | 0        | 1955     | 85      | 0            |
| 1   | D     | 1918  | 0        | 1955     | 84      | 0            |
| 1   | E     | 1918  | 0        | 1955     | 88      | 0            |
| 1   | F     | 1918  | 0        | 1955     | 83      | 0            |
| 1   | G     | 1918  | 0        | 1955     | 85      | 0            |
| 1   | H     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | I     | 1918  | 0        | 1955     | 89      | 0            |
| 1   | J     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | K     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | L     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | M     | 1918  | 0        | 1955     | 85      | 0            |
| 1   | N     | 1918  | 0        | 1955     | 88      | 0            |
| 1   | O     | 1918  | 0        | 1955     | 90      | 0            |
| 1   | P     | 1918  | 0        | 1955     | 84      | 0            |
| 1   | Q     | 1918  | 0        | 1955     | 87      | 0            |
| 1   | R     | 1918  | 0        | 1955     | 87      | 0            |
| 1   | S     | 1918  | 0        | 1955     | 87      | 0            |
| 1   | T     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | U     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | V     | 1918  | 0        | 1955     | 88      | 0            |
| 1   | W     | 1918  | 0        | 1955     | 84      | 0            |
| 1   | X     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | Y     | 1918  | 0        | 1955     | 84      | 0            |
| 1   | Z     | 1918  | 0        | 1955     | 82      | 0            |
| 1   | a     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | b     | 1918  | 0        | 1955     | 83      | 0            |
| 1   | c     | 1918  | 0        | 1955     | 86      | 0            |
| 1   | d     | 1918  | 0        | 1955     | 84      | 0            |
| All | All   | 57540 | 0        | 58650    | 2429    | 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 21.

All (2429) 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:L:143:VAL:O | 1:L:144:LEU:HG | 1.38                     | 1.22              |
| 1:U:143:VAL:O | 1:U:144:LEU:HG | 1.38                     | 1.22              |
| 1:V:143:VAL:O | 1:V:144:LEU:HG | 1.38                     | 1.22              |
| 1:W:143:VAL:O | 1:W:144:LEU:HG | 1.38                     | 1.22              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:M:143:VAL:O   | 1:M:144:LEU:HG   | 1.38                     | 1.22              |
| 1:N:143:VAL:O   | 1:N:144:LEU:HG   | 1.38                     | 1.21              |
| 1:X:143:VAL:O   | 1:X:144:LEU:HG   | 1.38                     | 1.21              |
| 1:O:143:VAL:O   | 1:O:144:LEU:HG   | 1.38                     | 1.21              |
| 1:Y:143:VAL:O   | 1:Y:144:LEU:HG   | 1.38                     | 1.21              |
| 1:P:143:VAL:O   | 1:P:144:LEU:HG   | 1.38                     | 1.20              |
| 1:Z:143:VAL:O   | 1:Z:144:LEU:HG   | 1.38                     | 1.20              |
| 1:Q:143:VAL:O   | 1:Q:144:LEU:HG   | 1.38                     | 1.19              |
| 1:a:143:VAL:O   | 1:a:144:LEU:HG   | 1.38                     | 1.19              |
| 1:R:143:VAL:O   | 1:R:144:LEU:HG   | 1.38                     | 1.18              |
| 1:C:143:VAL:O   | 1:C:144:LEU:HG   | 1.38                     | 1.18              |
| 1:I:143:VAL:O   | 1:I:144:LEU:HG   | 1.38                     | 1.18              |
| 1:J:143:VAL:O   | 1:J:144:LEU:HG   | 1.38                     | 1.18              |
| 1:K:143:VAL:O   | 1:K:144:LEU:HG   | 1.38                     | 1.18              |
| 1:T:143:VAL:O   | 1:T:144:LEU:HG   | 1.38                     | 1.18              |
| 1:A:143:VAL:O   | 1:A:144:LEU:HG   | 1.38                     | 1.18              |
| 1:B:143:VAL:O   | 1:B:144:LEU:HG   | 1.38                     | 1.18              |
| 1:b:143:VAL:O   | 1:b:144:LEU:HG   | 1.38                     | 1.18              |
| 1:d:143:VAL:O   | 1:d:144:LEU:HG   | 1.38                     | 1.18              |
| 1:D:143:VAL:O   | 1:D:144:LEU:HG   | 1.38                     | 1.18              |
| 1:E:143:VAL:O   | 1:E:144:LEU:HG   | 1.38                     | 1.18              |
| 1:H:143:VAL:O   | 1:H:144:LEU:HG   | 1.38                     | 1.18              |
| 1:S:143:VAL:O   | 1:S:144:LEU:HG   | 1.38                     | 1.18              |
| 1:G:143:VAL:O   | 1:G:144:LEU:HG   | 1.38                     | 1.18              |
| 1:c:143:VAL:O   | 1:c:144:LEU:HG   | 1.38                     | 1.17              |
| 1:F:143:VAL:O   | 1:F:144:LEU:HG   | 1.38                     | 1.17              |
| 1:X:36:LEU:HD23 | 1:X:155:LEU:HD21 | 1.45                     | 0.97              |
| 1:b:36:LEU:HD23 | 1:b:155:LEU:HD21 | 1.46                     | 0.97              |
| 1:Y:36:LEU:HD23 | 1:Y:155:LEU:HD21 | 1.46                     | 0.97              |
| 1:a:36:LEU:HD23 | 1:a:155:LEU:HD21 | 1.46                     | 0.97              |
| 1:U:36:LEU:HD23 | 1:U:155:LEU:HD21 | 1.46                     | 0.97              |
| 1:A:36:LEU:HD23 | 1:A:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:I:36:LEU:HD23 | 1:I:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:H:36:LEU:HD23 | 1:H:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:S:36:LEU:HD23 | 1:S:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:J:36:LEU:HD23 | 1:J:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:R:36:LEU:HD23 | 1:R:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:T:36:LEU:HD23 | 1:T:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:V:36:LEU:HD23 | 1:V:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:d:36:LEU:HD23 | 1:d:155:LEU:HD21 | 1.46                     | 0.96              |
| 1:K:36:LEU:HD23 | 1:K:155:LEU:HD21 | 1.46                     | 0.95              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:X:71:VAL:HB   | 1:X:124:ASP:HB2  | 1.48                     | 0.95              |
| 1:B:36:LEU:HD23 | 1:B:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:G:36:LEU:HD23 | 1:G:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:L:36:LEU:HD23 | 1:L:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:Z:71:VAL:HB   | 1:Z:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:Y:71:VAL:HB   | 1:Y:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:Q:36:LEU:HD23 | 1:Q:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:U:71:VAL:HB   | 1:U:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:W:36:LEU:HD23 | 1:W:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:W:71:VAL:HB   | 1:W:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:c:36:LEU:HD23 | 1:c:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:L:71:VAL:HB   | 1:L:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:V:71:VAL:HB   | 1:V:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:a:71:VAL:HB   | 1:a:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:M:71:VAL:HB   | 1:M:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:R:71:VAL:HB   | 1:R:124:ASP:HB2  | 1.48                     | 0.95              |
| 1:b:71:VAL:HB   | 1:b:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:B:71:VAL:HB   | 1:B:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:N:36:LEU:HD23 | 1:N:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:Q:71:VAL:HB   | 1:Q:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:D:36:LEU:HD23 | 1:D:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:P:71:VAL:HB   | 1:P:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:C:71:VAL:HB   | 1:C:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:E:36:LEU:HD23 | 1:E:155:LEU:HD21 | 1.45                     | 0.95              |
| 1:F:36:LEU:HD23 | 1:F:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:O:71:VAL:HB   | 1:O:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:P:36:LEU:HD23 | 1:P:155:LEU:HD21 | 1.46                     | 0.95              |
| 1:c:71:VAL:HB   | 1:c:124:ASP:HB2  | 1.49                     | 0.95              |
| 1:D:71:VAL:HB   | 1:D:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:O:36:LEU:HD23 | 1:O:155:LEU:HD21 | 1.46                     | 0.94              |
| 1:A:71:VAL:HB   | 1:A:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:d:71:VAL:HB   | 1:d:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:S:71:VAL:HB   | 1:S:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:Z:36:LEU:HD23 | 1:Z:155:LEU:HD21 | 1.46                     | 0.94              |
| 1:N:71:VAL:HB   | 1:N:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:E:71:VAL:HB   | 1:E:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:I:71:VAL:HB   | 1:I:124:ASP:HB2  | 1.48                     | 0.94              |
| 1:T:71:VAL:HB   | 1:T:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:H:71:VAL:HB   | 1:H:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:J:71:VAL:HB   | 1:J:124:ASP:HB2  | 1.49                     | 0.94              |
| 1:G:71:VAL:HB   | 1:G:124:ASP:HB2  | 1.49                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:71:VAL:HB    | 1:F:124:ASP:HB2  | 1.49                     | 0.93              |
| 1:C:36:LEU:HD23  | 1:C:155:LEU:HD21 | 1.46                     | 0.93              |
| 1:K:71:VAL:HB    | 1:K:124:ASP:HB2  | 1.49                     | 0.93              |
| 1:M:36:LEU:HD23  | 1:M:155:LEU:HD21 | 1.46                     | 0.93              |
| 1:N:13:VAL:HG21  | 1:N:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:P:13:VAL:HG21  | 1:P:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:W:13:VAL:HG21  | 1:W:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:L:13:VAL:HG21  | 1:L:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:R:13:VAL:HG21  | 1:R:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:U:13:VAL:HG21  | 1:U:78:VAL:HG21  | 1.61                     | 0.83              |
| 1:Y:13:VAL:HG21  | 1:Y:78:VAL:HG21  | 1.60                     | 0.83              |
| 1:K:13:VAL:HG21  | 1:K:78:VAL:HG21  | 1.61                     | 0.82              |
| 1:S:13:VAL:HG21  | 1:S:78:VAL:HG21  | 1.61                     | 0.82              |
| 1:M:13:VAL:HG21  | 1:M:78:VAL:HG21  | 1.61                     | 0.82              |
| 1:b:13:VAL:HG21  | 1:b:78:VAL:HG21  | 1.60                     | 0.82              |
| 1:Q:13:VAL:HG21  | 1:Q:78:VAL:HG21  | 1.60                     | 0.82              |
| 1:V:13:VAL:HG21  | 1:V:78:VAL:HG21  | 1.61                     | 0.82              |
| 1:I:13:VAL:HG21  | 1:I:78:VAL:HG21  | 1.61                     | 0.82              |
| 1:Z:13:VAL:HG21  | 1:Z:78:VAL:HG21  | 1.60                     | 0.82              |
| 1:H:13:VAL:HG21  | 1:H:78:VAL:HG21  | 1.60                     | 0.81              |
| 1:F:13:VAL:HG21  | 1:F:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:T:13:VAL:HG21  | 1:T:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:C:13:VAL:HG21  | 1:C:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:a:13:VAL:HG21  | 1:a:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:O:13:VAL:HG21  | 1:O:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:d:13:VAL:HG21  | 1:d:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:A:13:VAL:HG21  | 1:A:78:VAL:HG21  | 1.61                     | 0.81              |
| 1:J:13:VAL:HG21  | 1:J:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:B:13:VAL:HG21  | 1:B:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:D:13:VAL:HG21  | 1:D:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:X:13:VAL:HG21  | 1:X:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:E:128:LEU:HD21 | 1:E:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:I:128:LEU:HD21 | 1:I:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:N:128:LEU:HD21 | 1:N:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:R:128:LEU:HD21 | 1:R:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:S:128:LEU:HD21 | 1:S:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:D:128:LEU:HD21 | 1:D:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:O:128:LEU:HD21 | 1:O:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:E:13:VAL:HG21  | 1:E:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:J:128:LEU:HD21 | 1:J:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:F:128:LEU:HD21 | 1:F:222:ILE:HD11 | 1.64                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:128:LEU:HD21 | 1:M:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:c:13:VAL:HG21  | 1:c:78:VAL:HG21  | 1.61                     | 0.80              |
| 1:G:13:VAL:HG21  | 1:G:78:VAL:HG21  | 1.60                     | 0.80              |
| 1:W:128:LEU:HD21 | 1:W:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:c:128:LEU:HD21 | 1:c:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:d:128:LEU:HD21 | 1:d:222:ILE:HD11 | 1.64                     | 0.80              |
| 1:X:128:LEU:HD21 | 1:X:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:H:128:LEU:HD21 | 1:H:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:V:128:LEU:HD21 | 1:V:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:Q:128:LEU:HD21 | 1:Q:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:A:128:LEU:HD21 | 1:A:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:T:128:LEU:HD21 | 1:T:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:K:128:LEU:HD21 | 1:K:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:C:128:LEU:HD21 | 1:C:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:G:34:LEU:HD11  | 1:G:123:VAL:HG21 | 1.65                     | 0.79              |
| 1:I:34:LEU:HD11  | 1:I:123:VAL:HG21 | 1.65                     | 0.79              |
| 1:F:34:LEU:HD11  | 1:F:123:VAL:HG21 | 1.65                     | 0.79              |
| 1:Y:128:LEU:HD21 | 1:Y:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:b:128:LEU:HD21 | 1:b:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:P:128:LEU:HD21 | 1:P:222:ILE:HD11 | 1.64                     | 0.79              |
| 1:D:34:LEU:HD11  | 1:D:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:H:34:LEU:HD11  | 1:H:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:J:34:LEU:HD11  | 1:J:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:L:128:LEU:HD21 | 1:L:222:ILE:HD11 | 1.64                     | 0.78              |
| 1:T:34:LEU:HD11  | 1:T:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:W:34:LEU:HD11  | 1:W:123:VAL:HG21 | 1.64                     | 0.78              |
| 1:G:128:LEU:HD21 | 1:G:222:ILE:HD11 | 1.64                     | 0.78              |
| 1:K:34:LEU:HD11  | 1:K:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:E:34:LEU:HD11  | 1:E:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:C:34:LEU:HD11  | 1:C:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:A:34:LEU:HD11  | 1:A:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:M:34:LEU:HD11  | 1:M:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:V:34:LEU:HD11  | 1:V:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:B:34:LEU:HD11  | 1:B:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:R:34:LEU:HD11  | 1:R:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:U:128:LEU:HD21 | 1:U:222:ILE:HD11 | 1.64                     | 0.78              |
| 1:B:128:LEU:HD21 | 1:B:222:ILE:HD11 | 1.64                     | 0.78              |
| 1:S:34:LEU:HD11  | 1:S:123:VAL:HG21 | 1.65                     | 0.78              |
| 1:X:34:LEU:HD11  | 1:X:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:Z:34:LEU:HD11  | 1:Z:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:a:34:LEU:HD11  | 1:a:123:VAL:HG21 | 1.65                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:34:LEU:HD11  | 1:N:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:Q:34:LEU:HD11  | 1:Q:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:a:128:LEU:HD21 | 1:a:222:ILE:HD11 | 1.64                     | 0.77              |
| 1:Z:128:LEU:HD21 | 1:Z:222:ILE:HD11 | 1.64                     | 0.77              |
| 1:L:34:LEU:HD11  | 1:L:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:d:34:LEU:HD11  | 1:d:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:c:34:LEU:HD11  | 1:c:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:b:34:LEU:HD11  | 1:b:123:VAL:HG21 | 1.65                     | 0.77              |
| 1:O:34:LEU:HD11  | 1:O:123:VAL:HG21 | 1.65                     | 0.76              |
| 1:P:34:LEU:HD11  | 1:P:123:VAL:HG21 | 1.65                     | 0.76              |
| 1:U:34:LEU:HD11  | 1:U:123:VAL:HG21 | 1.65                     | 0.76              |
| 1:Y:34:LEU:HD11  | 1:Y:123:VAL:HG21 | 1.65                     | 0.76              |
| 1:S:58:LEU:HD21  | 1:S:157:VAL:HG21 | 1.70                     | 0.73              |
| 1:X:58:LEU:HD21  | 1:X:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:K:58:LEU:HD21  | 1:K:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:T:58:LEU:HD21  | 1:T:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:U:58:LEU:HD21  | 1:U:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:R:58:LEU:HD21  | 1:R:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:V:58:LEU:HD21  | 1:V:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:W:58:LEU:HD21  | 1:W:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:J:58:LEU:HD21  | 1:J:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:I:58:LEU:HD21  | 1:I:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:L:58:LEU:HD21  | 1:L:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:Y:58:LEU:HD21  | 1:Y:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:M:58:LEU:HD21  | 1:M:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:Q:58:LEU:HD21  | 1:Q:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:P:58:LEU:HD21  | 1:P:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:Z:58:LEU:HD21  | 1:Z:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:N:58:LEU:HD21  | 1:N:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:O:58:LEU:HD21  | 1:O:157:VAL:HG21 | 1.71                     | 0.73              |
| 1:E:58:LEU:HD21  | 1:E:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:H:58:LEU:HD21  | 1:H:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:b:58:LEU:HD21  | 1:b:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:c:58:LEU:HD21  | 1:c:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:F:58:LEU:HD21  | 1:F:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:G:58:LEU:HD21  | 1:G:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:a:58:LEU:HD21  | 1:a:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:D:58:LEU:HD21  | 1:D:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:d:58:LEU:HD21  | 1:d:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:A:58:LEU:HD21  | 1:A:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:C:58:LEU:HD21  | 1:C:157:VAL:HG21 | 1.71                     | 0.72              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:58:LEU:HD21 | 1:B:157:VAL:HG21 | 1.71                     | 0.72              |
| 1:Y:143:VAL:O   | 1:Y:144:LEU:CG   | 2.31                     | 0.69              |
| 1:A:10:LEU:HD11 | 1:A:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:E:10:LEU:HD11 | 1:E:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:Z:10:LEU:HD11 | 1:Z:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:a:10:LEU:HD11 | 1:a:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:W:10:LEU:HD11 | 1:W:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:d:10:LEU:HD11 | 1:d:218:ALA:HB2  | 1.75                     | 0.69              |
| 1:D:10:LEU:HD11 | 1:D:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:I:10:LEU:HD11 | 1:I:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:B:10:LEU:HD11 | 1:B:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:F:10:LEU:HD11 | 1:F:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:H:10:LEU:HD11 | 1:H:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:V:10:LEU:HD11 | 1:V:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:b:10:LEU:HD11 | 1:b:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:M:10:LEU:HD11 | 1:M:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:X:143:VAL:O   | 1:X:144:LEU:CG   | 2.32                     | 0.68              |
| 1:X:10:LEU:HD11 | 1:X:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:T:10:LEU:HD11 | 1:T:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:L:10:LEU:HD11 | 1:L:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:P:10:LEU:HD11 | 1:P:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:S:10:LEU:HD11 | 1:S:218:ALA:HB2  | 1.75                     | 0.68              |
| 1:c:10:LEU:HD11 | 1:c:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:C:10:LEU:HD11 | 1:C:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:J:10:LEU:HD11 | 1:J:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:Y:10:LEU:HD11 | 1:Y:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:Q:10:LEU:HD11 | 1:Q:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:K:10:LEU:HD11 | 1:K:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:W:143:VAL:O   | 1:W:144:LEU:CG   | 2.31                     | 0.67              |
| 1:G:10:LEU:HD11 | 1:G:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:N:10:LEU:HD11 | 1:N:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:X:126:GLN:NE2 | 1:Y:60:ASP:OD2   | 2.28                     | 0.67              |
| 1:D:126:GLN:NE2 | 1:E:60:ASP:OD2   | 2.29                     | 0.67              |
| 1:O:10:LEU:HD11 | 1:O:218:ALA:HB2  | 1.75                     | 0.67              |
| 1:c:36:LEU:HB3  | 1:c:155:LEU:HD11 | 1.77                     | 0.67              |
| 1:d:36:LEU:HB3  | 1:d:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:U:10:LEU:HD11 | 1:U:218:ALA:HB2  | 1.75                     | 0.66              |
| 1:a:36:LEU:HB3  | 1:a:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:R:60:ASP:OD2  | 1:S:126:GLN:NE2  | 2.29                     | 0.66              |
| 1:Y:36:LEU:HB3  | 1:Y:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:Z:36:LEU:HB3  | 1:Z:155:LEU:HD11 | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:36:LEU:HB3   | 1:b:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:A:36:LEU:HB3   | 1:A:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:U:126:GLN:NE2  | 1:V:60:ASP:OD2   | 2.28                     | 0.66              |
| 1:a:126:GLN:NE2  | 1:b:60:ASP:OD2   | 2.28                     | 0.66              |
| 1:B:36:LEU:HB3   | 1:B:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:G:126:GLN:NE2  | 1:H:60:ASP:OD2   | 2.29                     | 0.66              |
| 1:V:188:THR:HG22 | 1:V:189:LYS:N    | 2.11                     | 0.66              |
| 1:X:36:LEU:HB3   | 1:X:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:a:36:LEU:CD2   | 1:a:155:LEU:HD21 | 2.25                     | 0.66              |
| 1:A:60:ASP:OD2   | 1:d:126:GLN:NE2  | 2.29                     | 0.66              |
| 1:M:188:THR:HG22 | 1:M:189:LYS:N    | 2.11                     | 0.66              |
| 1:W:36:LEU:HB3   | 1:W:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:d:36:LEU:CD2   | 1:d:155:LEU:HD21 | 2.25                     | 0.66              |
| 1:J:126:GLN:NE2  | 1:K:60:ASP:OD2   | 2.29                     | 0.66              |
| 1:K:126:GLN:NE2  | 1:T:60:ASP:OD2   | 2.29                     | 0.66              |
| 1:Q:188:THR:HG22 | 1:Q:189:LYS:N    | 2.11                     | 0.66              |
| 1:Z:188:THR:HG22 | 1:Z:189:LYS:N    | 2.11                     | 0.66              |
| 1:C:36:LEU:HB3   | 1:C:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:N:188:THR:HG22 | 1:N:189:LYS:N    | 2.11                     | 0.66              |
| 1:Q:36:LEU:HB3   | 1:Q:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:R:10:LEU:HD11  | 1:R:218:ALA:HB2  | 1.75                     | 0.66              |
| 1:V:143:VAL:O    | 1:V:144:LEU:CG   | 2.31                     | 0.66              |
| 1:I:143:VAL:O    | 1:I:144:LEU:CG   | 2.31                     | 0.66              |
| 1:J:36:LEU:HB3   | 1:J:155:LEU:HD11 | 1.77                     | 0.66              |
| 1:R:188:THR:HG22 | 1:R:189:LYS:N    | 2.11                     | 0.65              |
| 1:U:36:LEU:HB3   | 1:U:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:d:143:VAL:O    | 1:d:144:LEU:CG   | 2.31                     | 0.65              |
| 1:D:36:LEU:HB3   | 1:D:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:E:143:VAL:O    | 1:E:144:LEU:CG   | 2.31                     | 0.65              |
| 1:F:143:VAL:O    | 1:F:144:LEU:CG   | 2.31                     | 0.65              |
| 1:H:126:GLN:NE2  | 1:I:60:ASP:OD2   | 2.29                     | 0.65              |
| 1:L:126:GLN:NE2  | 1:U:60:ASP:OD2   | 2.29                     | 0.65              |
| 1:M:60:ASP:OD2   | 1:N:126:GLN:NE2  | 2.29                     | 0.65              |
| 1:S:36:LEU:HB3   | 1:S:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:W:188:THR:HG22 | 1:W:189:LYS:N    | 2.11                     | 0.65              |
| 1:Y:188:THR:HG22 | 1:Y:189:LYS:N    | 2.11                     | 0.65              |
| 1:c:126:GLN:NE2  | 1:d:60:ASP:OD2   | 2.29                     | 0.65              |
| 1:B:126:GLN:NE2  | 1:C:60:ASP:OD2   | 2.29                     | 0.65              |
| 1:G:143:VAL:O    | 1:G:144:LEU:CG   | 2.31                     | 0.65              |
| 1:V:36:LEU:HB3   | 1:V:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:Y:36:LEU:CD2   | 1:Y:155:LEU:HD21 | 2.25                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:188:THR:HG22 | 1:a:189:LYS:N    | 2.11                     | 0.65              |
| 1:K:188:THR:HG22 | 1:K:189:LYS:N    | 2.11                     | 0.65              |
| 1:O:36:LEU:HB3   | 1:O:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:P:188:THR:HG22 | 1:P:189:LYS:N    | 2.11                     | 0.65              |
| 1:T:36:LEU:HB3   | 1:T:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:E:126:GLN:NE2  | 1:F:60:ASP:OD2   | 2.30                     | 0.65              |
| 1:H:36:LEU:HB3   | 1:H:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:H:143:VAL:O    | 1:H:144:LEU:CG   | 2.31                     | 0.65              |
| 1:L:36:LEU:HB3   | 1:L:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:d:188:THR:HG22 | 1:d:189:LYS:N    | 2.11                     | 0.65              |
| 1:E:36:LEU:HB3   | 1:E:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:U:188:THR:HG22 | 1:U:189:LYS:N    | 2.11                     | 0.65              |
| 1:F:36:LEU:HB3   | 1:F:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:J:188:THR:HG22 | 1:J:189:LYS:N    | 2.11                     | 0.65              |
| 1:M:36:LEU:HB3   | 1:M:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:D:143:VAL:O    | 1:D:144:LEU:CG   | 2.31                     | 0.65              |
| 1:K:36:LEU:HB3   | 1:K:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:A:126:GLN:NE2  | 1:B:60:ASP:OD2   | 2.30                     | 0.65              |
| 1:G:36:LEU:HB3   | 1:G:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:H:13:VAL:CG2   | 1:H:78:VAL:HG21  | 2.27                     | 0.65              |
| 1:N:36:LEU:HB3   | 1:N:155:LEU:HD11 | 1.77                     | 0.65              |
| 1:O:60:ASP:OD2   | 1:P:126:GLN:NE2  | 2.30                     | 0.65              |
| 1:Q:60:ASP:OD2   | 1:R:126:GLN:NE2  | 2.30                     | 0.65              |
| 1:T:188:THR:HG22 | 1:T:189:LYS:N    | 2.11                     | 0.65              |
| 1:c:188:THR:HG22 | 1:c:189:LYS:N    | 2.11                     | 0.65              |
| 1:L:188:THR:HG22 | 1:L:189:LYS:N    | 2.11                     | 0.65              |
| 1:O:188:THR:HG22 | 1:O:189:LYS:N    | 2.11                     | 0.65              |
| 1:U:13:VAL:CG2   | 1:U:78:VAL:HG21  | 2.27                     | 0.65              |
| 1:Z:13:VAL:CG2   | 1:Z:78:VAL:HG21  | 2.27                     | 0.65              |
| 1:b:36:LEU:CD2   | 1:b:155:LEU:HD21 | 2.25                     | 0.65              |
| 1:A:188:THR:HG22 | 1:A:189:LYS:N    | 2.11                     | 0.64              |
| 1:B:13:VAL:CG2   | 1:B:78:VAL:HG21  | 2.28                     | 0.64              |
| 1:C:13:VAL:CG2   | 1:C:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:L:13:VAL:CG2   | 1:L:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:P:60:ASP:OD2   | 1:Q:126:GLN:NE2  | 2.30                     | 0.64              |
| 1:a:13:VAL:CG2   | 1:a:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:G:13:VAL:CG2   | 1:G:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:C:143:VAL:O    | 1:C:144:LEU:CG   | 2.31                     | 0.64              |
| 1:I:13:VAL:CG2   | 1:I:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:T:13:VAL:CG2   | 1:T:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:U:143:VAL:O    | 1:U:144:LEU:CG   | 2.31                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:13:VAL:CG2   | 1:V:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:Y:13:VAL:CG2   | 1:Y:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:J:143:VAL:O    | 1:J:144:LEU:CG   | 2.32                     | 0.64              |
| 1:O:13:VAL:CG2   | 1:O:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:P:13:VAL:CG2   | 1:P:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:S:188:THR:HG22 | 1:S:189:LYS:N    | 2.11                     | 0.64              |
| 1:W:126:GLN:NE2  | 1:X:60:ASP:OD2   | 2.30                     | 0.64              |
| 1:A:13:VAL:CG2   | 1:A:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:A:36:LEU:CD2   | 1:A:155:LEU:HD21 | 2.25                     | 0.64              |
| 1:R:36:LEU:HB3   | 1:R:155:LEU:HD11 | 1.77                     | 0.64              |
| 1:S:13:VAL:CG2   | 1:S:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:X:188:THR:HG22 | 1:X:189:LYS:N    | 2.11                     | 0.64              |
| 1:b:13:VAL:CG2   | 1:b:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:D:13:VAL:CG2   | 1:D:78:VAL:HG21  | 2.28                     | 0.64              |
| 1:E:188:THR:HG22 | 1:E:189:LYS:N    | 2.11                     | 0.64              |
| 1:I:36:LEU:HB3   | 1:I:155:LEU:HD11 | 1.77                     | 0.64              |
| 1:N:36:LEU:CD2   | 1:N:155:LEU:HD21 | 2.25                     | 0.64              |
| 1:S:60:ASP:OD2   | 1:T:126:GLN:NE2  | 2.31                     | 0.64              |
| 1:L:60:ASP:OD2   | 1:M:126:GLN:NE2  | 2.31                     | 0.64              |
| 1:P:36:LEU:HB3   | 1:P:155:LEU:HD11 | 1.77                     | 0.64              |
| 1:F:13:VAL:CG2   | 1:F:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:F:188:THR:HG22 | 1:F:189:LYS:N    | 2.11                     | 0.64              |
| 1:I:188:THR:HG22 | 1:I:189:LYS:N    | 2.11                     | 0.64              |
| 1:K:13:VAL:CG2   | 1:K:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:Q:13:VAL:CG2   | 1:Q:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:W:36:LEU:CD2   | 1:W:155:LEU:HD21 | 2.25                     | 0.64              |
| 1:C:126:GLN:NE2  | 1:D:60:ASP:OD2   | 2.31                     | 0.64              |
| 1:M:13:VAL:CG2   | 1:M:78:VAL:HG21  | 2.28                     | 0.64              |
| 1:b:188:THR:HG22 | 1:b:189:LYS:N    | 2.11                     | 0.64              |
| 1:B:143:VAL:O    | 1:B:144:LEU:CG   | 2.31                     | 0.64              |
| 1:C:188:THR:HG22 | 1:C:189:LYS:N    | 2.11                     | 0.64              |
| 1:G:188:THR:HG22 | 1:G:189:LYS:N    | 2.11                     | 0.64              |
| 1:K:143:VAL:O    | 1:K:144:LEU:CG   | 2.31                     | 0.64              |
| 1:N:60:ASP:OD2   | 1:O:126:GLN:NE2  | 2.30                     | 0.64              |
| 1:X:13:VAL:CG2   | 1:X:78:VAL:HG21  | 2.27                     | 0.64              |
| 1:Z:126:GLN:NE2  | 1:a:60:ASP:OD2   | 2.31                     | 0.64              |
| 1:D:188:THR:HG22 | 1:D:189:LYS:N    | 2.11                     | 0.63              |
| 1:c:143:VAL:O    | 1:c:144:LEU:CG   | 2.31                     | 0.63              |
| 1:I:126:GLN:NE2  | 1:J:60:ASP:OD2   | 2.31                     | 0.63              |
| 1:B:188:THR:HG22 | 1:B:189:LYS:N    | 2.11                     | 0.63              |
| 1:D:36:LEU:CD2   | 1:D:155:LEU:HD21 | 2.25                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:13:VAL:CG2   | 1:d:78:VAL:HG21  | 2.28                     | 0.63              |
| 1:I:36:LEU:CD2   | 1:I:155:LEU:HD21 | 2.25                     | 0.63              |
| 1:L:143:VAL:O    | 1:L:144:LEU:CG   | 2.31                     | 0.63              |
| 1:C:237:LEU:HD23 | 1:D:146:GLN:HG3  | 1.80                     | 0.63              |
| 1:J:13:VAL:CG2   | 1:J:78:VAL:HG21  | 2.27                     | 0.63              |
| 1:H:188:THR:HG22 | 1:H:189:LYS:N    | 2.11                     | 0.63              |
| 1:T:143:VAL:O    | 1:T:144:LEU:CG   | 2.31                     | 0.63              |
| 1:E:13:VAL:CG2   | 1:E:78:VAL:HG21  | 2.27                     | 0.63              |
| 1:R:13:VAL:CG2   | 1:R:78:VAL:HG21  | 2.27                     | 0.63              |
| 1:A:143:VAL:O    | 1:A:144:LEU:CG   | 2.31                     | 0.63              |
| 1:N:13:VAL:CG2   | 1:N:78:VAL:HG21  | 2.27                     | 0.63              |
| 1:A:146:GLN:HG3  | 1:d:237:LEU:HD23 | 1.80                     | 0.62              |
| 1:F:126:GLN:NE2  | 1:G:60:ASP:OD2   | 2.32                     | 0.62              |
| 1:P:36:LEU:CD2   | 1:P:155:LEU:HD21 | 2.25                     | 0.62              |
| 1:W:13:VAL:CG2   | 1:W:78:VAL:HG21  | 2.27                     | 0.62              |
| 1:Z:36:LEU:CD2   | 1:Z:155:LEU:HD21 | 2.25                     | 0.62              |
| 1:V:126:GLN:NE2  | 1:W:60:ASP:OD2   | 2.32                     | 0.62              |
| 1:W:189:LYS:O    | 1:W:190:THR:HG22 | 1.99                     | 0.62              |
| 1:X:189:LYS:O    | 1:X:190:THR:HG22 | 1.99                     | 0.62              |
| 1:c:13:VAL:CG2   | 1:c:78:VAL:HG21  | 2.27                     | 0.62              |
| 1:A:65:ASP:HB3   | 1:A:136:THR:HG23 | 1.82                     | 0.62              |
| 1:B:65:ASP:HB3   | 1:B:136:THR:HG23 | 1.82                     | 0.62              |
| 1:Y:126:GLN:NE2  | 1:Z:60:ASP:OD2   | 2.32                     | 0.62              |
| 1:F:237:LEU:HD23 | 1:G:146:GLN:HG3  | 1.80                     | 0.62              |
| 1:Y:65:ASP:HB3   | 1:Y:136:THR:HG23 | 1.82                     | 0.62              |
| 1:d:65:ASP:HB3   | 1:d:136:THR:HG23 | 1.82                     | 0.62              |
| 1:I:189:LYS:O    | 1:I:190:THR:HG22 | 1.99                     | 0.62              |
| 1:Y:189:LYS:O    | 1:Y:190:THR:HG22 | 1.99                     | 0.62              |
| 1:Z:189:LYS:O    | 1:Z:190:THR:HG22 | 1.99                     | 0.62              |
| 1:a:65:ASP:HB3   | 1:a:136:THR:HG23 | 1.82                     | 0.62              |
| 1:a:189:LYS:O    | 1:a:190:THR:HG22 | 1.99                     | 0.62              |
| 1:c:65:ASP:HB3   | 1:c:136:THR:HG23 | 1.82                     | 0.62              |
| 1:E:237:LEU:HD23 | 1:F:146:GLN:HG3  | 1.81                     | 0.62              |
| 1:K:18:ASP:OD1   | 1:K:18:ASP:O     | 2.18                     | 0.62              |
| 1:M:143:VAL:O    | 1:M:144:LEU:CG   | 2.32                     | 0.62              |
| 1:S:143:VAL:O    | 1:S:144:LEU:CG   | 2.32                     | 0.62              |
| 1:X:65:ASP:HB3   | 1:X:136:THR:HG23 | 1.82                     | 0.62              |
| 1:Z:65:ASP:HB3   | 1:Z:136:THR:HG23 | 1.82                     | 0.62              |
| 1:b:189:LYS:O    | 1:b:190:THR:HG22 | 1.99                     | 0.62              |
| 1:H:189:LYS:O    | 1:H:190:THR:HG22 | 1.99                     | 0.62              |
| 1:J:189:LYS:O    | 1:J:190:THR:HG22 | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:189:LYS:O    | 1:V:190:THR:HG22 | 1.99                     | 0.62              |
| 1:a:143:VAL:C    | 1:a:144:LEU:HG   | 2.24                     | 0.62              |
| 1:c:189:LYS:O    | 1:c:190:THR:HG22 | 1.99                     | 0.62              |
| 1:J:18:ASP:O     | 1:J:18:ASP:OD1   | 2.18                     | 0.62              |
| 1:R:36:LEU:CD2   | 1:R:155:LEU:HD21 | 2.25                     | 0.62              |
| 1:T:18:ASP:OD1   | 1:T:18:ASP:O     | 2.18                     | 0.62              |
| 1:U:36:LEU:CD2   | 1:U:155:LEU:HD21 | 2.25                     | 0.62              |
| 1:D:65:ASP:HB3   | 1:D:136:THR:HG23 | 1.82                     | 0.61              |
| 1:E:189:LYS:O    | 1:E:190:THR:HG22 | 1.99                     | 0.61              |
| 1:F:65:ASP:HB3   | 1:F:136:THR:HG23 | 1.82                     | 0.61              |
| 1:G:36:LEU:CD2   | 1:G:155:LEU:HD21 | 2.25                     | 0.61              |
| 1:G:65:ASP:HB3   | 1:G:136:THR:HG23 | 1.82                     | 0.61              |
| 1:I:18:ASP:OD1   | 1:I:18:ASP:O     | 2.18                     | 0.61              |
| 1:L:146:GLN:HG3  | 1:M:237:LEU:HD23 | 1.82                     | 0.61              |
| 1:O:18:ASP:OD1   | 1:O:18:ASP:O     | 2.18                     | 0.61              |
| 1:V:237:LEU:HD23 | 1:W:146:GLN:HG3  | 1.81                     | 0.61              |
| 1:Z:143:VAL:C    | 1:Z:144:LEU:HG   | 2.24                     | 0.61              |
| 1:c:36:LEU:CD2   | 1:c:155:LEU:HD21 | 2.25                     | 0.61              |
| 1:C:18:ASP:OD1   | 1:C:18:ASP:O     | 2.18                     | 0.61              |
| 1:D:18:ASP:OD1   | 1:D:18:ASP:O     | 2.18                     | 0.61              |
| 1:E:65:ASP:HB3   | 1:E:136:THR:HG23 | 1.82                     | 0.61              |
| 1:F:189:LYS:O    | 1:F:190:THR:HG22 | 1.99                     | 0.61              |
| 1:G:189:LYS:O    | 1:G:190:THR:HG22 | 1.99                     | 0.61              |
| 1:I:237:LEU:HD23 | 1:J:146:GLN:HG3  | 1.81                     | 0.61              |
| 1:J:36:LEU:CD2   | 1:J:155:LEU:HD21 | 2.25                     | 0.61              |
| 1:N:18:ASP:OD1   | 1:N:18:ASP:O     | 2.18                     | 0.61              |
| 1:U:65:ASP:HB3   | 1:U:136:THR:HG23 | 1.82                     | 0.61              |
| 1:U:189:LYS:O    | 1:U:190:THR:HG22 | 1.99                     | 0.61              |
| 1:W:65:ASP:HB3   | 1:W:136:THR:HG23 | 1.82                     | 0.61              |
| 1:b:65:ASP:HB3   | 1:b:136:THR:HG23 | 1.82                     | 0.61              |
| 1:b:143:VAL:O    | 1:b:144:LEU:CG   | 2.32                     | 0.61              |
| 1:d:189:LYS:O    | 1:d:190:THR:HG22 | 1.99                     | 0.61              |
| 1:C:65:ASP:HB3   | 1:C:136:THR:HG23 | 1.82                     | 0.61              |
| 1:E:18:ASP:O     | 1:E:18:ASP:OD1   | 2.18                     | 0.61              |
| 1:L:65:ASP:HB3   | 1:L:136:THR:HG23 | 1.82                     | 0.61              |
| 1:O:189:LYS:O    | 1:O:190:THR:HG22 | 1.99                     | 0.61              |
| 1:P:18:ASP:O     | 1:P:18:ASP:OD1   | 2.18                     | 0.61              |
| 1:b:126:GLN:NE2  | 1:c:60:ASP:OD2   | 2.32                     | 0.61              |
| 1:B:18:ASP:O     | 1:B:18:ASP:OD1   | 2.18                     | 0.61              |
| 1:D:189:LYS:O    | 1:D:190:THR:HG22 | 1.99                     | 0.61              |
| 1:H:65:ASP:HB3   | 1:H:136:THR:HG23 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:189:LYS:O    | 1:L:190:THR:HG22 | 1.99                     | 0.61              |
| 1:N:189:LYS:O    | 1:N:190:THR:HG22 | 1.99                     | 0.61              |
| 1:S:18:ASP:OD1   | 1:S:18:ASP:O     | 2.18                     | 0.61              |
| 1:S:146:GLN:HG3  | 1:T:237:LEU:HD23 | 1.81                     | 0.61              |
| 1:U:237:LEU:HD23 | 1:V:146:GLN:HG3  | 1.82                     | 0.61              |
| 1:Y:143:VAL:C    | 1:Y:144:LEU:HG   | 2.24                     | 0.61              |
| 1:A:189:LYS:O    | 1:A:190:THR:HG22 | 1.99                     | 0.61              |
| 1:B:189:LYS:O    | 1:B:190:THR:HG22 | 1.99                     | 0.61              |
| 1:C:189:LYS:O    | 1:C:190:THR:HG22 | 1.99                     | 0.61              |
| 1:K:189:LYS:O    | 1:K:190:THR:HG22 | 1.99                     | 0.61              |
| 1:M:18:ASP:O     | 1:M:18:ASP:OD1   | 2.18                     | 0.61              |
| 1:M:65:ASP:HB3   | 1:M:136:THR:HG23 | 1.82                     | 0.61              |
| 1:N:65:ASP:HB3   | 1:N:136:THR:HG23 | 1.82                     | 0.61              |
| 1:O:146:GLN:HG3  | 1:P:237:LEU:HD23 | 1.81                     | 0.61              |
| 1:S:36:LEU:CD2   | 1:S:155:LEU:HD21 | 2.25                     | 0.61              |
| 1:V:65:ASP:HB3   | 1:V:136:THR:HG23 | 1.82                     | 0.61              |
| 1:N:146:GLN:HG3  | 1:O:237:LEU:HD23 | 1.82                     | 0.61              |
| 1:R:143:VAL:O    | 1:R:144:LEU:CG   | 2.31                     | 0.61              |
| 1:W:143:VAL:C    | 1:W:144:LEU:HG   | 2.24                     | 0.61              |
| 1:X:143:VAL:C    | 1:X:144:LEU:HG   | 2.24                     | 0.61              |
| 1:F:18:ASP:OD1   | 1:F:18:ASP:O     | 2.18                     | 0.61              |
| 1:H:18:ASP:O     | 1:H:18:ASP:OD1   | 2.18                     | 0.61              |
| 1:I:65:ASP:HB3   | 1:I:136:THR:HG23 | 1.82                     | 0.61              |
| 1:O:65:ASP:HB3   | 1:O:136:THR:HG23 | 1.82                     | 0.61              |
| 1:P:189:LYS:O    | 1:P:190:THR:HG22 | 1.99                     | 0.61              |
| 1:H:237:LEU:HD23 | 1:I:146:GLN:HG3  | 1.81                     | 0.61              |
| 1:L:18:ASP:OD1   | 1:L:18:ASP:O     | 2.18                     | 0.61              |
| 1:L:237:LEU:HD23 | 1:U:146:GLN:HG3  | 1.83                     | 0.61              |
| 1:M:189:LYS:O    | 1:M:190:THR:HG22 | 1.99                     | 0.61              |
| 1:Q:18:ASP:OD1   | 1:Q:18:ASP:O     | 2.18                     | 0.61              |
| 1:A:18:ASP:OD1   | 1:A:18:ASP:O     | 2.18                     | 0.61              |
| 1:B:36:LEU:CD2   | 1:B:155:LEU:HD21 | 2.25                     | 0.61              |
| 1:N:143:VAL:O    | 1:N:144:LEU:CG   | 2.31                     | 0.61              |
| 1:P:65:ASP:HB3   | 1:P:136:THR:HG23 | 1.82                     | 0.61              |
| 1:V:143:VAL:C    | 1:V:144:LEU:HG   | 2.24                     | 0.61              |
| 1:Y:237:LEU:HD23 | 1:Z:146:GLN:HG3  | 1.81                     | 0.61              |
| 1:c:237:LEU:HD23 | 1:d:146:GLN:HG3  | 1.82                     | 0.61              |
| 1:B:237:LEU:HD23 | 1:C:146:GLN:HG3  | 1.82                     | 0.60              |
| 1:J:65:ASP:HB3   | 1:J:136:THR:HG23 | 1.82                     | 0.60              |
| 1:L:143:VAL:C    | 1:L:144:LEU:HG   | 2.24                     | 0.60              |
| 1:Q:36:LEU:CD2   | 1:Q:155:LEU:HD21 | 2.25                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:189:LYS:O    | 1:Q:190:THR:HG22 | 1.99                     | 0.60              |
| 1:R:18:ASP:O     | 1:R:18:ASP:OD1   | 2.18                     | 0.60              |
| 1:U:143:VAL:C    | 1:U:144:LEU:HG   | 2.24                     | 0.60              |
| 1:Y:18:ASP:OD1   | 1:Y:18:ASP:O     | 2.18                     | 0.60              |
| 1:K:36:LEU:CD2   | 1:K:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:K:237:LEU:HD23 | 1:T:146:GLN:HG3  | 1.82                     | 0.60              |
| 1:M:146:GLN:HG3  | 1:N:237:LEU:HD23 | 1.83                     | 0.60              |
| 1:T:189:LYS:O    | 1:T:190:THR:HG22 | 1.99                     | 0.60              |
| 1:Z:18:ASP:OD1   | 1:Z:18:ASP:O     | 2.18                     | 0.60              |
| 1:G:18:ASP:OD1   | 1:G:18:ASP:O     | 2.18                     | 0.60              |
| 1:K:65:ASP:HB3   | 1:K:136:THR:HG23 | 1.82                     | 0.60              |
| 1:Q:65:ASP:HB3   | 1:Q:136:THR:HG23 | 1.82                     | 0.60              |
| 1:R:65:ASP:HB3   | 1:R:136:THR:HG23 | 1.82                     | 0.60              |
| 1:R:189:LYS:O    | 1:R:190:THR:HG22 | 1.99                     | 0.60              |
| 1:a:18:ASP:OD1   | 1:a:18:ASP:O     | 2.18                     | 0.60              |
| 1:A:127:GLN:OE1  | 1:A:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:B:127:GLN:OE1  | 1:B:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:M:143:VAL:C    | 1:M:144:LEU:HG   | 2.24                     | 0.60              |
| 1:N:127:GLN:OE1  | 1:N:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:Q:146:GLN:HG3  | 1:R:237:LEU:HD23 | 1.82                     | 0.60              |
| 1:S:65:ASP:HB3   | 1:S:136:THR:HG23 | 1.82                     | 0.60              |
| 1:S:127:GLN:OE1  | 1:S:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:X:18:ASP:O     | 1:X:18:ASP:OD1   | 2.18                     | 0.60              |
| 1:Z:127:GLN:OE1  | 1:Z:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:b:237:LEU:HD23 | 1:c:146:GLN:HG3  | 1.82                     | 0.60              |
| 1:H:36:LEU:CD2   | 1:H:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:M:127:GLN:OE1  | 1:M:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:T:127:GLN:OE1  | 1:T:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:U:18:ASP:O     | 1:U:18:ASP:OD1   | 2.18                     | 0.60              |
| 1:Y:127:GLN:OE1  | 1:Y:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:C:127:GLN:OE1  | 1:C:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:Q:143:VAL:O    | 1:Q:144:LEU:CG   | 2.32                     | 0.60              |
| 1:S:189:LYS:O    | 1:S:190:THR:HG22 | 1.99                     | 0.60              |
| 1:T:36:LEU:CD2   | 1:T:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:T:65:ASP:HB3   | 1:T:136:THR:HG23 | 1.82                     | 0.60              |
| 1:b:18:ASP:OD1   | 1:b:18:ASP:O     | 2.18                     | 0.60              |
| 1:d:18:ASP:OD1   | 1:d:18:ASP:O     | 2.18                     | 0.60              |
| 1:d:127:GLN:OE1  | 1:d:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:D:127:GLN:OE1  | 1:D:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:N:143:VAL:C    | 1:N:144:LEU:HG   | 2.24                     | 0.60              |
| 1:O:127:GLN:OE1  | 1:O:130:ARG:NH1  | 2.35                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:143:VAL:C    | 1:O:144:LEU:HG   | 2.24                     | 0.60              |
| 1:R:127:GLN:OE1  | 1:R:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:W:18:ASP:OD1   | 1:W:18:ASP:O     | 2.18                     | 0.60              |
| 1:X:36:LEU:CD2   | 1:X:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:X:127:GLN:OE1  | 1:X:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:A:9:PHE:HD2    | 1:A:10:LEU:HD12  | 1.67                     | 0.60              |
| 1:E:36:LEU:CD2   | 1:E:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:K:127:GLN:OE1  | 1:K:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:L:127:GLN:OE1  | 1:L:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:Q:9:PHE:HD2    | 1:Q:10:LEU:HD12  | 1.67                     | 0.60              |
| 1:Q:127:GLN:OE1  | 1:Q:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:R:146:GLN:HG3  | 1:S:237:LEU:HD23 | 1.82                     | 0.60              |
| 1:X:237:LEU:HD23 | 1:Y:146:GLN:HG3  | 1.82                     | 0.60              |
| 1:a:127:GLN:OE1  | 1:a:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:c:127:GLN:OE1  | 1:c:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:P:127:GLN:OE1  | 1:P:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:a:237:LEU:HD23 | 1:b:146:GLN:HG3  | 1.82                     | 0.60              |
| 1:D:9:PHE:HD2    | 1:D:10:LEU:HD12  | 1.67                     | 0.60              |
| 1:J:127:GLN:OE1  | 1:J:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:M:36:LEU:CD2   | 1:M:155:LEU:HD21 | 2.25                     | 0.60              |
| 1:P:143:VAL:C    | 1:P:144:LEU:HG   | 2.24                     | 0.60              |
| 1:W:127:GLN:OE1  | 1:W:130:ARG:NH1  | 2.35                     | 0.60              |
| 1:b:9:PHE:HD2    | 1:b:10:LEU:HD12  | 1.67                     | 0.60              |
| 1:c:18:ASP:OD1   | 1:c:18:ASP:O     | 2.18                     | 0.60              |
| 1:L:9:PHE:HD2    | 1:L:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:N:9:PHE:HD2    | 1:N:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:O:143:VAL:O    | 1:O:144:LEU:CG   | 2.31                     | 0.59              |
| 1:S:9:PHE:HD2    | 1:S:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:a:143:VAL:O    | 1:a:144:LEU:CG   | 2.31                     | 0.59              |
| 1:b:127:GLN:OE1  | 1:b:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:D:58:LEU:HD11  | 1:D:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:E:58:LEU:HD11  | 1:E:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:E:127:GLN:OE1  | 1:E:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:H:9:PHE:HD2    | 1:H:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:U:127:GLN:OE1  | 1:U:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:V:18:ASP:OD1   | 1:V:18:ASP:O     | 2.18                     | 0.59              |
| 1:W:58:LEU:HD11  | 1:W:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:Z:237:LEU:HD23 | 1:a:146:GLN:HG3  | 1.83                     | 0.59              |
| 1:a:9:PHE:HD2    | 1:a:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:C:58:LEU:HD11  | 1:C:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:E:9:PHE:HD2    | 1:E:10:LEU:HD12  | 1.67                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:58:LEU:HD11  | 1:F:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:F:127:GLN:OE1  | 1:F:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:I:127:GLN:OE1  | 1:I:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:X:9:PHE:HD2    | 1:X:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:Y:58:LEU:HD11  | 1:Y:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:d:58:LEU:HD11  | 1:d:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:A:58:LEU:HD11  | 1:A:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:F:36:LEU:CD2   | 1:F:155:LEU:HD21 | 2.25                     | 0.59              |
| 1:J:9:PHE:HD2    | 1:J:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:P:143:VAL:O    | 1:P:144:LEU:CG   | 2.31                     | 0.59              |
| 1:Q:143:VAL:C    | 1:Q:144:LEU:HG   | 2.24                     | 0.59              |
| 1:W:237:LEU:HD23 | 1:X:146:GLN:HG3  | 1.84                     | 0.59              |
| 1:X:58:LEU:HD11  | 1:X:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:b:58:LEU:HD11  | 1:b:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:c:58:LEU:HD11  | 1:c:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:G:127:GLN:OE1  | 1:G:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:O:9:PHE:HD2    | 1:O:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:P:146:GLN:HG3  | 1:Q:237:LEU:HD23 | 1.83                     | 0.59              |
| 1:Z:58:LEU:HD11  | 1:Z:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:K:9:PHE:HD2    | 1:K:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:G:58:LEU:HD11  | 1:G:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:J:237:LEU:HD23 | 1:K:146:GLN:HG3  | 1.84                     | 0.59              |
| 1:O:36:LEU:CD2   | 1:O:155:LEU:HD21 | 2.25                     | 0.59              |
| 1:V:58:LEU:HD11  | 1:V:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:a:58:LEU:HD11  | 1:a:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:B:9:PHE:HD2    | 1:B:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:J:58:LEU:HD11  | 1:J:157:VAL:HG11 | 1.84                     | 0.59              |
| 1:P:9:PHE:HD2    | 1:P:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:R:143:VAL:C    | 1:R:144:LEU:HG   | 2.24                     | 0.59              |
| 1:V:9:PHE:HD2    | 1:V:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:V:127:GLN:OE1  | 1:V:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:Y:9:PHE:HD2    | 1:Y:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:B:58:LEU:HD11  | 1:B:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:H:127:GLN:OE1  | 1:H:130:ARG:NH1  | 2.35                     | 0.59              |
| 1:T:9:PHE:HD2    | 1:T:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:d:9:PHE:HD2    | 1:d:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:F:9:PHE:HD2    | 1:F:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:G:9:PHE:HD2    | 1:G:10:LEU:HD12  | 1.67                     | 0.59              |
| 1:M:58:LEU:HD11  | 1:M:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:U:58:LEU:HD11  | 1:U:157:VAL:HG11 | 1.85                     | 0.59              |
| 1:D:237:LEU:HD23 | 1:E:146:GLN:HG3  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:58:LEU:HD11  | 1:H:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:O:58:LEU:HD11  | 1:O:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:T:58:LEU:HD11  | 1:T:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:U:9:PHE:HD2    | 1:U:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:W:9:PHE:HD2    | 1:W:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:I:58:LEU:HD11  | 1:I:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:Q:58:LEU:HD11  | 1:Q:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:R:58:LEU:HD11  | 1:R:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:S:143:VAL:C    | 1:S:144:LEU:HG   | 2.24                     | 0.58              |
| 1:Z:143:VAL:O    | 1:Z:144:LEU:CG   | 2.31                     | 0.58              |
| 1:c:9:PHE:HD2    | 1:c:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:I:9:PHE:HD2    | 1:I:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:K:58:LEU:HD11  | 1:K:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:L:58:LEU:HD11  | 1:L:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:N:58:LEU:HD11  | 1:N:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:P:58:LEU:HD11  | 1:P:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:S:58:LEU:HD11  | 1:S:157:VAL:HG11 | 1.85                     | 0.58              |
| 1:G:237:LEU:HD23 | 1:H:146:GLN:HG3  | 1.84                     | 0.58              |
| 1:T:143:VAL:C    | 1:T:144:LEU:HG   | 2.24                     | 0.58              |
| 1:L:36:LEU:CD2   | 1:L:155:LEU:HD21 | 2.25                     | 0.58              |
| 1:C:9:PHE:HD2    | 1:C:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:M:9:PHE:HD2    | 1:M:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:A:237:LEU:HD23 | 1:B:146:GLN:HG3  | 1.85                     | 0.58              |
| 1:R:9:PHE:HD2    | 1:R:10:LEU:HD12  | 1.67                     | 0.58              |
| 1:C:36:LEU:CD2   | 1:C:155:LEU:HD21 | 2.25                     | 0.57              |
| 1:Z:9:PHE:HD2    | 1:Z:10:LEU:HD12  | 1.67                     | 0.57              |
| 1:G:36:LEU:HD11  | 1:G:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:K:143:VAL:C    | 1:K:144:LEU:HG   | 2.24                     | 0.57              |
| 1:G:161:LYS:HE3  | 1:G:163:THR:CG2  | 2.35                     | 0.57              |
| 1:I:36:LEU:HD11  | 1:I:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:J:36:LEU:HD11  | 1:J:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:J:161:LYS:HE3  | 1:J:163:THR:CG2  | 2.34                     | 0.57              |
| 1:K:36:LEU:HD11  | 1:K:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:a:161:LYS:HE3  | 1:a:163:THR:CG2  | 2.35                     | 0.57              |
| 1:K:161:LYS:HE3  | 1:K:163:THR:CG2  | 2.35                     | 0.57              |
| 1:Z:161:LYS:HE3  | 1:Z:163:THR:CG2  | 2.35                     | 0.57              |
| 1:d:161:LYS:HE3  | 1:d:163:THR:CG2  | 2.35                     | 0.57              |
| 1:C:161:LYS:HE3  | 1:C:163:THR:CG2  | 2.34                     | 0.57              |
| 1:D:161:LYS:HE3  | 1:D:163:THR:CG2  | 2.35                     | 0.57              |
| 1:F:161:LYS:HE3  | 1:F:163:THR:CG2  | 2.35                     | 0.57              |
| 1:H:36:LEU:HD11  | 1:H:58:LEU:HD23  | 1.86                     | 0.57              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:161:LYS:HE3 | 1:H:163:THR:CG2  | 2.35                     | 0.57              |
| 1:J:143:VAL:C   | 1:J:144:LEU:HG   | 2.24                     | 0.57              |
| 1:W:161:LYS:HE3 | 1:W:163:THR:CG2  | 2.35                     | 0.57              |
| 1:F:36:LEU:HD11 | 1:F:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:T:36:LEU:HD11 | 1:T:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:E:161:LYS:HE3 | 1:E:163:THR:CG2  | 2.35                     | 0.57              |
| 1:E:36:LEU:HD11 | 1:E:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:I:161:LYS:HE3 | 1:I:163:THR:CG2  | 2.35                     | 0.57              |
| 1:R:36:LEU:HD11 | 1:R:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:R:161:LYS:HE3 | 1:R:163:THR:CG2  | 2.35                     | 0.57              |
| 1:S:36:LEU:HD11 | 1:S:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:X:161:LYS:HE3 | 1:X:163:THR:CG2  | 2.35                     | 0.57              |
| 1:Y:161:LYS:HE3 | 1:Y:163:THR:CG2  | 2.34                     | 0.57              |
| 1:a:36:LEU:HD11 | 1:a:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:b:161:LYS:HE3 | 1:b:163:THR:CG2  | 2.35                     | 0.57              |
| 1:A:161:LYS:HE3 | 1:A:163:THR:CG2  | 2.35                     | 0.57              |
| 1:B:138:ASN:ND2 | 1:B:140:ARG:O    | 2.38                     | 0.57              |
| 1:V:36:LEU:CD2  | 1:V:155:LEU:HD21 | 2.25                     | 0.57              |
| 1:c:161:LYS:HE3 | 1:c:163:THR:CG2  | 2.35                     | 0.57              |
| 1:F:138:ASN:ND2 | 1:F:140:ARG:O    | 2.38                     | 0.57              |
| 1:I:143:VAL:C   | 1:I:144:LEU:HG   | 2.24                     | 0.57              |
| 1:J:138:ASN:ND2 | 1:J:140:ARG:O    | 2.38                     | 0.57              |
| 1:O:36:LEU:HD11 | 1:O:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:R:138:ASN:ND2 | 1:R:140:ARG:O    | 2.38                     | 0.57              |
| 1:S:161:LYS:HE3 | 1:S:163:THR:CG2  | 2.35                     | 0.57              |
| 1:Z:36:LEU:HD11 | 1:Z:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:b:36:LEU:HD11 | 1:b:58:LEU:HD23  | 1.86                     | 0.57              |
| 1:D:36:LEU:HD11 | 1:D:58:LEU:HD23  | 1.86                     | 0.56              |
| 1:L:161:LYS:HE3 | 1:L:163:THR:CG2  | 2.35                     | 0.56              |
| 1:M:36:LEU:HD11 | 1:M:58:LEU:HD23  | 1.86                     | 0.56              |
| 1:O:138:ASN:ND2 | 1:O:140:ARG:O    | 2.38                     | 0.56              |
| 1:O:161:LYS:HE3 | 1:O:163:THR:CG2  | 2.35                     | 0.56              |
| 1:P:36:LEU:HD11 | 1:P:58:LEU:HD23  | 1.87                     | 0.56              |
| 1:Q:36:LEU:HD11 | 1:Q:58:LEU:HD23  | 1.87                     | 0.56              |
| 1:V:113:SER:HB3 | 1:V:115:PHE:HE2  | 1.70                     | 0.56              |
| 1:Y:36:LEU:HD11 | 1:Y:58:LEU:HD23  | 1.86                     | 0.56              |
| 1:b:138:ASN:ND2 | 1:b:140:ARG:O    | 2.38                     | 0.56              |
| 1:c:36:LEU:HD11 | 1:c:58:LEU:HD23  | 1.86                     | 0.56              |
| 1:c:113:SER:HB3 | 1:c:115:PHE:HE2  | 1.70                     | 0.56              |
| 1:c:138:ASN:ND2 | 1:c:140:ARG:O    | 2.38                     | 0.56              |
| 1:B:113:SER:HB3 | 1:B:115:PHE:HE2  | 1.71                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:138:ASN:ND2 | 1:I:140:ARG:O   | 2.38                     | 0.56              |
| 1:N:36:LEU:HD11 | 1:N:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:P:138:ASN:ND2 | 1:P:140:ARG:O   | 2.38                     | 0.56              |
| 1:U:138:ASN:ND2 | 1:U:140:ARG:O   | 2.38                     | 0.56              |
| 1:V:138:ASN:ND2 | 1:V:140:ARG:O   | 2.38                     | 0.56              |
| 1:B:161:LYS:HE3 | 1:B:163:THR:CG2 | 2.34                     | 0.56              |
| 1:C:138:ASN:ND2 | 1:C:140:ARG:O   | 2.38                     | 0.56              |
| 1:E:138:ASN:ND2 | 1:E:140:ARG:O   | 2.38                     | 0.56              |
| 1:F:113:SER:HB3 | 1:F:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:H:143:VAL:C   | 1:H:144:LEU:HG  | 2.24                     | 0.56              |
| 1:M:161:LYS:HE3 | 1:M:163:THR:CG2 | 2.35                     | 0.56              |
| 1:N:138:ASN:ND2 | 1:N:140:ARG:O   | 2.38                     | 0.56              |
| 1:R:113:SER:HB3 | 1:R:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:X:36:LEU:HD11 | 1:X:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:X:138:ASN:ND2 | 1:X:140:ARG:O   | 2.38                     | 0.56              |
| 1:Y:113:SER:HB3 | 1:Y:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:C:36:LEU:HD11 | 1:C:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:G:138:ASN:ND2 | 1:G:140:ARG:O   | 2.38                     | 0.56              |
| 1:I:113:SER:HB3 | 1:I:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:M:113:SER:HB3 | 1:M:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:N:161:LYS:HE3 | 1:N:163:THR:CG2 | 2.35                     | 0.56              |
| 1:S:138:ASN:ND2 | 1:S:140:ARG:O   | 2.38                     | 0.56              |
| 1:U:113:SER:HB3 | 1:U:115:PHE:HE2 | 1.70                     | 0.56              |
| 1:U:161:LYS:HE3 | 1:U:163:THR:CG2 | 2.35                     | 0.56              |
| 1:W:138:ASN:ND2 | 1:W:140:ARG:O   | 2.38                     | 0.56              |
| 1:Y:138:ASN:ND2 | 1:Y:140:ARG:O   | 2.38                     | 0.56              |
| 1:d:36:LEU:HD11 | 1:d:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:138:ASN:ND2 | 1:A:140:ARG:O   | 2.38                     | 0.56              |
| 1:C:113:SER:HB3 | 1:C:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:K:138:ASN:ND2 | 1:K:140:ARG:O   | 2.38                     | 0.56              |
| 1:L:36:LEU:HD11 | 1:L:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:P:161:LYS:HE3 | 1:P:163:THR:CG2 | 2.34                     | 0.56              |
| 1:Q:138:ASN:ND2 | 1:Q:140:ARG:O   | 2.38                     | 0.56              |
| 1:S:113:SER:HB3 | 1:S:115:PHE:HE2 | 1.70                     | 0.56              |
| 1:T:161:LYS:HE3 | 1:T:163:THR:CG2 | 2.35                     | 0.56              |
| 1:Z:138:ASN:ND2 | 1:Z:140:ARG:O   | 2.38                     | 0.56              |
| 1:a:138:ASN:ND2 | 1:a:140:ARG:O   | 2.38                     | 0.56              |
| 1:G:143:VAL:C   | 1:G:144:LEU:HG  | 2.24                     | 0.56              |
| 1:M:76:ASP:HB3  | 1:M:119:ARG:HG2 | 1.88                     | 0.56              |
| 1:N:113:SER:HB3 | 1:N:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:T:138:ASN:ND2 | 1:T:140:ARG:O   | 2.38                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:V:161:LYS:HE3 | 1:V:163:THR:CG2 | 2.35                     | 0.56              |
| 1:W:36:LEU:HD11 | 1:W:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:b:113:SER:HB3 | 1:b:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:E:113:SER:HB3 | 1:E:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:H:113:SER:HB3 | 1:H:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:J:113:SER:HB3 | 1:J:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:L:138:ASN:ND2 | 1:L:140:ARG:O   | 2.38                     | 0.56              |
| 1:M:138:ASN:ND2 | 1:M:140:ARG:O   | 2.38                     | 0.56              |
| 1:N:76:ASP:HB3  | 1:N:119:ARG:HG2 | 1.88                     | 0.56              |
| 1:Q:113:SER:HB3 | 1:Q:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:Z:113:SER:HB3 | 1:Z:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:b:71:VAL:HB   | 1:b:124:ASP:CB  | 2.32                     | 0.56              |
| 1:A:36:LEU:HD11 | 1:A:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:B:36:LEU:HD11 | 1:B:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:D:138:ASN:ND2 | 1:D:140:ARG:O   | 2.38                     | 0.56              |
| 1:L:113:SER:HB3 | 1:L:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:O:76:ASP:HB3  | 1:O:119:ARG:HG2 | 1.88                     | 0.56              |
| 1:T:113:SER:HB3 | 1:T:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:C:188:THR:CG2 | 1:C:189:LYS:N   | 2.69                     | 0.56              |
| 1:E:188:THR:CG2 | 1:E:189:LYS:N   | 2.69                     | 0.56              |
| 1:L:76:ASP:HB3  | 1:L:119:ARG:HG2 | 1.88                     | 0.56              |
| 1:Q:161:LYS:HE3 | 1:Q:163:THR:CG2 | 2.35                     | 0.56              |
| 1:V:36:LEU:HD11 | 1:V:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:O:188:THR:CG2 | 1:O:189:LYS:N   | 2.69                     | 0.56              |
| 1:P:113:SER:HB3 | 1:P:115:PHE:HE2 | 1.71                     | 0.56              |
| 1:U:36:LEU:HD11 | 1:U:58:LEU:HD23 | 1.86                     | 0.56              |
| 1:d:138:ASN:ND2 | 1:d:140:ARG:O   | 2.38                     | 0.56              |
| 1:A:188:THR:CG2 | 1:A:189:LYS:N   | 2.69                     | 0.55              |
| 1:F:143:VAL:C   | 1:F:144:LEU:HG  | 2.24                     | 0.55              |
| 1:M:188:THR:CG2 | 1:M:189:LYS:N   | 2.69                     | 0.55              |
| 1:P:76:ASP:HB3  | 1:P:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:Q:188:THR:CG2 | 1:Q:189:LYS:N   | 2.69                     | 0.55              |
| 1:W:113:SER:HB3 | 1:W:115:PHE:HE2 | 1.71                     | 0.55              |
| 1:X:113:SER:HB3 | 1:X:115:PHE:HE2 | 1.71                     | 0.55              |
| 1:d:113:SER:HB3 | 1:d:115:PHE:HE2 | 1.71                     | 0.55              |
| 1:E:76:ASP:HB3  | 1:E:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:F:76:ASP:HB3  | 1:F:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:G:188:THR:CG2 | 1:G:189:LYS:N   | 2.69                     | 0.55              |
| 1:H:138:ASN:ND2 | 1:H:140:ARG:O   | 2.38                     | 0.55              |
| 1:V:76:ASP:HB3  | 1:V:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:b:188:THR:CG2 | 1:b:189:LYS:N   | 2.69                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:d:188:THR:CG2 | 1:d:189:LYS:N   | 2.69                     | 0.55              |
| 1:D:113:SER:HB3 | 1:D:115:PHE:HE2 | 1.70                     | 0.55              |
| 1:E:143:VAL:C   | 1:E:144:LEU:HG  | 2.24                     | 0.55              |
| 1:G:76:ASP:HB3  | 1:G:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:H:76:ASP:HB3  | 1:H:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:L:188:THR:CG2 | 1:L:189:LYS:N   | 2.69                     | 0.55              |
| 1:Q:76:ASP:HB3  | 1:Q:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:S:188:THR:CG2 | 1:S:189:LYS:N   | 2.69                     | 0.55              |
| 1:U:76:ASP:HB3  | 1:U:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:V:188:THR:CG2 | 1:V:189:LYS:N   | 2.69                     | 0.55              |
| 1:A:113:SER:HB3 | 1:A:115:PHE:HE2 | 1.71                     | 0.55              |
| 1:N:188:THR:CG2 | 1:N:189:LYS:N   | 2.69                     | 0.55              |
| 1:d:71:VAL:HB   | 1:d:124:ASP:CB  | 2.32                     | 0.55              |
| 1:X:188:THR:CG2 | 1:X:189:LYS:N   | 2.69                     | 0.55              |
| 1:B:188:THR:CG2 | 1:B:189:LYS:N   | 2.69                     | 0.55              |
| 1:D:76:ASP:HB3  | 1:D:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:K:113:SER:HB3 | 1:K:115:PHE:HE2 | 1.70                     | 0.55              |
| 1:U:188:THR:CG2 | 1:U:189:LYS:N   | 2.69                     | 0.55              |
| 1:G:113:SER:HB3 | 1:G:115:PHE:HE2 | 1.71                     | 0.55              |
| 1:H:188:THR:CG2 | 1:H:189:LYS:N   | 2.69                     | 0.55              |
| 1:I:76:ASP:HB3  | 1:I:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:J:188:THR:CG2 | 1:J:189:LYS:N   | 2.69                     | 0.55              |
| 1:P:188:THR:CG2 | 1:P:189:LYS:N   | 2.69                     | 0.55              |
| 1:Z:188:THR:CG2 | 1:Z:189:LYS:N   | 2.69                     | 0.55              |
| 1:c:188:THR:CG2 | 1:c:189:LYS:N   | 2.69                     | 0.55              |
| 1:J:76:ASP:HB3  | 1:J:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:R:76:ASP:HB3  | 1:R:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:T:188:THR:CG2 | 1:T:189:LYS:N   | 2.69                     | 0.55              |
| 1:W:76:ASP:HB3  | 1:W:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:C:76:ASP:HB3  | 1:C:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:H:150:GLY:O   | 1:H:151:ARG:C   | 2.50                     | 0.55              |
| 1:K:188:THR:CG2 | 1:K:189:LYS:N   | 2.69                     | 0.55              |
| 1:S:168:CYS:HB2 | 1:S:211:ILE:HB  | 1.89                     | 0.55              |
| 1:X:76:ASP:HB3  | 1:X:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:d:168:CYS:HB2 | 1:d:211:ILE:HB  | 1.89                     | 0.55              |
| 1:B:76:ASP:HB3  | 1:B:119:ARG:HG2 | 1.88                     | 0.55              |
| 1:G:71:VAL:HB   | 1:G:124:ASP:CB  | 2.32                     | 0.55              |
| 1:O:113:SER:HB3 | 1:O:115:PHE:HE2 | 1.70                     | 0.55              |
| 1:T:168:CYS:HB2 | 1:T:211:ILE:HB  | 1.89                     | 0.55              |
| 1:b:168:CYS:HB2 | 1:b:211:ILE:HB  | 1.89                     | 0.55              |
| 1:c:168:CYS:HB2 | 1:c:211:ILE:HB  | 1.90                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:143:VAL:C   | 1:D:144:LEU:HG  | 2.24                     | 0.54              |
| 1:D:188:THR:CG2 | 1:D:189:LYS:N   | 2.69                     | 0.54              |
| 1:F:188:THR:CG2 | 1:F:189:LYS:N   | 2.69                     | 0.54              |
| 1:I:150:GLY:O   | 1:I:151:ARG:C   | 2.50                     | 0.54              |
| 1:R:168:CYS:HB2 | 1:R:211:ILE:HB  | 1.90                     | 0.54              |
| 1:R:188:THR:CG2 | 1:R:189:LYS:N   | 2.69                     | 0.54              |
| 1:S:76:ASP:HB3  | 1:S:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:U:150:GLY:O   | 1:U:151:ARG:C   | 2.50                     | 0.54              |
| 1:V:150:GLY:O   | 1:V:151:ARG:C   | 2.50                     | 0.54              |
| 1:a:168:CYS:HB2 | 1:a:211:ILE:HB  | 1.90                     | 0.54              |
| 1:c:76:ASP:HB3  | 1:c:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:d:76:ASP:HB3  | 1:d:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:A:168:CYS:HB2 | 1:A:211:ILE:HB  | 1.90                     | 0.54              |
| 1:G:150:GLY:O   | 1:G:151:ARG:C   | 2.50                     | 0.54              |
| 1:I:188:THR:CG2 | 1:I:189:LYS:N   | 2.69                     | 0.54              |
| 1:K:76:ASP:HB3  | 1:K:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:Q:168:CYS:HB2 | 1:Q:211:ILE:HB  | 1.89                     | 0.54              |
| 1:Z:168:CYS:HB2 | 1:Z:211:ILE:HB  | 1.89                     | 0.54              |
| 1:b:76:ASP:HB3  | 1:b:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:A:76:ASP:HB3  | 1:A:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:C:143:VAL:C   | 1:C:144:LEU:HG  | 2.24                     | 0.54              |
| 1:J:150:GLY:O   | 1:J:151:ARG:C   | 2.50                     | 0.54              |
| 1:K:168:CYS:HB2 | 1:K:211:ILE:HB  | 1.90                     | 0.54              |
| 1:L:150:GLY:O   | 1:L:151:ARG:C   | 2.50                     | 0.54              |
| 1:W:188:THR:CG2 | 1:W:189:LYS:N   | 2.69                     | 0.54              |
| 1:a:76:ASP:HB3  | 1:a:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:a:113:SER:HB3 | 1:a:115:PHE:HE2 | 1.71                     | 0.54              |
| 1:B:71:VAL:HB   | 1:B:124:ASP:CB  | 2.32                     | 0.54              |
| 1:B:168:CYS:HB2 | 1:B:211:ILE:HB  | 1.90                     | 0.54              |
| 1:F:150:GLY:O   | 1:F:151:ARG:C   | 2.50                     | 0.54              |
| 1:W:150:GLY:O   | 1:W:151:ARG:C   | 2.50                     | 0.54              |
| 1:Y:76:ASP:HB3  | 1:Y:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:Y:188:THR:CG2 | 1:Y:189:LYS:N   | 2.69                     | 0.54              |
| 1:S:71:VAL:HB   | 1:S:124:ASP:CB  | 2.32                     | 0.54              |
| 1:Z:76:ASP:HB3  | 1:Z:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:a:150:GLY:O   | 1:a:151:ARG:C   | 2.50                     | 0.54              |
| 1:a:188:THR:CG2 | 1:a:189:LYS:N   | 2.69                     | 0.54              |
| 1:b:150:GLY:O   | 1:b:151:ARG:C   | 2.50                     | 0.54              |
| 1:c:150:GLY:O   | 1:c:151:ARG:C   | 2.50                     | 0.54              |
| 1:E:228:LEU:HG  | 1:E:245:GLU:HA  | 1.90                     | 0.54              |
| 1:J:168:CYS:HB2 | 1:J:211:ILE:HB  | 1.90                     | 0.54              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:228:LEU:HG  | 1:J:245:GLU:HA  | 1.90                     | 0.54              |
| 1:K:150:GLY:O   | 1:K:151:ARG:C   | 2.50                     | 0.54              |
| 1:P:168:CYS:HB2 | 1:P:211:ILE:HB  | 1.90                     | 0.54              |
| 1:C:168:CYS:HB2 | 1:C:211:ILE:HB  | 1.89                     | 0.54              |
| 1:D:228:LEU:HG  | 1:D:245:GLU:HA  | 1.90                     | 0.54              |
| 1:F:228:LEU:HG  | 1:F:245:GLU:HA  | 1.90                     | 0.54              |
| 1:I:168:CYS:HB2 | 1:I:211:ILE:HB  | 1.90                     | 0.54              |
| 1:L:71:VAL:HB   | 1:L:124:ASP:CB  | 2.32                     | 0.54              |
| 1:L:165:MET:HA  | 1:L:165:MET:HE3 | 1.90                     | 0.54              |
| 1:M:150:GLY:O   | 1:M:151:ARG:C   | 2.50                     | 0.54              |
| 1:O:165:MET:HA  | 1:O:165:MET:HE3 | 1.90                     | 0.54              |
| 1:R:165:MET:HE3 | 1:R:165:MET:HA  | 1.90                     | 0.54              |
| 1:T:71:VAL:HB   | 1:T:124:ASP:CB  | 2.32                     | 0.54              |
| 1:T:76:ASP:HB3  | 1:T:119:ARG:HG2 | 1.88                     | 0.54              |
| 1:B:143:VAL:C   | 1:B:144:LEU:HG  | 2.24                     | 0.54              |
| 1:I:165:MET:HA  | 1:I:165:MET:HE3 | 1.90                     | 0.54              |
| 1:I:228:LEU:HG  | 1:I:245:GLU:HA  | 1.90                     | 0.54              |
| 1:M:71:VAL:HB   | 1:M:124:ASP:CB  | 2.32                     | 0.54              |
| 1:N:165:MET:HA  | 1:N:165:MET:HE3 | 1.90                     | 0.54              |
| 1:O:168:CYS:HB2 | 1:O:211:ILE:HB  | 1.90                     | 0.54              |
| 1:T:165:MET:HA  | 1:T:165:MET:HE3 | 1.90                     | 0.54              |
| 1:X:168:CYS:HB2 | 1:X:211:ILE:HB  | 1.89                     | 0.54              |
| 1:Y:168:CYS:HB2 | 1:Y:211:ILE:HB  | 1.90                     | 0.54              |
| 1:Z:150:GLY:O   | 1:Z:151:ARG:C   | 2.50                     | 0.54              |
| 1:d:150:GLY:O   | 1:d:151:ARG:C   | 2.50                     | 0.54              |
| 1:A:143:VAL:C   | 1:A:144:LEU:HG  | 2.24                     | 0.54              |
| 1:E:150:GLY:O   | 1:E:151:ARG:C   | 2.50                     | 0.54              |
| 1:F:71:VAL:HB   | 1:F:124:ASP:CB  | 2.32                     | 0.54              |
| 1:K:165:MET:HA  | 1:K:165:MET:HE3 | 1.90                     | 0.54              |
| 1:K:228:LEU:HG  | 1:K:245:GLU:HA  | 1.90                     | 0.54              |
| 1:Q:165:MET:HA  | 1:Q:165:MET:HE3 | 1.90                     | 0.54              |
| 1:S:165:MET:HA  | 1:S:165:MET:HE3 | 1.90                     | 0.54              |
| 1:X:150:GLY:O   | 1:X:151:ARG:C   | 2.50                     | 0.54              |
| 1:D:168:CYS:HB2 | 1:D:211:ILE:HB  | 1.89                     | 0.54              |
| 1:G:228:LEU:HG  | 1:G:245:GLU:HA  | 1.90                     | 0.54              |
| 1:J:165:MET:HE3 | 1:J:165:MET:HA  | 1.90                     | 0.54              |
| 1:M:165:MET:HA  | 1:M:165:MET:HE3 | 1.90                     | 0.54              |
| 1:V:165:MET:HA  | 1:V:165:MET:HE3 | 1.90                     | 0.54              |
| 1:W:168:CYS:HB2 | 1:W:211:ILE:HB  | 1.89                     | 0.54              |
| 1:A:150:GLY:O   | 1:A:151:ARG:C   | 2.50                     | 0.53              |
| 1:F:165:MET:HA  | 1:F:165:MET:HE3 | 1.90                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:165:MET:HA  | 1:G:165:MET:HE3 | 1.90                     | 0.53              |
| 1:H:165:MET:HA  | 1:H:165:MET:HE3 | 1.90                     | 0.53              |
| 1:H:168:CYS:HB2 | 1:H:211:ILE:HB  | 1.90                     | 0.53              |
| 1:H:228:LEU:HG  | 1:H:245:GLU:HA  | 1.90                     | 0.53              |
| 1:N:168:CYS:HB2 | 1:N:211:ILE:HB  | 1.90                     | 0.53              |
| 1:P:165:MET:HA  | 1:P:165:MET:HE3 | 1.90                     | 0.53              |
| 1:U:165:MET:HA  | 1:U:165:MET:HE3 | 1.90                     | 0.53              |
| 1:W:165:MET:HA  | 1:W:165:MET:HE3 | 1.90                     | 0.53              |
| 1:d:143:VAL:C   | 1:d:144:LEU:HG  | 2.24                     | 0.53              |
| 1:B:228:LEU:HG  | 1:B:245:GLU:HA  | 1.90                     | 0.53              |
| 1:N:150:GLY:O   | 1:N:151:ARG:C   | 2.50                     | 0.53              |
| 1:P:150:GLY:O   | 1:P:151:ARG:C   | 2.50                     | 0.53              |
| 1:T:228:LEU:HG  | 1:T:245:GLU:HA  | 1.90                     | 0.53              |
| 1:Y:165:MET:HA  | 1:Y:165:MET:HE3 | 1.90                     | 0.53              |
| 1:d:228:LEU:HG  | 1:d:245:GLU:HA  | 1.90                     | 0.53              |
| 1:B:150:GLY:O   | 1:B:151:ARG:C   | 2.50                     | 0.53              |
| 1:C:228:LEU:HG  | 1:C:245:GLU:HA  | 1.90                     | 0.53              |
| 1:Q:150:GLY:O   | 1:Q:151:ARG:C   | 2.50                     | 0.53              |
| 1:X:165:MET:HA  | 1:X:165:MET:HE3 | 1.90                     | 0.53              |
| 1:D:150:GLY:O   | 1:D:151:ARG:C   | 2.50                     | 0.53              |
| 1:O:150:GLY:O   | 1:O:151:ARG:C   | 2.50                     | 0.53              |
| 1:R:150:GLY:O   | 1:R:151:ARG:C   | 2.50                     | 0.53              |
| 1:Y:150:GLY:O   | 1:Y:151:ARG:C   | 2.50                     | 0.53              |
| 1:Z:165:MET:HE3 | 1:Z:165:MET:HA  | 1.90                     | 0.53              |
| 1:c:143:VAL:C   | 1:c:144:LEU:HG  | 2.24                     | 0.53              |
| 1:A:228:LEU:HG  | 1:A:245:GLU:HA  | 1.90                     | 0.53              |
| 1:C:165:MET:HA  | 1:C:165:MET:HE3 | 1.90                     | 0.53              |
| 1:D:165:MET:HA  | 1:D:165:MET:HE3 | 1.90                     | 0.53              |
| 1:E:165:MET:HA  | 1:E:165:MET:HE3 | 1.90                     | 0.53              |
| 1:E:168:CYS:HB2 | 1:E:211:ILE:HB  | 1.89                     | 0.53              |
| 1:G:168:CYS:HB2 | 1:G:211:ILE:HB  | 1.89                     | 0.53              |
| 1:Q:228:LEU:HG  | 1:Q:245:GLU:HA  | 1.90                     | 0.53              |
| 1:R:228:LEU:HG  | 1:R:245:GLU:HA  | 1.90                     | 0.53              |
| 1:V:168:CYS:HB2 | 1:V:211:ILE:HB  | 1.89                     | 0.53              |
| 1:a:165:MET:HA  | 1:a:165:MET:HE3 | 1.90                     | 0.53              |
| 1:B:165:MET:HE3 | 1:B:165:MET:HA  | 1.90                     | 0.53              |
| 1:M:168:CYS:HB2 | 1:M:211:ILE:HB  | 1.90                     | 0.53              |
| 1:P:228:LEU:HG  | 1:P:245:GLU:HA  | 1.90                     | 0.53              |
| 1:S:228:LEU:HG  | 1:S:245:GLU:HA  | 1.90                     | 0.53              |
| 1:U:71:VAL:HB   | 1:U:124:ASP:CB  | 2.32                     | 0.53              |
| 1:c:228:LEU:HG  | 1:c:245:GLU:HA  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:165:MET:HA   | 1:d:165:MET:HE3 | 1.90                     | 0.53              |
| 1:S:150:GLY:O    | 1:S:151:ARG:C   | 2.50                     | 0.53              |
| 1:U:168:CYS:HB2  | 1:U:211:ILE:HB  | 1.89                     | 0.53              |
| 1:b:228:LEU:HG   | 1:b:245:GLU:HA  | 1.90                     | 0.53              |
| 1:K:71:VAL:HB    | 1:K:124:ASP:CB  | 2.32                     | 0.53              |
| 1:L:168:CYS:HB2  | 1:L:211:ILE:HB  | 1.89                     | 0.53              |
| 1:P:98:LYS:HE2   | 1:P:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:Y:98:LYS:HE2   | 1:Y:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:a:78:VAL:HG22  | 1:a:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:A:165:MET:HA   | 1:A:165:MET:HE3 | 1.90                     | 0.53              |
| 1:L:98:LYS:HE2   | 1:L:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:O:228:LEU:HG   | 1:O:245:GLU:HA  | 1.90                     | 0.53              |
| 1:V:98:LYS:HE2   | 1:V:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:W:98:LYS:HE2   | 1:W:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:Z:78:VAL:HG22  | 1:Z:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:a:228:LEU:HG   | 1:a:245:GLU:HA  | 1.90                     | 0.53              |
| 1:b:78:VAL:HG22  | 1:b:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:c:98:LYS:HE2   | 1:c:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:c:165:MET:HA   | 1:c:165:MET:HE3 | 1.90                     | 0.53              |
| 1:A:78:VAL:HG22  | 1:A:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:D:71:VAL:HB    | 1:D:124:ASP:CB  | 2.32                     | 0.53              |
| 1:F:168:CYS:HB2  | 1:F:211:ILE:HB  | 1.89                     | 0.53              |
| 1:I:71:VAL:HB    | 1:I:124:ASP:CB  | 2.32                     | 0.53              |
| 1:M:98:LYS:HE2   | 1:M:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:N:98:LYS:HE2   | 1:N:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:O:98:LYS:HE2   | 1:O:187:GLN:HG2 | 1.91                     | 0.53              |
| 1:T:150:GLY:O    | 1:T:151:ARG:C   | 2.50                     | 0.53              |
| 1:Z:98:LYS:HE2   | 1:Z:187:GLN:HG2 | 1.92                     | 0.53              |
| 1:c:78:VAL:HG22  | 1:c:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:d:78:VAL:HG22  | 1:d:80:TYR:HB2  | 1.91                     | 0.53              |
| 1:B:78:VAL:HG22  | 1:B:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:N:228:LEU:HG   | 1:N:245:GLU:HA  | 1.90                     | 0.52              |
| 1:Y:78:VAL:HG22  | 1:Y:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:b:143:VAL:C    | 1:b:144:LEU:HG  | 2.24                     | 0.52              |
| 1:b:165:MET:HE3  | 1:b:165:MET:HA  | 1.90                     | 0.52              |
| 1:b:186:ILE:HG12 | 1:b:193:VAL:HB  | 1.91                     | 0.52              |
| 1:c:186:ILE:HG12 | 1:c:193:VAL:HB  | 1.91                     | 0.52              |
| 1:M:228:LEU:HG   | 1:M:245:GLU:HA  | 1.90                     | 0.52              |
| 1:R:98:LYS:HE2   | 1:R:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:U:98:LYS:HE2   | 1:U:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:X:78:VAL:HG22  | 1:X:80:TYR:HB2  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:186:ILE:HG12 | 1:d:193:VAL:HB  | 1.92                     | 0.52              |
| 1:A:186:ILE:HG12 | 1:A:193:VAL:HB  | 1.92                     | 0.52              |
| 1:C:150:GLY:O    | 1:C:151:ARG:C   | 2.50                     | 0.52              |
| 1:Q:98:LYS:HE2   | 1:Q:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:R:71:VAL:HB    | 1:R:124:ASP:CB  | 2.32                     | 0.52              |
| 1:R:78:VAL:HG22  | 1:R:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:X:98:LYS:HE2   | 1:X:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:Z:228:LEU:HG   | 1:Z:245:GLU:HA  | 1.90                     | 0.52              |
| 1:a:98:LYS:HE2   | 1:a:187:GLN:HG2 | 1.92                     | 0.52              |
| 1:b:98:LYS:HE2   | 1:b:187:GLN:HG2 | 1.92                     | 0.52              |
| 1:d:98:LYS:HE2   | 1:d:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:B:186:ILE:HG12 | 1:B:193:VAL:HB  | 1.91                     | 0.52              |
| 1:P:78:VAL:HG22  | 1:P:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:S:78:VAL:HG22  | 1:S:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:W:71:VAL:HB    | 1:W:124:ASP:CB  | 2.32                     | 0.52              |
| 1:B:98:LYS:HE2   | 1:B:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:C:78:VAL:HG22  | 1:C:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:K:78:VAL:HG22  | 1:K:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:Y:228:LEU:HG   | 1:Y:245:GLU:HA  | 1.90                     | 0.52              |
| 1:a:186:ILE:HG12 | 1:a:193:VAL:HB  | 1.91                     | 0.52              |
| 1:J:78:VAL:HG22  | 1:J:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:O:78:VAL:HG22  | 1:O:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:Q:78:VAL:HG22  | 1:Q:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:S:98:LYS:HE2   | 1:S:187:GLN:HG2 | 1.92                     | 0.52              |
| 1:T:78:VAL:HG22  | 1:T:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:T:98:LYS:HE2   | 1:T:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:U:228:LEU:HG   | 1:U:245:GLU:HA  | 1.90                     | 0.52              |
| 1:W:78:VAL:HG22  | 1:W:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:A:24:ASN:HB3   | 1:d:15:ALA:H    | 1.75                     | 0.52              |
| 1:A:71:VAL:HB    | 1:A:124:ASP:CB  | 2.32                     | 0.52              |
| 1:A:98:LYS:HE2   | 1:A:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:D:78:VAL:HG22  | 1:D:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:L:228:LEU:HG   | 1:L:245:GLU:HA  | 1.90                     | 0.52              |
| 1:N:71:VAL:HB    | 1:N:124:ASP:CB  | 2.32                     | 0.52              |
| 1:X:228:LEU:HG   | 1:X:245:GLU:HA  | 1.90                     | 0.52              |
| 1:C:186:ILE:HG12 | 1:C:193:VAL:HB  | 1.92                     | 0.52              |
| 1:E:98:LYS:HE2   | 1:E:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:P:34:LEU:HD23  | 1:P:58:LEU:HD12 | 1.92                     | 0.52              |
| 1:V:228:LEU:HG   | 1:V:245:GLU:HA  | 1.90                     | 0.52              |
| 1:J:98:LYS:HE2   | 1:J:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:K:98:LYS:HE2   | 1:K:187:GLN:HG2 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:N:34:LEU:HD23  | 1:N:58:LEU:HD12 | 1.92                     | 0.52              |
| 1:U:34:LEU:HD23  | 1:U:58:LEU:HD12 | 1.92                     | 0.52              |
| 1:V:78:VAL:HG22  | 1:V:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:W:228:LEU:HG   | 1:W:245:GLU:HA  | 1.90                     | 0.52              |
| 1:Z:186:ILE:HG12 | 1:Z:193:VAL:HB  | 1.91                     | 0.52              |
| 1:a:15:ALA:H     | 1:b:24:ASN:HB3  | 1.75                     | 0.52              |
| 1:C:98:LYS:HE2   | 1:C:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:G:98:LYS:HE2   | 1:G:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:H:98:LYS:HE2   | 1:H:187:GLN:HG2 | 1.91                     | 0.52              |
| 1:I:78:VAL:HG22  | 1:I:80:TYR:HB2  | 1.91                     | 0.52              |
| 1:L:186:ILE:HG12 | 1:L:193:VAL:HB  | 1.91                     | 0.52              |
| 1:M:186:ILE:HG12 | 1:M:193:VAL:HB  | 1.91                     | 0.52              |
| 1:R:34:LEU:HD23  | 1:R:58:LEU:HD12 | 1.92                     | 0.52              |
| 1:U:186:ILE:HG12 | 1:U:193:VAL:HB  | 1.91                     | 0.52              |
| 1:V:186:ILE:HG12 | 1:V:193:VAL:HB  | 1.91                     | 0.52              |
| 1:W:34:LEU:HD23  | 1:W:58:LEU:HD12 | 1.92                     | 0.52              |
| 1:D:98:LYS:HE2   | 1:D:187:GLN:HG2 | 1.92                     | 0.51              |
| 1:H:78:VAL:HG22  | 1:H:80:TYR:HB2  | 1.91                     | 0.51              |
| 1:M:131:ASP:OD1  | 1:M:132:SER:N   | 2.44                     | 0.51              |
| 1:N:78:VAL:HG22  | 1:N:80:TYR:HB2  | 1.91                     | 0.51              |
| 1:V:131:ASP:OD1  | 1:V:132:SER:N   | 2.44                     | 0.51              |
| 1:Y:71:VAL:HB    | 1:Y:124:ASP:CB  | 2.32                     | 0.51              |
| 1:D:186:ILE:HG12 | 1:D:193:VAL:HB  | 1.92                     | 0.51              |
| 1:F:98:LYS:HE2   | 1:F:187:GLN:HG2 | 1.91                     | 0.51              |
| 1:L:131:ASP:OD1  | 1:L:132:SER:N   | 2.44                     | 0.51              |
| 1:M:34:LEU:HD23  | 1:M:58:LEU:HD12 | 1.92                     | 0.51              |
| 1:N:131:ASP:OD1  | 1:N:132:SER:N   | 2.44                     | 0.51              |
| 1:N:186:ILE:HG12 | 1:N:193:VAL:HB  | 1.91                     | 0.51              |
| 1:S:131:ASP:OD1  | 1:S:132:SER:N   | 2.44                     | 0.51              |
| 1:U:78:VAL:HG22  | 1:U:80:TYR:HB2  | 1.91                     | 0.51              |
| 1:U:131:ASP:OD1  | 1:U:132:SER:N   | 2.44                     | 0.51              |
| 1:W:131:ASP:OD1  | 1:W:132:SER:N   | 2.44                     | 0.51              |
| 1:C:131:ASP:OD1  | 1:C:132:SER:N   | 2.44                     | 0.51              |
| 1:D:131:ASP:OD1  | 1:D:132:SER:N   | 2.44                     | 0.51              |
| 1:E:131:ASP:OD1  | 1:E:132:SER:N   | 2.44                     | 0.51              |
| 1:G:15:ALA:H     | 1:H:24:ASN:HB3  | 1.75                     | 0.51              |
| 1:I:98:LYS:HE2   | 1:I:187:GLN:HG2 | 1.91                     | 0.51              |
| 1:R:131:ASP:OD1  | 1:R:132:SER:N   | 2.44                     | 0.51              |
| 1:T:131:ASP:OD1  | 1:T:132:SER:N   | 2.44                     | 0.51              |
| 1:X:131:ASP:OD1  | 1:X:132:SER:N   | 2.44                     | 0.51              |
| 1:A:131:ASP:OD1  | 1:A:132:SER:N   | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:ASP:OD1  | 1:B:132:SER:N    | 2.44                     | 0.51              |
| 1:E:78:VAL:HG22  | 1:E:80:TYR:HB2   | 1.91                     | 0.51              |
| 1:F:131:ASP:OD1  | 1:F:132:SER:N    | 2.44                     | 0.51              |
| 1:K:34:LEU:HD23  | 1:K:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:K:131:ASP:OD1  | 1:K:132:SER:N    | 2.44                     | 0.51              |
| 1:L:78:VAL:HG22  | 1:L:80:TYR:HB2   | 1.91                     | 0.51              |
| 1:O:131:ASP:OD1  | 1:O:132:SER:N    | 2.44                     | 0.51              |
| 1:O:186:ILE:HG12 | 1:O:193:VAL:HB   | 1.91                     | 0.51              |
| 1:R:24:ASN:HB3   | 1:S:15:ALA:H     | 1.75                     | 0.51              |
| 1:S:186:ILE:HG12 | 1:S:193:VAL:HB   | 1.91                     | 0.51              |
| 1:T:186:ILE:HG12 | 1:T:193:VAL:HB   | 1.91                     | 0.51              |
| 1:Y:186:ILE:HG12 | 1:Y:193:VAL:HB   | 1.91                     | 0.51              |
| 1:a:131:ASP:OD1  | 1:a:132:SER:N    | 2.43                     | 0.51              |
| 1:d:131:ASP:OD1  | 1:d:132:SER:N    | 2.44                     | 0.51              |
| 1:E:186:ILE:HG12 | 1:E:193:VAL:HB   | 1.91                     | 0.51              |
| 1:F:78:VAL:HG22  | 1:F:80:TYR:HB2   | 1.91                     | 0.51              |
| 1:G:78:VAL:HG22  | 1:G:80:TYR:HB2   | 1.91                     | 0.51              |
| 1:G:131:ASP:OD1  | 1:G:132:SER:N    | 2.44                     | 0.51              |
| 1:L:34:LEU:HD23  | 1:L:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:M:78:VAL:HG22  | 1:M:80:TYR:HB2   | 1.91                     | 0.51              |
| 1:O:24:ASN:HB3   | 1:P:15:ALA:H     | 1.76                     | 0.51              |
| 1:P:131:ASP:OD1  | 1:P:132:SER:N    | 2.44                     | 0.51              |
| 1:P:186:ILE:HG12 | 1:P:193:VAL:HB   | 1.91                     | 0.51              |
| 1:Q:131:ASP:OD1  | 1:Q:132:SER:N    | 2.44                     | 0.51              |
| 1:W:186:ILE:HG12 | 1:W:193:VAL:HB   | 1.92                     | 0.51              |
| 1:Y:34:LEU:HD23  | 1:Y:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:Y:131:ASP:OD1  | 1:Y:132:SER:N    | 2.44                     | 0.51              |
| 1:Z:131:ASP:OD1  | 1:Z:132:SER:N    | 2.44                     | 0.51              |
| 1:c:131:ASP:OD1  | 1:c:132:SER:N    | 2.44                     | 0.51              |
| 1:J:131:ASP:OD1  | 1:J:132:SER:N    | 2.44                     | 0.51              |
| 1:P:33:LEU:HA    | 1:P:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:Q:186:ILE:HG12 | 1:Q:193:VAL:HB   | 1.91                     | 0.51              |
| 1:S:33:LEU:HA    | 1:S:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:U:36:LEU:HG    | 1:U:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:W:36:LEU:HG    | 1:W:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:Z:34:LEU:HD23  | 1:Z:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:b:131:ASP:OD1  | 1:b:132:SER:N    | 2.44                     | 0.51              |
| 1:H:15:ALA:H     | 1:I:24:ASN:HB3   | 1.76                     | 0.51              |
| 1:J:33:LEU:HA    | 1:J:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:L:36:LEU:HG    | 1:L:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:M:36:LEU:HG    | 1:M:157:VAL:HG22 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:36:LEU:HG    | 1:N:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:R:33:LEU:HA    | 1:R:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:S:34:LEU:HD23  | 1:S:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:T:34:LEU:HD23  | 1:T:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:U:15:ALA:H     | 1:V:24:ASN:HB3   | 1.75                     | 0.51              |
| 1:X:186:ILE:HG12 | 1:X:193:VAL:HB   | 1.91                     | 0.51              |
| 1:H:131:ASP:OD1  | 1:H:132:SER:N    | 2.44                     | 0.51              |
| 1:I:34:LEU:HD23  | 1:I:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:J:186:ILE:HG12 | 1:J:193:VAL:HB   | 1.91                     | 0.51              |
| 1:M:24:ASN:HB3   | 1:N:15:ALA:H     | 1.76                     | 0.51              |
| 1:R:186:ILE:HG12 | 1:R:193:VAL:HB   | 1.91                     | 0.51              |
| 1:V:36:LEU:HG    | 1:V:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:X:36:LEU:HG    | 1:X:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:c:15:ALA:H     | 1:d:24:ASN:HB3   | 1.76                     | 0.51              |
| 1:D:37:VAL:HG12  | 1:D:38:THR:N     | 2.26                     | 0.51              |
| 1:H:33:LEU:HA    | 1:H:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:K:15:ALA:H     | 1:T:24:ASN:HB3   | 1.76                     | 0.51              |
| 1:K:33:LEU:HA    | 1:K:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:K:186:ILE:HG12 | 1:K:193:VAL:HB   | 1.91                     | 0.51              |
| 1:M:33:LEU:HA    | 1:M:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:O:34:LEU:HD23  | 1:O:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:O:36:LEU:HG    | 1:O:157:VAL:HG22 | 1.93                     | 0.51              |
| 1:X:15:ALA:H     | 1:Y:24:ASN:HB3   | 1.75                     | 0.51              |
| 1:a:71:VAL:HB    | 1:a:124:ASP:CB   | 2.32                     | 0.51              |
| 1:b:34:LEU:HD23  | 1:b:58:LEU:HD12  | 1.92                     | 0.51              |
| 1:d:37:VAL:HG12  | 1:d:38:THR:N     | 2.26                     | 0.51              |
| 1:C:37:VAL:HG12  | 1:C:38:THR:N     | 2.26                     | 0.51              |
| 1:I:131:ASP:OD1  | 1:I:132:SER:N    | 2.44                     | 0.51              |
| 1:U:33:LEU:HA    | 1:U:158:LEU:HD22 | 1.93                     | 0.51              |
| 1:c:37:VAL:HG12  | 1:c:38:THR:N     | 2.26                     | 0.51              |
| 1:F:186:ILE:HG12 | 1:F:193:VAL:HB   | 1.91                     | 0.50              |
| 1:I:186:ILE:HG12 | 1:I:193:VAL:HB   | 1.92                     | 0.50              |
| 1:O:33:LEU:HA    | 1:O:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:P:36:LEU:HG    | 1:P:157:VAL:HG22 | 1.93                     | 0.50              |
| 1:X:34:LEU:HD23  | 1:X:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:b:37:VAL:HG12  | 1:b:38:THR:N     | 2.26                     | 0.50              |
| 1:D:15:ALA:H     | 1:E:24:ASN:HB3   | 1.75                     | 0.50              |
| 1:J:15:ALA:H     | 1:K:24:ASN:HB3   | 1.76                     | 0.50              |
| 1:a:37:VAL:HG12  | 1:a:38:THR:N     | 2.26                     | 0.50              |
| 1:N:33:LEU:HA    | 1:N:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:P:71:VAL:HB    | 1:P:124:ASP:CB   | 2.32                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:36:LEU:HG    | 1:Y:157:VAL:HG22 | 1.93                     | 0.50              |
| 1:B:34:LEU:HD23  | 1:B:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:E:33:LEU:HA    | 1:E:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:F:33:LEU:HA    | 1:F:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:F:34:LEU:HD23  | 1:F:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:G:37:VAL:HG12  | 1:G:38:THR:N     | 2.26                     | 0.50              |
| 1:H:37:VAL:HG12  | 1:H:38:THR:N     | 2.26                     | 0.50              |
| 1:H:186:ILE:HG12 | 1:H:193:VAL:HB   | 1.91                     | 0.50              |
| 1:L:15:ALA:H     | 1:U:24:ASN:HB3   | 1.76                     | 0.50              |
| 1:V:33:LEU:HA    | 1:V:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:V:34:LEU:HD23  | 1:V:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:A:34:LEU:HD23  | 1:A:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:B:15:ALA:H     | 1:C:24:ASN:HB3   | 1.76                     | 0.50              |
| 1:C:33:LEU:HA    | 1:C:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:T:62:LEU:HD22  | 1:T:136:THR:HG22 | 1.93                     | 0.50              |
| 1:W:15:ALA:H     | 1:X:24:ASN:HB3   | 1.77                     | 0.50              |
| 1:B:37:VAL:HG12  | 1:B:38:THR:N     | 2.26                     | 0.50              |
| 1:C:34:LEU:HD23  | 1:C:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:D:34:LEU:HD23  | 1:D:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:E:34:LEU:HD23  | 1:E:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:G:33:LEU:HA    | 1:G:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:G:186:ILE:HG12 | 1:G:193:VAL:HB   | 1.91                     | 0.50              |
| 1:H:34:LEU:HD23  | 1:H:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:Q:34:LEU:HD23  | 1:Q:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:Q:36:LEU:HG    | 1:Q:157:VAL:HG22 | 1.93                     | 0.50              |
| 1:Y:37:VAL:HG12  | 1:Y:38:THR:N     | 2.26                     | 0.50              |
| 1:b:58:LEU:O     | 1:b:62:LEU:HG    | 2.12                     | 0.50              |
| 1:c:71:VAL:HB    | 1:c:124:ASP:CB   | 2.32                     | 0.50              |
| 1:I:33:LEU:HA    | 1:I:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:S:62:LEU:HD22  | 1:S:136:THR:HG22 | 1.94                     | 0.50              |
| 1:Z:36:LEU:HG    | 1:Z:157:VAL:HG22 | 1.93                     | 0.50              |
| 1:D:129:ILE:HD12 | 1:D:132:SER:OG   | 2.12                     | 0.50              |
| 1:F:66:GLN:NE2   | 1:F:67:PHE:H     | 2.10                     | 0.50              |
| 1:L:58:LEU:O     | 1:L:62:LEU:HG    | 2.12                     | 0.50              |
| 1:M:58:LEU:O     | 1:M:62:LEU:HG    | 2.12                     | 0.50              |
| 1:P:37:VAL:HG12  | 1:P:38:THR:N     | 2.26                     | 0.50              |
| 1:Q:33:LEU:HA    | 1:Q:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:X:33:LEU:HA    | 1:X:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:Z:62:LEU:HD22  | 1:Z:136:THR:HG22 | 1.94                     | 0.50              |
| 1:a:58:LEU:O     | 1:a:62:LEU:HG    | 2.12                     | 0.50              |
| 1:c:62:LEU:HD22  | 1:c:136:THR:HG22 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:34:LEU:HD23  | 1:d:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:A:33:LEU:HA    | 1:A:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:C:129:ILE:HD12 | 1:C:132:SER:OG   | 2.12                     | 0.50              |
| 1:G:34:LEU:HD23  | 1:G:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:K:62:LEU:HD22  | 1:K:136:THR:HG22 | 1.94                     | 0.50              |
| 1:L:24:ASN:HB3   | 1:M:15:ALA:H     | 1.77                     | 0.50              |
| 1:L:33:LEU:HA    | 1:L:158:LEU:HD22 | 1.93                     | 0.50              |
| 1:L:37:VAL:HG12  | 1:L:38:THR:N     | 2.26                     | 0.50              |
| 1:P:24:ASN:HB3   | 1:Q:15:ALA:H     | 1.77                     | 0.50              |
| 1:Q:37:VAL:HG12  | 1:Q:38:THR:N     | 2.26                     | 0.50              |
| 1:Z:15:ALA:H     | 1:a:24:ASN:HB3   | 1.77                     | 0.50              |
| 1:Z:37:VAL:HG12  | 1:Z:38:THR:N     | 2.26                     | 0.50              |
| 1:Z:58:LEU:O     | 1:Z:62:LEU:HG    | 2.12                     | 0.50              |
| 1:a:34:LEU:HD23  | 1:a:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:b:62:LEU:HD22  | 1:b:136:THR:HG22 | 1.93                     | 0.50              |
| 1:c:34:LEU:HD23  | 1:c:58:LEU:HD12  | 1.92                     | 0.50              |
| 1:C:15:ALA:H     | 1:D:24:ASN:HB3   | 1.77                     | 0.49              |
| 1:E:37:VAL:HG12  | 1:E:38:THR:N     | 2.26                     | 0.49              |
| 1:E:129:ILE:HD12 | 1:E:132:SER:OG   | 2.12                     | 0.49              |
| 1:N:58:LEU:O     | 1:N:62:LEU:HG    | 2.12                     | 0.49              |
| 1:N:66:GLN:NE2   | 1:N:67:PHE:H     | 2.10                     | 0.49              |
| 1:R:62:LEU:HD22  | 1:R:136:THR:HG22 | 1.94                     | 0.49              |
| 1:W:58:LEU:O     | 1:W:62:LEU:HG    | 2.12                     | 0.49              |
| 1:X:37:VAL:HG12  | 1:X:38:THR:N     | 2.26                     | 0.49              |
| 1:X:58:LEU:O     | 1:X:62:LEU:HG    | 2.12                     | 0.49              |
| 1:Y:58:LEU:O     | 1:Y:62:LEU:HG    | 2.12                     | 0.49              |
| 1:Z:33:LEU:HA    | 1:Z:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:a:36:LEU:HG    | 1:a:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:D:66:GLN:NE2   | 1:D:67:PHE:H     | 2.10                     | 0.49              |
| 1:R:36:LEU:HG    | 1:R:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:S:24:ASN:HB3   | 1:T:15:ALA:H     | 1.77                     | 0.49              |
| 1:T:33:LEU:HA    | 1:T:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:V:66:GLN:NE2   | 1:V:67:PHE:H     | 2.10                     | 0.49              |
| 1:W:33:LEU:HA    | 1:W:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:c:58:LEU:O     | 1:c:62:LEU:HG    | 2.12                     | 0.49              |
| 1:d:62:LEU:HD22  | 1:d:136:THR:HG22 | 1.94                     | 0.49              |
| 1:A:37:VAL:HG12  | 1:A:38:THR:N     | 2.26                     | 0.49              |
| 1:B:6:THR:HG22   | 1:B:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:B:129:ILE:HD12 | 1:B:132:SER:OG   | 2.12                     | 0.49              |
| 1:I:37:VAL:HG12  | 1:I:38:THR:N     | 2.26                     | 0.49              |
| 1:J:62:LEU:HD22  | 1:J:136:THR:HG22 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:37:VAL:HG12  | 1:M:38:THR:N     | 2.26                     | 0.49              |
| 1:O:58:LEU:O     | 1:O:62:LEU:HG    | 2.12                     | 0.49              |
| 1:V:58:LEU:O     | 1:V:62:LEU:HG    | 2.12                     | 0.49              |
| 1:Z:71:VAL:HB    | 1:Z:124:ASP:CB   | 2.32                     | 0.49              |
| 1:a:62:LEU:HD22  | 1:a:136:THR:HG22 | 1.94                     | 0.49              |
| 1:A:36:LEU:HG    | 1:A:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:B:36:LEU:HG    | 1:B:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:D:36:LEU:HG    | 1:D:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:E:15:ALA:H     | 1:F:24:ASN:HB3   | 1.76                     | 0.49              |
| 1:F:6:THR:HG22   | 1:F:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:F:37:VAL:HG12  | 1:F:38:THR:N     | 2.26                     | 0.49              |
| 1:F:129:ILE:HD12 | 1:F:132:SER:OG   | 2.12                     | 0.49              |
| 1:H:66:GLN:NE2   | 1:H:67:PHE:H     | 2.10                     | 0.49              |
| 1:K:66:GLN:NE2   | 1:K:67:PHE:H     | 2.10                     | 0.49              |
| 1:N:24:ASN:HB3   | 1:O:15:ALA:H     | 1.77                     | 0.49              |
| 1:R:37:VAL:HG12  | 1:R:38:THR:N     | 2.26                     | 0.49              |
| 1:U:58:LEU:O     | 1:U:62:LEU:HG    | 2.12                     | 0.49              |
| 1:Y:62:LEU:HD22  | 1:Y:136:THR:HG22 | 1.94                     | 0.49              |
| 1:b:33:LEU:HA    | 1:b:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:d:58:LEU:O     | 1:d:62:LEU:HG    | 2.12                     | 0.49              |
| 1:B:33:LEU:HA    | 1:B:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:B:62:LEU:HD22  | 1:B:136:THR:HG22 | 1.94                     | 0.49              |
| 1:C:36:LEU:HG    | 1:C:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:C:62:LEU:HD22  | 1:C:136:THR:HG22 | 1.94                     | 0.49              |
| 1:F:36:LEU:HG    | 1:F:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:G:66:GLN:NE2   | 1:G:67:PHE:H     | 2.10                     | 0.49              |
| 1:H:36:LEU:HG    | 1:H:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:I:66:GLN:NE2   | 1:I:67:PHE:H     | 2.10                     | 0.49              |
| 1:Q:62:LEU:HD22  | 1:Q:136:THR:HG22 | 1.94                     | 0.49              |
| 1:S:36:LEU:HG    | 1:S:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:U:129:ILE:HD12 | 1:U:132:SER:OG   | 2.12                     | 0.49              |
| 1:V:15:ALA:H     | 1:W:24:ASN:HB3   | 1.78                     | 0.49              |
| 1:c:33:LEU:HA    | 1:c:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:d:33:LEU:HA    | 1:d:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:A:6:THR:HG22   | 1:A:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:D:33:LEU:HA    | 1:D:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:E:6:THR:HG22   | 1:E:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:E:36:LEU:HG    | 1:E:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:G:36:LEU:HG    | 1:G:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:I:62:LEU:HD22  | 1:I:136:THR:HG22 | 1.94                     | 0.49              |
| 1:J:6:THR:HG22   | 1:J:217:ILE:HD13 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:34:LEU:HD23  | 1:J:58:LEU:HD12  | 1.92                     | 0.49              |
| 1:M:66:GLN:NE2   | 1:M:67:PHE:H     | 2.10                     | 0.49              |
| 1:U:66:GLN:NE2   | 1:U:67:PHE:H     | 2.10                     | 0.49              |
| 1:V:129:ILE:HD12 | 1:V:132:SER:OG   | 2.12                     | 0.49              |
| 1:W:62:LEU:HD22  | 1:W:136:THR:HG22 | 1.94                     | 0.49              |
| 1:Y:66:GLN:NE2   | 1:Y:67:PHE:H     | 2.10                     | 0.49              |
| 1:Z:66:GLN:NE2   | 1:Z:67:PHE:H     | 2.10                     | 0.49              |
| 1:A:66:GLN:NE2   | 1:A:67:PHE:H     | 2.10                     | 0.49              |
| 1:E:66:GLN:NE2   | 1:E:67:PHE:H     | 2.10                     | 0.49              |
| 1:G:129:ILE:HD12 | 1:G:132:SER:OG   | 2.12                     | 0.49              |
| 1:I:15:ALA:H     | 1:J:24:ASN:HB3   | 1.77                     | 0.49              |
| 1:I:36:LEU:HG    | 1:I:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:L:129:ILE:HD12 | 1:L:132:SER:OG   | 2.12                     | 0.49              |
| 1:O:37:VAL:HG12  | 1:O:38:THR:N     | 2.26                     | 0.49              |
| 1:T:37:VAL:HG12  | 1:T:38:THR:N     | 2.26                     | 0.49              |
| 1:T:129:ILE:HD12 | 1:T:132:SER:OG   | 2.12                     | 0.49              |
| 1:U:37:VAL:HG12  | 1:U:38:THR:N     | 2.26                     | 0.49              |
| 1:W:129:ILE:HD12 | 1:W:132:SER:OG   | 2.12                     | 0.49              |
| 1:X:129:ILE:HD12 | 1:X:132:SER:OG   | 2.12                     | 0.49              |
| 1:c:66:GLN:NE2   | 1:c:67:PHE:H     | 2.10                     | 0.49              |
| 1:d:36:LEU:HG    | 1:d:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:d:227:LYS:HD2  | 1:d:229:ASP:HB2  | 1.95                     | 0.49              |
| 1:A:15:ALA:H     | 1:B:24:ASN:HB3   | 1.77                     | 0.49              |
| 1:A:62:LEU:HD22  | 1:A:136:THR:HG22 | 1.94                     | 0.49              |
| 1:A:129:ILE:HD12 | 1:A:132:SER:OG   | 2.12                     | 0.49              |
| 1:A:227:LYS:HD2  | 1:A:229:ASP:HB2  | 1.95                     | 0.49              |
| 1:C:6:THR:HG22   | 1:C:217:ILE:HD13 | 1.94                     | 0.49              |
| 1:J:66:GLN:NE2   | 1:J:67:PHE:H     | 2.10                     | 0.49              |
| 1:K:6:THR:HG22   | 1:K:217:ILE:HD13 | 1.94                     | 0.49              |
| 1:K:37:VAL:HG12  | 1:K:38:THR:N     | 2.26                     | 0.49              |
| 1:K:129:ILE:HD12 | 1:K:132:SER:OG   | 2.12                     | 0.49              |
| 1:M:129:ILE:HD12 | 1:M:132:SER:OG   | 2.12                     | 0.49              |
| 1:Q:24:ASN:HB3   | 1:R:15:ALA:H     | 1.77                     | 0.49              |
| 1:V:62:LEU:HD22  | 1:V:136:THR:HG22 | 1.94                     | 0.49              |
| 1:X:62:LEU:HD22  | 1:X:136:THR:HG22 | 1.94                     | 0.49              |
| 1:a:33:LEU:HA    | 1:a:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:b:6:THR:HG22   | 1:b:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:b:36:LEU:HG    | 1:b:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:c:36:LEU:HG    | 1:c:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:B:66:GLN:NE2   | 1:B:67:PHE:H     | 2.10                     | 0.49              |
| 1:C:66:GLN:NE2   | 1:C:67:PHE:H     | 2.10                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:58:LEU:O     | 1:E:62:LEU:HG    | 2.12                     | 0.49              |
| 1:G:6:THR:HG22   | 1:G:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:H:129:ILE:HD12 | 1:H:132:SER:OG   | 2.12                     | 0.49              |
| 1:J:36:LEU:HG    | 1:J:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:J:129:ILE:HD12 | 1:J:132:SER:OG   | 2.12                     | 0.49              |
| 1:N:37:VAL:HG12  | 1:N:38:THR:N     | 2.26                     | 0.49              |
| 1:O:66:GLN:NE2   | 1:O:67:PHE:H     | 2.10                     | 0.49              |
| 1:P:58:LEU:O     | 1:P:62:LEU:HG    | 2.12                     | 0.49              |
| 1:P:62:LEU:HD22  | 1:P:136:THR:HG22 | 1.94                     | 0.49              |
| 1:S:66:GLN:NE2   | 1:S:67:PHE:H     | 2.10                     | 0.49              |
| 1:S:129:ILE:HD12 | 1:S:132:SER:OG   | 2.12                     | 0.49              |
| 1:Z:227:LYS:HD2  | 1:Z:229:ASP:HB2  | 1.95                     | 0.49              |
| 1:a:6:THR:HG22   | 1:a:217:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:58:LEU:O     | 1:A:62:LEU:HG    | 2.12                     | 0.49              |
| 1:D:58:LEU:O     | 1:D:62:LEU:HG    | 2.12                     | 0.49              |
| 1:E:62:LEU:HD22  | 1:E:136:THR:HG22 | 1.94                     | 0.49              |
| 1:H:58:LEU:O     | 1:H:62:LEU:HG    | 2.12                     | 0.49              |
| 1:J:37:VAL:HG12  | 1:J:38:THR:N     | 2.26                     | 0.49              |
| 1:K:36:LEU:HG    | 1:K:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:N:129:ILE:HD12 | 1:N:132:SER:OG   | 2.12                     | 0.49              |
| 1:O:129:ILE:HD12 | 1:O:132:SER:OG   | 2.12                     | 0.49              |
| 1:Y:33:LEU:HA    | 1:Y:158:LEU:HD22 | 1.93                     | 0.49              |
| 1:Y:129:ILE:HD12 | 1:Y:132:SER:OG   | 2.12                     | 0.49              |
| 1:b:227:LYS:HD2  | 1:b:229:ASP:HB2  | 1.95                     | 0.49              |
| 1:c:227:LYS:HD2  | 1:c:229:ASP:HB2  | 1.95                     | 0.49              |
| 1:B:227:LYS:HD2  | 1:B:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:D:227:LYS:HD2  | 1:D:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:F:58:LEU:O     | 1:F:62:LEU:HG    | 2.12                     | 0.48              |
| 1:G:58:LEU:O     | 1:G:62:LEU:HG    | 2.12                     | 0.48              |
| 1:Q:66:GLN:NE2   | 1:Q:67:PHE:H     | 2.10                     | 0.48              |
| 1:R:66:GLN:NE2   | 1:R:67:PHE:H     | 2.10                     | 0.48              |
| 1:S:113:SER:HB3  | 1:S:115:PHE:CE2  | 2.48                     | 0.48              |
| 1:W:66:GLN:NE2   | 1:W:67:PHE:H     | 2.10                     | 0.48              |
| 1:Z:129:ILE:HD12 | 1:Z:132:SER:OG   | 2.12                     | 0.48              |
| 1:a:227:LYS:HD2  | 1:a:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:d:129:ILE:HD12 | 1:d:132:SER:OG   | 2.12                     | 0.48              |
| 1:C:227:LYS:HD2  | 1:C:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:D:62:LEU:HD22  | 1:D:136:THR:HG22 | 1.94                     | 0.48              |
| 1:F:15:ALA:H     | 1:G:24:ASN:HB3   | 1.78                     | 0.48              |
| 1:H:62:LEU:HD22  | 1:H:136:THR:HG22 | 1.94                     | 0.48              |
| 1:P:113:SER:HB3  | 1:P:115:PHE:CE2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:129:ILE:HD12 | 1:R:132:SER:OG   | 2.12                     | 0.48              |
| 1:R:227:LYS:HD2  | 1:R:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:S:37:VAL:HG12  | 1:S:38:THR:N     | 2.26                     | 0.48              |
| 1:T:227:LYS:HD2  | 1:T:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:V:37:VAL:HG12  | 1:V:38:THR:N     | 2.26                     | 0.48              |
| 1:X:66:GLN:NE2   | 1:X:67:PHE:H     | 2.10                     | 0.48              |
| 1:Y:227:LYS:HD2  | 1:Y:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:E:227:LYS:HD2  | 1:E:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:I:6:THR:HG22   | 1:I:217:ILE:HD13 | 1.94                     | 0.48              |
| 1:L:66:GLN:NE2   | 1:L:67:PHE:H     | 2.10                     | 0.48              |
| 1:O:62:LEU:HD22  | 1:O:136:THR:HG22 | 1.94                     | 0.48              |
| 1:O:227:LYS:HD2  | 1:O:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:Q:58:LEU:O     | 1:Q:62:LEU:HG    | 2.12                     | 0.48              |
| 1:S:227:LYS:HD2  | 1:S:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:W:37:VAL:HG12  | 1:W:38:THR:N     | 2.26                     | 0.48              |
| 1:B:58:LEU:O     | 1:B:62:LEU:HG    | 2.12                     | 0.48              |
| 1:B:81:GLU:OE2   | 1:B:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:H:71:VAL:HB    | 1:H:124:ASP:CB   | 2.32                     | 0.48              |
| 1:I:58:LEU:O     | 1:I:62:LEU:HG    | 2.12                     | 0.48              |
| 1:I:129:ILE:HD12 | 1:I:132:SER:OG   | 2.12                     | 0.48              |
| 1:L:62:LEU:HD22  | 1:L:136:THR:HG22 | 1.94                     | 0.48              |
| 1:N:81:GLU:OE2   | 1:N:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:P:66:GLN:NE2   | 1:P:67:PHE:H     | 2.10                     | 0.48              |
| 1:P:227:LYS:HD2  | 1:P:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:Q:227:LYS:HD2  | 1:Q:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:Z:6:THR:HG22   | 1:Z:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:a:129:ILE:HD12 | 1:a:132:SER:OG   | 2.12                     | 0.48              |
| 1:c:129:ILE:HD12 | 1:c:132:SER:OG   | 2.12                     | 0.48              |
| 1:F:62:LEU:HD22  | 1:F:136:THR:HG22 | 1.94                     | 0.48              |
| 1:I:113:SER:HB3  | 1:I:115:PHE:CE2  | 2.49                     | 0.48              |
| 1:O:167:LYS:HE2  | 1:O:167:LYS:HB2  | 1.47                     | 0.48              |
| 1:P:129:ILE:HD12 | 1:P:132:SER:OG   | 2.12                     | 0.48              |
| 1:P:167:LYS:HE2  | 1:P:167:LYS:HB2  | 1.47                     | 0.48              |
| 1:Q:129:ILE:HD12 | 1:Q:132:SER:OG   | 2.12                     | 0.48              |
| 1:T:36:LEU:HG    | 1:T:157:VAL:HG22 | 1.93                     | 0.48              |
| 1:T:52:GLN:NE2   | 1:T:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:V:39:LYS:HB2   | 1:V:39:LYS:HE3   | 1.46                     | 0.48              |
| 1:Y:81:GLU:OE2   | 1:Y:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:C:58:LEU:O     | 1:C:62:LEU:HG    | 2.12                     | 0.48              |
| 1:F:227:LYS:HD2  | 1:F:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:J:58:LEU:O     | 1:J:62:LEU:HG    | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:227:LYS:HD2  | 1:K:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:M:113:SER:HB3  | 1:M:115:PHE:CE2  | 2.48                     | 0.48              |
| 1:O:52:GLN:NE2   | 1:O:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:Q:81:GLU:OE2   | 1:Q:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:Q:167:LYS:HB2  | 1:Q:167:LYS:HE2  | 1.46                     | 0.48              |
| 1:T:113:SER:HB3  | 1:T:115:PHE:CE2  | 2.48                     | 0.48              |
| 1:W:52:GLN:NE2   | 1:W:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:X:227:LYS:HD2  | 1:X:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:a:66:GLN:NE2   | 1:a:67:PHE:H     | 2.10                     | 0.48              |
| 1:b:129:ILE:HD12 | 1:b:132:SER:OG   | 2.12                     | 0.48              |
| 1:E:81:GLU:OE2   | 1:E:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:G:52:GLN:NE2   | 1:G:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:K:52:GLN:NE2   | 1:K:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:L:81:GLU:OE2   | 1:L:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:N:227:LYS:HD2  | 1:N:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:P:52:GLN:NE2   | 1:P:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:S:81:GLU:OE2   | 1:S:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:S:167:LYS:HE2  | 1:S:167:LYS:HB2  | 1.46                     | 0.48              |
| 1:U:62:LEU:HD22  | 1:U:136:THR:HG22 | 1.94                     | 0.48              |
| 1:Y:15:ALA:H     | 1:Z:24:ASN:HB3   | 1.78                     | 0.48              |
| 1:Z:1:MET:HE2    | 1:Z:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:Z:52:GLN:NE2   | 1:Z:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:a:52:GLN:NE2   | 1:a:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:a:81:GLU:OE2   | 1:a:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:b:66:GLN:NE2   | 1:b:67:PHE:H     | 2.10                     | 0.48              |
| 1:d:6:THR:HG22   | 1:d:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:d:52:GLN:NE2   | 1:d:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:d:81:GLU:OE2   | 1:d:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:A:52:GLN:NE2   | 1:A:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:D:6:THR:HG22   | 1:D:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:D:81:GLU:OE2   | 1:D:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:G:62:LEU:HD22  | 1:G:136:THR:HG22 | 1.94                     | 0.48              |
| 1:G:81:GLU:OE2   | 1:G:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:J:81:GLU:OE2   | 1:J:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:M:6:THR:HG22   | 1:M:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:N:62:LEU:HD22  | 1:N:136:THR:HG22 | 1.94                     | 0.48              |
| 1:P:6:THR:HG22   | 1:P:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:T:6:THR:HG22   | 1:T:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:T:58:LEU:O     | 1:T:62:LEU:HG    | 2.12                     | 0.48              |
| 1:V:1:MET:HE2    | 1:V:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:W:1:MET:HE2    | 1:W:3:ALA:HB3    | 1.96                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:W:81:GLU:OE2  | 1:W:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:c:6:THR:HG22  | 1:c:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:D:52:GLN:NE2  | 1:D:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:F:52:GLN:NE2  | 1:F:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:H:52:GLN:NE2  | 1:H:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:J:227:LYS:HD2 | 1:J:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:K:58:LEU:O    | 1:K:62:LEU:HG    | 2.12                     | 0.48              |
| 1:M:52:GLN:NE2  | 1:M:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:M:62:LEU:HD22 | 1:M:136:THR:HG22 | 1.94                     | 0.48              |
| 1:M:227:LYS:HD2 | 1:M:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:N:39:LYS:HB2  | 1:N:39:LYS:HE3   | 1.46                     | 0.48              |
| 1:P:81:GLU:OE2  | 1:P:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:S:52:GLN:NE2  | 1:S:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:V:6:THR:HG22  | 1:V:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:V:52:GLN:NE2  | 1:V:153:GLU:OE1  | 2.47                     | 0.48              |
| 1:Y:1:MET:HE2   | 1:Y:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:c:81:GLU:OE2  | 1:c:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:d:66:GLN:NE2  | 1:d:67:PHE:H     | 2.10                     | 0.48              |
| 1:L:227:LYS:HD2 | 1:L:229:ASP:HB2  | 1.95                     | 0.48              |
| 1:N:167:LYS:HE2 | 1:N:167:LYS:HB2  | 1.47                     | 0.48              |
| 1:Q:6:THR:HG22  | 1:Q:217:ILE:HD13 | 1.95                     | 0.48              |
| 1:R:58:LEU:O    | 1:R:62:LEU:HG    | 2.12                     | 0.48              |
| 1:T:66:GLN:NE2  | 1:T:67:PHE:H     | 2.10                     | 0.48              |
| 1:U:1:MET:HE2   | 1:U:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:U:81:GLU:OE2  | 1:U:83:LYS:HG3   | 2.14                     | 0.48              |
| 1:X:1:MET:HE2   | 1:X:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:a:1:MET:HE2   | 1:a:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:b:1:MET:HE2   | 1:b:3:ALA:HB3    | 1.96                     | 0.48              |
| 1:c:113:SER:HB3 | 1:c:115:PHE:CE2  | 2.48                     | 0.48              |
| 1:B:151:ARG:HA  | 1:B:151:ARG:HD2  | 1.37                     | 0.47              |
| 1:G:227:LYS:HD2 | 1:G:229:ASP:HB2  | 1.95                     | 0.47              |
| 1:I:39:LYS:HE3  | 1:I:39:LYS:HB2   | 1.46                     | 0.47              |
| 1:L:1:MET:HE2   | 1:L:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:M:1:MET:HE2   | 1:M:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:N:1:MET:HE2   | 1:N:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:N:6:THR:HG22  | 1:N:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:N:52:GLN:NE2  | 1:N:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:O:6:THR:HG22  | 1:O:217:ILE:HD13 | 1.94                     | 0.47              |
| 1:Q:113:SER:HB3 | 1:Q:115:PHE:CE2  | 2.49                     | 0.47              |
| 1:S:58:LEU:O    | 1:S:62:LEU:HG    | 2.12                     | 0.47              |
| 1:U:6:THR:HG22  | 1:U:217:ILE:HD13 | 1.95                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:U:52:GLN:NE2  | 1:U:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:V:81:GLU:OE2  | 1:V:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:X:52:GLN:NE2  | 1:X:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:c:1:MET:HE2   | 1:c:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:C:52:GLN:NE2  | 1:C:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:E:39:LYS:HB2  | 1:E:39:LYS:HE3   | 1.46                     | 0.47              |
| 1:E:52:GLN:NE2  | 1:E:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:J:52:GLN:NE2  | 1:J:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:L:52:GLN:NE2  | 1:L:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:b:81:GLU:OE2  | 1:b:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:A:113:SER:HB3 | 1:A:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:B:52:GLN:NE2  | 1:B:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:C:71:VAL:HB   | 1:C:124:ASP:CB   | 2.32                     | 0.47              |
| 1:H:81:GLU:OE2  | 1:H:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:H:227:LYS:HD2 | 1:H:229:ASP:HB2  | 1.95                     | 0.47              |
| 1:I:227:LYS:HD2 | 1:I:229:ASP:HB2  | 1.95                     | 0.47              |
| 1:O:81:GLU:OE2  | 1:O:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:P:1:MET:HE2   | 1:P:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:T:81:GLU:OE2  | 1:T:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:W:6:THR:HG22  | 1:W:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:c:52:GLN:NE2  | 1:c:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:F:39:LYS:HB2  | 1:F:39:LYS:HE3   | 1.45                     | 0.47              |
| 1:H:6:THR:HG22  | 1:H:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:Q:52:GLN:NE2  | 1:Q:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:U:227:LYS:HD2 | 1:U:229:ASP:HB2  | 1.95                     | 0.47              |
| 1:W:227:LYS:HD2 | 1:W:229:ASP:HB2  | 1.95                     | 0.47              |
| 1:a:151:ARG:HA  | 1:a:151:ARG:HD2  | 1.37                     | 0.47              |
| 1:b:52:GLN:NE2  | 1:b:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:C:81:GLU:OE2  | 1:C:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:E:151:ARG:HA  | 1:E:151:ARG:HD2  | 1.37                     | 0.47              |
| 1:H:39:LYS:HB2  | 1:H:39:LYS:HE3   | 1.46                     | 0.47              |
| 1:H:113:SER:HB3 | 1:H:115:PHE:CE2  | 2.49                     | 0.47              |
| 1:I:167:LYS:HE2 | 1:I:167:LYS:HB2  | 1.47                     | 0.47              |
| 1:O:1:MET:HE2   | 1:O:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:R:52:GLN:NE2  | 1:R:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:X:113:SER:HB3 | 1:X:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:Z:113:SER:HB3 | 1:Z:115:PHE:CE2  | 2.49                     | 0.47              |
| 1:A:1:MET:HE2   | 1:A:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:A:81:GLU:OE2  | 1:A:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:F:237:LEU:HG  | 1:F:238:ARG:N    | 2.30                     | 0.47              |
| 1:G:39:LYS:HE3  | 1:G:39:LYS:HB2   | 1.46                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:237:LEU:HG  | 1:G:238:ARG:N    | 2.30                     | 0.47              |
| 1:I:52:GLN:NE2  | 1:I:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:K:81:GLU:OE2  | 1:K:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:L:6:THR:HG22  | 1:L:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:M:81:GLU:OE2  | 1:M:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:N:40:LYS:HB3  | 1:N:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:V:113:SER:HB3 | 1:V:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:X:81:GLU:OE2  | 1:X:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:b:113:SER:HB3 | 1:b:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:d:1:MET:HE2   | 1:d:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:B:1:MET:HE2   | 1:B:3:ALA:HB3    | 1.96                     | 0.47              |
| 1:B:113:SER:HB3 | 1:B:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:B:234:PHE:N   | 1:B:234:PHE:CD1  | 2.83                     | 0.47              |
| 1:B:237:LEU:HG  | 1:B:238:ARG:N    | 2.30                     | 0.47              |
| 1:C:234:PHE:N   | 1:C:234:PHE:CD1  | 2.83                     | 0.47              |
| 1:D:113:SER:HB3 | 1:D:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:D:237:LEU:HG  | 1:D:238:ARG:N    | 2.30                     | 0.47              |
| 1:E:237:LEU:HG  | 1:E:238:ARG:N    | 2.30                     | 0.47              |
| 1:F:40:LYS:HB3  | 1:F:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:G:40:LYS:HB3  | 1:G:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:I:81:GLU:OE2  | 1:I:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:I:237:LEU:HG  | 1:I:238:ARG:N    | 2.30                     | 0.47              |
| 1:J:234:PHE:N   | 1:J:234:PHE:CD1  | 2.83                     | 0.47              |
| 1:K:113:SER:HB3 | 1:K:115:PHE:CE2  | 2.48                     | 0.47              |
| 1:L:40:LYS:HB3  | 1:L:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:M:40:LYS:HB3  | 1:M:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:N:113:SER:HB3 | 1:N:115:PHE:CE2  | 2.49                     | 0.47              |
| 1:O:40:LYS:HB3  | 1:O:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:P:40:LYS:HB3  | 1:P:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:R:6:THR:HG22  | 1:R:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:R:167:LYS:HE2 | 1:R:167:LYS:HB2  | 1.47                     | 0.47              |
| 1:S:6:THR:HG22  | 1:S:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:X:6:THR:HG22  | 1:X:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:Y:6:THR:HG22  | 1:Y:217:ILE:HD13 | 1.95                     | 0.47              |
| 1:Y:52:GLN:NE2  | 1:Y:153:GLU:OE1  | 2.47                     | 0.47              |
| 1:Z:81:GLU:OE2  | 1:Z:83:LYS:HG3   | 2.14                     | 0.47              |
| 1:a:113:SER:HB3 | 1:a:115:PHE:CE2  | 2.49                     | 0.47              |
| 1:b:15:ALA:H    | 1:c:24:ASN:HB3   | 1.78                     | 0.47              |
| 1:C:237:LEU:HG  | 1:C:238:ARG:N    | 2.30                     | 0.47              |
| 1:E:40:LYS:HB3  | 1:E:50:LYS:HB3   | 1.97                     | 0.47              |
| 1:H:40:LYS:HB3  | 1:H:50:LYS:HB3   | 1.97                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:237:LEU:HG  | 1:H:238:ARG:N   | 2.30                     | 0.47              |
| 1:K:237:LEU:HG  | 1:K:238:ARG:N   | 2.30                     | 0.47              |
| 1:Q:237:LEU:HG  | 1:Q:238:ARG:N   | 2.30                     | 0.47              |
| 1:S:1:MET:HE2   | 1:S:3:ALA:HB3   | 1.96                     | 0.47              |
| 1:T:237:LEU:HG  | 1:T:238:ARG:N   | 2.30                     | 0.47              |
| 1:V:227:LYS:HD2 | 1:V:229:ASP:HB2 | 1.95                     | 0.47              |
| 1:W:151:ARG:HA  | 1:W:151:ARG:HD2 | 1.37                     | 0.47              |
| 1:a:234:PHE:N   | 1:a:234:PHE:CD1 | 2.83                     | 0.47              |
| 1:D:40:LYS:HB3  | 1:D:50:LYS:HB3  | 1.97                     | 0.47              |
| 1:F:81:GLU:OE2  | 1:F:83:LYS:HG3  | 2.14                     | 0.47              |
| 1:G:6:THR:HG22  | 1:G:217:ILE:CD1 | 2.45                     | 0.47              |
| 1:J:237:LEU:HG  | 1:J:238:ARG:N   | 2.30                     | 0.47              |
| 1:M:167:LYS:HE2 | 1:M:167:LYS:HB2 | 1.47                     | 0.47              |
| 1:Q:1:MET:HE2   | 1:Q:3:ALA:HB3   | 1.96                     | 0.47              |
| 1:R:1:MET:HE2   | 1:R:3:ALA:HB3   | 1.96                     | 0.47              |
| 1:U:40:LYS:HB3  | 1:U:50:LYS:HB3  | 1.97                     | 0.47              |
| 1:c:6:THR:HG22  | 1:c:217:ILE:CD1 | 2.45                     | 0.47              |
| 1:d:6:THR:HG22  | 1:d:217:ILE:CD1 | 2.45                     | 0.47              |
| 1:C:113:SER:HB3 | 1:C:115:PHE:CE2 | 2.48                     | 0.47              |
| 1:F:6:THR:HG22  | 1:F:217:ILE:CD1 | 2.45                     | 0.47              |
| 1:I:40:LYS:HB3  | 1:I:50:LYS:HB3  | 1.97                     | 0.47              |
| 1:I:234:PHE:N   | 1:I:234:PHE:CD1 | 2.83                     | 0.47              |
| 1:L:39:LYS:HB2  | 1:L:39:LYS:HE3  | 1.46                     | 0.47              |
| 1:O:39:LYS:HE3  | 1:O:39:LYS:HB2  | 1.45                     | 0.47              |
| 1:Q:40:LYS:HB3  | 1:Q:50:LYS:HB3  | 1.97                     | 0.47              |
| 1:R:234:PHE:N   | 1:R:234:PHE:CD1 | 2.83                     | 0.47              |
| 1:S:237:LEU:HG  | 1:S:238:ARG:N   | 2.30                     | 0.47              |
| 1:X:234:PHE:CD1 | 1:X:234:PHE:N   | 2.83                     | 0.47              |
| 1:d:234:PHE:N   | 1:d:234:PHE:CD1 | 2.83                     | 0.47              |
| 1:A:6:THR:HG22  | 1:A:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:A:237:LEU:HG  | 1:A:238:ARG:N   | 2.30                     | 0.46              |
| 1:C:1:MET:HE2   | 1:C:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:C:40:LYS:HB3  | 1:C:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:E:1:MET:HE2   | 1:E:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:H:6:THR:HG22  | 1:H:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:Q:234:PHE:N   | 1:Q:234:PHE:CD1 | 2.83                     | 0.46              |
| 1:R:81:GLU:OE2  | 1:R:83:LYS:HG3  | 2.14                     | 0.46              |
| 1:R:237:LEU:HG  | 1:R:238:ARG:N   | 2.30                     | 0.46              |
| 1:V:40:LYS:HB3  | 1:V:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:D:1:MET:HE2   | 1:D:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:E:6:THR:HG22  | 1:E:217:ILE:CD1 | 2.45                     | 0.46              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:1:MET:HE2   | 1:F:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:F:113:SER:HB3 | 1:F:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:J:40:LYS:HB3  | 1:J:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:O:6:THR:HG22  | 1:O:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:P:237:LEU:HG  | 1:P:238:ARG:N   | 2.30                     | 0.46              |
| 1:c:237:LEU:HG  | 1:c:238:ARG:N   | 2.30                     | 0.46              |
| 1:A:234:PHE:N   | 1:A:234:PHE:CD1 | 2.83                     | 0.46              |
| 1:B:40:LYS:HB3  | 1:B:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:D:87:HIS:HB3  | 1:E:202:THR:HB  | 1.97                     | 0.46              |
| 1:G:110:GLU:OE1 | 1:G:110:GLU:O   | 2.34                     | 0.46              |
| 1:H:110:GLU:OE1 | 1:H:110:GLU:O   | 2.34                     | 0.46              |
| 1:M:6:THR:HG22  | 1:M:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:N:6:THR:HG22  | 1:N:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:R:40:LYS:HB3  | 1:R:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:R:113:SER:HB3 | 1:R:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:U:234:PHE:N   | 1:U:234:PHE:CD1 | 2.83                     | 0.46              |
| 1:W:40:LYS:HB3  | 1:W:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:b:6:THR:HG22  | 1:b:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:d:237:LEU:HG  | 1:d:238:ARG:N   | 2.30                     | 0.46              |
| 1:B:6:THR:HG22  | 1:B:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:F:110:GLU:OE1 | 1:F:110:GLU:O   | 2.34                     | 0.46              |
| 1:I:110:GLU:OE1 | 1:I:110:GLU:O   | 2.34                     | 0.46              |
| 1:L:6:THR:HG22  | 1:L:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:P:6:THR:HG22  | 1:P:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:S:40:LYS:HB3  | 1:S:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:T:1:MET:HE2   | 1:T:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:U:110:GLU:OE1 | 1:U:110:GLU:O   | 2.34                     | 0.46              |
| 1:X:6:THR:HG22  | 1:X:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:Y:113:SER:HB3 | 1:Y:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:b:237:LEU:HG  | 1:b:238:ARG:N   | 2.30                     | 0.46              |
| 1:E:110:GLU:OE1 | 1:E:110:GLU:O   | 2.34                     | 0.46              |
| 1:G:1:MET:HE2   | 1:G:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:G:76:ASP:HA   | 1:G:119:ARG:HA  | 1.97                     | 0.46              |
| 1:H:234:PHE:CD1 | 1:H:234:PHE:N   | 2.83                     | 0.46              |
| 1:J:110:GLU:OE1 | 1:J:110:GLU:O   | 2.34                     | 0.46              |
| 1:K:1:MET:HE2   | 1:K:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:K:40:LYS:HB3  | 1:K:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:K:234:PHE:N   | 1:K:234:PHE:CD1 | 2.83                     | 0.46              |
| 1:L:110:GLU:OE1 | 1:L:110:GLU:O   | 2.34                     | 0.46              |
| 1:M:110:GLU:OE1 | 1:M:110:GLU:O   | 2.34                     | 0.46              |
| 1:N:110:GLU:OE1 | 1:N:110:GLU:O   | 2.34                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:110:GLU:OE1  | 1:O:110:GLU:O   | 2.34                     | 0.46              |
| 1:Q:6:THR:HG22   | 1:Q:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:T:6:THR:HG22   | 1:T:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:U:6:THR:HG22   | 1:U:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:V:110:GLU:OE1  | 1:V:110:GLU:O   | 2.34                     | 0.46              |
| 1:X:110:GLU:OE1  | 1:X:110:GLU:O   | 2.34                     | 0.46              |
| 1:d:113:SER:HB3  | 1:d:115:PHE:CE2 | 2.49                     | 0.46              |
| 1:A:40:LYS:HB3   | 1:A:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:A:241:GLN:OE1  | 1:A:241:GLN:N   | 2.49                     | 0.46              |
| 1:B:241:GLN:OE1  | 1:B:241:GLN:N   | 2.49                     | 0.46              |
| 1:D:76:ASP:HA    | 1:D:119:ARG:HA  | 1.97                     | 0.46              |
| 1:E:241:GLN:OE1  | 1:E:241:GLN:N   | 2.49                     | 0.46              |
| 1:F:76:ASP:HA    | 1:F:119:ARG:HA  | 1.98                     | 0.46              |
| 1:F:241:GLN:OE1  | 1:F:241:GLN:N   | 2.49                     | 0.46              |
| 1:I:6:THR:HG22   | 1:I:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:J:1:MET:HE2    | 1:J:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:K:110:GLU:OE1  | 1:K:110:GLU:O   | 2.34                     | 0.46              |
| 1:M:169:VAL:HG22 | 1:M:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:O:237:LEU:HG   | 1:O:238:ARG:N   | 2.30                     | 0.46              |
| 1:P:110:GLU:OE1  | 1:P:110:GLU:O   | 2.34                     | 0.46              |
| 1:R:6:THR:HG22   | 1:R:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:T:169:VAL:HG22 | 1:T:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:W:110:GLU:OE1  | 1:W:110:GLU:O   | 2.34                     | 0.46              |
| 1:Y:6:THR:HG22   | 1:Y:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:Z:110:GLU:OE1  | 1:Z:110:GLU:O   | 2.34                     | 0.46              |
| 1:a:237:LEU:HG   | 1:a:238:ARG:N   | 2.30                     | 0.46              |
| 1:c:151:ARG:HA   | 1:c:151:ARG:HD2 | 1.37                     | 0.46              |
| 1:C:110:GLU:O    | 1:C:110:GLU:OE1 | 2.34                     | 0.46              |
| 1:C:241:GLN:OE1  | 1:C:241:GLN:N   | 2.49                     | 0.46              |
| 1:D:110:GLU:OE1  | 1:D:110:GLU:O   | 2.34                     | 0.46              |
| 1:H:1:MET:HE2    | 1:H:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:J:169:VAL:HG22 | 1:J:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:K:6:THR:HG22   | 1:K:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:K:169:VAL:HG22 | 1:K:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:L:76:ASP:HA    | 1:L:119:ARG:HA  | 1.97                     | 0.46              |
| 1:L:169:VAL:HG22 | 1:L:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:N:62:LEU:O     | 1:N:64:GLU:N    | 2.44                     | 0.46              |
| 1:S:6:THR:HG22   | 1:S:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:U:113:SER:HB3  | 1:U:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:V:6:THR:HG22   | 1:V:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:W:113:SER:HB3  | 1:W:115:PHE:CE2 | 2.48                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:X:71:VAL:HB    | 1:X:124:ASP:CB  | 2.32                     | 0.46              |
| 1:Y:110:GLU:OE1  | 1:Y:110:GLU:O   | 2.34                     | 0.46              |
| 1:a:110:GLU:OE1  | 1:a:110:GLU:O   | 2.34                     | 0.46              |
| 1:B:110:GLU:OE1  | 1:B:110:GLU:O   | 2.34                     | 0.46              |
| 1:C:76:ASP:HA    | 1:C:119:ARG:HA  | 1.97                     | 0.46              |
| 1:D:6:THR:HG22   | 1:D:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:E:167:LYS:HE2  | 1:E:167:LYS:HB2 | 1.47                     | 0.46              |
| 1:G:87:HIS:HB3   | 1:H:202:THR:HB  | 1.97                     | 0.46              |
| 1:I:1:MET:HE2    | 1:I:3:ALA:HB3   | 1.96                     | 0.46              |
| 1:I:76:ASP:HA    | 1:I:119:ARG:HA  | 1.98                     | 0.46              |
| 1:N:169:VAL:HG22 | 1:N:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:N:234:PHE:N    | 1:N:234:PHE:CD1 | 2.83                     | 0.46              |
| 1:O:151:ARG:HA   | 1:O:151:ARG:HD2 | 1.37                     | 0.46              |
| 1:R:169:VAL:HG22 | 1:R:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:S:169:VAL:HG22 | 1:S:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:T:110:GLU:OE1  | 1:T:110:GLU:O   | 2.34                     | 0.46              |
| 1:V:169:VAL:HG22 | 1:V:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:X:169:VAL:HG22 | 1:X:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:Y:169:VAL:HG22 | 1:Y:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:Z:169:VAL:HG22 | 1:Z:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:Z:237:LEU:HG   | 1:Z:238:ARG:N   | 2.30                     | 0.46              |
| 1:Z:241:GLN:N    | 1:Z:241:GLN:OE1 | 2.49                     | 0.46              |
| 1:a:169:VAL:HG22 | 1:a:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:b:110:GLU:OE1  | 1:b:110:GLU:O   | 2.34                     | 0.46              |
| 1:d:241:GLN:OE1  | 1:d:241:GLN:N   | 2.49                     | 0.46              |
| 1:A:110:GLU:OE1  | 1:A:110:GLU:O   | 2.34                     | 0.46              |
| 1:E:76:ASP:HA    | 1:E:119:ARG:HA  | 1.98                     | 0.46              |
| 1:H:76:ASP:HA    | 1:H:119:ARG:HA  | 1.98                     | 0.46              |
| 1:J:76:ASP:HA    | 1:J:119:ARG:HA  | 1.97                     | 0.46              |
| 1:K:39:LYS:HB2   | 1:K:39:LYS:HE3  | 1.46                     | 0.46              |
| 1:M:237:LEU:HG   | 1:M:238:ARG:N   | 2.30                     | 0.46              |
| 1:N:76:ASP:HA    | 1:N:119:ARG:HA  | 1.98                     | 0.46              |
| 1:O:76:ASP:HA    | 1:O:119:ARG:HA  | 1.98                     | 0.46              |
| 1:Q:110:GLU:OE1  | 1:Q:110:GLU:O   | 2.34                     | 0.46              |
| 1:S:110:GLU:OE1  | 1:S:110:GLU:O   | 2.34                     | 0.46              |
| 1:T:40:LYS:HB3   | 1:T:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:U:169:VAL:HG22 | 1:U:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:V:71:VAL:HB    | 1:V:124:ASP:CB  | 2.32                     | 0.46              |
| 1:W:6:THR:HG22   | 1:W:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:X:40:LYS:HB3   | 1:X:50:LYS:HB3  | 1.97                     | 0.46              |
| 1:Y:237:LEU:HG   | 1:Y:238:ARG:N   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:a:241:GLN:OE1  | 1:a:241:GLN:N   | 2.49                     | 0.46              |
| 1:c:110:GLU:OE1  | 1:c:110:GLU:O   | 2.34                     | 0.46              |
| 1:c:167:LYS:HE2  | 1:c:167:LYS:HB2 | 1.46                     | 0.46              |
| 1:d:110:GLU:OE1  | 1:d:110:GLU:O   | 2.34                     | 0.46              |
| 1:I:169:VAL:HG22 | 1:I:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:J:113:SER:HB3  | 1:J:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:M:76:ASP:HA    | 1:M:119:ARG:HA  | 1.98                     | 0.46              |
| 1:O:113:SER:HB3  | 1:O:115:PHE:CE2 | 2.48                     | 0.46              |
| 1:O:169:VAL:HG22 | 1:O:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:Q:169:VAL:HG22 | 1:Q:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:R:110:GLU:OE1  | 1:R:110:GLU:O   | 2.34                     | 0.46              |
| 1:W:169:VAL:HG22 | 1:W:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:W:237:LEU:HG   | 1:W:238:ARG:N   | 2.30                     | 0.46              |
| 1:Y:241:GLN:OE1  | 1:Y:241:GLN:N   | 2.49                     | 0.46              |
| 1:Z:6:THR:HG22   | 1:Z:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:a:6:THR:HG22   | 1:a:217:ILE:CD1 | 2.45                     | 0.46              |
| 1:b:169:VAL:HG22 | 1:b:210:GLU:OE2 | 2.16                     | 0.46              |
| 1:D:241:GLN:N    | 1:D:241:GLN:OE1 | 2.49                     | 0.45              |
| 1:G:113:SER:HB3  | 1:G:115:PHE:CE2 | 2.49                     | 0.45              |
| 1:L:237:LEU:HG   | 1:L:238:ARG:N   | 2.30                     | 0.45              |
| 1:P:76:ASP:HA    | 1:P:119:ARG:HA  | 1.98                     | 0.45              |
| 1:U:76:ASP:HA    | 1:U:119:ARG:HA  | 1.98                     | 0.45              |
| 1:X:87:HIS:HB3   | 1:Y:202:THR:HB  | 1.97                     | 0.45              |
| 1:c:169:VAL:HG22 | 1:c:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:d:40:LYS:HB3   | 1:d:50:LYS:HB3  | 1.97                     | 0.45              |
| 1:B:76:ASP:HA    | 1:B:119:ARG:HA  | 1.98                     | 0.45              |
| 1:C:6:THR:HG22   | 1:C:217:ILE:CD1 | 2.45                     | 0.45              |
| 1:E:113:SER:HB3  | 1:E:115:PHE:CE2 | 2.49                     | 0.45              |
| 1:F:234:PHE:N    | 1:F:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:G:234:PHE:N    | 1:G:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:G:241:GLN:N    | 1:G:241:GLN:OE1 | 2.49                     | 0.45              |
| 1:H:169:VAL:HG22 | 1:H:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:J:6:THR:HG22   | 1:J:217:ILE:CD1 | 2.45                     | 0.45              |
| 1:J:71:VAL:HB    | 1:J:124:ASP:CB  | 2.32                     | 0.45              |
| 1:J:241:GLN:OE1  | 1:J:241:GLN:N   | 2.49                     | 0.45              |
| 1:L:113:SER:HB3  | 1:L:115:PHE:CE2 | 2.48                     | 0.45              |
| 1:L:167:LYS:HB2  | 1:L:167:LYS:HE2 | 1.47                     | 0.45              |
| 1:N:241:GLN:OE1  | 1:N:241:GLN:N   | 2.49                     | 0.45              |
| 1:U:87:HIS:HB3   | 1:V:202:THR:HB  | 1.98                     | 0.45              |
| 1:V:234:PHE:N    | 1:V:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:c:40:LYS:HB3   | 1:c:50:LYS:HB3  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:169:VAL:HG22 | 1:d:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:A:76:ASP:HA    | 1:A:119:ARG:HA  | 1.98                     | 0.45              |
| 1:B:39:LYS:HB2   | 1:B:39:LYS:HE3  | 1.46                     | 0.45              |
| 1:L:241:GLN:N    | 1:L:241:GLN:OE1 | 2.49                     | 0.45              |
| 1:M:241:GLN:OE1  | 1:M:241:GLN:N   | 2.49                     | 0.45              |
| 1:P:169:VAL:HG22 | 1:P:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:b:40:LYS:HB3   | 1:b:50:LYS:HB3  | 1.97                     | 0.45              |
| 1:d:76:ASP:HA    | 1:d:119:ARG:HA  | 1.98                     | 0.45              |
| 1:A:169:VAL:HG22 | 1:A:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:E:71:VAL:HB    | 1:E:124:ASP:CB  | 2.32                     | 0.45              |
| 1:F:169:VAL:HG22 | 1:F:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:G:169:VAL:HG22 | 1:G:210:GLU:OE2 | 2.16                     | 0.45              |
| 1:H:167:LYS:HE2  | 1:H:167:LYS:HB2 | 1.47                     | 0.45              |
| 1:I:241:GLN:OE1  | 1:I:241:GLN:N   | 2.49                     | 0.45              |
| 1:J:62:LEU:O     | 1:J:64:GLU:N    | 2.44                     | 0.45              |
| 1:K:76:ASP:HA    | 1:K:119:ARG:HA  | 1.98                     | 0.45              |
| 1:K:241:GLN:OE1  | 1:K:241:GLN:N   | 2.49                     | 0.45              |
| 1:S:234:PHE:N    | 1:S:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:U:237:LEU:HG   | 1:U:238:ARG:N   | 2.30                     | 0.45              |
| 1:V:76:ASP:HA    | 1:V:119:ARG:HA  | 1.98                     | 0.45              |
| 1:X:237:LEU:HG   | 1:X:238:ARG:N   | 2.30                     | 0.45              |
| 1:Y:40:LYS:HB3   | 1:Y:50:LYS:HB3  | 1.97                     | 0.45              |
| 1:b:234:PHE:N    | 1:b:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:c:76:ASP:HA    | 1:c:119:ARG:HA  | 1.97                     | 0.45              |
| 1:I:37:VAL:HG11  | 1:I:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:K:37:VAL:HG11  | 1:K:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:L:37:VAL:HG11  | 1:L:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:O:241:GLN:N    | 1:O:241:GLN:OE1 | 2.49                     | 0.45              |
| 1:Q:76:ASP:HA    | 1:Q:119:ARG:HA  | 1.98                     | 0.45              |
| 1:R:62:LEU:O     | 1:R:64:GLU:N    | 2.44                     | 0.45              |
| 1:T:234:PHE:N    | 1:T:234:PHE:CD1 | 2.83                     | 0.45              |
| 1:U:151:ARG:HA   | 1:U:151:ARG:HD2 | 1.37                     | 0.45              |
| 1:V:237:LEU:HG   | 1:V:238:ARG:N   | 2.30                     | 0.45              |
| 1:Z:40:LYS:HB3   | 1:Z:50:LYS:HB3  | 1.97                     | 0.45              |
| 1:a:37:VAL:HG11  | 1:a:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:a:39:LYS:HB2   | 1:a:39:LYS:HE3  | 1.46                     | 0.45              |
| 1:c:241:GLN:OE1  | 1:c:241:GLN:N   | 2.49                     | 0.45              |
| 1:C:76:ASP:OD1   | 1:C:76:ASP:N    | 2.50                     | 0.45              |
| 1:N:37:VAL:HG11  | 1:N:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:P:37:VAL:HG11  | 1:P:51:TYR:HD1  | 1.82                     | 0.45              |
| 1:T:76:ASP:HA    | 1:T:119:ARG:HA  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:241:GLN:N    | 1:T:241:GLN:OE1  | 2.49                     | 0.45              |
| 1:W:76:ASP:HA    | 1:W:119:ARG:HA   | 1.98                     | 0.45              |
| 1:W:234:PHE:N    | 1:W:234:PHE:CD1  | 2.83                     | 0.45              |
| 1:X:241:GLN:OE1  | 1:X:241:GLN:N    | 2.49                     | 0.45              |
| 1:a:40:LYS:HB3   | 1:a:50:LYS:HB3   | 1.97                     | 0.45              |
| 1:a:76:ASP:HA    | 1:a:119:ARG:HA   | 1.97                     | 0.45              |
| 1:b:76:ASP:HA    | 1:b:119:ARG:HA   | 1.98                     | 0.45              |
| 1:b:241:GLN:N    | 1:b:241:GLN:OE1  | 2.49                     | 0.45              |
| 1:c:37:VAL:HG11  | 1:c:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:B:169:VAL:HG22 | 1:B:210:GLU:OE2  | 2.16                     | 0.45              |
| 1:D:234:PHE:N    | 1:D:234:PHE:CD1  | 2.83                     | 0.45              |
| 1:E:169:VAL:HG22 | 1:E:210:GLU:OE2  | 2.16                     | 0.45              |
| 1:N:237:LEU:HG   | 1:N:238:ARG:N    | 2.30                     | 0.45              |
| 1:P:39:LYS:HB2   | 1:P:39:LYS:HE3   | 1.46                     | 0.45              |
| 1:S:37:VAL:HG11  | 1:S:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:S:241:GLN:OE1  | 1:S:241:GLN:N    | 2.49                     | 0.45              |
| 1:V:37:VAL:HG11  | 1:V:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:B:76:ASP:OD1   | 1:B:76:ASP:N     | 2.50                     | 0.45              |
| 1:B:87:HIS:HB3   | 1:C:202:THR:HB   | 1.99                     | 0.45              |
| 1:E:37:VAL:HG11  | 1:E:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:Q:71:VAL:HB    | 1:Q:124:ASP:CB   | 2.32                     | 0.45              |
| 1:R:76:ASP:HA    | 1:R:119:ARG:HA   | 1.97                     | 0.45              |
| 1:R:241:GLN:OE1  | 1:R:241:GLN:N    | 2.49                     | 0.45              |
| 1:U:241:GLN:OE1  | 1:U:241:GLN:N    | 2.49                     | 0.45              |
| 1:W:241:GLN:N    | 1:W:241:GLN:OE1  | 2.49                     | 0.45              |
| 1:X:37:VAL:HG11  | 1:X:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:D:37:VAL:HG11  | 1:D:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:D:169:VAL:HG22 | 1:D:210:GLU:OE2  | 2.16                     | 0.45              |
| 1:F:37:VAL:HG11  | 1:F:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:F:161:LYS:HE3  | 1:F:163:THR:HG22 | 1.99                     | 0.45              |
| 1:G:161:LYS:HE3  | 1:G:163:THR:HG22 | 1.99                     | 0.45              |
| 1:H:161:LYS:HE3  | 1:H:163:THR:HG22 | 1.99                     | 0.45              |
| 1:H:241:GLN:OE1  | 1:H:241:GLN:N    | 2.49                     | 0.45              |
| 1:I:161:LYS:HE3  | 1:I:163:THR:HG22 | 1.99                     | 0.45              |
| 1:M:202:THR:HB   | 1:N:87:HIS:HB3   | 1.98                     | 0.45              |
| 1:P:241:GLN:OE1  | 1:P:241:GLN:N    | 2.49                     | 0.45              |
| 1:R:37:VAL:HG11  | 1:R:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:V:241:GLN:OE1  | 1:V:241:GLN:N    | 2.49                     | 0.45              |
| 1:X:76:ASP:HA    | 1:X:119:ARG:HA   | 1.97                     | 0.45              |
| 1:Y:37:VAL:HG11  | 1:Y:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:Y:234:PHE:N    | 1:Y:234:PHE:CD1  | 2.83                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:VAL:HG11  | 1:B:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:D:151:ARG:HA   | 1:D:151:ARG:HD2  | 1.37                     | 0.45              |
| 1:J:87:HIS:HB3   | 1:K:202:THR:HB   | 1.97                     | 0.45              |
| 1:J:161:LYS:HE3  | 1:J:163:THR:HG22 | 1.99                     | 0.45              |
| 1:L:87:HIS:HB3   | 1:U:202:THR:HB   | 1.99                     | 0.45              |
| 1:W:87:HIS:HB3   | 1:X:202:THR:HB   | 1.98                     | 0.45              |
| 1:Z:76:ASP:HA    | 1:Z:119:ARG:HA   | 1.97                     | 0.45              |
| 1:a:87:HIS:HB3   | 1:b:202:THR:HB   | 1.98                     | 0.45              |
| 1:c:234:PHE:CD1  | 1:c:234:PHE:N    | 2.83                     | 0.45              |
| 1:d:37:VAL:HG11  | 1:d:51:TYR:HD1   | 1.82                     | 0.45              |
| 1:d:62:LEU:O     | 1:d:64:GLU:N     | 2.44                     | 0.45              |
| 1:C:37:VAL:HG11  | 1:C:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:C:169:VAL:HG22 | 1:C:210:GLU:OE2  | 2.16                     | 0.44              |
| 1:E:161:LYS:HE3  | 1:E:163:THR:HG22 | 1.99                     | 0.44              |
| 1:G:37:VAL:HG11  | 1:G:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:K:161:LYS:HE3  | 1:K:163:THR:HG22 | 1.99                     | 0.44              |
| 1:M:36:LEU:HD11  | 1:M:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:Q:37:VAL:HG11  | 1:Q:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:S:76:ASP:HA    | 1:S:119:ARG:HA   | 1.98                     | 0.44              |
| 1:A:37:VAL:HG11  | 1:A:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:A:87:HIS:HB3   | 1:B:202:THR:HB   | 1.99                     | 0.44              |
| 1:D:161:LYS:HE3  | 1:D:163:THR:HG22 | 1.99                     | 0.44              |
| 1:E:62:LEU:O     | 1:E:64:GLU:N     | 2.44                     | 0.44              |
| 1:E:234:PHE:N    | 1:E:234:PHE:CD1  | 2.83                     | 0.44              |
| 1:H:37:VAL:HG11  | 1:H:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:H:87:HIS:HB3   | 1:I:202:THR:HB   | 1.99                     | 0.44              |
| 1:L:36:LEU:HD11  | 1:L:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:N:36:LEU:HD11  | 1:N:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:T:37:VAL:HG11  | 1:T:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:T:161:LYS:HE3  | 1:T:163:THR:HG22 | 1.99                     | 0.44              |
| 1:U:79:LYS:HE2   | 1:V:210:GLU:HG3  | 1.99                     | 0.44              |
| 1:Z:37:VAL:HG11  | 1:Z:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:a:98:LYS:NZ    | 1:a:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:A:98:LYS:NZ    | 1:A:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:O:224:LEU:HG   | 1:O:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:Q:241:GLN:OE1  | 1:Q:241:GLN:N    | 2.49                     | 0.44              |
| 1:R:202:THR:HB   | 1:S:87:HIS:HB3   | 1.98                     | 0.44              |
| 1:U:62:LEU:O     | 1:U:64:GLU:N     | 2.44                     | 0.44              |
| 1:c:224:LEU:HG   | 1:c:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:d:98:LYS:NZ    | 1:d:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:B:161:LYS:HE3  | 1:B:163:THR:HG22 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:161:LYS:HE3  | 1:C:163:THR:HG22 | 1.99                     | 0.44              |
| 1:H:151:ARG:HA   | 1:H:151:ARG:HD2  | 1.37                     | 0.44              |
| 1:O:139:LEU:HD22 | 1:O:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:R:161:LYS:HE3  | 1:R:163:THR:HG22 | 1.99                     | 0.44              |
| 1:S:161:LYS:HE3  | 1:S:163:THR:HG22 | 1.99                     | 0.44              |
| 1:U:36:LEU:HD11  | 1:U:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:U:224:LEU:HG   | 1:U:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:V:36:LEU:HD11  | 1:V:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:V:98:LYS:NZ    | 1:V:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:W:37:VAL:HG11  | 1:W:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:Y:76:ASP:OD1   | 1:Y:76:ASP:N     | 2.50                     | 0.44              |
| 1:Y:98:LYS:NZ    | 1:Y:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:Y:224:LEU:HG   | 1:Y:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:Z:98:LYS:NZ    | 1:Z:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:b:37:VAL:HG11  | 1:b:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:b:167:LYS:HE2  | 1:b:167:LYS:HB2  | 1.47                     | 0.44              |
| 1:d:224:LEU:HG   | 1:d:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:D:36:LEU:HD11  | 1:D:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:D:98:LYS:NZ    | 1:D:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:E:36:LEU:HD11  | 1:E:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:G:151:ARG:HA   | 1:G:151:ARG:HD2  | 1.37                     | 0.44              |
| 1:L:234:PHE:N    | 1:L:234:PHE:CD1  | 2.83                     | 0.44              |
| 1:M:234:PHE:N    | 1:M:234:PHE:CD1  | 2.83                     | 0.44              |
| 1:O:36:LEU:HD11  | 1:O:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:W:98:LYS:NZ    | 1:W:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:Y:62:LEU:O     | 1:Y:64:GLU:N     | 2.44                     | 0.44              |
| 1:b:98:LYS:NZ    | 1:b:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:c:98:LYS:NZ    | 1:c:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:A:161:LYS:HE3  | 1:A:163:THR:HG22 | 1.99                     | 0.44              |
| 1:A:202:THR:HB   | 1:d:87:HIS:HB3   | 1.99                     | 0.44              |
| 1:B:128:LEU:CD2  | 1:B:222:ILE:HD11 | 2.43                     | 0.44              |
| 1:C:36:LEU:HD11  | 1:C:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:C:224:LEU:HG   | 1:C:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:D:167:LYS:HE2  | 1:D:167:LYS:HB2  | 1.47                     | 0.44              |
| 1:D:224:LEU:HG   | 1:D:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:E:98:LYS:NZ    | 1:E:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:G:36:LEU:HD11  | 1:G:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:J:37:VAL:HG11  | 1:J:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:L:139:LEU:HD22 | 1:L:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:M:139:LEU:HD22 | 1:M:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:O:161:LYS:HE3  | 1:O:163:THR:HG22 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:139:LEU:HD22 | 1:P:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:P:161:LYS:HE3  | 1:P:163:THR:HG22 | 1.99                     | 0.44              |
| 1:P:224:LEU:HG   | 1:P:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:R:39:LYS:HE3   | 1:R:39:LYS:HB2   | 1.46                     | 0.44              |
| 1:R:224:LEU:HG   | 1:R:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:S:224:LEU:HG   | 1:S:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:W:36:LEU:HD11  | 1:W:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:X:36:LEU:HD11  | 1:X:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:X:79:LYS:HE2   | 1:Y:210:GLU:HG3  | 1.99                     | 0.44              |
| 1:X:98:LYS:NZ    | 1:X:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:X:139:LEU:HD22 | 1:X:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:X:203:LYS:HZ1  | 1:X:205:SER:HB2  | 1.83                     | 0.44              |
| 1:X:224:LEU:HG   | 1:X:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:Y:76:ASP:HA    | 1:Y:119:ARG:HA   | 1.98                     | 0.44              |
| 1:Z:139:LEU:HD22 | 1:Z:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:Z:234:PHE:N    | 1:Z:234:PHE:CD1  | 2.83                     | 0.44              |
| 1:b:139:LEU:HD22 | 1:b:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:c:87:HIS:HB3   | 1:d:202:THR:HB   | 1.99                     | 0.44              |
| 1:C:167:LYS:HE2  | 1:C:167:LYS:HB2  | 1.46                     | 0.44              |
| 1:E:128:LEU:CD2  | 1:E:222:ILE:HD11 | 2.43                     | 0.44              |
| 1:F:36:LEU:HD11  | 1:F:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:F:224:LEU:HG   | 1:F:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:J:224:LEU:HG   | 1:J:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:L:151:ARG:HA   | 1:L:151:ARG:HD2  | 1.37                     | 0.44              |
| 1:M:98:LYS:NZ    | 1:M:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:Q:139:LEU:HD22 | 1:Q:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:Q:161:LYS:HE3  | 1:Q:163:THR:HG22 | 1.99                     | 0.44              |
| 1:U:139:LEU:HD22 | 1:U:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:V:224:LEU:HG   | 1:V:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:W:139:LEU:HD22 | 1:W:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:X:76:ASP:OD1   | 1:X:76:ASP:N     | 2.50                     | 0.44              |
| 1:b:224:LEU:HG   | 1:b:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:B:36:LEU:HD11  | 1:B:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:B:224:LEU:HG   | 1:B:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:E:87:HIS:HB3   | 1:F:202:THR:HB   | 2.00                     | 0.44              |
| 1:E:224:LEU:HG   | 1:E:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:J:76:ASP:OD1   | 1:J:76:ASP:N     | 2.50                     | 0.44              |
| 1:L:224:LEU:HG   | 1:L:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:M:161:LYS:HE3  | 1:M:163:THR:HG22 | 1.99                     | 0.44              |
| 1:N:139:LEU:HD22 | 1:N:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:N:224:LEU:HG   | 1:N:234:PHE:CD1  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:37:VAL:HG11  | 1:O:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:O:234:PHE:CD1  | 1:O:234:PHE:N    | 2.83                     | 0.44              |
| 1:P:36:LEU:HD11  | 1:P:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:Q:224:LEU:HG   | 1:Q:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:U:37:VAL:HG11  | 1:U:51:TYR:HD1   | 1.82                     | 0.44              |
| 1:U:161:LYS:HE3  | 1:U:163:THR:HG22 | 1.99                     | 0.44              |
| 1:U:167:LYS:HE2  | 1:U:167:LYS:HB2  | 1.47                     | 0.44              |
| 1:Y:139:LEU:HD22 | 1:Y:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:Z:224:LEU:HG   | 1:Z:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:a:139:LEU:HD22 | 1:a:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:a:203:LYS:HZ1  | 1:a:205:SER:HB2  | 1.83                     | 0.44              |
| 1:d:39:LYS:HB2   | 1:d:39:LYS:HE3   | 1.46                     | 0.44              |
| 1:G:224:LEU:HG   | 1:G:234:PHE:CD1  | 2.53                     | 0.44              |
| 1:H:36:LEU:HD11  | 1:H:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:I:76:ASP:OD1   | 1:I:76:ASP:N     | 2.50                     | 0.44              |
| 1:L:161:LYS:HE3  | 1:L:163:THR:HG22 | 1.99                     | 0.44              |
| 1:M:210:GLU:HG3  | 1:N:79:LYS:HE2   | 2.00                     | 0.44              |
| 1:N:98:LYS:NZ    | 1:N:187:GLN:HG2  | 2.33                     | 0.44              |
| 1:N:161:LYS:HE3  | 1:N:163:THR:HG22 | 2.00                     | 0.44              |
| 1:R:139:LEU:HD22 | 1:R:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:S:139:LEU:HD22 | 1:S:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:T:203:LYS:HZ1  | 1:T:205:SER:HB2  | 1.83                     | 0.44              |
| 1:V:139:LEU:HD22 | 1:V:230:GLY:HA2  | 2.00                     | 0.44              |
| 1:V:161:LYS:HE3  | 1:V:163:THR:HG22 | 1.99                     | 0.44              |
| 1:W:161:LYS:HE3  | 1:W:163:THR:HG22 | 1.99                     | 0.44              |
| 1:Y:36:LEU:HD11  | 1:Y:58:LEU:CD2   | 2.48                     | 0.44              |
| 1:c:203:LYS:HZ1  | 1:c:205:SER:HB2  | 1.83                     | 0.44              |
| 1:B:39:LYS:HB3   | 1:B:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:B:98:LYS:NZ    | 1:B:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:G:39:LYS:HB3   | 1:G:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:H:39:LYS:HB3   | 1:H:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:H:98:LYS:NZ    | 1:H:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:H:203:LYS:HZ1  | 1:H:205:SER:HB2  | 1.83                     | 0.43              |
| 1:I:36:LEU:HD11  | 1:I:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:I:39:LYS:HB3   | 1:I:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:K:39:LYS:HB3   | 1:K:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:K:76:ASP:OD1   | 1:K:76:ASP:N     | 2.50                     | 0.43              |
| 1:M:37:VAL:HG11  | 1:M:51:TYR:HD1   | 1.82                     | 0.43              |
| 1:Z:36:LEU:HD11  | 1:Z:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:a:39:LYS:HB3   | 1:a:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:c:161:LYS:HE3  | 1:c:163:THR:HG22 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:161:LYS:HE3  | 1:d:163:THR:HG22 | 1.99                     | 0.43              |
| 1:F:39:LYS:HB3   | 1:F:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:H:128:LEU:CD2  | 1:H:222:ILE:HD11 | 2.43                     | 0.43              |
| 1:J:39:LYS:HB3   | 1:J:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:M:151:ARG:HA   | 1:M:151:ARG:HD2  | 1.37                     | 0.43              |
| 1:Q:36:LEU:HD11  | 1:Q:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:Q:39:LYS:HB2   | 1:Q:39:LYS:HE3   | 1.46                     | 0.43              |
| 1:Q:98:LYS:NZ    | 1:Q:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:S:39:LYS:HB3   | 1:S:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:T:76:ASP:OD1   | 1:T:76:ASP:N     | 2.50                     | 0.43              |
| 1:T:224:LEU:HG   | 1:T:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:U:98:LYS:NZ    | 1:U:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:V:203:LYS:HZ1  | 1:V:205:SER:HB2  | 1.83                     | 0.43              |
| 1:X:161:LYS:HE3  | 1:X:163:THR:HG22 | 1.99                     | 0.43              |
| 1:c:39:LYS:HB3   | 1:c:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:c:139:LEU:HD22 | 1:c:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:d:139:LEU:HD22 | 1:d:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:A:224:LEU:HG   | 1:A:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:C:98:LYS:NZ    | 1:C:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:D:39:LYS:HB3   | 1:D:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:E:39:LYS:HB3   | 1:E:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:I:224:LEU:HG   | 1:I:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:K:224:LEU:HG   | 1:K:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:O:62:LEU:O     | 1:O:64:GLU:N     | 2.44                     | 0.43              |
| 1:P:234:PHE:CD1  | 1:P:234:PHE:N    | 2.83                     | 0.43              |
| 1:W:76:ASP:OD1   | 1:W:76:ASP:N     | 2.50                     | 0.43              |
| 1:Y:161:LYS:HE3  | 1:Y:163:THR:HG22 | 1.99                     | 0.43              |
| 1:Y:203:LYS:HZ1  | 1:Y:205:SER:HB2  | 1.83                     | 0.43              |
| 1:a:36:LEU:HD11  | 1:a:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:d:39:LYS:HB3   | 1:d:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:B:167:LYS:HE2  | 1:B:167:LYS:HB2  | 1.47                     | 0.43              |
| 1:E:203:LYS:HZ1  | 1:E:205:SER:HB2  | 1.83                     | 0.43              |
| 1:F:203:LYS:HZ1  | 1:F:205:SER:HB2  | 1.83                     | 0.43              |
| 1:G:79:LYS:HE2   | 1:H:210:GLU:HG3  | 2.00                     | 0.43              |
| 1:G:203:LYS:HZ1  | 1:G:205:SER:HB2  | 1.83                     | 0.43              |
| 1:H:224:LEU:HG   | 1:H:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:L:79:LYS:HE2   | 1:U:210:GLU:HG3  | 2.01                     | 0.43              |
| 1:Q:39:LYS:HB3   | 1:Q:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:T:39:LYS:HB3   | 1:T:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:A:151:ARG:HA   | 1:A:151:ARG:HD2  | 1.37                     | 0.43              |
| 1:C:39:LYS:HB3   | 1:C:51:TYR:CE2   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:98:LYS:NZ    | 1:G:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:I:98:LYS:NZ    | 1:I:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:J:36:LEU:HD11  | 1:J:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:K:87:HIS:HB3   | 1:T:202:THR:HB   | 1.99                     | 0.43              |
| 1:L:98:LYS:NZ    | 1:L:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:M:224:LEU:HG   | 1:M:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:N:39:LYS:HB3   | 1:N:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:O:71:VAL:HB    | 1:O:124:ASP:CB   | 2.32                     | 0.43              |
| 1:O:203:LYS:HZ1  | 1:O:205:SER:HB2  | 1.83                     | 0.43              |
| 1:P:98:LYS:NZ    | 1:P:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:Q:203:LYS:HZ1  | 1:Q:205:SER:HB2  | 1.83                     | 0.43              |
| 1:R:39:LYS:HB3   | 1:R:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:T:98:LYS:NZ    | 1:T:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:T:139:LEU:HD22 | 1:T:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:W:224:LEU:HG   | 1:W:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:Y:39:LYS:HB2   | 1:Y:39:LYS:HE3   | 1.46                     | 0.43              |
| 1:Z:161:LYS:HE3  | 1:Z:163:THR:HG22 | 1.99                     | 0.43              |
| 1:b:36:LEU:HD11  | 1:b:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:F:98:LYS:NZ    | 1:F:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:I:139:LEU:HD22 | 1:I:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:J:128:LEU:CD2  | 1:J:222:ILE:HD11 | 2.43                     | 0.43              |
| 1:J:203:LYS:HZ1  | 1:J:205:SER:HB2  | 1.84                     | 0.43              |
| 1:K:36:LEU:HD11  | 1:K:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:K:139:LEU:HD22 | 1:K:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:M:39:LYS:HB3   | 1:M:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:P:39:LYS:HB3   | 1:P:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:X:39:LYS:HB3   | 1:X:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:a:224:LEU:HG   | 1:a:234:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:39:LYS:HB3   | 1:A:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:B:203:LYS:HZ1  | 1:B:205:SER:HB2  | 1.83                     | 0.43              |
| 1:C:128:LEU:CD2  | 1:C:222:ILE:HD11 | 2.43                     | 0.43              |
| 1:C:203:LYS:HZ1  | 1:C:205:SER:HB2  | 1.84                     | 0.43              |
| 1:D:139:LEU:HD22 | 1:D:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:D:203:LYS:HZ1  | 1:D:205:SER:HB2  | 1.83                     | 0.43              |
| 1:K:98:LYS:NZ    | 1:K:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:N:202:THR:HB   | 1:O:87:HIS:HB3   | 1.99                     | 0.43              |
| 1:a:79:LYS:HE2   | 1:b:210:GLU:HG3  | 1.99                     | 0.43              |
| 1:A:139:LEU:HD22 | 1:A:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:C:139:LEU:HD22 | 1:C:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:F:128:LEU:CD2  | 1:F:222:ILE:HD11 | 2.43                     | 0.43              |
| 1:H:139:LEU:HD22 | 1:H:230:GLY:HA2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:79:LYS:HE2   | 1:K:210:GLU:HG3  | 2.00                     | 0.43              |
| 1:J:139:LEU:HD22 | 1:J:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:L:39:LYS:HB3   | 1:L:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:O:39:LYS:HB3   | 1:O:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:U:39:LYS:HB3   | 1:U:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:V:39:LYS:HB3   | 1:V:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:W:39:LYS:HB3   | 1:W:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:c:36:LEU:HD11  | 1:c:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:B:139:LEU:HD22 | 1:B:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:C:39:LYS:HB2   | 1:C:39:LYS:HE3   | 1.46                     | 0.43              |
| 1:D:79:LYS:HE2   | 1:E:210:GLU:HG3  | 2.00                     | 0.43              |
| 1:I:62:LEU:O     | 1:I:64:GLU:N     | 2.44                     | 0.43              |
| 1:N:203:LYS:HZ1  | 1:N:205:SER:HB2  | 1.83                     | 0.43              |
| 1:O:33:LEU:HD12  | 1:O:161:LYS:HD2  | 2.01                     | 0.43              |
| 1:O:129:ILE:HD12 | 1:O:129:ILE:HA   | 1.87                     | 0.43              |
| 1:O:202:THR:HB   | 1:P:87:HIS:HB3   | 1.99                     | 0.43              |
| 1:P:33:LEU:HD12  | 1:P:161:LYS:HD2  | 2.01                     | 0.43              |
| 1:Q:33:LEU:HD12  | 1:Q:161:LYS:HD2  | 2.01                     | 0.43              |
| 1:T:36:LEU:HD11  | 1:T:58:LEU:CD2   | 2.48                     | 0.43              |
| 1:V:76:ASP:OD1   | 1:V:76:ASP:N     | 2.50                     | 0.43              |
| 1:W:203:LYS:HZ1  | 1:W:205:SER:HB2  | 1.83                     | 0.43              |
| 1:Y:39:LYS:HB3   | 1:Y:51:TYR:CE2   | 2.54                     | 0.43              |
| 1:Z:39:LYS:HB3   | 1:Z:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:a:161:LYS:HE3  | 1:a:163:THR:HG22 | 1.99                     | 0.43              |
| 1:b:203:LYS:HZ1  | 1:b:205:SER:HB2  | 1.83                     | 0.43              |
| 1:A:39:LYS:HB2   | 1:A:39:LYS:HE3   | 1.46                     | 0.43              |
| 1:E:139:LEU:HD22 | 1:E:230:GLY:HA2  | 2.00                     | 0.43              |
| 1:L:31:LEU:HD21  | 1:L:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:N:31:LEU:HD21  | 1:N:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:N:33:LEU:HD12  | 1:N:161:LYS:HD2  | 2.01                     | 0.43              |
| 1:P:202:THR:HB   | 1:Q:87:HIS:HB3   | 2.00                     | 0.43              |
| 1:Q:202:THR:HB   | 1:R:87:HIS:HB3   | 2.00                     | 0.43              |
| 1:R:33:LEU:HD12  | 1:R:161:LYS:HD2  | 2.01                     | 0.43              |
| 1:R:98:LYS:NZ    | 1:R:187:GLN:HG2  | 2.33                     | 0.43              |
| 1:S:31:LEU:HD21  | 1:S:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:S:151:ARG:HA   | 1:S:151:ARG:HD2  | 1.37                     | 0.43              |
| 1:T:167:LYS:HE2  | 1:T:167:LYS:HB2  | 1.47                     | 0.43              |
| 1:V:31:LEU:HD21  | 1:V:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:X:31:LEU:HD21  | 1:X:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:a:31:LEU:HD21  | 1:a:53:PHE:CE1   | 2.54                     | 0.43              |
| 1:a:167:LYS:HE2  | 1:a:167:LYS:HB2  | 1.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:39:LYS:HB3   | 1:b:51:TYR:CE2   | 2.53                     | 0.43              |
| 1:d:203:LYS:HZ1  | 1:d:205:SER:HB2  | 1.83                     | 0.43              |
| 1:A:167:LYS:HB2  | 1:A:167:LYS:HE2  | 1.46                     | 0.42              |
| 1:L:202:THR:HB   | 1:M:87:HIS:HB3   | 2.00                     | 0.42              |
| 1:M:203:LYS:HZ1  | 1:M:205:SER:HB2  | 1.83                     | 0.42              |
| 1:R:203:LYS:HZ1  | 1:R:205:SER:HB2  | 1.83                     | 0.42              |
| 1:S:203:LYS:HZ1  | 1:S:205:SER:HB2  | 1.83                     | 0.42              |
| 1:S:211:ILE:HD13 | 1:S:211:ILE:HA   | 1.93                     | 0.42              |
| 1:Y:31:LEU:HD21  | 1:Y:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:Z:87:HIS:HB3   | 1:a:202:THR:HB   | 2.00                     | 0.42              |
| 1:a:62:LEU:O     | 1:a:64:GLU:N     | 2.44                     | 0.42              |
| 1:c:33:LEU:HD12  | 1:c:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:A:203:LYS:HZ1  | 1:A:205:SER:HB2  | 1.84                     | 0.42              |
| 1:H:79:LYS:HE2   | 1:I:210:GLU:HG3  | 2.00                     | 0.42              |
| 1:H:129:ILE:HD12 | 1:H:129:ILE:HA   | 1.87                     | 0.42              |
| 1:I:203:LYS:HZ1  | 1:I:205:SER:HB2  | 1.83                     | 0.42              |
| 1:J:98:LYS:NZ    | 1:J:187:GLN:HG2  | 2.33                     | 0.42              |
| 1:J:151:ARG:HA   | 1:J:151:ARG:HD2  | 1.37                     | 0.42              |
| 1:L:203:LYS:HZ1  | 1:L:205:SER:HB2  | 1.84                     | 0.42              |
| 1:O:98:LYS:NZ    | 1:O:187:GLN:HG2  | 2.33                     | 0.42              |
| 1:Q:31:LEU:HD21  | 1:Q:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:U:31:LEU:HD21  | 1:U:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:b:33:LEU:HD12  | 1:b:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:b:161:LYS:HE3  | 1:b:163:THR:HG22 | 1.99                     | 0.42              |
| 1:d:36:LEU:HD11  | 1:d:58:LEU:CD2   | 2.48                     | 0.42              |
| 1:F:139:LEU:HD22 | 1:F:230:GLY:HA2  | 2.00                     | 0.42              |
| 1:G:33:LEU:HD12  | 1:G:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:I:33:LEU:HD12  | 1:I:161:LYS:HD2  | 2.00                     | 0.42              |
| 1:I:151:ARG:HA   | 1:I:151:ARG:HD2  | 1.37                     | 0.42              |
| 1:P:31:LEU:HD21  | 1:P:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:S:33:LEU:HD12  | 1:S:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:S:62:LEU:O     | 1:S:64:GLU:N     | 2.44                     | 0.42              |
| 1:V:98:LYS:CE    | 1:V:187:GLN:HG2  | 2.50                     | 0.42              |
| 1:W:79:LYS:HE2   | 1:X:210:GLU:HG3  | 2.01                     | 0.42              |
| 1:c:31:LEU:HD21  | 1:c:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:d:128:LEU:CD2  | 1:d:222:ILE:HD11 | 2.43                     | 0.42              |
| 1:F:33:LEU:HD12  | 1:F:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:G:139:LEU:HD22 | 1:G:230:GLY:HA2  | 2.00                     | 0.42              |
| 1:J:37:VAL:CG1   | 1:J:38:THR:N     | 2.83                     | 0.42              |
| 1:K:31:LEU:HD21  | 1:K:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:K:128:LEU:CD2  | 1:K:222:ILE:HD11 | 2.43                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:36:LEU:HD11  | 1:S:58:LEU:CD2   | 2.48                     | 0.42              |
| 1:U:76:ASP:OD1   | 1:U:76:ASP:N     | 2.50                     | 0.42              |
| 1:V:87:HIS:HB3   | 1:W:202:THR:HB   | 2.01                     | 0.42              |
| 1:W:31:LEU:HD21  | 1:W:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:Y:33:LEU:HD12  | 1:Y:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:c:62:LEU:O     | 1:c:64:GLU:N     | 2.44                     | 0.42              |
| 1:A:210:GLU:HG3  | 1:d:79:LYS:HE2   | 2.00                     | 0.42              |
| 1:C:87:HIS:HB3   | 1:D:202:THR:HB   | 2.01                     | 0.42              |
| 1:D:62:LEU:O     | 1:D:64:GLU:N     | 2.44                     | 0.42              |
| 1:G:167:LYS:HE2  | 1:G:167:LYS:HB2  | 1.47                     | 0.42              |
| 1:H:33:LEU:HD12  | 1:H:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:K:37:VAL:CG1   | 1:K:38:THR:N     | 2.83                     | 0.42              |
| 1:M:31:LEU:HD21  | 1:M:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:O:129:ILE:HD13 | 1:O:234:PHE:O    | 2.20                     | 0.42              |
| 1:O:210:GLU:HG3  | 1:P:79:LYS:HE2   | 2.01                     | 0.42              |
| 1:R:210:GLU:HG3  | 1:S:79:LYS:HE2   | 2.00                     | 0.42              |
| 1:S:98:LYS:NZ    | 1:S:187:GLN:HG2  | 2.33                     | 0.42              |
| 1:X:37:VAL:CG1   | 1:X:38:THR:N     | 2.83                     | 0.42              |
| 1:Y:98:LYS:CE    | 1:Y:187:GLN:HG2  | 2.49                     | 0.42              |
| 1:Z:31:LEU:HD21  | 1:Z:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:Z:33:LEU:HD12  | 1:Z:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:Z:98:LYS:CE    | 1:Z:187:GLN:HG2  | 2.50                     | 0.42              |
| 1:d:31:LEU:HD21  | 1:d:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:A:33:LEU:HD12  | 1:A:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:B:31:LEU:HD21  | 1:B:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:E:33:LEU:HD12  | 1:E:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:E:129:ILE:HD12 | 1:E:129:ILE:HA   | 1.87                     | 0.42              |
| 1:I:128:LEU:CD2  | 1:I:222:ILE:HD11 | 2.43                     | 0.42              |
| 1:I:129:ILE:HD13 | 1:I:234:PHE:O    | 2.20                     | 0.42              |
| 1:J:31:LEU:HD21  | 1:J:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:J:129:ILE:HD13 | 1:J:234:PHE:O    | 2.20                     | 0.42              |
| 1:M:31:LEU:O     | 1:M:161:LYS:NZ   | 2.51                     | 0.42              |
| 1:M:33:LEU:HD12  | 1:M:161:LYS:HD2  | 2.01                     | 0.42              |
| 1:N:98:LYS:CE    | 1:N:187:GLN:HG2  | 2.49                     | 0.42              |
| 1:N:129:ILE:HD13 | 1:N:234:PHE:O    | 2.20                     | 0.42              |
| 1:N:210:GLU:HG3  | 1:O:79:LYS:HE2   | 2.01                     | 0.42              |
| 1:O:31:LEU:HD21  | 1:O:53:PHE:CE1   | 2.54                     | 0.42              |
| 1:O:37:VAL:CG1   | 1:O:38:THR:N     | 2.83                     | 0.42              |
| 1:O:211:ILE:HD13 | 1:O:211:ILE:HA   | 1.93                     | 0.42              |
| 1:R:31:LEU:O     | 1:R:161:LYS:NZ   | 2.51                     | 0.42              |
| 1:T:37:VAL:CG1   | 1:T:38:THR:N     | 2.83                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:T:129:ILE:HD12 | 1:T:129:ILE:HA  | 1.87                     | 0.42              |
| 1:U:98:LYS:CE    | 1:U:187:GLN:HG2 | 2.50                     | 0.42              |
| 1:V:129:ILE:HD12 | 1:V:129:ILE:HA  | 1.87                     | 0.42              |
| 1:W:37:VAL:CG1   | 1:W:38:THR:N    | 2.83                     | 0.42              |
| 1:W:167:LYS:HE2  | 1:W:167:LYS:HB2 | 1.47                     | 0.42              |
| 1:X:129:ILE:HD13 | 1:X:234:PHE:O   | 2.20                     | 0.42              |
| 1:Y:37:VAL:CG1   | 1:Y:38:THR:N    | 2.83                     | 0.42              |
| 1:a:33:LEU:HD12  | 1:a:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:c:39:LYS:HB2   | 1:c:39:LYS:HE3  | 1.46                     | 0.42              |
| 1:d:98:LYS:CE    | 1:d:187:GLN:HG2 | 2.49                     | 0.42              |
| 1:A:31:LEU:HD21  | 1:A:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:36:LEU:HD11  | 1:A:58:LEU:CD2  | 2.48                     | 0.42              |
| 1:C:62:LEU:O     | 1:C:64:GLU:N    | 2.44                     | 0.42              |
| 1:H:129:ILE:HD13 | 1:H:234:PHE:O   | 2.20                     | 0.42              |
| 1:L:31:LEU:O     | 1:L:161:LYS:NZ  | 2.51                     | 0.42              |
| 1:L:33:LEU:HD12  | 1:L:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:N:31:LEU:O     | 1:N:161:LYS:NZ  | 2.51                     | 0.42              |
| 1:N:37:VAL:CG1   | 1:N:38:THR:N    | 2.83                     | 0.42              |
| 1:P:129:ILE:HD13 | 1:P:234:PHE:O   | 2.20                     | 0.42              |
| 1:S:39:LYS:HB2   | 1:S:39:LYS:HE3  | 1.46                     | 0.42              |
| 1:T:33:LEU:HD12  | 1:T:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:b:129:ILE:HD13 | 1:b:234:PHE:O   | 2.20                     | 0.42              |
| 1:d:33:LEU:HD12  | 1:d:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:B:33:LEU:HD12  | 1:B:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:B:98:LYS:CE    | 1:B:187:GLN:HG2 | 2.50                     | 0.42              |
| 1:D:37:VAL:CG1   | 1:D:38:THR:N    | 2.83                     | 0.42              |
| 1:E:31:LEU:HD21  | 1:E:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:F:31:LEU:HD21  | 1:F:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:F:87:HIS:HB3   | 1:G:202:THR:HB  | 2.02                     | 0.42              |
| 1:H:31:LEU:HD21  | 1:H:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:I:37:VAL:CG1   | 1:I:38:THR:N    | 2.83                     | 0.42              |
| 1:K:79:LYS:HE2   | 1:T:210:GLU:HG3 | 2.01                     | 0.42              |
| 1:K:203:LYS:HZ1  | 1:K:205:SER:HB2 | 1.83                     | 0.42              |
| 1:M:37:VAL:CG1   | 1:M:38:THR:N    | 2.83                     | 0.42              |
| 1:P:37:VAL:CG1   | 1:P:38:THR:N    | 2.83                     | 0.42              |
| 1:R:36:LEU:HD11  | 1:R:58:LEU:CD2  | 2.48                     | 0.42              |
| 1:U:203:LYS:HZ1  | 1:U:205:SER:HB2 | 1.83                     | 0.42              |
| 1:V:37:VAL:CG1   | 1:V:38:THR:N    | 2.83                     | 0.42              |
| 1:V:167:LYS:HE2  | 1:V:167:LYS:HB2 | 1.47                     | 0.42              |
| 1:V:211:ILE:HD13 | 1:V:211:ILE:HA  | 1.93                     | 0.42              |
| 1:W:33:LEU:HD12  | 1:W:161:LYS:HD2 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:W:98:LYS:CE    | 1:W:187:GLN:HG2 | 2.50                     | 0.42              |
| 1:X:33:LEU:HD12  | 1:X:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:a:98:LYS:CE    | 1:a:187:GLN:HG2 | 2.50                     | 0.42              |
| 1:b:31:LEU:HD21  | 1:b:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:B:129:ILE:HD12 | 1:B:129:ILE:HA  | 1.87                     | 0.42              |
| 1:B:129:ILE:HD13 | 1:B:234:PHE:O   | 2.20                     | 0.42              |
| 1:B:211:ILE:HD13 | 1:B:211:ILE:HA  | 1.93                     | 0.42              |
| 1:C:37:VAL:CG1   | 1:C:38:THR:N    | 2.83                     | 0.42              |
| 1:D:31:LEU:HD21  | 1:D:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:D:33:LEU:HD12  | 1:D:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:I:211:ILE:HD13 | 1:I:211:ILE:HA  | 1.93                     | 0.42              |
| 1:K:129:ILE:HD13 | 1:K:234:PHE:O   | 2.20                     | 0.42              |
| 1:L:98:LYS:CE    | 1:L:187:GLN:HG2 | 2.49                     | 0.42              |
| 1:L:129:ILE:HD13 | 1:L:234:PHE:O   | 2.20                     | 0.42              |
| 1:M:129:ILE:HD13 | 1:M:234:PHE:O   | 2.20                     | 0.42              |
| 1:Q:129:ILE:HD13 | 1:Q:234:PHE:O   | 2.20                     | 0.42              |
| 1:R:31:LEU:HD21  | 1:R:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:U:31:LEU:O     | 1:U:161:LYS:NZ  | 2.51                     | 0.42              |
| 1:V:33:LEU:HD12  | 1:V:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:Z:37:VAL:CG1   | 1:Z:38:THR:N    | 2.83                     | 0.42              |
| 1:c:79:LYS:HE2   | 1:d:210:GLU:HG3 | 2.01                     | 0.42              |
| 1:c:98:LYS:CE    | 1:c:187:GLN:HG2 | 2.49                     | 0.42              |
| 1:c:129:ILE:HD13 | 1:c:234:PHE:O   | 2.20                     | 0.42              |
| 1:A:98:LYS:CE    | 1:A:187:GLN:HG2 | 2.50                     | 0.42              |
| 1:B:79:LYS:HE2   | 1:C:210:GLU:HG3 | 2.01                     | 0.42              |
| 1:G:129:ILE:HD13 | 1:G:234:PHE:O   | 2.20                     | 0.42              |
| 1:I:87:HIS:HB3   | 1:J:202:THR:HB  | 2.01                     | 0.42              |
| 1:J:33:LEU:HD12  | 1:J:161:LYS:HD2 | 2.01                     | 0.42              |
| 1:J:39:LYS:HB2   | 1:J:39:LYS:HE3  | 1.45                     | 0.42              |
| 1:O:98:LYS:CE    | 1:O:187:GLN:HG2 | 2.49                     | 0.42              |
| 1:T:31:LEU:HD21  | 1:T:53:PHE:CE1  | 2.54                     | 0.42              |
| 1:X:167:LYS:HE2  | 1:X:167:LYS:HB2 | 1.47                     | 0.42              |
| 1:Y:129:ILE:HD13 | 1:Y:234:PHE:O   | 2.20                     | 0.42              |
| 1:Z:203:LYS:HZ1  | 1:Z:205:SER:HB2 | 1.84                     | 0.42              |
| 1:A:129:ILE:HD13 | 1:A:234:PHE:O   | 2.20                     | 0.41              |
| 1:B:37:VAL:CG1   | 1:B:38:THR:N    | 2.83                     | 0.41              |
| 1:B:62:LEU:O     | 1:B:64:GLU:N    | 2.44                     | 0.41              |
| 1:C:31:LEU:HD21  | 1:C:53:PHE:CE1  | 2.54                     | 0.41              |
| 1:I:31:LEU:HD21  | 1:I:53:PHE:CE1  | 2.54                     | 0.41              |
| 1:J:98:LYS:CE    | 1:J:187:GLN:HG2 | 2.50                     | 0.41              |
| 1:L:76:ASP:OD1   | 1:L:76:ASP:N    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:98:LYS:CE    | 1:M:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:N:151:ARG:HA   | 1:N:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:O:31:LEU:O     | 1:O:161:LYS:NZ   | 2.51                     | 0.41              |
| 1:S:37:VAL:CG1   | 1:S:38:THR:N     | 2.83                     | 0.41              |
| 1:S:128:LEU:CD2  | 1:S:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:U:129:ILE:HD13 | 1:U:234:PHE:O    | 2.20                     | 0.41              |
| 1:V:151:ARG:HA   | 1:V:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:X:151:ARG:HA   | 1:X:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:a:128:LEU:CD2  | 1:a:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:a:129:ILE:HD13 | 1:a:234:PHE:O    | 2.20                     | 0.41              |
| 1:d:129:ILE:HD13 | 1:d:234:PHE:O    | 2.20                     | 0.41              |
| 1:d:167:LYS:HE2  | 1:d:167:LYS:HB2  | 1.47                     | 0.41              |
| 1:A:37:VAL:CG1   | 1:A:38:THR:N     | 2.83                     | 0.41              |
| 1:C:33:LEU:HD12  | 1:C:161:LYS:HD2  | 2.01                     | 0.41              |
| 1:E:37:VAL:CG1   | 1:E:38:THR:N     | 2.83                     | 0.41              |
| 1:E:98:LYS:CE    | 1:E:187:GLN:HG2  | 2.49                     | 0.41              |
| 1:F:37:VAL:CG1   | 1:F:38:THR:N     | 2.83                     | 0.41              |
| 1:F:98:LYS:CE    | 1:F:187:GLN:HG2  | 2.49                     | 0.41              |
| 1:K:33:LEU:HD12  | 1:K:161:LYS:HD2  | 2.01                     | 0.41              |
| 1:L:37:VAL:CG1   | 1:L:38:THR:N     | 2.83                     | 0.41              |
| 1:Q:31:LEU:O     | 1:Q:161:LYS:NZ   | 2.51                     | 0.41              |
| 1:U:33:LEU:HD12  | 1:U:161:LYS:HD2  | 2.01                     | 0.41              |
| 1:W:129:ILE:HD13 | 1:W:234:PHE:O    | 2.20                     | 0.41              |
| 1:Z:167:LYS:HE2  | 1:Z:167:LYS:HB2  | 1.46                     | 0.41              |
| 1:C:129:ILE:HD13 | 1:C:234:PHE:O    | 2.20                     | 0.41              |
| 1:G:31:LEU:HD21  | 1:G:53:PHE:CE1   | 2.54                     | 0.41              |
| 1:H:37:VAL:CG1   | 1:H:38:THR:N     | 2.83                     | 0.41              |
| 1:K:98:LYS:CE    | 1:K:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:Q:37:VAL:CG1   | 1:Q:38:THR:N     | 2.83                     | 0.41              |
| 1:R:98:LYS:CE    | 1:R:187:GLN:HG2  | 2.49                     | 0.41              |
| 1:S:202:THR:HB   | 1:T:87:HIS:HB3   | 2.01                     | 0.41              |
| 1:V:31:LEU:O     | 1:V:161:LYS:NZ   | 2.51                     | 0.41              |
| 1:Y:87:HIS:HB3   | 1:Z:202:THR:HB   | 2.01                     | 0.41              |
| 1:Y:167:LYS:HE2  | 1:Y:167:LYS:HB2  | 1.47                     | 0.41              |
| 1:a:37:VAL:CG1   | 1:a:38:THR:N     | 2.83                     | 0.41              |
| 1:c:129:ILE:HD12 | 1:c:129:ILE:HA   | 1.87                     | 0.41              |
| 1:D:128:LEU:CD2  | 1:D:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:I:98:LYS:CE    | 1:I:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:P:31:LEU:O     | 1:P:161:LYS:NZ   | 2.51                     | 0.41              |
| 1:P:210:GLU:HG3  | 1:Q:79:LYS:HE2   | 2.02                     | 0.41              |
| 1:Q:98:LYS:CE    | 1:Q:187:GLN:HG2  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:98:LYS:CE    | 1:C:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:D:98:LYS:CE    | 1:D:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:D:129:ILE:HD13 | 1:D:234:PHE:O    | 2.20                     | 0.41              |
| 1:F:129:ILE:HD13 | 1:F:234:PHE:O    | 2.20                     | 0.41              |
| 1:M:76:ASP:OD1   | 1:M:76:ASP:N     | 2.50                     | 0.41              |
| 1:P:203:LYS:HZ1  | 1:P:205:SER:HB2  | 1.84                     | 0.41              |
| 1:R:129:ILE:HD13 | 1:R:234:PHE:O    | 2.20                     | 0.41              |
| 1:T:129:ILE:HD13 | 1:T:234:PHE:O    | 2.20                     | 0.41              |
| 1:U:37:VAL:CG1   | 1:U:38:THR:N     | 2.83                     | 0.41              |
| 1:X:62:LEU:O     | 1:X:64:GLU:N     | 2.44                     | 0.41              |
| 1:b:87:HIS:HB3   | 1:c:202:THR:HB   | 2.01                     | 0.41              |
| 1:G:37:VAL:CG1   | 1:G:38:THR:N     | 2.83                     | 0.41              |
| 1:G:128:LEU:CD2  | 1:G:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:K:151:ARG:HA   | 1:K:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:L:62:LEU:O     | 1:L:64:GLU:N     | 2.44                     | 0.41              |
| 1:L:210:GLU:HG3  | 1:M:79:LYS:HE2   | 2.03                     | 0.41              |
| 1:N:129:ILE:HD12 | 1:N:129:ILE:HA   | 1.87                     | 0.41              |
| 1:R:37:VAL:CG1   | 1:R:38:THR:N     | 2.83                     | 0.41              |
| 1:T:151:ARG:HA   | 1:T:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:X:98:LYS:CE    | 1:X:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:Z:151:ARG:HA   | 1:Z:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:d:37:VAL:CG1   | 1:d:38:THR:N     | 2.83                     | 0.41              |
| 1:E:79:LYS:HE2   | 1:F:210:GLU:HG3  | 2.02                     | 0.41              |
| 1:E:129:ILE:HD13 | 1:E:234:PHE:O    | 2.20                     | 0.41              |
| 1:Q:151:ARG:HD2  | 1:Q:151:ARG:HA   | 1.37                     | 0.41              |
| 1:Q:210:GLU:HG3  | 1:R:79:LYS:HE2   | 2.02                     | 0.41              |
| 1:A:128:LEU:CD2  | 1:A:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:F:151:ARG:HA   | 1:F:151:ARG:HD2  | 1.37                     | 0.41              |
| 1:S:129:ILE:HD13 | 1:S:234:PHE:O    | 2.20                     | 0.41              |
| 1:V:79:LYS:HE2   | 1:W:210:GLU:HG3  | 2.03                     | 0.41              |
| 1:b:37:VAL:CG1   | 1:b:38:THR:N     | 2.83                     | 0.41              |
| 1:A:79:LYS:HE2   | 1:B:210:GLU:HG3  | 2.02                     | 0.41              |
| 1:C:151:ARG:NH1  | 1:C:243:GLY:C    | 2.79                     | 0.41              |
| 1:G:98:LYS:CE    | 1:G:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:M:39:LYS:H     | 1:M:39:LYS:HG3   | 1.79                     | 0.41              |
| 1:N:76:ASP:OD1   | 1:N:76:ASP:N     | 2.50                     | 0.41              |
| 1:P:98:LYS:CE    | 1:P:187:GLN:HG2  | 2.49                     | 0.41              |
| 1:Q:128:LEU:CD2  | 1:Q:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:S:129:ILE:HD12 | 1:S:129:ILE:HA   | 1.87                     | 0.41              |
| 1:X:128:LEU:CD2  | 1:X:222:ILE:HD11 | 2.43                     | 0.41              |
| 1:Y:151:ARG:NH1  | 1:Y:243:GLY:C    | 2.79                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:129:ILE:HD13 | 1:Z:234:PHE:O    | 2.20                     | 0.41              |
| 1:b:39:LYS:HB2   | 1:b:39:LYS:HE3   | 1.46                     | 0.41              |
| 1:b:98:LYS:CE    | 1:b:187:GLN:HG2  | 2.50                     | 0.41              |
| 1:c:37:VAL:CG1   | 1:c:38:THR:N     | 2.83                     | 0.41              |
| 1:E:39:LYS:H     | 1:E:39:LYS:HG3   | 1.79                     | 0.41              |
| 1:I:151:ARG:NH1  | 1:I:243:GLY:C    | 2.79                     | 0.41              |
| 1:N:151:ARG:NH1  | 1:N:243:GLY:C    | 2.79                     | 0.41              |
| 1:U:151:ARG:NH1  | 1:U:243:GLY:C    | 2.79                     | 0.41              |
| 1:b:151:ARG:NH1  | 1:b:243:GLY:C    | 2.79                     | 0.41              |
| 1:H:98:LYS:CE    | 1:H:187:GLN:HG2  | 2.50                     | 0.40              |
| 1:H:151:ARG:NH1  | 1:H:243:GLY:C    | 2.80                     | 0.40              |
| 1:O:151:ARG:NH1  | 1:O:243:GLY:C    | 2.79                     | 0.40              |
| 1:R:151:ARG:NH1  | 1:R:243:GLY:C    | 2.79                     | 0.40              |
| 1:S:151:ARG:NH1  | 1:S:243:GLY:C    | 2.79                     | 0.40              |
| 1:T:39:LYS:HB2   | 1:T:39:LYS:HE3   | 1.46                     | 0.40              |
| 1:T:128:LEU:CD2  | 1:T:222:ILE:HD11 | 2.43                     | 0.40              |
| 1:c:151:ARG:NH1  | 1:c:243:GLY:C    | 2.79                     | 0.40              |
| 1:D:151:ARG:NH1  | 1:D:243:GLY:C    | 2.80                     | 0.40              |
| 1:G:211:ILE:HD13 | 1:G:211:ILE:HA   | 1.93                     | 0.40              |
| 1:I:79:LYS:HE2   | 1:J:210:GLU:HG3  | 2.03                     | 0.40              |
| 1:R:151:ARG:HD2  | 1:R:151:ARG:HA   | 1.37                     | 0.40              |
| 1:V:129:ILE:HD13 | 1:V:234:PHE:O    | 2.20                     | 0.40              |
| 1:V:151:ARG:NH1  | 1:V:243:GLY:C    | 2.79                     | 0.40              |
| 1:X:151:ARG:NH1  | 1:X:243:GLY:C    | 2.79                     | 0.40              |
| 1:Z:129:ILE:HD12 | 1:Z:129:ILE:HA   | 1.87                     | 0.40              |
| 1:B:151:ARG:NH1  | 1:B:243:GLY:C    | 2.80                     | 0.40              |
| 1:F:62:LEU:O     | 1:F:64:GLU:N     | 2.44                     | 0.40              |
| 1:G:151:ARG:NH1  | 1:G:243:GLY:C    | 2.79                     | 0.40              |
| 1:O:76:ASP:OD1   | 1:O:76:ASP:N     | 2.50                     | 0.40              |
| 1:T:98:LYS:CE    | 1:T:187:GLN:HG2  | 2.49                     | 0.40              |
| 1:E:211:ILE:HD13 | 1:E:211:ILE:HA   | 1.93                     | 0.40              |
| 1:J:151:ARG:NH1  | 1:J:243:GLY:C    | 2.79                     | 0.40              |
| 1:R:128:LEU:CD2  | 1:R:222:ILE:HD11 | 2.43                     | 0.40              |
| 1:S:98:LYS:CE    | 1:S:187:GLN:HG2  | 2.50                     | 0.40              |
| 1:W:225:TYR:HD2  | 1:W:233:GLU:HB2  | 1.87                     | 0.40              |
| 1:Z:79:LYS:HE2   | 1:a:210:GLU:HG3  | 2.02                     | 0.40              |
| 1:b:128:LEU:CD2  | 1:b:222:ILE:HD11 | 2.43                     | 0.40              |
| 1:c:211:ILE:HD13 | 1:c:211:ILE:HA   | 1.93                     | 0.40              |
| 1:I:129:ILE:HD12 | 1:I:129:ILE:HA   | 1.87                     | 0.40              |
| 1:K:167:LYS:HE2  | 1:K:167:LYS:HB2  | 1.47                     | 0.40              |
| 1:K:225:TYR:HD2  | 1:K:233:GLU:HB2  | 1.87                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:128:LEU:CD2 | 1:O:222:ILE:HD11 | 2.43                     | 0.40              |
| 1:P:151:ARG:HA  | 1:P:151:ARG:HD2  | 1.37                     | 0.40              |
| 1:Q:151:ARG:NH1 | 1:Q:243:GLY:C    | 2.79                     | 0.40              |
| 1:Q:225:TYR:HD2 | 1:Q:233:GLU:HB2  | 1.87                     | 0.40              |
| 1:T:151:ARG:NH1 | 1:T:243:GLY:C    | 2.80                     | 0.40              |
| 1:a:225:TYR:HD2 | 1:a:233:GLU:HB2  | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | B     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | C     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | D     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | E     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | F     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | G     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | H     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | I     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | J     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | K     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | L     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | M     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |
| 1   | N     | 243/245 (99%) | 225 (93%) | 17 (7%) | 1 (0%)   | 30          | 63 |
| 1   | O     | 243/245 (99%) | 226 (93%) | 16 (7%) | 1 (0%)   | 30          | 63 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | P     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | Q     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | R     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | S     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | T     | 243/245 (99%)   | 226 (93%)  | 16 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | U     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | V     | 243/245 (99%)   | 226 (93%)  | 16 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | W     | 243/245 (99%)   | 226 (93%)  | 16 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | X     | 243/245 (99%)   | 226 (93%)  | 16 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | Y     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | Z     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | a     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | b     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | c     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| 1   | d     | 243/245 (99%)   | 225 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 63 |
| All | All   | 7290/7350 (99%) | 6761 (93%) | 499 (7%) | 30 (0%)  | 32          | 63 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 152 | ASN  |
| 1   | B     | 152 | ASN  |
| 1   | C     | 152 | ASN  |
| 1   | D     | 152 | ASN  |
| 1   | E     | 152 | ASN  |
| 1   | F     | 152 | ASN  |
| 1   | G     | 152 | ASN  |
| 1   | H     | 152 | ASN  |
| 1   | I     | 152 | ASN  |
| 1   | J     | 152 | ASN  |
| 1   | K     | 152 | ASN  |
| 1   | L     | 152 | ASN  |
| 1   | M     | 152 | ASN  |
| 1   | N     | 152 | ASN  |
| 1   | O     | 152 | ASN  |
| 1   | P     | 152 | ASN  |
| 1   | Q     | 152 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 152 | ASN  |
| 1   | S     | 152 | ASN  |
| 1   | T     | 152 | ASN  |
| 1   | U     | 152 | ASN  |
| 1   | V     | 152 | ASN  |
| 1   | W     | 152 | ASN  |
| 1   | X     | 152 | ASN  |
| 1   | Y     | 152 | ASN  |
| 1   | Z     | 152 | ASN  |
| 1   | a     | 152 | ASN  |
| 1   | b     | 152 | ASN  |
| 1   | c     | 152 | ASN  |
| 1   | d     | 152 | ASN  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | B     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | C     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | D     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | E     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | F     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | G     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | H     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | I     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | J     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | K     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | L     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | M     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |
| 1   | N     | 216/216 (100%) | 201 (93%) | 15 (7%)  | 13          | 40 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | O     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | P     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | Q     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | R     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | S     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | T     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | U     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | V     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | W     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | X     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | Y     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | Z     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | a     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | b     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | c     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| 1   | d     | 216/216 (100%)   | 201 (93%)  | 15 (7%)  | 13          | 40 |
| All | All   | 6480/6480 (100%) | 6030 (93%) | 450 (7%) | 15          | 40 |

All (450) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ARG  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 79  | LYS  |
| 1   | A     | 120 | LYS  |
| 1   | A     | 129 | ILE  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 151 | ARG  |
| 1   | A     | 167 | LYS  |
| 1   | A     | 183 | ILE  |
| 1   | A     | 186 | ILE  |
| 1   | A     | 190 | THR  |
| 1   | A     | 215 | THR  |
| 1   | A     | 236 | LEU  |
| 1   | A     | 240 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 7   | ARG  |
| 1   | B     | 39  | LYS  |
| 1   | B     | 79  | LYS  |
| 1   | B     | 120 | LYS  |
| 1   | B     | 129 | ILE  |
| 1   | B     | 143 | VAL  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 151 | ARG  |
| 1   | B     | 167 | LYS  |
| 1   | B     | 183 | ILE  |
| 1   | B     | 186 | ILE  |
| 1   | B     | 190 | THR  |
| 1   | B     | 215 | THR  |
| 1   | B     | 236 | LEU  |
| 1   | B     | 240 | LYS  |
| 1   | C     | 7   | ARG  |
| 1   | C     | 39  | LYS  |
| 1   | C     | 79  | LYS  |
| 1   | C     | 120 | LYS  |
| 1   | C     | 129 | ILE  |
| 1   | C     | 143 | VAL  |
| 1   | C     | 146 | GLN  |
| 1   | C     | 151 | ARG  |
| 1   | C     | 167 | LYS  |
| 1   | C     | 183 | ILE  |
| 1   | C     | 186 | ILE  |
| 1   | C     | 190 | THR  |
| 1   | C     | 215 | THR  |
| 1   | C     | 236 | LEU  |
| 1   | C     | 240 | LYS  |
| 1   | D     | 7   | ARG  |
| 1   | D     | 39  | LYS  |
| 1   | D     | 79  | LYS  |
| 1   | D     | 120 | LYS  |
| 1   | D     | 129 | ILE  |
| 1   | D     | 143 | VAL  |
| 1   | D     | 146 | GLN  |
| 1   | D     | 151 | ARG  |
| 1   | D     | 167 | LYS  |
| 1   | D     | 183 | ILE  |
| 1   | D     | 186 | ILE  |
| 1   | D     | 190 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 215 | THR  |
| 1   | D     | 236 | LEU  |
| 1   | D     | 240 | LYS  |
| 1   | E     | 7   | ARG  |
| 1   | E     | 39  | LYS  |
| 1   | E     | 79  | LYS  |
| 1   | E     | 120 | LYS  |
| 1   | E     | 129 | ILE  |
| 1   | E     | 143 | VAL  |
| 1   | E     | 146 | GLN  |
| 1   | E     | 151 | ARG  |
| 1   | E     | 167 | LYS  |
| 1   | E     | 183 | ILE  |
| 1   | E     | 186 | ILE  |
| 1   | E     | 190 | THR  |
| 1   | E     | 215 | THR  |
| 1   | E     | 236 | LEU  |
| 1   | E     | 240 | LYS  |
| 1   | F     | 7   | ARG  |
| 1   | F     | 39  | LYS  |
| 1   | F     | 79  | LYS  |
| 1   | F     | 120 | LYS  |
| 1   | F     | 129 | ILE  |
| 1   | F     | 143 | VAL  |
| 1   | F     | 146 | GLN  |
| 1   | F     | 151 | ARG  |
| 1   | F     | 167 | LYS  |
| 1   | F     | 183 | ILE  |
| 1   | F     | 186 | ILE  |
| 1   | F     | 190 | THR  |
| 1   | F     | 215 | THR  |
| 1   | F     | 236 | LEU  |
| 1   | F     | 240 | LYS  |
| 1   | G     | 7   | ARG  |
| 1   | G     | 39  | LYS  |
| 1   | G     | 79  | LYS  |
| 1   | G     | 120 | LYS  |
| 1   | G     | 129 | ILE  |
| 1   | G     | 143 | VAL  |
| 1   | G     | 146 | GLN  |
| 1   | G     | 151 | ARG  |
| 1   | G     | 167 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 183 | ILE  |
| 1   | G     | 186 | ILE  |
| 1   | G     | 190 | THR  |
| 1   | G     | 215 | THR  |
| 1   | G     | 236 | LEU  |
| 1   | G     | 240 | LYS  |
| 1   | H     | 7   | ARG  |
| 1   | H     | 39  | LYS  |
| 1   | H     | 79  | LYS  |
| 1   | H     | 120 | LYS  |
| 1   | H     | 129 | ILE  |
| 1   | H     | 143 | VAL  |
| 1   | H     | 146 | GLN  |
| 1   | H     | 151 | ARG  |
| 1   | H     | 167 | LYS  |
| 1   | H     | 183 | ILE  |
| 1   | H     | 186 | ILE  |
| 1   | H     | 190 | THR  |
| 1   | H     | 215 | THR  |
| 1   | H     | 236 | LEU  |
| 1   | H     | 240 | LYS  |
| 1   | I     | 7   | ARG  |
| 1   | I     | 39  | LYS  |
| 1   | I     | 79  | LYS  |
| 1   | I     | 120 | LYS  |
| 1   | I     | 129 | ILE  |
| 1   | I     | 143 | VAL  |
| 1   | I     | 146 | GLN  |
| 1   | I     | 151 | ARG  |
| 1   | I     | 167 | LYS  |
| 1   | I     | 183 | ILE  |
| 1   | I     | 186 | ILE  |
| 1   | I     | 190 | THR  |
| 1   | I     | 215 | THR  |
| 1   | I     | 236 | LEU  |
| 1   | I     | 240 | LYS  |
| 1   | J     | 7   | ARG  |
| 1   | J     | 39  | LYS  |
| 1   | J     | 79  | LYS  |
| 1   | J     | 120 | LYS  |
| 1   | J     | 129 | ILE  |
| 1   | J     | 143 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 146 | GLN  |
| 1   | J     | 151 | ARG  |
| 1   | J     | 167 | LYS  |
| 1   | J     | 183 | ILE  |
| 1   | J     | 186 | ILE  |
| 1   | J     | 190 | THR  |
| 1   | J     | 215 | THR  |
| 1   | J     | 236 | LEU  |
| 1   | J     | 240 | LYS  |
| 1   | K     | 7   | ARG  |
| 1   | K     | 39  | LYS  |
| 1   | K     | 79  | LYS  |
| 1   | K     | 120 | LYS  |
| 1   | K     | 129 | ILE  |
| 1   | K     | 143 | VAL  |
| 1   | K     | 146 | GLN  |
| 1   | K     | 151 | ARG  |
| 1   | K     | 167 | LYS  |
| 1   | K     | 183 | ILE  |
| 1   | K     | 186 | ILE  |
| 1   | K     | 190 | THR  |
| 1   | K     | 215 | THR  |
| 1   | K     | 236 | LEU  |
| 1   | K     | 240 | LYS  |
| 1   | L     | 7   | ARG  |
| 1   | L     | 39  | LYS  |
| 1   | L     | 79  | LYS  |
| 1   | L     | 120 | LYS  |
| 1   | L     | 129 | ILE  |
| 1   | L     | 143 | VAL  |
| 1   | L     | 146 | GLN  |
| 1   | L     | 151 | ARG  |
| 1   | L     | 167 | LYS  |
| 1   | L     | 183 | ILE  |
| 1   | L     | 186 | ILE  |
| 1   | L     | 190 | THR  |
| 1   | L     | 215 | THR  |
| 1   | L     | 236 | LEU  |
| 1   | L     | 240 | LYS  |
| 1   | M     | 7   | ARG  |
| 1   | M     | 39  | LYS  |
| 1   | M     | 79  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 120 | LYS  |
| 1   | M     | 129 | ILE  |
| 1   | M     | 143 | VAL  |
| 1   | M     | 146 | GLN  |
| 1   | M     | 151 | ARG  |
| 1   | M     | 167 | LYS  |
| 1   | M     | 183 | ILE  |
| 1   | M     | 186 | ILE  |
| 1   | M     | 190 | THR  |
| 1   | M     | 215 | THR  |
| 1   | M     | 236 | LEU  |
| 1   | M     | 240 | LYS  |
| 1   | N     | 7   | ARG  |
| 1   | N     | 39  | LYS  |
| 1   | N     | 79  | LYS  |
| 1   | N     | 120 | LYS  |
| 1   | N     | 129 | ILE  |
| 1   | N     | 143 | VAL  |
| 1   | N     | 146 | GLN  |
| 1   | N     | 151 | ARG  |
| 1   | N     | 167 | LYS  |
| 1   | N     | 183 | ILE  |
| 1   | N     | 186 | ILE  |
| 1   | N     | 190 | THR  |
| 1   | N     | 215 | THR  |
| 1   | N     | 236 | LEU  |
| 1   | N     | 240 | LYS  |
| 1   | O     | 7   | ARG  |
| 1   | O     | 39  | LYS  |
| 1   | O     | 79  | LYS  |
| 1   | O     | 120 | LYS  |
| 1   | O     | 129 | ILE  |
| 1   | O     | 143 | VAL  |
| 1   | O     | 146 | GLN  |
| 1   | O     | 151 | ARG  |
| 1   | O     | 167 | LYS  |
| 1   | O     | 183 | ILE  |
| 1   | O     | 186 | ILE  |
| 1   | O     | 190 | THR  |
| 1   | O     | 215 | THR  |
| 1   | O     | 236 | LEU  |
| 1   | O     | 240 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 7   | ARG  |
| 1   | P     | 39  | LYS  |
| 1   | P     | 79  | LYS  |
| 1   | P     | 120 | LYS  |
| 1   | P     | 129 | ILE  |
| 1   | P     | 143 | VAL  |
| 1   | P     | 146 | GLN  |
| 1   | P     | 151 | ARG  |
| 1   | P     | 167 | LYS  |
| 1   | P     | 183 | ILE  |
| 1   | P     | 186 | ILE  |
| 1   | P     | 190 | THR  |
| 1   | P     | 215 | THR  |
| 1   | P     | 236 | LEU  |
| 1   | P     | 240 | LYS  |
| 1   | Q     | 7   | ARG  |
| 1   | Q     | 39  | LYS  |
| 1   | Q     | 79  | LYS  |
| 1   | Q     | 120 | LYS  |
| 1   | Q     | 129 | ILE  |
| 1   | Q     | 143 | VAL  |
| 1   | Q     | 146 | GLN  |
| 1   | Q     | 151 | ARG  |
| 1   | Q     | 167 | LYS  |
| 1   | Q     | 183 | ILE  |
| 1   | Q     | 186 | ILE  |
| 1   | Q     | 190 | THR  |
| 1   | Q     | 215 | THR  |
| 1   | Q     | 236 | LEU  |
| 1   | Q     | 240 | LYS  |
| 1   | R     | 7   | ARG  |
| 1   | R     | 39  | LYS  |
| 1   | R     | 79  | LYS  |
| 1   | R     | 120 | LYS  |
| 1   | R     | 129 | ILE  |
| 1   | R     | 143 | VAL  |
| 1   | R     | 146 | GLN  |
| 1   | R     | 151 | ARG  |
| 1   | R     | 167 | LYS  |
| 1   | R     | 183 | ILE  |
| 1   | R     | 186 | ILE  |
| 1   | R     | 190 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 215 | THR  |
| 1   | R     | 236 | LEU  |
| 1   | R     | 240 | LYS  |
| 1   | S     | 7   | ARG  |
| 1   | S     | 39  | LYS  |
| 1   | S     | 79  | LYS  |
| 1   | S     | 120 | LYS  |
| 1   | S     | 129 | ILE  |
| 1   | S     | 143 | VAL  |
| 1   | S     | 146 | GLN  |
| 1   | S     | 151 | ARG  |
| 1   | S     | 167 | LYS  |
| 1   | S     | 183 | ILE  |
| 1   | S     | 186 | ILE  |
| 1   | S     | 190 | THR  |
| 1   | S     | 215 | THR  |
| 1   | S     | 236 | LEU  |
| 1   | S     | 240 | LYS  |
| 1   | T     | 7   | ARG  |
| 1   | T     | 39  | LYS  |
| 1   | T     | 79  | LYS  |
| 1   | T     | 120 | LYS  |
| 1   | T     | 129 | ILE  |
| 1   | T     | 143 | VAL  |
| 1   | T     | 146 | GLN  |
| 1   | T     | 151 | ARG  |
| 1   | T     | 167 | LYS  |
| 1   | T     | 183 | ILE  |
| 1   | T     | 186 | ILE  |
| 1   | T     | 190 | THR  |
| 1   | T     | 215 | THR  |
| 1   | T     | 236 | LEU  |
| 1   | T     | 240 | LYS  |
| 1   | U     | 7   | ARG  |
| 1   | U     | 39  | LYS  |
| 1   | U     | 79  | LYS  |
| 1   | U     | 120 | LYS  |
| 1   | U     | 129 | ILE  |
| 1   | U     | 143 | VAL  |
| 1   | U     | 146 | GLN  |
| 1   | U     | 151 | ARG  |
| 1   | U     | 167 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 183 | ILE  |
| 1   | U     | 186 | ILE  |
| 1   | U     | 190 | THR  |
| 1   | U     | 215 | THR  |
| 1   | U     | 236 | LEU  |
| 1   | U     | 240 | LYS  |
| 1   | V     | 7   | ARG  |
| 1   | V     | 39  | LYS  |
| 1   | V     | 79  | LYS  |
| 1   | V     | 120 | LYS  |
| 1   | V     | 129 | ILE  |
| 1   | V     | 143 | VAL  |
| 1   | V     | 146 | GLN  |
| 1   | V     | 151 | ARG  |
| 1   | V     | 167 | LYS  |
| 1   | V     | 183 | ILE  |
| 1   | V     | 186 | ILE  |
| 1   | V     | 190 | THR  |
| 1   | V     | 215 | THR  |
| 1   | V     | 236 | LEU  |
| 1   | V     | 240 | LYS  |
| 1   | W     | 7   | ARG  |
| 1   | W     | 39  | LYS  |
| 1   | W     | 79  | LYS  |
| 1   | W     | 120 | LYS  |
| 1   | W     | 129 | ILE  |
| 1   | W     | 143 | VAL  |
| 1   | W     | 146 | GLN  |
| 1   | W     | 151 | ARG  |
| 1   | W     | 167 | LYS  |
| 1   | W     | 183 | ILE  |
| 1   | W     | 186 | ILE  |
| 1   | W     | 190 | THR  |
| 1   | W     | 215 | THR  |
| 1   | W     | 236 | LEU  |
| 1   | W     | 240 | LYS  |
| 1   | X     | 7   | ARG  |
| 1   | X     | 39  | LYS  |
| 1   | X     | 79  | LYS  |
| 1   | X     | 120 | LYS  |
| 1   | X     | 129 | ILE  |
| 1   | X     | 143 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 146 | GLN  |
| 1   | X     | 151 | ARG  |
| 1   | X     | 167 | LYS  |
| 1   | X     | 183 | ILE  |
| 1   | X     | 186 | ILE  |
| 1   | X     | 190 | THR  |
| 1   | X     | 215 | THR  |
| 1   | X     | 236 | LEU  |
| 1   | X     | 240 | LYS  |
| 1   | Y     | 7   | ARG  |
| 1   | Y     | 39  | LYS  |
| 1   | Y     | 79  | LYS  |
| 1   | Y     | 120 | LYS  |
| 1   | Y     | 129 | ILE  |
| 1   | Y     | 143 | VAL  |
| 1   | Y     | 146 | GLN  |
| 1   | Y     | 151 | ARG  |
| 1   | Y     | 167 | LYS  |
| 1   | Y     | 183 | ILE  |
| 1   | Y     | 186 | ILE  |
| 1   | Y     | 190 | THR  |
| 1   | Y     | 215 | THR  |
| 1   | Y     | 236 | LEU  |
| 1   | Y     | 240 | LYS  |
| 1   | Z     | 7   | ARG  |
| 1   | Z     | 39  | LYS  |
| 1   | Z     | 79  | LYS  |
| 1   | Z     | 120 | LYS  |
| 1   | Z     | 129 | ILE  |
| 1   | Z     | 143 | VAL  |
| 1   | Z     | 146 | GLN  |
| 1   | Z     | 151 | ARG  |
| 1   | Z     | 167 | LYS  |
| 1   | Z     | 183 | ILE  |
| 1   | Z     | 186 | ILE  |
| 1   | Z     | 190 | THR  |
| 1   | Z     | 215 | THR  |
| 1   | Z     | 236 | LEU  |
| 1   | Z     | 240 | LYS  |
| 1   | a     | 7   | ARG  |
| 1   | a     | 39  | LYS  |
| 1   | a     | 79  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 120 | LYS  |
| 1   | a     | 129 | ILE  |
| 1   | a     | 143 | VAL  |
| 1   | a     | 146 | GLN  |
| 1   | a     | 151 | ARG  |
| 1   | a     | 167 | LYS  |
| 1   | a     | 183 | ILE  |
| 1   | a     | 186 | ILE  |
| 1   | a     | 190 | THR  |
| 1   | a     | 215 | THR  |
| 1   | a     | 236 | LEU  |
| 1   | a     | 240 | LYS  |
| 1   | b     | 7   | ARG  |
| 1   | b     | 39  | LYS  |
| 1   | b     | 79  | LYS  |
| 1   | b     | 120 | LYS  |
| 1   | b     | 129 | ILE  |
| 1   | b     | 143 | VAL  |
| 1   | b     | 146 | GLN  |
| 1   | b     | 151 | ARG  |
| 1   | b     | 167 | LYS  |
| 1   | b     | 183 | ILE  |
| 1   | b     | 186 | ILE  |
| 1   | b     | 190 | THR  |
| 1   | b     | 215 | THR  |
| 1   | b     | 236 | LEU  |
| 1   | b     | 240 | LYS  |
| 1   | c     | 7   | ARG  |
| 1   | c     | 39  | LYS  |
| 1   | c     | 79  | LYS  |
| 1   | c     | 120 | LYS  |
| 1   | c     | 129 | ILE  |
| 1   | c     | 143 | VAL  |
| 1   | c     | 146 | GLN  |
| 1   | c     | 151 | ARG  |
| 1   | c     | 167 | LYS  |
| 1   | c     | 183 | ILE  |
| 1   | c     | 186 | ILE  |
| 1   | c     | 190 | THR  |
| 1   | c     | 215 | THR  |
| 1   | c     | 236 | LEU  |
| 1   | c     | 240 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | d     | 7   | ARG  |
| 1   | d     | 39  | LYS  |
| 1   | d     | 79  | LYS  |
| 1   | d     | 120 | LYS  |
| 1   | d     | 129 | ILE  |
| 1   | d     | 143 | VAL  |
| 1   | d     | 146 | GLN  |
| 1   | d     | 151 | ARG  |
| 1   | d     | 167 | LYS  |
| 1   | d     | 183 | ILE  |
| 1   | d     | 186 | ILE  |
| 1   | d     | 190 | THR  |
| 1   | d     | 215 | THR  |
| 1   | d     | 236 | LEU  |
| 1   | d     | 240 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | ASN  |
| 1   | A     | 32  | GLN  |
| 1   | A     | 66  | GLN  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 66  | GLN  |
| 1   | C     | 32  | GLN  |
| 1   | C     | 66  | GLN  |
| 1   | D     | 32  | GLN  |
| 1   | D     | 66  | GLN  |
| 1   | E     | 32  | GLN  |
| 1   | E     | 66  | GLN  |
| 1   | E     | 160 | GLN  |
| 1   | F     | 26  | ASN  |
| 1   | F     | 32  | GLN  |
| 1   | F     | 66  | GLN  |
| 1   | F     | 160 | GLN  |
| 1   | G     | 26  | ASN  |
| 1   | G     | 32  | GLN  |
| 1   | G     | 66  | GLN  |
| 1   | G     | 160 | GLN  |
| 1   | H     | 26  | ASN  |
| 1   | H     | 32  | GLN  |
| 1   | H     | 66  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 160 | GLN  |
| 1   | I     | 26  | ASN  |
| 1   | I     | 32  | GLN  |
| 1   | I     | 66  | GLN  |
| 1   | J     | 66  | GLN  |
| 1   | J     | 160 | GLN  |
| 1   | K     | 26  | ASN  |
| 1   | K     | 66  | GLN  |
| 1   | L     | 32  | GLN  |
| 1   | L     | 66  | GLN  |
| 1   | M     | 32  | GLN  |
| 1   | M     | 66  | GLN  |
| 1   | N     | 32  | GLN  |
| 1   | N     | 66  | GLN  |
| 1   | O     | 32  | GLN  |
| 1   | O     | 66  | GLN  |
| 1   | P     | 32  | GLN  |
| 1   | P     | 66  | GLN  |
| 1   | Q     | 32  | GLN  |
| 1   | Q     | 66  | GLN  |
| 1   | R     | 32  | GLN  |
| 1   | R     | 66  | GLN  |
| 1   | S     | 32  | GLN  |
| 1   | S     | 66  | GLN  |
| 1   | T     | 32  | GLN  |
| 1   | T     | 66  | GLN  |
| 1   | U     | 32  | GLN  |
| 1   | U     | 66  | GLN  |
| 1   | V     | 32  | GLN  |
| 1   | V     | 66  | GLN  |
| 1   | W     | 32  | GLN  |
| 1   | W     | 66  | GLN  |
| 1   | X     | 32  | GLN  |
| 1   | X     | 66  | GLN  |
| 1   | Y     | 32  | GLN  |
| 1   | Y     | 66  | GLN  |
| 1   | Z     | 32  | GLN  |
| 1   | Z     | 66  | GLN  |
| 1   | a     | 32  | GLN  |
| 1   | a     | 66  | GLN  |
| 1   | a     | 160 | GLN  |
| 1   | b     | 32  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 66  | GLN  |
| 1   | c     | 32  | GLN  |
| 1   | c     | 66  | GLN  |
| 1   | d     | 32  | GLN  |
| 1   | d     | 66  | GLN  |
| 1   | d     | 160 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

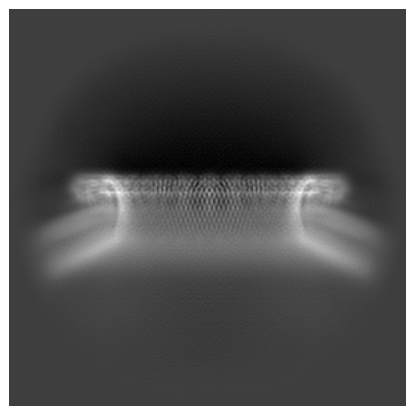
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51889. These allow visual inspection of the internal detail of the map and identification of artifacts.

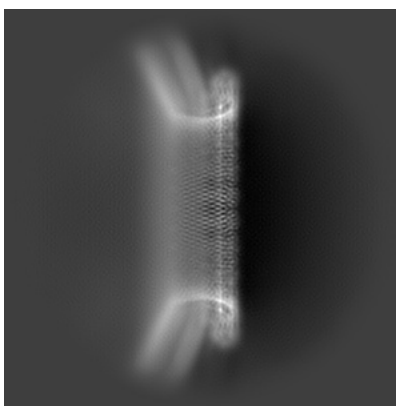
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

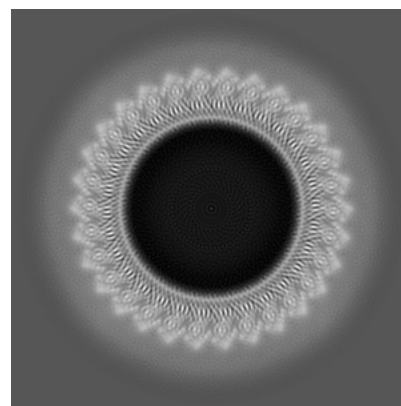
#### 6.1.1 Primary map



X

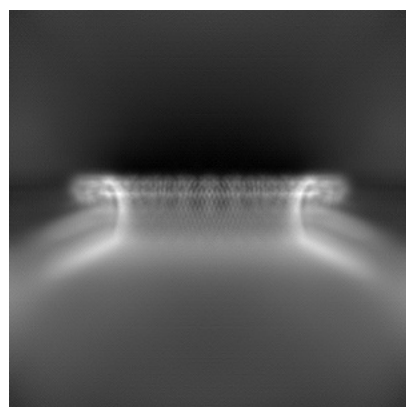


Y

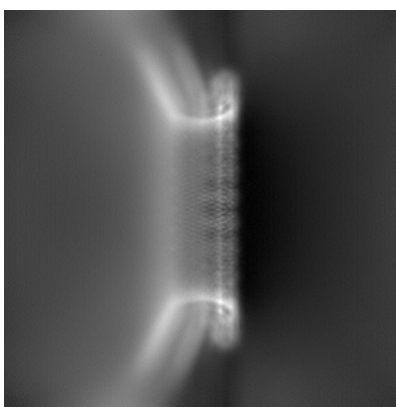


Z

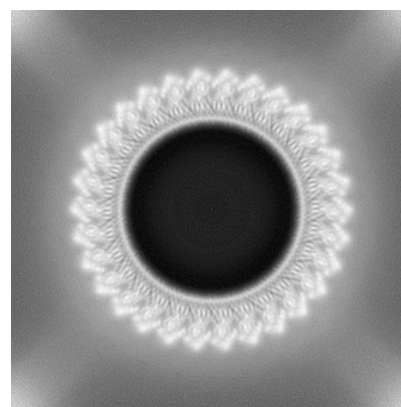
#### 6.1.2 Raw map



X



Y

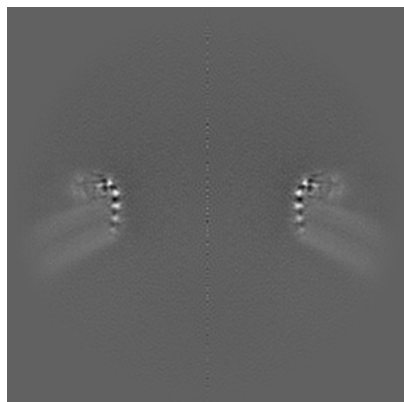


Z

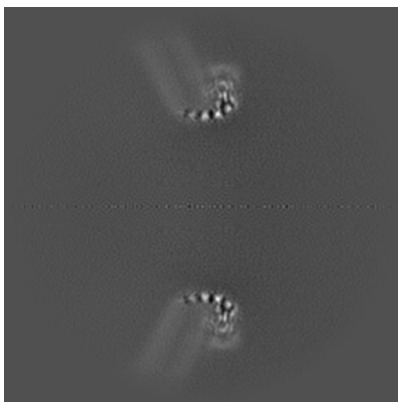
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

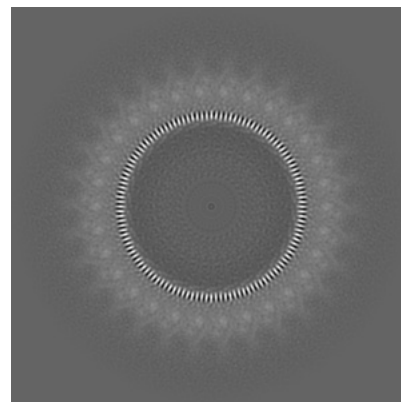
### 6.2.1 Primary map



X Index: 250

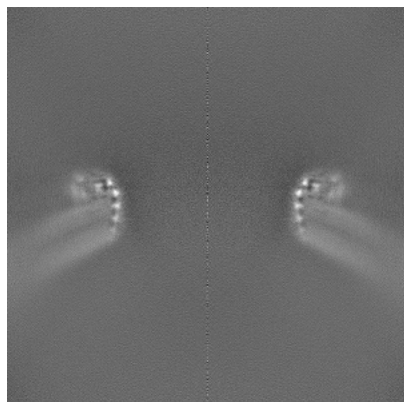


Y Index: 250



Z Index: 250

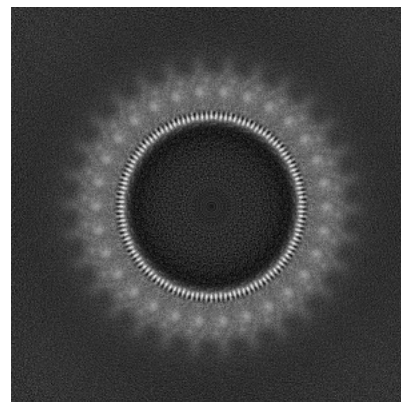
### 6.2.2 Raw map



X Index: 250



Y Index: 250

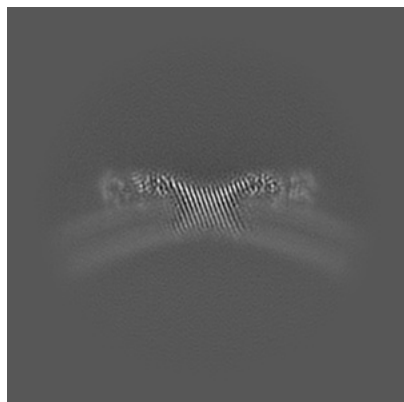


Z Index: 250

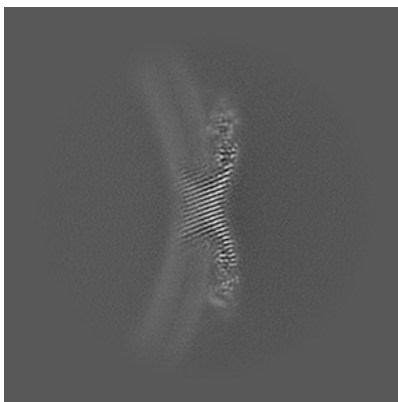
The images above show central slices of the map in three orthogonal directions.

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

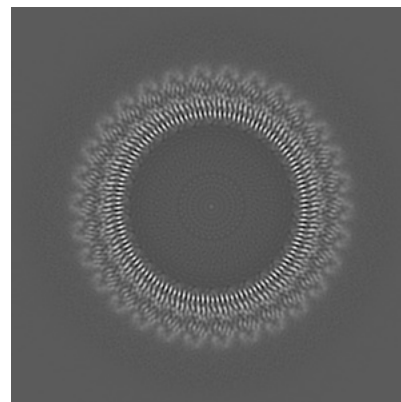
### 6.3.1 Primary map



X Index: 137

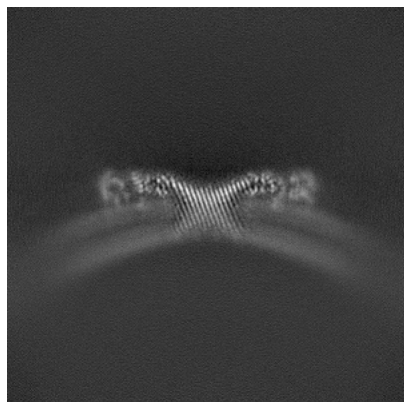


Y Index: 137

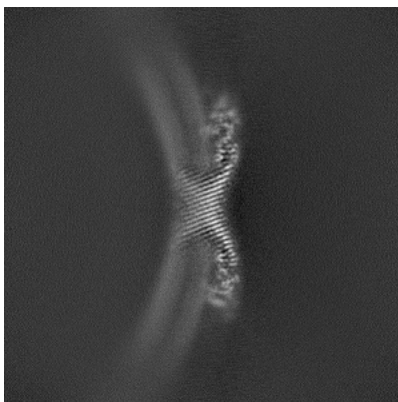


Z Index: 271

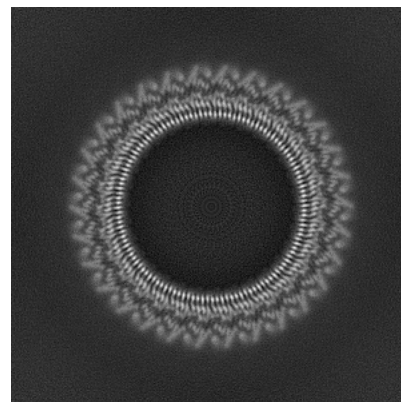
### 6.3.2 Raw map



X Index: 137



Y Index: 138

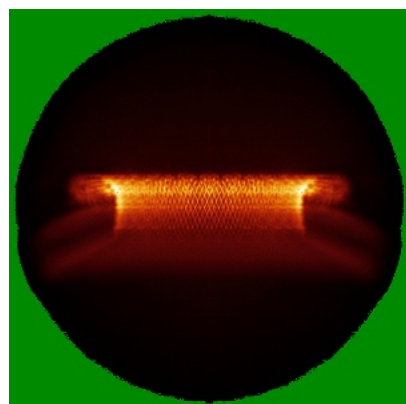


Z Index: 270

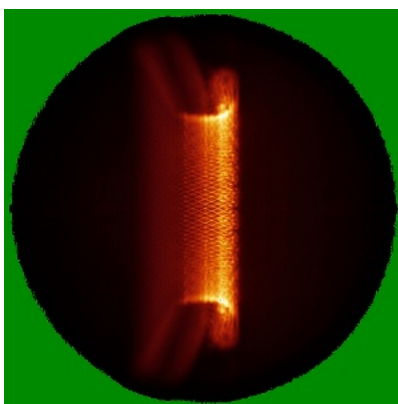
The images above show the largest variance slices of the map in three orthogonal directions.

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

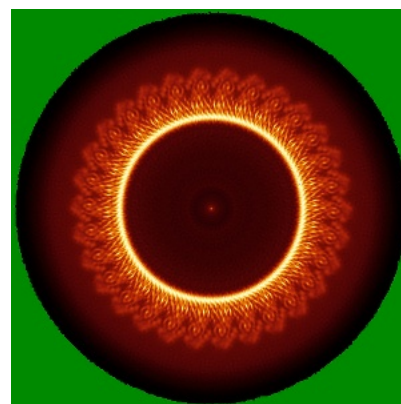
### 6.4.1 Primary map



X

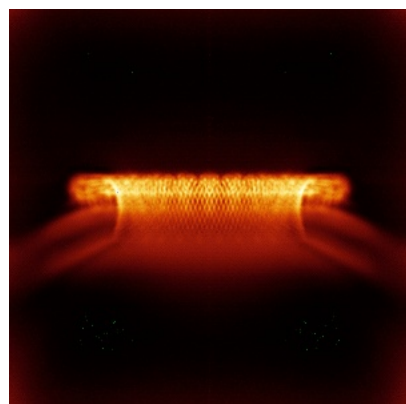


Y

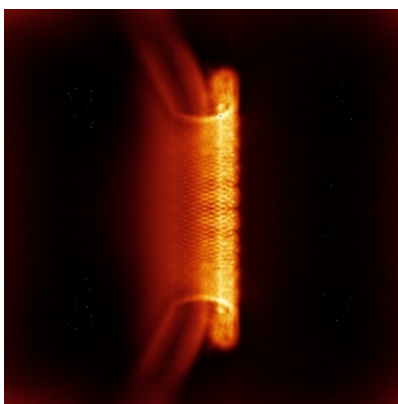


Z

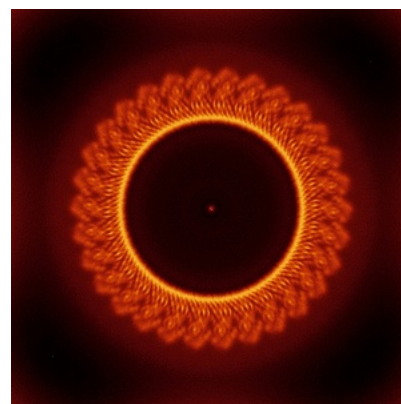
### 6.4.2 Raw map



X



Y

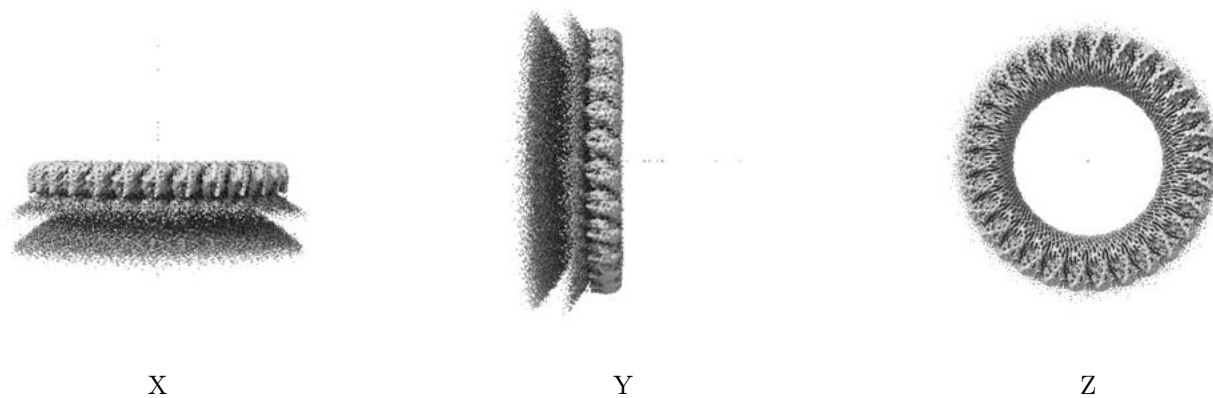


Z

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

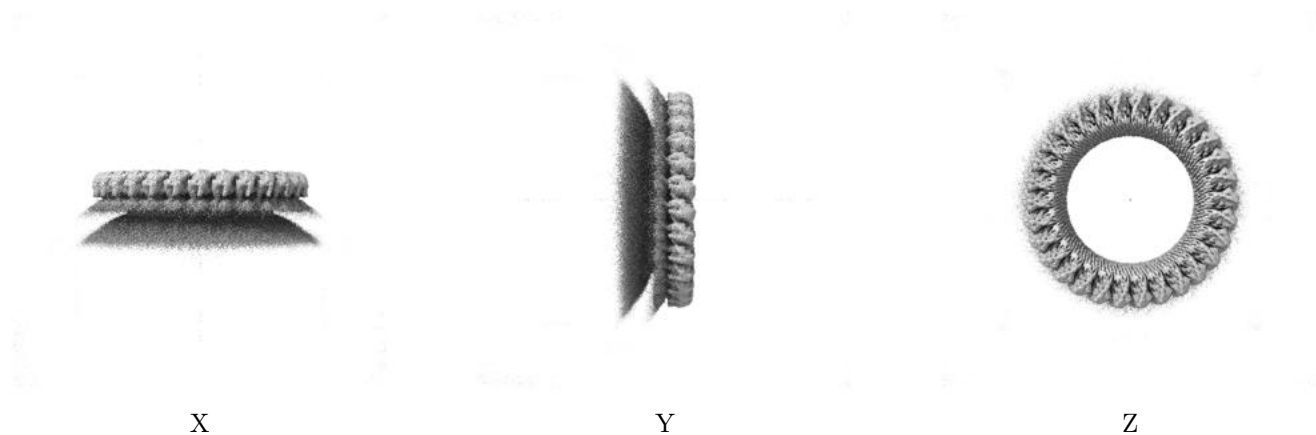
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

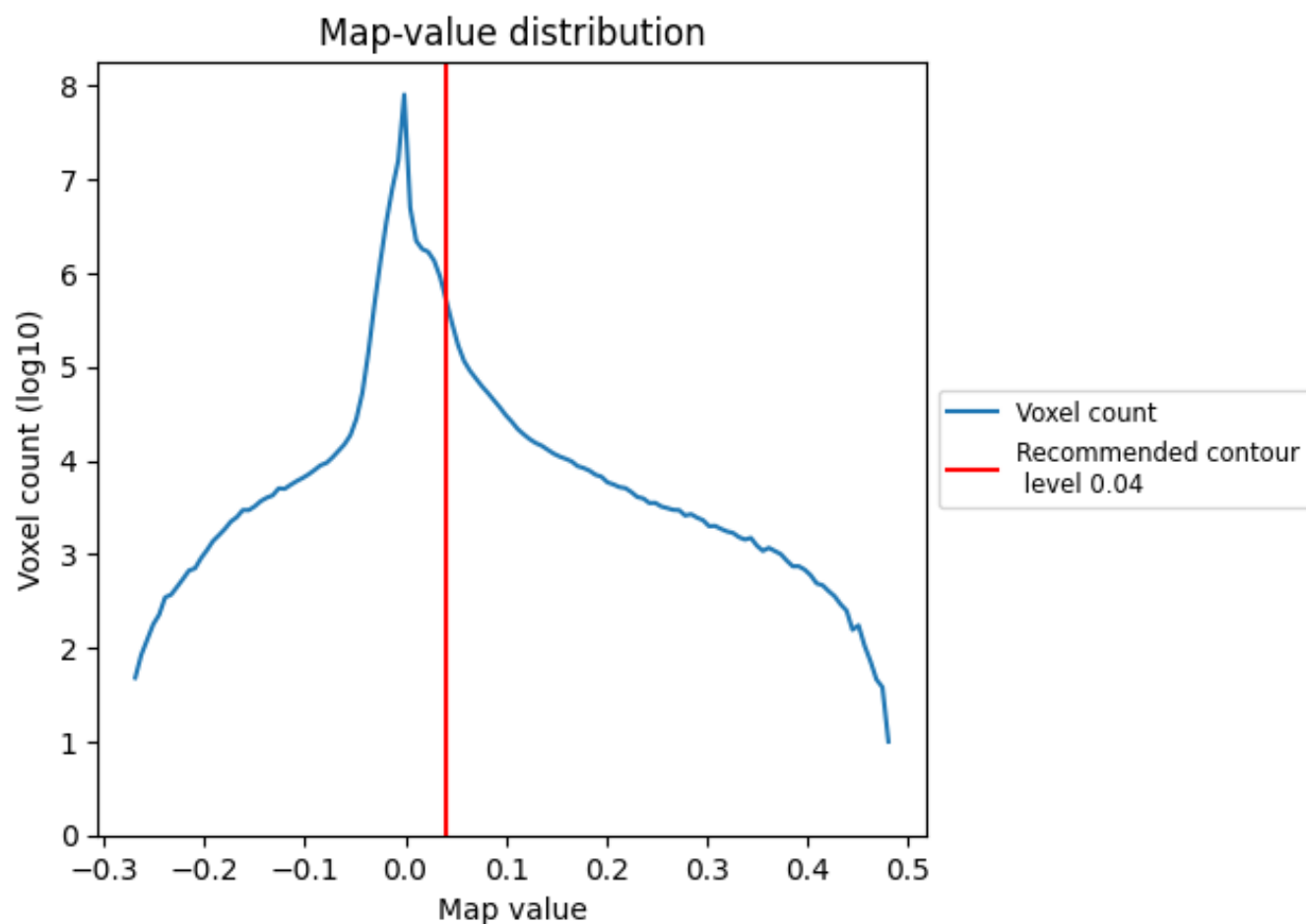
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

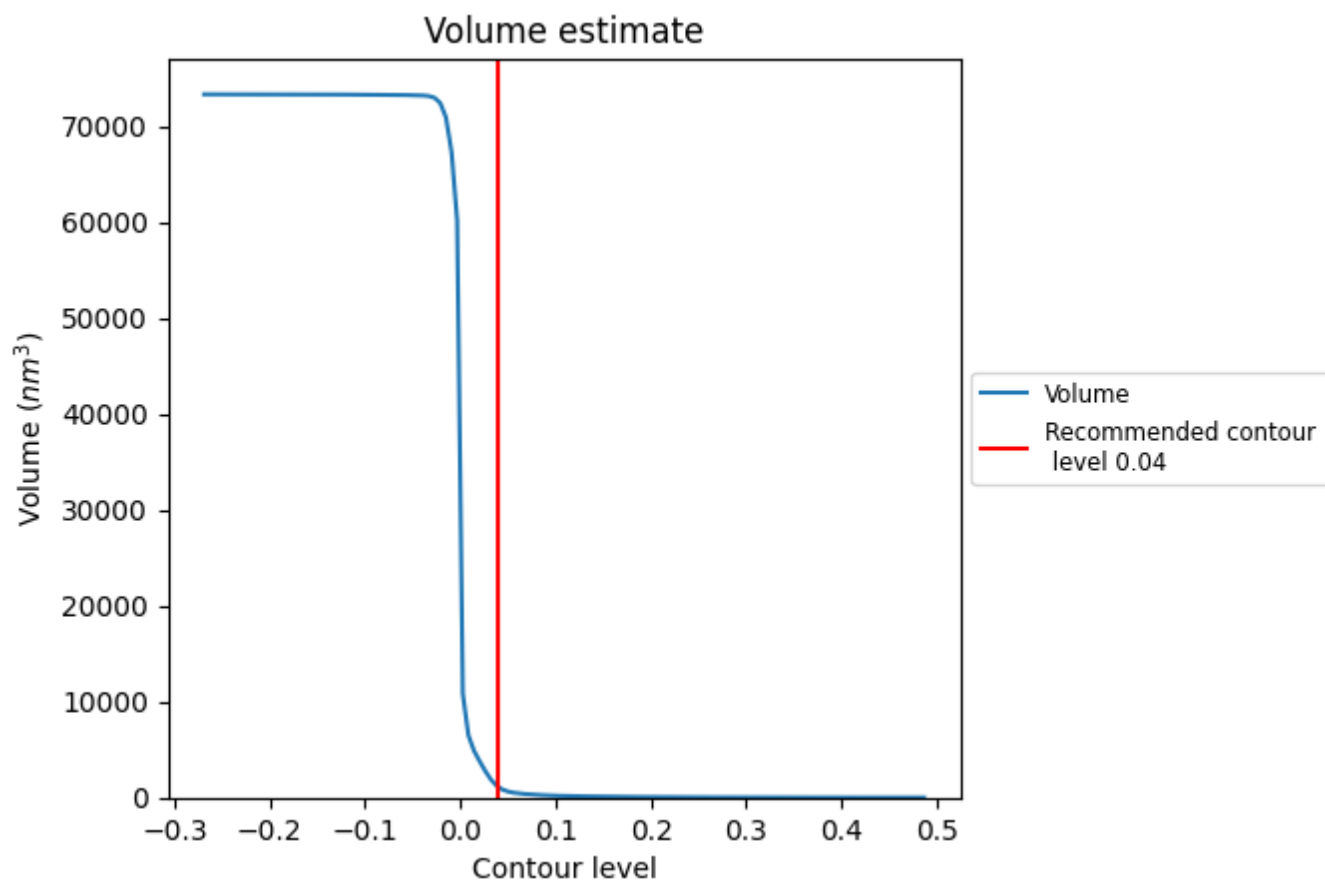
This section contains the results of statistical analysis of the map.

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



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

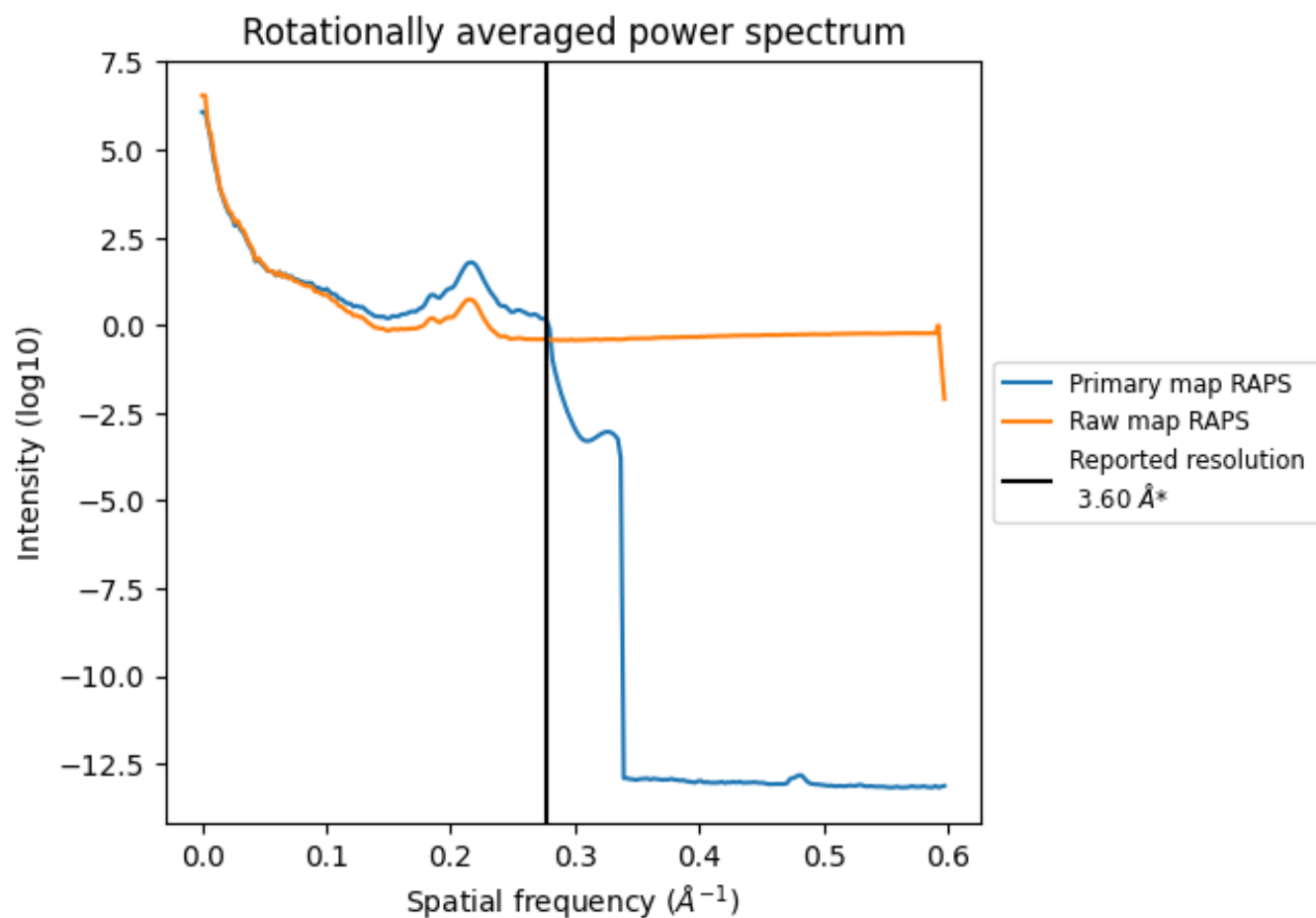
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1112  $\text{nm}^3$ ; this corresponds to an approximate mass of 1005 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

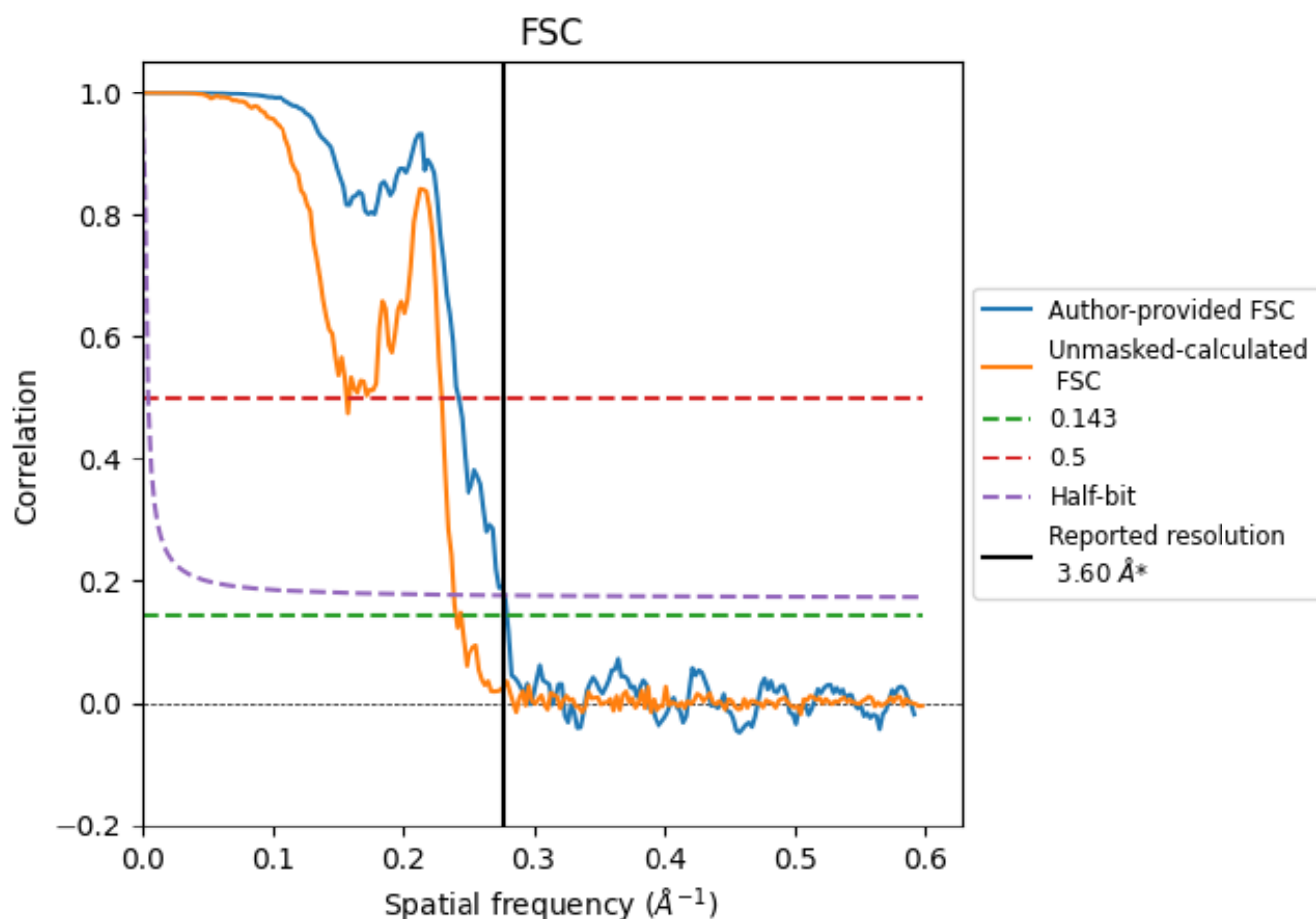


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.278 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

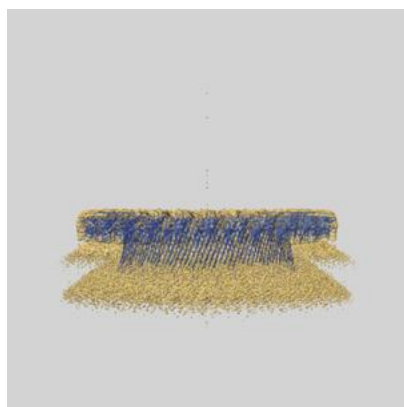
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.60                               | -    | -        |
| Author-provided FSC curve | 3.58                               | 4.13 | 3.60     |
| Unmasked-calculated*      | 4.16                               | 6.38 | 4.19     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.6 by more than 10 %

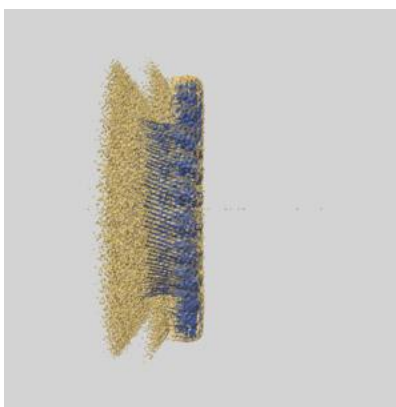
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51889 and PDB model 9H5M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



X



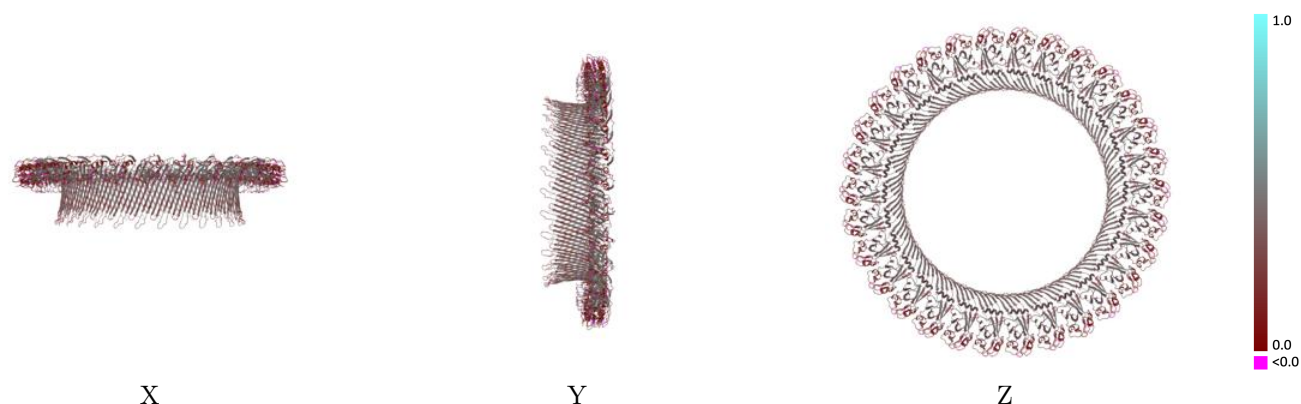
Y



Z

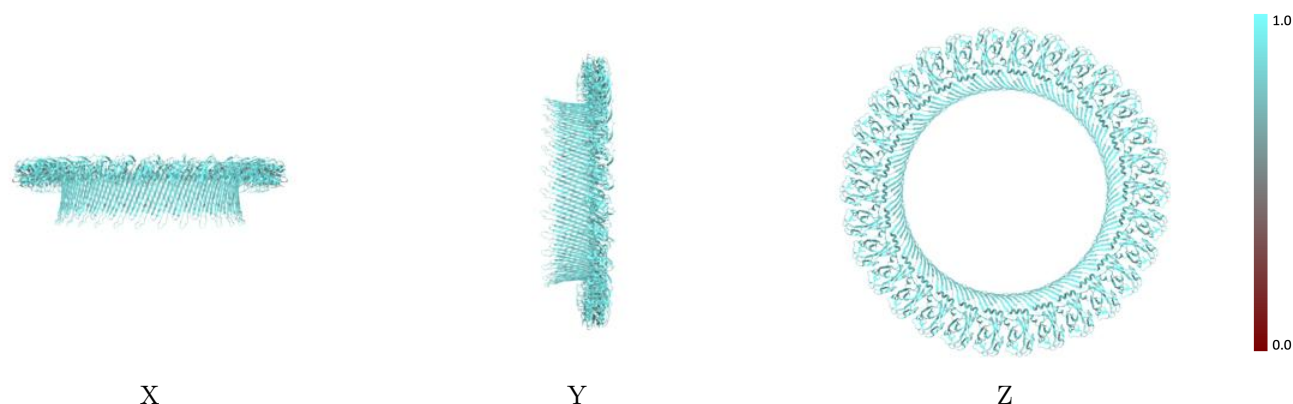
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



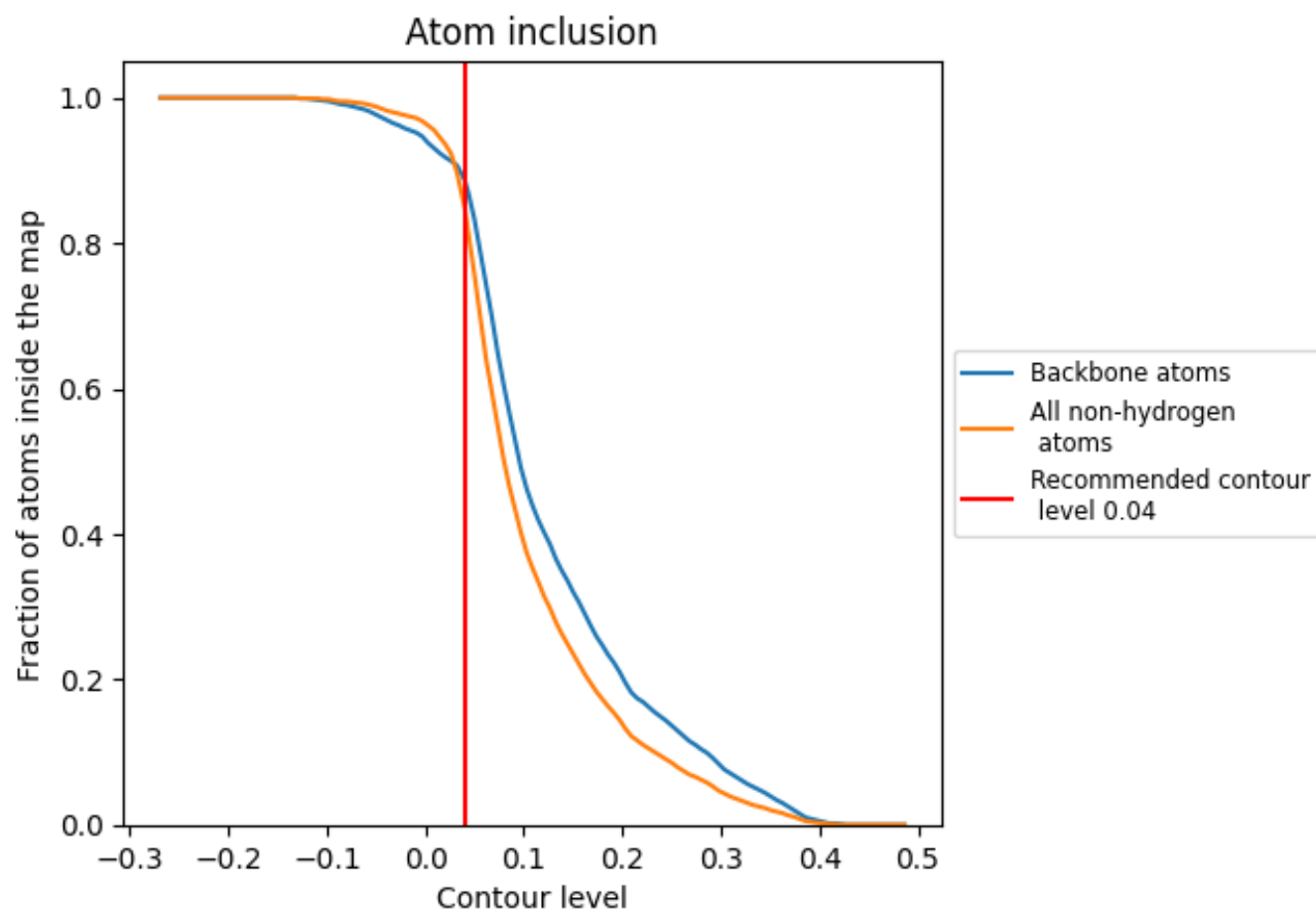
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8490   |  0.3090   |
| A     |  0.8460   |  0.3070   |
| B     |  0.8480   |  0.3060   |
| C     |  0.8510   |  0.3060   |
| D     |  0.8510   |  0.3090   |
| E     |  0.8500   |  0.3080   |
| F     |  0.8480   |  0.3090   |
| G     |  0.8480   |  0.3090   |
| H     |  0.8480   |  0.3100   |
| I     |  0.8520   |  0.3110   |
| J     |  0.8490   |  0.3140   |
| K     |  0.8500   |  0.3130   |
| L     |  0.8490   |  0.3080   |
| M     |  0.8510   |  0.3110   |
| N     |  0.8520  |  0.3090  |
| O     |  0.8490 |  0.3100 |
| P     |  0.8460 |  0.3090 |
| Q     |  0.8490 |  0.3110 |
| R     |  0.8460 |  0.3100 |
| S     |  0.8500 |  0.3120 |
| T     |  0.8510 |  0.3120 |
| U     |  0.8470 |  0.3110 |
| V     |  0.8480 |  0.3100 |
| W     |  0.8500 |  0.3090 |
| X     |  0.8500 |  0.3080 |
| Y     |  0.8530 |  0.3080 |
| Z     |  0.8500 |  0.3080 |
| a     |  0.8490 |  0.3060 |
| b     |  0.8490 |  0.3040 |
| c     |  0.8430 |  0.3060 |
| d     |  0.8480 |  0.3070 |

