



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:58 PM UTC

PDB ID : 3ZBJ / pdb\_00003zbj  
EMDB ID : EMD-2233  
Title : Fitting results in the I-layer of the subnanometer structure of the bacterial pKM101 type IV secretion system core complex digested with elastase  
Authors : Rivera-Calzada, A.; Fronzes, R.; Savva, C.G.; Chandran, V.; Lian, P.W.; Laeremans, T.; Pardon, E.; Steyaert, J.; Remaut, H.; Waksman, G.; Orlova, E.V.  
Deposited on : 2012-11-10  
Resolution : 8.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

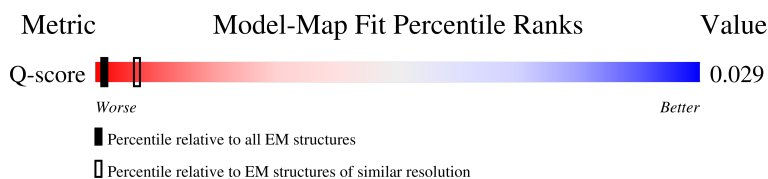
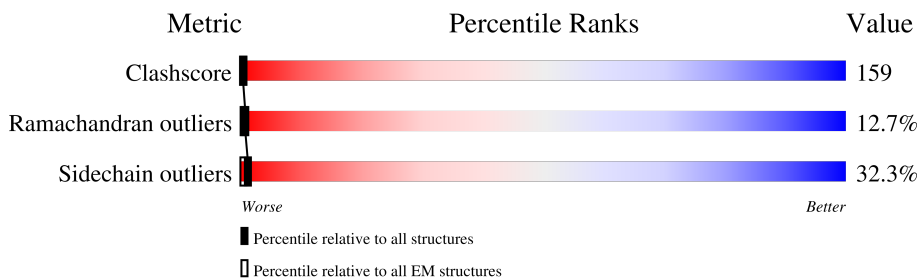
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 328 ( 8.00 - 9.00 )                                      |

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     | 112    |                  |
| 1   | B     | 112    |                  |
| 1   | C     | 112    |                  |
| 1   | D     | 112    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 112    |                  |
| 1   | F     | 112    |                  |
| 1   | G     | 112    |                  |
| 1   | H     | 112    |                  |
| 1   | I     | 112    |                  |
| 1   | J     | 112    |                  |
| 1   | K     | 112    |                  |
| 1   | L     | 112    |                  |
| 1   | M     | 112    |                  |
| 1   | N     | 112    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12404 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.

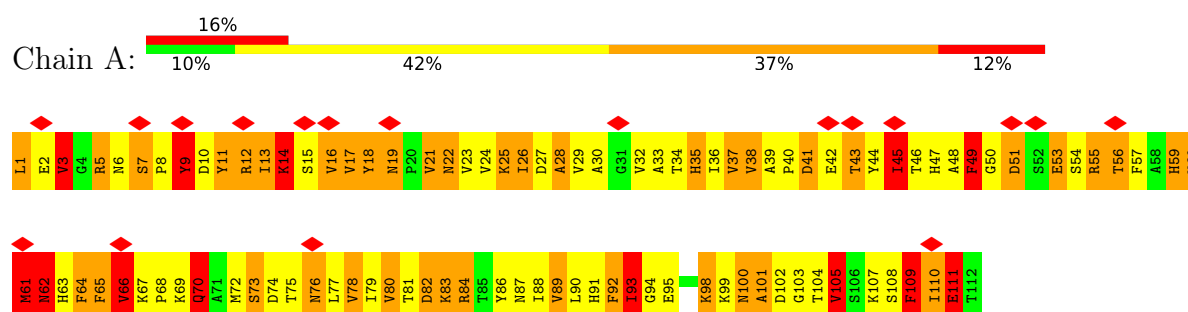
- Molecule 1 is a protein called TRA0 PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | B     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | C     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | D     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | E     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | F     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | G     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | H     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | I     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | J     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | K     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | L     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | M     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |
| 1   | N     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 564 | 151 | 169 | 2 |         |       |

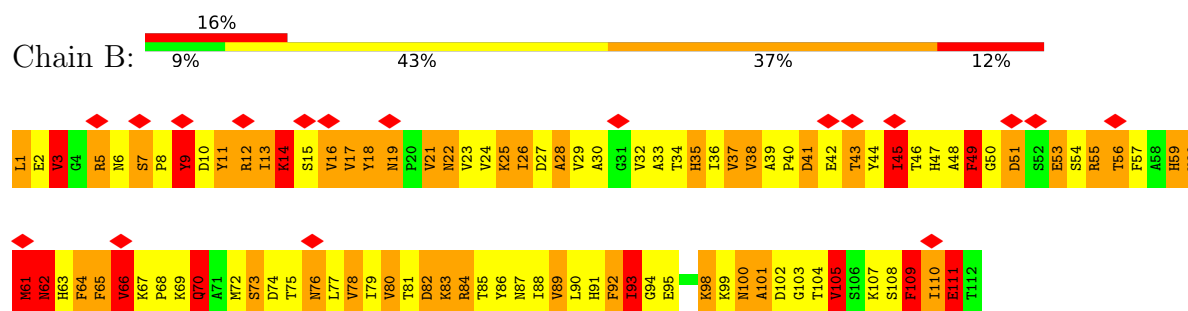
### 3 Residue-property plots [i](#)

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

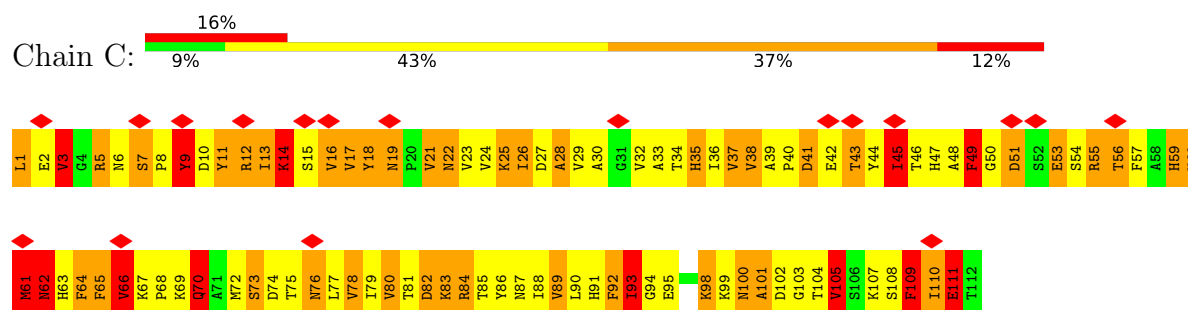
#### • Molecule 1: TRA0 PROTEIN



#### • Molecule 1: TRA0 PROTEIN

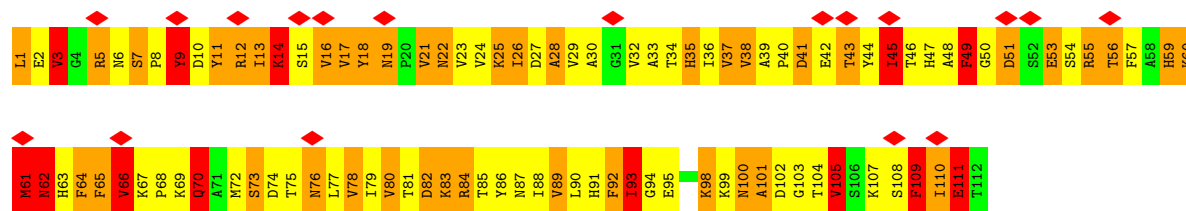


#### • Molecule 1: TRA0 PROTEIN

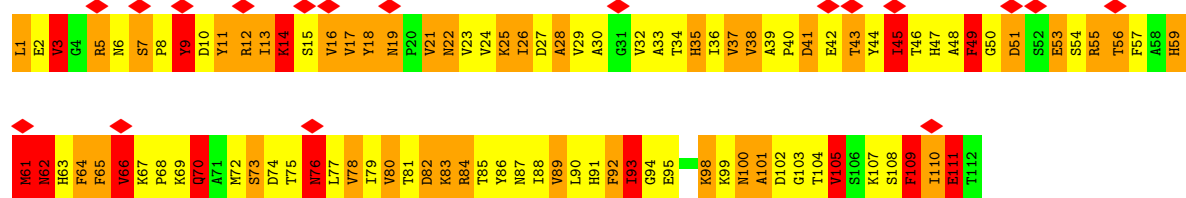


#### • Molecule 1: TRA0 PROTEIN

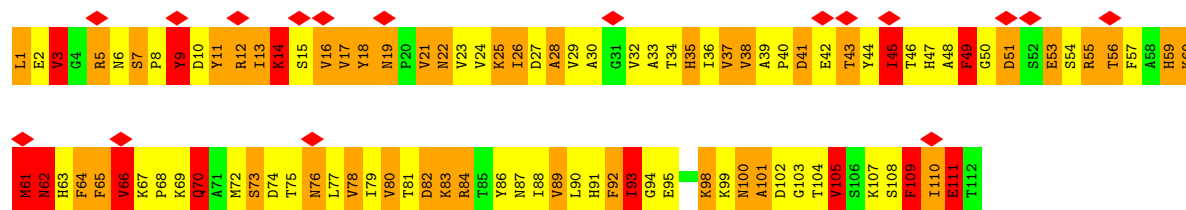




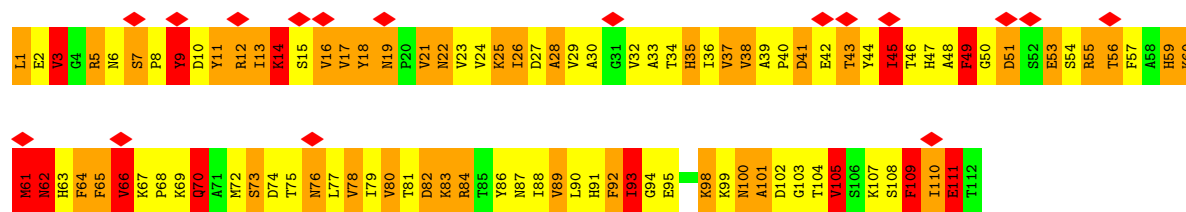
• Molecule 1: TRAO PROTEIN



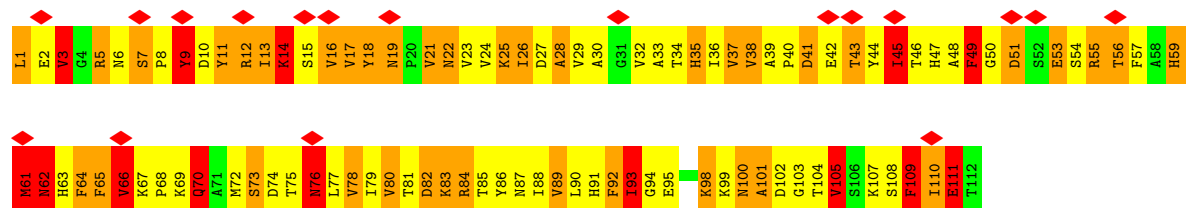
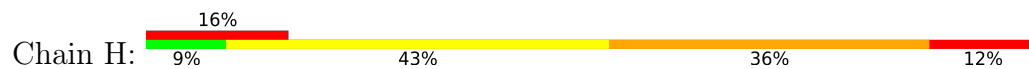
• Molecule 1: TRAO PROTEIN



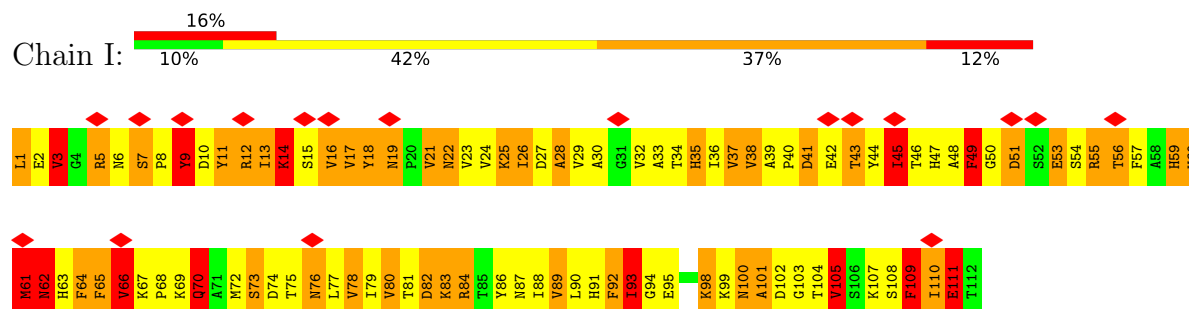
• Molecule 1: TRAO PROTEIN



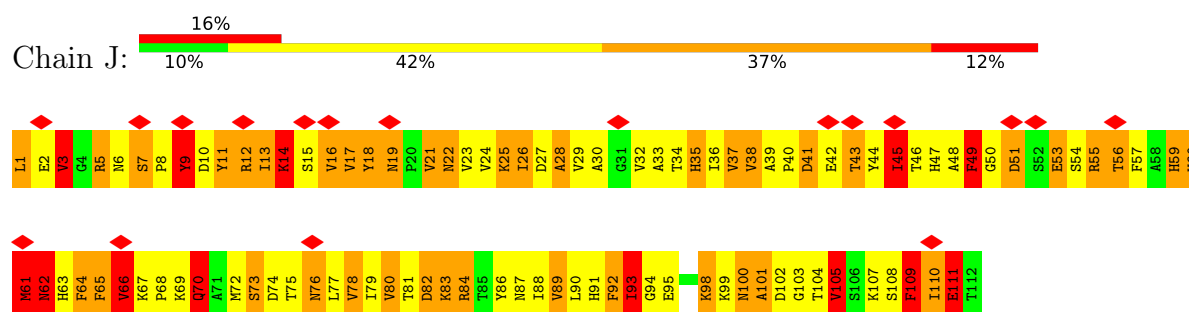
• Molecule 1: TRAO PROTEIN



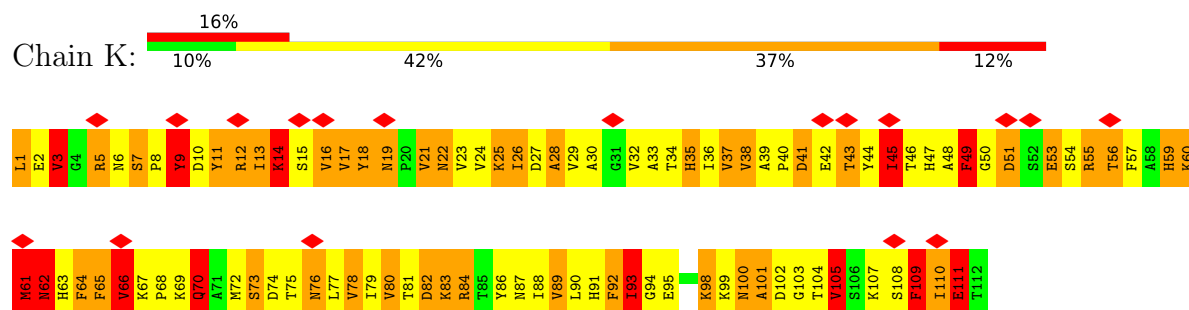
## ● Molecule 1: TRA0 PROTEIN



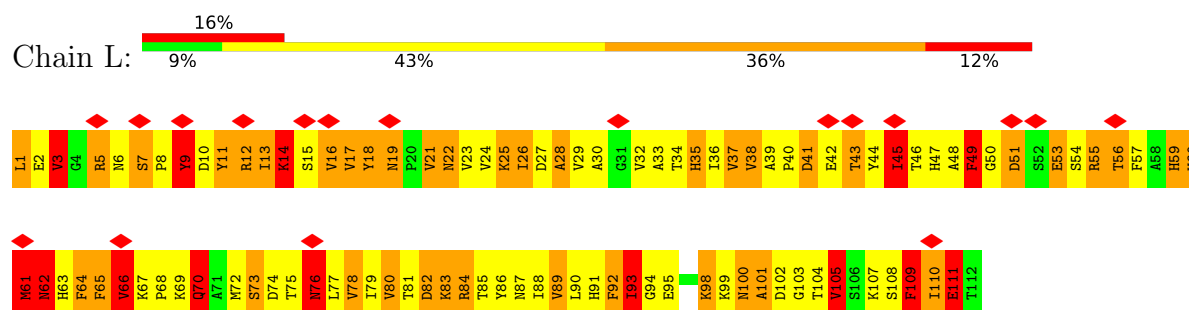
## ● Molecule 1: TRA0 PROTEIN



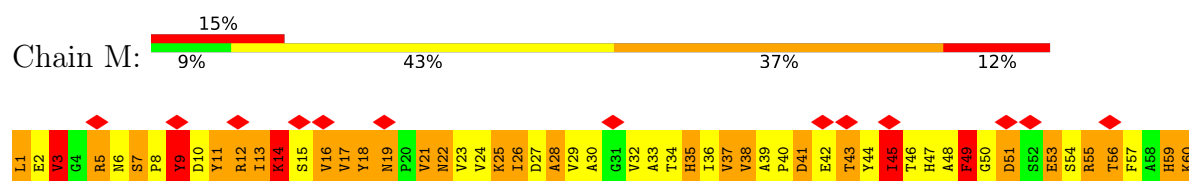
## ● Molecule 1: TRA0 PROTEIN

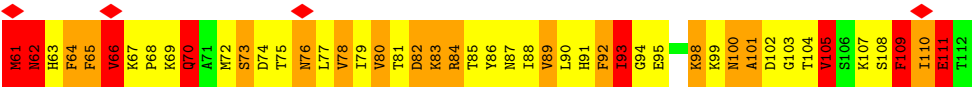


## ● Molecule 1: TRA0 PROTEIN

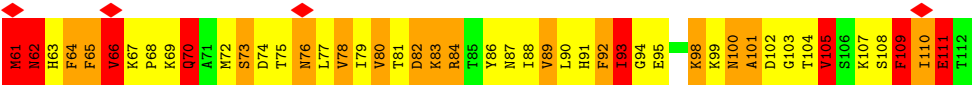
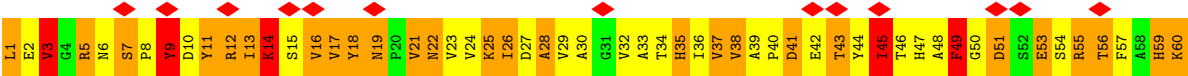


## ● Molecule 1: TRA0 PROTEIN





• Molecule 1: TRA0 PROTEIN



## 4 Experimental information

| Property                             | Value                          | Source    |
|--------------------------------------|--------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                | Depositor |
| Imposed symmetry                     | POINT, C14                     | Depositor |
| Number of particles used             | 5430                           | Depositor |
| Resolution determination method      | Not provided                   |           |
| CTF correction method                | PHASE FLIPPING, EACH CCD IMAGE | Depositor |
| Microscope                           | FEI TECNAI 12                  | Depositor |
| Voltage (kV)                         | 200                            | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                             | Depositor |
| Minimum defocus (nm)                 | 1500                           | Depositor |
| Maximum defocus (nm)                 | 3500                           | Depositor |
| Magnification                        | 68100                          | Depositor |
| Image detector                       | GENERIC GATAN                  | Depositor |
| Maximum map value                    | 5.163                          | Depositor |
| Minimum map value                    | -3.082                         | Depositor |
| Average map value                    | 0.019                          | Depositor |
| Map value standard deviation         | 0.223                          | Depositor |
| Recommended contour level            | 0.23                           | Depositor |
| Map size ( $\text{\AA}$ )            | 332.8, 332.8, 332.8            | wwPDB     |
| Map dimensions                       | 160, 160, 160                  | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0               | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.08, 2.08, 2.08               | 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     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | B     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | C     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | D     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | E     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | F     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | G     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | H     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | I     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | J     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | K     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | L     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | M     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| 1   | N     | 1.50         | 0/905       | 1.85        | 28/1227 (2.3%)   |
| All | All   | 1.50         | 0/12670     | 1.85        | 392/17178 (2.3%) |

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                   | 7                   |
| 1   | B     | 0                   | 7                   |
| 1   | C     | 0                   | 7                   |
| 1   | D     | 0                   | 7                   |
| 1   | E     | 0                   | 7                   |
| 1   | F     | 0                   | 7                   |
| 1   | G     | 0                   | 7                   |
| 1   | H     | 0                   | 7                   |
| 1   | I     | 0                   | 7                   |
| 1   | J     | 0                   | 7                   |
| 1   | K     | 0                   | 7                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | L     | 0                   | 7                   |
| 1   | M     | 0                   | 7                   |
| 1   | N     | 0                   | 7                   |
| All | All   | 0                   | 98                  |

There are no bond length outliers.

All (392) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 92  | PHE  | CA-CB-CG | -9.38 | 104.42      | 113.80   |
| 1   | N     | 92  | PHE  | CA-CB-CG | -9.38 | 104.42      | 113.80   |
| 1   | B     | 92  | PHE  | CA-CB-CG | -9.37 | 104.43      | 113.80   |
| 1   | I     | 92  | PHE  | CA-CB-CG | -9.37 | 104.43      | 113.80   |
| 1   | C     | 92  | PHE  | CA-CB-CG | -9.37 | 104.43      | 113.80   |
| 1   | J     | 92  | PHE  | CA-CB-CG | -9.37 | 104.43      | 113.80   |
| 1   | F     | 92  | PHE  | CA-CB-CG | -9.36 | 104.44      | 113.80   |
| 1   | M     | 92  | PHE  | CA-CB-CG | -9.36 | 104.44      | 113.80   |
| 1   | A     | 92  | PHE  | CA-CB-CG | -9.36 | 104.44      | 113.80   |
| 1   | H     | 92  | PHE  | CA-CB-CG | -9.36 | 104.44      | 113.80   |
| 1   | D     | 92  | PHE  | CA-CB-CG | -9.35 | 104.45      | 113.80   |
| 1   | K     | 92  | PHE  | CA-CB-CG | -9.35 | 104.45      | 113.80   |
| 1   | E     | 92  | PHE  | CA-CB-CG | -9.33 | 104.47      | 113.80   |
| 1   | L     | 92  | PHE  | CA-CB-CG | -9.33 | 104.47      | 113.80   |
| 1   | C     | 66  | VAL  | CA-C-N   | -7.98 | 115.26      | 122.28   |
| 1   | C     | 66  | VAL  | C-N-CA   | -7.98 | 115.26      | 122.28   |
| 1   | J     | 66  | VAL  | CA-C-N   | -7.98 | 115.26      | 122.28   |
| 1   | J     | 66  | VAL  | C-N-CA   | -7.98 | 115.26      | 122.28   |
| 1   | G     | 66  | VAL  | CA-C-N   | -7.97 | 115.27      | 122.28   |
| 1   | G     | 66  | VAL  | C-N-CA   | -7.97 | 115.27      | 122.28   |
| 1   | N     | 66  | VAL  | CA-C-N   | -7.97 | 115.27      | 122.28   |
| 1   | N     | 66  | VAL  | C-N-CA   | -7.97 | 115.27      | 122.28   |
| 1   | B     | 66  | VAL  | CA-C-N   | -7.96 | 115.28      | 122.28   |
| 1   | B     | 66  | VAL  | C-N-CA   | -7.96 | 115.28      | 122.28   |
| 1   | I     | 66  | VAL  | CA-C-N   | -7.96 | 115.28      | 122.28   |
| 1   | I     | 66  | VAL  | C-N-CA   | -7.96 | 115.28      | 122.28   |
| 1   | D     | 66  | VAL  | CA-C-N   | -7.94 | 115.30      | 122.28   |
| 1   | D     | 66  | VAL  | C-N-CA   | -7.94 | 115.30      | 122.28   |
| 1   | K     | 66  | VAL  | CA-C-N   | -7.94 | 115.30      | 122.28   |
| 1   | K     | 66  | VAL  | C-N-CA   | -7.94 | 115.30      | 122.28   |
| 1   | F     | 66  | VAL  | CA-C-N   | -7.93 | 115.30      | 122.28   |
| 1   | F     | 66  | VAL  | C-N-CA   | -7.93 | 115.30      | 122.28   |
| 1   | M     | 66  | VAL  | CA-C-N   | -7.93 | 115.30      | 122.28   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | M     | 66  | VAL  | C-N-CA   | -7.93 | 115.30      | 122.28   |
| 1   | A     | 66  | VAL  | CA-C-N   | -7.93 | 115.30      | 122.28   |
| 1   | A     | 66  | VAL  | C-N-CA   | -7.93 | 115.30      | 122.28   |
| 1   | H     | 66  | VAL  | CA-C-N   | -7.93 | 115.30      | 122.28   |
| 1   | H     | 66  | VAL  | C-N-CA   | -7.93 | 115.30      | 122.28   |
| 1   | E     | 66  | VAL  | CA-C-N   | -7.88 | 115.35      | 122.28   |
| 1   | E     | 66  | VAL  | C-N-CA   | -7.88 | 115.35      | 122.28   |
| 1   | L     | 66  | VAL  | CA-C-N   | -7.88 | 115.35      | 122.28   |
| 1   | L     | 66  | VAL  | C-N-CA   | -7.88 | 115.35      | 122.28   |
| 1   | G     | 76  | ASN  | CA-CB-CG | -7.44 | 105.16      | 112.60   |
| 1   | N     | 76  | ASN  | CA-CB-CG | -7.44 | 105.16      | 112.60   |
| 1   | A     | 76  | ASN  | CA-CB-CG | -7.44 | 105.16      | 112.60   |
| 1   | H     | 76  | ASN  | CA-CB-CG | -7.44 | 105.16      | 112.60   |
| 1   | B     | 76  | ASN  | CA-CB-CG | -7.43 | 105.17      | 112.60   |
| 1   | I     | 76  | ASN  | CA-CB-CG | -7.43 | 105.17      | 112.60   |
| 1   | D     | 76  | ASN  | CA-CB-CG | -7.43 | 105.17      | 112.60   |
| 1   | K     | 76  | ASN  | CA-CB-CG | -7.43 | 105.17      | 112.60   |
| 1   | F     | 76  | ASN  | CA-CB-CG | -7.42 | 105.18      | 112.60   |
| 1   | M     | 76  | ASN  | CA-CB-CG | -7.42 | 105.18      | 112.60   |
| 1   | E     | 76  | ASN  | CA-CB-CG | -7.41 | 105.19      | 112.60   |
| 1   | L     | 76  | ASN  | CA-CB-CG | -7.41 | 105.19      | 112.60   |
| 1   | C     | 76  | ASN  | CA-CB-CG | -7.40 | 105.20      | 112.60   |
| 1   | J     | 76  | ASN  | CA-CB-CG | -7.40 | 105.20      | 112.60   |
| 1   | G     | 51  | ASP  | CA-CB-CG | -7.30 | 105.30      | 112.60   |
| 1   | N     | 51  | ASP  | CA-CB-CG | -7.30 | 105.30      | 112.60   |
| 1   | C     | 51  | ASP  | CA-CB-CG | -7.29 | 105.31      | 112.60   |
| 1   | J     | 51  | ASP  | CA-CB-CG | -7.29 | 105.31      | 112.60   |
| 1   | F     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | M     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | A     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | D     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | H     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | K     | 51  | ASP  | CA-CB-CG | -7.28 | 105.32      | 112.60   |
| 1   | E     | 51  | ASP  | CA-CB-CG | -7.26 | 105.33      | 112.60   |
| 1   | L     | 51  | ASP  | CA-CB-CG | -7.26 | 105.33      | 112.60   |
| 1   | B     | 51  | ASP  | CA-CB-CG | -7.26 | 105.34      | 112.60   |
| 1   | I     | 51  | ASP  | CA-CB-CG | -7.26 | 105.34      | 112.60   |
| 1   | C     | 82  | ASP  | N-CA-C   | -6.60 | 103.90      | 112.68   |
| 1   | J     | 82  | ASP  | N-CA-C   | -6.60 | 103.90      | 112.68   |
| 1   | B     | 82  | ASP  | N-CA-C   | -6.60 | 103.91      | 112.68   |
| 1   | I     | 82  | ASP  | N-CA-C   | -6.60 | 103.91      | 112.68   |
| 1   | G     | 82  | ASP  | N-CA-C   | -6.58 | 103.92      | 112.68   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 82  | ASP  | N-CA-C  | -6.58 | 103.92      | 112.68   |
| 1   | A     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | H     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | D     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | K     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | F     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | M     | 82  | ASP  | N-CA-C  | -6.57 | 103.94      | 112.68   |
| 1   | E     | 82  | ASP  | N-CA-C  | -6.55 | 103.97      | 112.68   |
| 1   | L     | 82  | ASP  | N-CA-C  | -6.55 | 103.97      | 112.68   |
| 1   | E     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | L     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | F     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | M     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | B     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | I     | 61  | MET  | CB-CA-C | -6.22 | 106.62      | 114.40   |
| 1   | A     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | H     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | C     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | D     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | G     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | J     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | K     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | N     | 61  | MET  | CB-CA-C | -6.22 | 106.63      | 114.40   |
| 1   | B     | 101 | ALA  | N-CA-C  | -6.11 | 105.86      | 113.38   |
| 1   | I     | 101 | ALA  | N-CA-C  | -6.11 | 105.86      | 113.38   |
| 1   | C     | 72  | MET  | N-CA-C  | -6.10 | 105.67      | 113.23   |
| 1   | J     | 72  | MET  | N-CA-C  | -6.10 | 105.67      | 113.23   |
| 1   | A     | 101 | ALA  | N-CA-C  | -6.09 | 105.89      | 113.38   |
| 1   | H     | 101 | ALA  | N-CA-C  | -6.09 | 105.89      | 113.38   |
| 1   | E     | 101 | ALA  | N-CA-C  | -6.09 | 105.89      | 113.38   |
| 1   | L     | 101 | ALA  | N-CA-C  | -6.09 | 105.89      | 113.38   |
| 1   | G     | 101 | ALA  | N-CA-C  | -6.08 | 105.90      | 113.38   |
| 1   | N     | 101 | ALA  | N-CA-C  | -6.08 | 105.90      | 113.38   |
| 1   | D     | 101 | ALA  | N-CA-C  | -6.07 | 105.91      | 113.38   |
| 1   | K     | 101 | ALA  | N-CA-C  | -6.07 | 105.91      | 113.38   |
| 1   | C     | 101 | ALA  | N-CA-C  | -6.06 | 105.92      | 113.38   |
| 1   | F     | 72  | MET  | N-CA-C  | -6.06 | 105.71      | 113.23   |
| 1   | J     | 101 | ALA  | N-CA-C  | -6.06 | 105.92      | 113.38   |
| 1   | M     | 72  | MET  | N-CA-C  | -6.06 | 105.71      | 113.23   |
| 1   | A     | 72  | MET  | N-CA-C  | -6.06 | 105.72      | 113.23   |
| 1   | H     | 72  | MET  | N-CA-C  | -6.06 | 105.72      | 113.23   |
| 1   | F     | 101 | ALA  | N-CA-C  | -6.05 | 105.93      | 113.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 101 | ALA  | N-CA-C  | -6.05 | 105.93      | 113.38   |
| 1   | B     | 72  | MET  | N-CA-C  | -6.05 | 105.73      | 113.23   |
| 1   | I     | 72  | MET  | N-CA-C  | -6.05 | 105.73      | 113.23   |
| 1   | B     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | I     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | D     | 72  | MET  | N-CA-C  | -6.04 | 105.74      | 113.23   |
| 1   | G     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | K     | 72  | MET  | N-CA-C  | -6.04 | 105.74      | 113.23   |
| 1   | N     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | E     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | L     | 111 | GLU  | N-CA-C  | -6.04 | 104.65      | 112.68   |
| 1   | A     | 111 | GLU  | N-CA-C  | -6.03 | 104.65      | 112.68   |
| 1   | H     | 111 | GLU  | N-CA-C  | -6.03 | 104.65      | 112.68   |
| 1   | G     | 72  | MET  | N-CA-C  | -6.03 | 105.76      | 113.23   |
| 1   | N     | 72  | MET  | N-CA-C  | -6.03 | 105.76      | 113.23   |
| 1   | E     | 72  | MET  | N-CA-C  | -6.02 | 105.76      | 113.23   |
| 1   | L     | 72  | MET  | N-CA-C  | -6.02 | 105.76      | 113.23   |
| 1   | F     | 111 | GLU  | N-CA-C  | -6.02 | 104.67      | 112.68   |
| 1   | M     | 111 | GLU  | N-CA-C  | -6.02 | 104.67      | 112.68   |
| 1   | C     | 111 | GLU  | N-CA-C  | -6.02 | 104.67      | 112.68   |
| 1   | J     | 111 | GLU  | N-CA-C  | -6.02 | 104.67      | 112.68   |
| 1   | D     | 111 | GLU  | N-CA-C  | -6.01 | 104.68      | 112.68   |
| 1   | K     | 111 | GLU  | N-CA-C  | -6.01 | 104.68      | 112.68   |
| 1   | F     | 19  | ASN  | N-CA-C  | -5.84 | 103.31      | 110.31   |
| 1   | M     | 19  | ASN  | N-CA-C  | -5.84 | 103.31      | 110.31   |
| 1   | G     | 13  | ILE  | CB-CA-C | -5.83 | 101.73      | 111.29   |
| 1   | N     | 13  | ILE  | CB-CA-C | -5.83 | 101.73      | 111.29   |
| 1   | A     | 19  | ASN  | N-CA-C  | -5.83 | 103.32      | 110.31   |
| 1   | B     | 19  | ASN  | N-CA-C  | -5.83 | 103.32      | 110.31   |
| 1   | H     | 19  | ASN  | N-CA-C  | -5.83 | 103.32      | 110.31   |
| 1   | I     | 19  | ASN  | N-CA-C  | -5.83 | 103.32      | 110.31   |
| 1   | F     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | M     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | A     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | B     | 13  | ILE  | CB-CA-C | -5.82 | 101.75      | 111.29   |
| 1   | E     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | H     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | I     | 13  | ILE  | CB-CA-C | -5.82 | 101.75      | 111.29   |
| 1   | L     | 13  | ILE  | CB-CA-C | -5.82 | 101.74      | 111.29   |
| 1   | E     | 19  | ASN  | N-CA-C  | -5.82 | 103.33      | 110.31   |
| 1   | L     | 19  | ASN  | N-CA-C  | -5.82 | 103.33      | 110.31   |
| 1   | D     | 13  | ILE  | CB-CA-C | -5.82 | 101.75      | 111.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | K     | 13  | ILE  | CB-CA-C  | -5.82 | 101.75      | 111.29   |
| 1   | G     | 19  | ASN  | N-CA-C   | -5.81 | 103.33      | 110.31   |
| 1   | N     | 19  | ASN  | N-CA-C   | -5.81 | 103.33      | 110.31   |
| 1   | C     | 13  | ILE  | CB-CA-C  | -5.81 | 101.76      | 111.29   |
| 1   | J     | 13  | ILE  | CB-CA-C  | -5.81 | 101.76      | 111.29   |
| 1   | C     | 19  | ASN  | N-CA-C   | -5.81 | 103.34      | 110.31   |
| 1   | J     | 19  | ASN  | N-CA-C   | -5.81 | 103.34      | 110.31   |
| 1   | D     | 19  | ASN  | N-CA-C   | -5.79 | 103.36      | 110.31   |
| 1   | K     | 19  | ASN  | N-CA-C   | -5.79 | 103.36      | 110.31   |
| 1   | E     | 41  | ASP  | CA-CB-CG | -5.79 | 106.81      | 112.60   |
| 1   | L     | 41  | ASP  | CA-CB-CG | -5.79 | 106.81      | 112.60   |
| 1   | B     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | G     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | I     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | N     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | A     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | H     | 41  | ASP  | CA-CB-CG | -5.77 | 106.83      | 112.60   |
| 1   | C     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | J     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | B     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | D     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | F     | 41  | ASP  | CA-CB-CG | -5.76 | 106.84      | 112.60   |
| 1   | I     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | K     | 9   | TYR  | N-CA-CB  | 5.76  | 118.32      | 109.91   |
| 1   | M     | 41  | ASP  | CA-CB-CG | -5.76 | 106.84      | 112.60   |
| 1   | A     | 9   | TYR  | N-CA-CB  | 5.75  | 118.31      | 109.91   |
| 1   | H     | 9   | TYR  | N-CA-CB  | 5.75  | 118.31      | 109.91   |
| 1   | G     | 9   | TYR  | N-CA-CB  | 5.75  | 118.30      | 109.91   |
| 1   | N     | 9   | TYR  | N-CA-CB  | 5.75  | 118.30      | 109.91   |
| 1   | E     | 9   | TYR  | N-CA-CB  | 5.75  | 118.30      | 109.91   |
| 1   | L     | 9   | TYR  | N-CA-CB  | 5.75  | 118.30      | 109.91   |
| 1   | F     | 9   | TYR  | N-CA-CB  | 5.74  | 118.30      | 109.91   |
| 1   | M     | 9   | TYR  | N-CA-CB  | 5.74  | 118.30      | 109.91   |
| 1   | C     | 41  | ASP  | CA-CB-CG | -5.74 | 106.86      | 112.60   |
| 1   | J     | 41  | ASP  | CA-CB-CG | -5.74 | 106.86      | 112.60   |
| 1   | D     | 41  | ASP  | CA-CB-CG | -5.73 | 106.87      | 112.60   |
| 1   | K     | 41  | ASP  | CA-CB-CG | -5.73 | 106.87      | 112.60   |
| 1   | F     | 9   | TYR  | CA-C-N   | 5.71  | 131.99      | 121.70   |
| 1   | F     | 9   | TYR  | C-N-CA   | 5.71  | 131.99      | 121.70   |
| 1   | M     | 9   | TYR  | CA-C-N   | 5.71  | 131.99      | 121.70   |
| 1   | M     | 9   | TYR  | C-N-CA   | 5.71  | 131.99      | 121.70   |
| 1   | B     | 9   | TYR  | CA-C-N   | 5.71  | 131.98      | 121.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 9   | TYR  | C-N-CA   | 5.71  | 131.98      | 121.70   |
| 1   | I     | 9   | TYR  | CA-C-N   | 5.71  | 131.98      | 121.70   |
| 1   | I     | 9   | TYR  | C-N-CA   | 5.71  | 131.98      | 121.70   |
| 1   | D     | 9   | TYR  | CA-C-N   | 5.70  | 131.95      | 121.70   |
| 1   | D     | 9   | TYR  | C-N-CA   | 5.70  | 131.95      | 121.70   |
| 1   | K     | 9   | TYR  | CA-C-N   | 5.70  | 131.95      | 121.70   |
| 1   | K     | 9   | TYR  | C-N-CA   | 5.70  | 131.95      | 121.70   |
| 1   | C     | 9   | TYR  | CA-C-N   | 5.69  | 131.94      | 121.70   |
| 1   | C     | 9   | TYR  | C-N-CA   | 5.69  | 131.94      | 121.70   |
| 1   | J     | 9   | TYR  | CA-C-N   | 5.69  | 131.94      | 121.70   |
| 1   | J     | 9   | TYR  | C-N-CA   | 5.69  | 131.94      | 121.70   |
| 1   | A     | 9   | TYR  | CA-C-N   | 5.69  | 131.94      | 121.70   |
| 1   | A     | 9   | TYR  | C-N-CA   | 5.69  | 131.94      | 121.70   |
| 1   | H     | 9   | TYR  | CA-C-N   | 5.69  | 131.94      | 121.70   |
| 1   | H     | 9   | TYR  | C-N-CA   | 5.69  | 131.94      | 121.70   |
| 1   | G     | 9   | TYR  | CA-C-N   | 5.68  | 131.92      | 121.70   |
| 1   | G     | 9   | TYR  | C-N-CA   | 5.68  | 131.92      | 121.70   |
| 1   | N     | 9   | TYR  | CA-C-N   | 5.68  | 131.92      | 121.70   |
| 1   | N     | 9   | TYR  | C-N-CA   | 5.68  | 131.92      | 121.70   |
| 1   | E     | 9   | TYR  | CA-C-N   | 5.67  | 131.91      | 121.70   |
| 1   | E     | 9   | TYR  | C-N-CA   | 5.67  | 131.91      | 121.70   |
| 1   | L     | 9   | TYR  | CA-C-N   | 5.67  | 131.91      | 121.70   |
| 1   | L     | 9   | TYR  | C-N-CA   | 5.67  | 131.91      | 121.70   |
| 1   | D     | 74  | ASP  | CA-CB-CG | -5.51 | 107.09      | 112.60   |
| 1   | K     | 74  | ASP  | CA-CB-CG | -5.51 | 107.09      | 112.60   |
| 1   | A     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | H     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | F     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | M     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | C     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | J     | 74  | ASP  | CA-CB-CG | -5.50 | 107.10      | 112.60   |
| 1   | E     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | L     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | G     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | N     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | B     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | I     | 74  | ASP  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 1   | C     | 105 | VAL  | CB-CA-C  | -5.49 | 102.29      | 111.29   |
| 1   | J     | 105 | VAL  | CB-CA-C  | -5.49 | 102.29      | 111.29   |
| 1   | F     | 105 | VAL  | CB-CA-C  | -5.48 | 102.31      | 111.29   |
| 1   | M     | 105 | VAL  | CB-CA-C  | -5.48 | 102.31      | 111.29   |
| 1   | G     | 105 | VAL  | CB-CA-C  | -5.47 | 102.31      | 111.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 105 | VAL  | CB-CA-C | -5.47 | 102.31      | 111.29   |
| 1   | A     | 105 | VAL  | CB-CA-C | -5.46 | 102.33      | 111.29   |
| 1   | H     | 105 | VAL  | CB-CA-C | -5.46 | 102.33      | 111.29   |
| 1   | E     | 105 | VAL  | CB-CA-C | -5.46 | 102.33      | 111.29   |
| 1   | L     | 105 | VAL  | CB-CA-C | -5.46 | 102.33      | 111.29   |
| 1   | B     | 41  | ASP  | N-CA-C  | -5.46 | 106.12      | 112.89   |
| 1   | I     | 41  | ASP  | N-CA-C  | -5.46 | 106.12      | 112.89   |
| 1   | D     | 105 | VAL  | CB-CA-C | -5.46 | 102.34      | 111.29   |
| 1   | K     | 105 | VAL  | CB-CA-C | -5.46 | 102.34      | 111.29   |
| 1   | B     | 105 | VAL  | CB-CA-C | -5.45 | 102.35      | 111.29   |
| 1   | I     | 105 | VAL  | CB-CA-C | -5.45 | 102.35      | 111.29   |
| 1   | G     | 41  | ASP  | N-CA-C  | -5.45 | 106.13      | 112.89   |
| 1   | N     | 41  | ASP  | N-CA-C  | -5.45 | 106.13      | 112.89   |
| 1   | C     | 16  | VAL  | CA-C-N  | -5.44 | 113.74      | 121.85   |
| 1   | C     | 16  | VAL  | C-N-CA  | -5.44 | 113.74      | 121.85   |
| 1   | J     | 16  | VAL  | CA-C-N  | -5.44 | 113.74      | 121.85   |
| 1   | J     | 16  | VAL  | C-N-CA  | -5.44 | 113.74      | 121.85   |
| 1   | E     | 41  | ASP  | N-CA-C  | -5.44 | 106.15      | 112.89   |
| 1   | L     | 41  | ASP  | N-CA-C  | -5.44 | 106.15      | 112.89   |
| 1   | C     | 41  | ASP  | N-CA-C  | -5.43 | 106.16      | 112.89   |
| 1   | J     | 41  | ASP  | N-CA-C  | -5.43 | 106.16      | 112.89   |
| 1   | A     | 41  | ASP  | N-CA-C  | -5.42 | 106.17      | 112.89   |
| 1   | H     | 41  | ASP  | N-CA-C  | -5.42 | 106.17      | 112.89   |
| 1   | D     | 16  | VAL  | CA-C-N  | -5.42 | 113.78      | 121.85   |
| 1   | D     | 16  | VAL  | C-N-CA  | -5.42 | 113.78      | 121.85   |
| 1   | K     | 16  | VAL  | CA-C-N  | -5.42 | 113.78      | 121.85   |
| 1   | K     | 16  | VAL  | C-N-CA  | -5.42 | 113.78      | 121.85   |
| 1   | A     | 16  | VAL  | CA-C-N  | -5.42 | 113.78      | 121.85   |
| 1   | A     | 16  | VAL  | C-N-CA  | -5.42 | 113.78      | 121.85   |
| 1   | H     | 16  | VAL  | CA-C-N  | -5.42 | 113.78      | 121.85   |
| 1   | H     | 16  | VAL  | C-N-CA  | -5.42 | 113.78      | 121.85   |
| 1   | D     | 41  | ASP  | N-CA-C  | -5.41 | 106.18      | 112.89   |
| 1   | F     | 41  | ASP  | N-CA-C  | -5.41 | 106.18      | 112.89   |
| 1   | K     | 41  | ASP  | N-CA-C  | -5.41 | 106.18      | 112.89   |
| 1   | M     | 41  | ASP  | N-CA-C  | -5.41 | 106.18      | 112.89   |
| 1   | G     | 16  | VAL  | CA-C-N  | -5.41 | 113.79      | 121.85   |
| 1   | G     | 16  | VAL  | C-N-CA  | -5.41 | 113.79      | 121.85   |
| 1   | N     | 16  | VAL  | CA-C-N  | -5.41 | 113.79      | 121.85   |
| 1   | N     | 16  | VAL  | C-N-CA  | -5.41 | 113.79      | 121.85   |
| 1   | B     | 16  | VAL  | CA-C-N  | -5.41 | 113.79      | 121.85   |
| 1   | B     | 16  | VAL  | C-N-CA  | -5.41 | 113.79      | 121.85   |
| 1   | I     | 16  | VAL  | CA-C-N  | -5.41 | 113.79      | 121.85   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | I     | 16  | VAL  | C-N-CA   | -5.41 | 113.79      | 121.85   |
| 1   | E     | 16  | VAL  | CA-C-N   | -5.39 | 113.81      | 121.85   |
| 1   | E     | 16  | VAL  | C-N-CA   | -5.39 | 113.81      | 121.85   |
| 1   | L     | 16  | VAL  | CA-C-N   | -5.39 | 113.81      | 121.85   |
| 1   | L     | 16  | VAL  | C-N-CA   | -5.39 | 113.81      | 121.85   |
| 1   | G     | 5   | ARG  | N-CA-C   | -5.38 | 105.31      | 111.07   |
| 1   | N     | 5   | ARG  | N-CA-C   | -5.38 | 105.31      | 111.07   |
| 1   | F     | 16  | VAL  | CA-C-N   | -5.38 | 113.84      | 121.85   |
| 1   | F     | 16  | VAL  | C-N-CA   | -5.38 | 113.84      | 121.85   |
| 1   | M     | 16  | VAL  | CA-C-N   | -5.38 | 113.84      | 121.85   |
| 1   | M     | 16  | VAL  | C-N-CA   | -5.38 | 113.84      | 121.85   |
| 1   | C     | 5   | ARG  | N-CA-C   | -5.35 | 105.34      | 111.07   |
| 1   | J     | 5   | ARG  | N-CA-C   | -5.35 | 105.34      | 111.07   |
| 1   | D     | 5   | ARG  | N-CA-C   | -5.34 | 105.36      | 111.07   |
| 1   | K     | 5   | ARG  | N-CA-C   | -5.34 | 105.36      | 111.07   |
| 1   | A     | 5   | ARG  | N-CA-C   | -5.33 | 105.36      | 111.07   |
| 1   | H     | 5   | ARG  | N-CA-C   | -5.33 | 105.36      | 111.07   |
| 1   | F     | 5   | ARG  | N-CA-C   | -5.31 | 105.39      | 111.07   |
| 1   | M     | 5   | ARG  | N-CA-C   | -5.31 | 105.39      | 111.07   |
| 1   | C     | 22  | ASN  | CA-CB-CG | -5.30 | 107.30      | 112.60   |
| 1   | J     | 22  | ASN  | CA-CB-CG | -5.30 | 107.30      | 112.60   |
| 1   | B     | 5   | ARG  | N-CA-C   | -5.29 | 105.41      | 111.07   |
| 1   | E     | 5   | ARG  | N-CA-C   | -5.29 | 105.41      | 111.07   |
| 1   | I     | 5   | ARG  | N-CA-C   | -5.29 | 105.41      | 111.07   |
| 1   | L     | 5   | ARG  | N-CA-C   | -5.29 | 105.41      | 111.07   |
| 1   | E     | 22  | ASN  | CA-CB-CG | -5.29 | 107.31      | 112.60   |
| 1   | L     | 22  | ASN  | CA-CB-CG | -5.29 | 107.31      | 112.60   |
| 1   | A     | 22  | ASN  | CA-CB-CG | -5.27 | 107.33      | 112.60   |
| 1   | H     | 22  | ASN  | CA-CB-CG | -5.27 | 107.33      | 112.60   |
| 1   | D     | 100 | ASN  | CA-CB-CG | -5.27 | 107.33      | 112.60   |
| 1   | K     | 100 | ASN  | CA-CB-CG | -5.27 | 107.33      | 112.60   |
| 1   | F     | 100 | ASN  | CA-CB-CG | -5.26 | 107.34      | 112.60   |
| 1   | M     | 100 | ASN  | CA-CB-CG | -5.26 | 107.34      | 112.60   |
| 1   | F     | 22  | ASN  | CA-CB-CG | -5.26 | 107.34      | 112.60   |
| 1   | M     | 22  | ASN  | CA-CB-CG | -5.26 | 107.34      | 112.60   |
| 1   | G     | 22  | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | N     | 22  | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | E     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | L     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | A     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | H     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | B     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | I     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | N     | 100 | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | D     | 22  | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | K     | 22  | ASN  | CA-CB-CG | -5.25 | 107.35      | 112.60   |
| 1   | C     | 100 | ASN  | CA-CB-CG | -5.24 | 107.36      | 112.60   |
| 1   | J     | 100 | ASN  | CA-CB-CG | -5.24 | 107.36      | 112.60   |
| 1   | B     | 22  | ASN  | CA-CB-CG | -5.22 | 107.38      | 112.60   |
| 1   | I     | 22  | ASN  | CA-CB-CG | -5.22 | 107.38      | 112.60   |
| 1   | E     | 13  | ILE  | CA-C-N   | 5.19  | 131.45      | 121.54   |
| 1   | E     | 13  | ILE  | C-N-CA   | 5.19  | 131.45      | 121.54   |
| 1   | L     | 13  | ILE  | CA-C-N   | 5.19  | 131.45      | 121.54   |
| 1   | L     | 13  | ILE  | C-N-CA   | 5.19  | 131.45      | 121.54   |
| 1   | B     | 13  | ILE  | CA-C-N   | 5.17  | 131.43      | 121.54   |
| 1   | B     | 13  | ILE  | C-N-CA   | 5.17  | 131.43      | 121.54   |
| 1   | F     | 13  | ILE  | CA-C-N   | 5.17  | 131.42      | 121.54   |
| 1   | F     | 13  | ILE  | C-N-CA   | 5.17  | 131.42      | 121.54   |
| 1   | I     | 13  | ILE  | CA-C-N   | 5.17  | 131.43      | 121.54   |
| 1   | I     | 13  | ILE  | C-N-CA   | 5.17  | 131.43      | 121.54   |
| 1   | M     | 13  | ILE  | CA-C-N   | 5.17  | 131.42      | 121.54   |
| 1   | M     | 13  | ILE  | C-N-CA   | 5.17  | 131.42      | 121.54   |
| 1   | A     | 13  | ILE  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 1   | A     | 13  | ILE  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 1   | H     | 13  | ILE  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 1   | H     | 13  | ILE  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 1   | C     | 13  | ILE  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 1   | C     | 13  | ILE  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 1   | J     | 13  | ILE  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 1   | J     | 13  | ILE  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 1   | D     | 13  | ILE  | CA-C-N   | 5.16  | 131.40      | 121.54   |
| 1   | D     | 13  | ILE  | C-N-CA   | 5.16  | 131.40      | 121.54   |
| 1   | K     | 13  | ILE  | CA-C-N   | 5.16  | 131.40      | 121.54   |
| 1   | K     | 13  | ILE  | C-N-CA   | 5.16  | 131.40      | 121.54   |
| 1   | G     | 13  | ILE  | CA-C-N   | 5.16  | 131.39      | 121.54   |
| 1   | G     | 13  | ILE  | C-N-CA   | 5.16  | 131.39      | 121.54   |
| 1   | N     | 13  | ILE  | CA-C-N   | 5.16  | 131.39      | 121.54   |
| 1   | N     | 13  | ILE  | C-N-CA   | 5.16  | 131.39      | 121.54   |
| 1   | F     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | M     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | B     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | I     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | D     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | K     | 49  | PHE  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | G     | 49  | PHE  | CA-CB-CG | -5.12 | 108.68      | 113.80   |
| 1   | N     | 49  | PHE  | CA-CB-CG | -5.12 | 108.68      | 113.80   |
| 1   | A     | 49  | PHE  | CA-CB-CG | -5.11 | 108.69      | 113.80   |
| 1   | H     | 49  | PHE  | CA-CB-CG | -5.11 | 108.69      | 113.80   |
| 1   | C     | 49  | PHE  | CA-CB-CG | -5.11 | 108.69      | 113.80   |
| 1   | J     | 49  | PHE  | CA-CB-CG | -5.11 | 108.69      | 113.80   |
| 1   | E     | 49  | PHE  | CA-CB-CG | -5.10 | 108.70      | 113.80   |
| 1   | L     | 49  | PHE  | CA-CB-CG | -5.10 | 108.70      | 113.80   |
| 1   | F     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | M     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | B     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | E     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | I     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | L     | 82  | ASP  | CB-CA-C  | -5.08 | 101.75      | 110.24   |
| 1   | C     | 82  | ASP  | CB-CA-C  | -5.08 | 101.76      | 110.24   |
| 1   | J     | 82  | ASP  | CB-CA-C  | -5.08 | 101.76      | 110.24   |
| 1   | A     | 82  | ASP  | CB-CA-C  | -5.08 | 101.76      | 110.24   |
| 1   | H     | 82  | ASP  | CB-CA-C  | -5.08 | 101.76      | 110.24   |
| 1   | D     | 82  | ASP  | CB-CA-C  | -5.07 | 101.77      | 110.24   |
| 1   | K     | 82  | ASP  | CB-CA-C  | -5.07 | 101.77      | 110.24   |
| 1   | G     | 82  | ASP  | CB-CA-C  | -5.07 | 101.77      | 110.24   |
| 1   | N     | 82  | ASP  | CB-CA-C  | -5.07 | 101.77      | 110.24   |

There are no chirality outliers.

All (98) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 12  | ARG  | Sidechain |
| 1   | A     | 18  | TYR  | Peptide   |
| 1   | A     | 45  | ILE  | Peptide   |
| 1   | A     | 56  | THR  | Peptide   |
| 1   | A     | 65  | PHE  | Peptide   |
| 1   | A     | 7   | SER  | Peptide   |
| 1   | A     | 99  | LYS  | Peptide   |
| 1   | B     | 12  | ARG  | Sidechain |
| 1   | B     | 18  | TYR  | Peptide   |
| 1   | B     | 45  | ILE  | Peptide   |
| 1   | B     | 56  | THR  | Peptide   |
| 1   | B     | 65  | PHE  | Peptide   |
| 1   | B     | 7   | SER  | Peptide   |
| 1   | B     | 99  | LYS  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 12  | ARG  | Sidechain |
| 1   | C     | 18  | TYR  | Peptide   |
| 1   | C     | 45  | ILE  | Peptide   |
| 1   | C     | 56  | THR  | Peptide   |
| 1   | C     | 65  | PHE  | Peptide   |
| 1   | C     | 7   | SER  | Peptide   |
| 1   | C     | 99  | LYS  | Peptide   |
| 1   | D     | 12  | ARG  | Sidechain |
| 1   | D     | 18  | TYR  | Peptide   |
| 1   | D     | 45  | ILE  | Peptide   |
| 1   | D     | 56  | THR  | Peptide   |
| 1   | D     | 65  | PHE  | Peptide   |
| 1   | D     | 7   | SER  | Peptide   |
| 1   | D     | 99  | LYS  | Peptide   |
| 1   | E     | 12  | ARG  | Sidechain |
| 1   | E     | 18  | TYR  | Peptide   |
| 1   | E     | 45  | ILE  | Peptide   |
| 1   | E     | 56  | THR  | Peptide   |
| 1   | E     | 65  | PHE  | Peptide   |
| 1   | E     | 7   | SER  | Peptide   |
| 1   | E     | 99  | LYS  | Peptide   |
| 1   | F     | 12  | ARG  | Sidechain |
| 1   | F     | 18  | TYR  | Peptide   |
| 1   | F     | 45  | ILE  | Peptide   |
| 1   | F     | 56  | THR  | Peptide   |
| 1   | F     | 65  | PHE  | Peptide   |
| 1   | F     | 7   | SER  | Peptide   |
| 1   | F     | 99  | LYS  | Peptide   |
| 1   | G     | 12  | ARG  | Sidechain |
| 1   | G     | 18  | TYR  | Peptide   |
| 1   | G     | 45  | ILE  | Peptide   |
| 1   | G     | 56  | THR  | Peptide   |
| 1   | G     | 65  | PHE  | Peptide   |
| 1   | G     | 7   | SER  | Peptide   |
| 1   | G     | 99  | LYS  | Peptide   |
| 1   | H     | 12  | ARG  | Sidechain |
| 1   | H     | 18  | TYR  | Peptide   |
| 1   | H     | 45  | ILE  | Peptide   |
| 1   | H     | 56  | THR  | Peptide   |
| 1   | H     | 65  | PHE  | Peptide   |
| 1   | H     | 7   | SER  | Peptide   |
| 1   | H     | 99  | LYS  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | I     | 12  | ARG  | Sidechain |
| 1   | I     | 18  | TYR  | Peptide   |
| 1   | I     | 45  | ILE  | Peptide   |
| 1   | I     | 56  | THR  | Peptide   |
| 1   | I     | 65  | PHE  | Peptide   |
| 1   | I     | 7   | SER  | Peptide   |
| 1   | I     | 99  | LYS  | Peptide   |
| 1   | J     | 12  | ARG  | Sidechain |
| 1   | J     | 18  | TYR  | Peptide   |
| 1   | J     | 45  | ILE  | Peptide   |
| 1   | J     | 56  | THR  | Peptide   |
| 1   | J     | 65  | PHE  | Peptide   |
| 1   | J     | 7   | SER  | Peptide   |
| 1   | J     | 99  | LYS  | Peptide   |
| 1   | K     | 12  | ARG  | Sidechain |
| 1   | K     | 18  | TYR  | Peptide   |
| 1   | K     | 45  | ILE  | Peptide   |
| 1   | K     | 56  | THR  | Peptide   |
| 1   | K     | 65  | PHE  | Peptide   |
| 1   | K     | 7   | SER  | Peptide   |
| 1   | K     | 99  | LYS  | Peptide   |
| 1   | L     | 12  | ARG  | Sidechain |
| 1   | L     | 18  | TYR  | Peptide   |
| 1   | L     | 45  | ILE  | Peptide   |
| 1   | L     | 56  | THR  | Peptide   |
| 1   | L     | 65  | PHE  | Peptide   |
| 1   | L     | 7   | SER  | Peptide   |
| 1   | L     | 99  | LYS  | Peptide   |
| 1   | M     | 12  | ARG  | Sidechain |
| 1   | M     | 18  | TYR  | Peptide   |
| 1   | M     | 45  | ILE  | Peptide   |
| 1   | M     | 56  | THR  | Peptide   |
| 1   | M     | 65  | PHE  | Peptide   |
| 1   | M     | 7   | SER  | Peptide   |
| 1   | M     | 99  | LYS  | Peptide   |
| 1   | N     | 12  | ARG  | Sidechain |
| 1   | N     | 18  | TYR  | Peptide   |
| 1   | N     | 45  | ILE  | Peptide   |
| 1   | N     | 56  | THR  | Peptide   |
| 1   | N     | 65  | PHE  | Peptide   |
| 1   | N     | 7   | SER  | Peptide   |
| 1   | N     | 99  | LYS  | Peptide   |

## 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     | 886   | 0        | 881      | 309     | 0            |
| 1   | B     | 886   | 0        | 881      | 312     | 0            |
| 1   | C     | 886   | 0        | 881      | 313     | 0            |
| 1   | D     | 886   | 0        | 881      | 309     | 0            |
| 1   | E     | 886   | 0        | 881      | 311     | 0            |
| 1   | F     | 886   | 0        | 881      | 310     | 0            |
| 1   | G     | 886   | 0        | 881      | 310     | 0            |
| 1   | H     | 886   | 0        | 881      | 314     | 0            |
| 1   | I     | 886   | 0        | 881      | 312     | 0            |
| 1   | J     | 886   | 0        | 881      | 306     | 0            |
| 1   | K     | 886   | 0        | 881      | 309     | 0            |
| 1   | L     | 886   | 0        | 881      | 318     | 0            |
| 1   | M     | 886   | 0        | 881      | 313     | 0            |
| 1   | N     | 886   | 0        | 881      | 313     | 0            |
| All | All   | 12404 | 0        | 12334    | 3944    | 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 159.

All (3944) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:91:HIS:HA   | 1:M:104:THR:HB  | 1.24                     | 1.18              |
| 1:F:1:LEU:HD12  | 1:F:16:VAL:HG23 | 1.23                     | 1.18              |
| 1:A:91:HIS:HA   | 1:A:104:THR:HB  | 1.24                     | 1.17              |
| 1:E:1:LEU:HD12  | 1:E:16:VAL:HG23 | 1.24                     | 1.16              |
| 1:G:1:LEU:HD12  | 1:G:16:VAL:HG23 | 1.24                     | 1.16              |
| 1:H:1:LEU:HD12  | 1:H:16:VAL:HG23 | 1.24                     | 1.16              |
| 1:I:1:LEU:HD12  | 1:I:16:VAL:HG23 | 1.23                     | 1.16              |
| 1:B:91:HIS:HA   | 1:B:104:THR:HB  | 1.24                     | 1.15              |
| 1:G:80:VAL:HG13 | 1:G:88:ILE:HG22 | 1.30                     | 1.14              |
| 1:F:80:VAL:HG13 | 1:F:88:ILE:HG22 | 1.30                     | 1.14              |
| 1:H:80:VAL:HG13 | 1:H:88:ILE:HG22 | 1.30                     | 1.14              |
| 1:I:80:VAL:HG13 | 1:I:88:ILE:HG22 | 1.30                     | 1.14              |
| 1:D:91:HIS:HA   | 1:D:104:THR:HB  | 1.24                     | 1.13              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:80:VAL:HG13 | 1:J:88:ILE:HG22 | 1.30                     | 1.13              |
| 1:L:91:HIS:HA   | 1:L:104:THR:HB  | 1.24                     | 1.13              |
| 1:C:1:LEU:HD12  | 1:C:16:VAL:HG23 | 1.23                     | 1.13              |
| 1:E:80:VAL:HG13 | 1:E:88:ILE:HG22 | 1.30                     | 1.13              |
| 1:J:91:HIS:HA   | 1:J:104:THR:HB  | 1.24                     | 1.13              |
| 1:D:1:LEU:HD12  | 1:D:16:VAL:HG23 | 1.24                     | 1.12              |
| 1:K:91:HIS:HA   | 1:K:104:THR:HB  | 1.24                     | 1.12              |
| 1:J:1:LEU:HD12  | 1:J:16:VAL:HG23 | 1.23                     | 1.12              |
| 1:K:80:VAL:HG13 | 1:K:88:ILE:HG22 | 1.30                     | 1.12              |
| 1:M:1:LEU:HD11  | 1:M:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:D:80:VAL:HG13 | 1:D:88:ILE:HG22 | 1.30                     | 1.11              |
| 1:G:1:LEU:HD11  | 1:G:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:H:1:LEU:HD11  | 1:H:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:L:1:LEU:HD11  | 1:L:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:L:80:VAL:HG13 | 1:L:88:ILE:HG22 | 1.30                     | 1.11              |
| 1:F:1:LEU:HD11  | 1:F:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:I:1:LEU:HD11  | 1:I:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:M:80:VAL:HG13 | 1:M:88:ILE:HG22 | 1.30                     | 1.11              |
| 1:C:80:VAL:HG13 | 1:C:88:ILE:HG22 | 1.30                     | 1.11              |
| 1:H:63:HIS:HA   | 1:H:82:ASP:HB2  | 1.13                     | 1.11              |
| 1:I:63:HIS:HA   | 1:I:82:ASP:HB2  | 1.13                     | 1.11              |
| 1:J:1:LEU:HD11  | 1:J:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:K:1:LEU:HD11  | 1:K:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:K:1:LEU:HD12  | 1:K:16:VAL:HG23 | 1.24                     | 1.11              |
| 1:N:1:LEU:HD11  | 1:N:13:ILE:HD11 | 1.33                     | 1.11              |
| 1:B:80:VAL:HG13 | 1:B:88:ILE:HG22 | 1.30                     | 1.10              |
| 1:N:80:VAL:HG13 | 1:N:88:ILE:HG22 | 1.30                     | 1.10              |
| 1:N:91:HIS:HA   | 1:N:104:THR:HB  | 1.24                     | 1.10              |
| 1:A:80:VAL:HG13 | 1:A:88:ILE:HG22 | 1.30                     | 1.10              |
| 1:G:63:HIS:HA   | 1:G:82:ASP:HB2  | 1.13                     | 1.10              |
| 1:C:91:HIS:HA   | 1:C:104:THR:HB  | 1.24                     | 1.10              |
| 1:J:63:HIS:HA   | 1:J:82:ASP:HB2  | 1.13                     | 1.10              |
| 1:A:1:LEU:HD11  | 1:A:13:ILE:HD11 | 1.33                     | 1.10              |
| 1:B:1:LEU:HD12  | 1:B:16:VAL:HG23 | 1.23                     | 1.10              |
| 1:E:1:LEU:HD11  | 1:E:13:ILE:HD11 | 1.33                     | 1.10              |
| 1:K:63:HIS:HA   | 1:K:82:ASP:HB2  | 1.13                     | 1.10              |
| 1:F:91:HIS:HA   | 1:F:104:THR:HB  | 1.24                     | 1.09              |
| 1:H:91:HIS:HA   | 1:H:104:THR:HB  | 1.24                     | 1.09              |
| 1:B:1:LEU:HD11  | 1:B:13:ILE:HD11 | 1.33                     | 1.09              |
| 1:D:1:LEU:HD11  | 1:D:13:ILE:HD11 | 1.33                     | 1.09              |
| 1:F:63:HIS:HA   | 1:F:82:ASP:HB2  | 1.13                     | 1.09              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:L:63:HIS:HA  | 1:L:82:ASP:HB2  | 1.13                     | 1.09              |
| 1:A:1:LEU:HD12 | 1:A:16:VAL:HG23 | 1.24                     | 1.09              |
| 1:C:1:LEU:HD11 | 1:C:13:ILE:HD11 | 1.33                     | 1.09              |
| 1:L:1:LEU:HD12 | 1:L:16:VAL:HG23 | 1.24                     | 1.09              |
| 1:M:63:HIS:HA  | 1:M:82:ASP:HB2  | 1.13                     | 1.09              |
| 1:G:18:TYR:HE2 | 1:G:22:ASN:HB3  | 1.18                     | 1.08              |
| 1:E:63:HIS:HA  | 1:E:82:ASP:HB2  | 1.13                     | 1.08              |
| 1:N:63:HIS:HA  | 1:N:82:ASP:HB2  | 1.13                     | 1.08              |
| 1:G:91:HIS:HA  | 1:G:104:THR:HB  | 1.24                     | 1.08              |
| 1:K:18:TYR:HE2 | 1:K:22:ASN:HB3  | 1.18                     | 1.08              |
| 1:M:1:LEU:HD12 | 1:M:16:VAL:HG23 | 1.23                     | 1.08              |
| 1:A:63:HIS:HA  | 1:A:82:ASP:HB2  | 1.13                     | 1.07              |
| 1:D:63:HIS:HA  | 1:D:82:ASP:HB2  | 1.13                     | 1.07              |
| 1:J:18:TYR:HE2 | 1:J:22:ASN:HB3  | 1.18                     | 1.07              |
| 1:B:63:HIS:HA  | 1:B:82:ASP:HB2  | 1.13                     | 1.07              |
| 1:I:91:HIS:HA  | 1:I:104:THR:HB  | 1.24                     | 1.07              |
| 1:C:63:HIS:HA  | 1:C:82:ASP:HB2  | 1.13                     | 1.07              |
| 1:H:18:TYR:HE2 | 1:H:22:ASN:HB3  | 1.18                     | 1.07              |
| 1:N:1:LEU:HD12 | 1:N:16:VAL:HG23 | 1.24                     | 1.07              |
| 1:E:91:HIS:HA  | 1:E:104:THR:HB  | 1.24                     | 1.06              |
| 1:F:18:TYR:HE2 | 1:F:22:ASN:HB3  | 1.18                     | 1.06              |
| 1:D:18:TYR:HE2 | 1:D:22:ASN:HB3  | 1.18                     | 1.05              |
| 1:H:86:TYR:HB3 | 1:H:109:PHE:HB3 | 1.39                     | 1.05              |
| 1:I:86:TYR:HB3 | 1:I:109:PHE:HB3 | 1.39                     | 1.05              |
| 1:G:86:TYR:HB3 | 1:G:109:PHE:HB3 | 1.39                     | 1.05              |
| 1:N:18:TYR:HE2 | 1:N:22:ASN:HB3  | 1.18                     | 1.05              |
| 1:L:18:TYR:HE2 | 1:L:22:ASN:HB3  | 1.18                     | 1.04              |
| 1:J:86:TYR:HB3 | 1:J:109:PHE:HB3 | 1.39                     | 1.04              |
| 1:C:18:TYR:HE2 | 1:C:22:ASN:HB3  | 1.18                     | 1.04              |
| 1:F:86:TYR:HB3 | 1:F:109:PHE:HB3 | 1.39                     | 1.04              |
| 1:K:86:TYR:HB3 | 1:K:109:PHE:HB3 | 1.39                     | 1.04              |
| 1:L:86:TYR:HB3 | 1:L:109:PHE:HB3 | 1.39                     | 1.04              |
| 1:I:18:TYR:HE2 | 1:I:22:ASN:HB3  | 1.18                     | 1.03              |
| 1:A:18:TYR:HE2 | 1:A:22:ASN:HB3  | 1.18                     | 1.03              |
| 1:M:18:TYR:HE2 | 1:M:22:ASN:HB3  | 1.18                     | 1.03              |
| 1:M:86:TYR:HB3 | 1:M:109:PHE:HB3 | 1.39                     | 1.03              |
| 1:E:18:TYR:HE2 | 1:E:22:ASN:HB3  | 1.18                     | 1.03              |
| 1:E:86:TYR:HB3 | 1:E:109:PHE:HB3 | 1.39                     | 1.02              |
| 1:N:86:TYR:HB3 | 1:N:109:PHE:HB3 | 1.39                     | 1.02              |
| 1:D:41:ASP:HA  | 1:D:83:LYS:HE3  | 1.42                     | 1.01              |
| 1:E:60:LYS:H   | 1:E:64:PHE:HB2  | 1.24                     | 1.01              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:60:LYS:H    | 1:H:64:PHE:HB2  | 1.24                     | 1.01              |
| 1:B:18:TYR:HE2  | 1:B:22:ASN:HB3  | 1.18                     | 1.01              |
| 1:A:46:THR:CB   | 1:B:13:ILE:HG22 | 1.90                     | 1.01              |
| 1:A:86:TYR:HB3  | 1:A:109:PHE:HB3 | 1.39                     | 1.01              |
| 1:B:46:THR:CB   | 1:C:13:ILE:HG22 | 1.90                     | 1.01              |
| 1:F:41:ASP:HA   | 1:F:83:LYS:HE3  | 1.42                     | 1.01              |
| 1:A:13:ILE:HG22 | 1:N:46:THR:CB   | 1.90                     | 1.01              |
| 1:C:46:THR:CB   | 1:D:13:ILE:HG22 | 1.90                     | 1.01              |
| 1:C:60:LYS:H    | 1:C:64:PHE:HB2  | 1.24                     | 1.01              |
| 1:B:60:LYS:H    | 1:B:64:PHE:HB2  | 1.24                     | 1.01              |
| 1:D:86:TYR:HB3  | 1:D:109:PHE:HB3 | 1.39                     | 1.01              |
| 1:E:41:ASP:HA   | 1:E:83:LYS:HE3  | 1.42                     | 1.01              |
| 1:G:60:LYS:H    | 1:G:64:PHE:HB2  | 1.24                     | 1.01              |
| 1:B:41:ASP:HA   | 1:B:83:LYS:HE3  | 1.42                     | 1.00              |
| 1:D:46:THR:CB   | 1:E:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:D:60:LYS:H    | 1:D:64:PHE:HB2  | 1.24                     | 1.00              |
| 1:B:86:TYR:HB3  | 1:B:109:PHE:HB3 | 1.39                     | 1.00              |
| 1:C:26:ILE:HA   | 1:C:107:LYS:HE2 | 1.43                     | 1.00              |
| 1:C:41:ASP:HA   | 1:C:83:LYS:HE3  | 1.42                     | 1.00              |
| 1:G:41:ASP:HA   | 1:G:83:LYS:HE3  | 1.42                     | 1.00              |
| 1:I:46:THR:CB   | 1:J:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:J:46:THR:CB   | 1:K:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:M:46:THR:CB   | 1:N:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:B:26:ILE:HA   | 1:B:107:LYS:HE2 | 1.43                     | 1.00              |
| 1:D:26:ILE:HA   | 1:D:107:LYS:HE2 | 1.43                     | 1.00              |
| 1:K:46:THR:CB   | 1:L:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:H:46:THR:CB   | 1:I:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:E:46:THR:CB   | 1:F:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:L:46:THR:CB   | 1:M:13:ILE:HG22 | 1.90                     | 1.00              |
| 1:C:86:TYR:HB3  | 1:C:109:PHE:HB3 | 1.39                     | 1.00              |
| 1:E:26:ILE:HA   | 1:E:107:LYS:HE2 | 1.43                     | 0.99              |
| 1:N:18:TYR:CE2  | 1:N:22:ASN:HB3  | 1.98                     | 0.99              |
| 1:A:18:TYR:CE2  | 1:A:22:ASN:HB3  | 1.97                     | 0.99              |
| 1:H:41:ASP:HA   | 1:H:83:LYS:HE3  | 1.42                     | 0.99              |
| 1:J:57:PHE:HB3  | 1:K:103:GLY:HA3 | 1.44                     | 0.99              |
| 1:K:60:LYS:H    | 1:K:64:PHE:HB2  | 1.24                     | 0.99              |
| 1:M:18:TYR:CE2  | 1:M:22:ASN:HB3  | 1.98                     | 0.99              |
| 1:A:60:LYS:H    | 1:A:64:PHE:HB2  | 1.24                     | 0.99              |
| 1:F:60:LYS:H    | 1:F:64:PHE:HB2  | 1.24                     | 0.99              |
| 1:L:18:TYR:CE2  | 1:L:22:ASN:HB3  | 1.97                     | 0.99              |
| 1:A:26:ILE:HA   | 1:A:107:LYS:HE2 | 1.43                     | 0.99              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:18:TYR:CE2  | 1:B:22:ASN:HB3  | 1.98                     | 0.99              |
| 1:C:18:TYR:CE2  | 1:C:22:ASN:HB3  | 1.97                     | 0.99              |
| 1:N:60:LYS:H    | 1:N:64:PHE:HB2  | 1.24                     | 0.99              |
| 1:L:57:PHE:HB3  | 1:M:103:GLY:HA3 | 1.44                     | 0.99              |
| 1:K:18:TYR:CE2  | 1:K:22:ASN:HB3  | 1.98                     | 0.99              |
| 1:F:46:THR:CB   | 1:G:13:ILE:HG22 | 1.90                     | 0.99              |
| 1:A:41:ASP:HA   | 1:A:83:LYS:HE3  | 1.42                     | 0.99              |
| 1:D:18:TYR:CE2  | 1:D:22:ASN:HB3  | 1.98                     | 0.99              |
| 1:G:46:THR:CB   | 1:H:13:ILE:HG22 | 1.90                     | 0.99              |
| 1:H:57:PHE:HB3  | 1:I:103:GLY:HA3 | 1.44                     | 0.99              |
| 1:I:57:PHE:HB3  | 1:J:103:GLY:HA3 | 1.44                     | 0.99              |
| 1:K:57:PHE:HB3  | 1:L:103:GLY:HA3 | 1.44                     | 0.99              |
| 1:J:18:TYR:CE2  | 1:J:22:ASN:HB3  | 1.97                     | 0.98              |
| 1:F:26:ILE:HA   | 1:F:107:LYS:HE2 | 1.43                     | 0.98              |
| 1:I:60:LYS:H    | 1:I:64:PHE:HB2  | 1.24                     | 0.98              |
| 1:L:60:LYS:H    | 1:L:64:PHE:HB2  | 1.24                     | 0.98              |
| 1:N:26:ILE:HA   | 1:N:107:LYS:HE2 | 1.43                     | 0.98              |
| 1:E:18:TYR:CE2  | 1:E:22:ASN:HB3  | 1.97                     | 0.98              |
| 1:G:80:VAL:HG22 | 1:G:88:ILE:HG23 | 1.46                     | 0.98              |
| 1:M:57:PHE:HB3  | 1:N:103:GLY:HA3 | 1.44                     | 0.98              |
| 1:N:41:ASP:HA   | 1:N:83:LYS:HE3  | 1.42                     | 0.98              |
| 1:I:18:TYR:CE2  | 1:I:22:ASN:HB3  | 1.98                     | 0.98              |
| 1:L:41:ASP:HA   | 1:L:83:LYS:HE3  | 1.42                     | 0.98              |
| 1:M:26:ILE:HA   | 1:M:107:LYS:HE2 | 1.43                     | 0.98              |
| 1:I:80:VAL:HG22 | 1:I:88:ILE:HG23 | 1.46                     | 0.98              |
| 1:M:60:LYS:H    | 1:M:64:PHE:HB2  | 1.24                     | 0.98              |
| 1:A:103:GLY:HA3 | 1:N:57:PHE:HB3  | 1.44                     | 0.98              |
| 1:D:80:VAL:HG22 | 1:D:88:ILE:HG23 | 1.46                     | 0.97              |
| 1:J:41:ASP:HA   | 1:J:83:LYS:HE3  | 1.42                     | 0.97              |
| 1:F:18:TYR:CE2  | 1:F:22:ASN:HB3  | 1.98                     | 0.97              |
| 1:H:18:TYR:CE2  | 1:H:22:ASN:HB3  | 1.97                     | 0.97              |
| 1:I:41:ASP:HA   | 1:I:83:LYS:HE3  | 1.42                     | 0.97              |
| 1:J:60:LYS:H    | 1:J:64:PHE:HB2  | 1.24                     | 0.97              |
| 1:J:80:VAL:HG22 | 1:J:88:ILE:HG23 | 1.46                     | 0.97              |
| 1:M:41:ASP:HA   | 1:M:83:LYS:HE3  | 1.42                     | 0.97              |
| 1:G:57:PHE:HB3  | 1:H:103:GLY:HA3 | 1.44                     | 0.97              |
| 1:G:18:TYR:CE2  | 1:G:22:ASN:HB3  | 1.98                     | 0.97              |
| 1:G:26:ILE:HA   | 1:G:107:LYS:HE2 | 1.43                     | 0.97              |
| 1:K:41:ASP:HA   | 1:K:83:LYS:HE3  | 1.42                     | 0.97              |
| 1:L:26:ILE:HA   | 1:L:107:LYS:HE2 | 1.43                     | 0.97              |
| 1:F:80:VAL:HG22 | 1:F:88:ILE:HG23 | 1.46                     | 0.97              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:63:HIS:HA   | 1:L:82:ASP:CB   | 1.95                     | 0.97              |
| 1:L:80:VAL:HG22 | 1:L:88:ILE:HG23 | 1.46                     | 0.97              |
| 1:E:80:VAL:HG22 | 1:E:88:ILE:HG23 | 1.46                     | 0.97              |
| 1:K:63:HIS:HA   | 1:K:82:ASP:CB   | 1.95                     | 0.96              |
| 1:B:80:VAL:HG22 | 1:B:88:ILE:HG23 | 1.46                     | 0.96              |
| 1:F:57:PHE:HB3  | 1:G:103:GLY:HA3 | 1.44                     | 0.96              |
| 1:H:63:HIS:HA   | 1:H:82:ASP:CB   | 1.95                     | 0.96              |
| 1:I:63:HIS:HA   | 1:I:82:ASP:CB   | 1.95                     | 0.96              |
| 1:M:63:HIS:HA   | 1:M:82:ASP:CB   | 1.95                     | 0.96              |
| 1:B:57:PHE:HB3  | 1:C:103:GLY:HA3 | 1.44                     | 0.96              |
| 1:J:26:ILE:HA   | 1:J:107:LYS:HE2 | 1.43                     | 0.96              |
| 1:K:26:ILE:HA   | 1:K:107:LYS:HE2 | 1.43                     | 0.96              |
| 1:E:57:PHE:HB3  | 1:F:103:GLY:HA3 | 1.44                     | 0.96              |
| 1:I:26:ILE:HA   | 1:I:107:LYS:HE2 | 1.43                     | 0.96              |
| 1:N:80:VAL:HG22 | 1:N:88:ILE:HG23 | 1.46                     | 0.96              |
| 1:A:63:HIS:HA   | 1:A:82:ASP:CB   | 1.95                     | 0.96              |
| 1:C:57:PHE:HB3  | 1:D:103:GLY:HA3 | 1.44                     | 0.96              |
| 1:D:63:HIS:HA   | 1:D:82:ASP:CB   | 1.95                     | 0.96              |
| 1:A:57:PHE:HB3  | 1:B:103:GLY:HA3 | 1.44                     | 0.95              |
| 1:B:63:HIS:HA   | 1:B:82:ASP:CB   | 1.95                     | 0.95              |
| 1:G:63:HIS:HA   | 1:G:82:ASP:CB   | 1.95                     | 0.95              |
| 1:K:80:VAL:HG22 | 1:K:88:ILE:HG23 | 1.46                     | 0.95              |
| 1:L:32:VAL:HB   | 1:L:51:ASP:HA   | 1.47                     | 0.95              |
| 1:K:32:VAL:HB   | 1:K:51:ASP:HA   | 1.48                     | 0.95              |
| 1:H:80:VAL:HG22 | 1:H:88:ILE:HG23 | 1.46                     | 0.95              |
| 1:H:26:ILE:HA   | 1:H:107:LYS:HE2 | 1.43                     | 0.95              |
| 1:J:63:HIS:HA   | 1:J:82:ASP:CB   | 1.95                     | 0.95              |
| 1:N:63:HIS:HA   | 1:N:82:ASP:CB   | 1.95                     | 0.95              |
| 1:C:63:HIS:HA   | 1:C:82:ASP:CB   | 1.95                     | 0.95              |
| 1:N:32:VAL:HB   | 1:N:51:ASP:HA   | 1.48                     | 0.95              |
| 1:F:63:HIS:HA   | 1:F:82:ASP:CB   | 1.95                     | 0.95              |
| 1:E:63:HIS:HA   | 1:E:82:ASP:CB   | 1.95                     | 0.95              |
| 1:E:32:VAL:HB   | 1:E:51:ASP:HA   | 1.47                     | 0.95              |
| 1:J:32:VAL:HB   | 1:J:51:ASP:HA   | 1.48                     | 0.95              |
| 1:M:32:VAL:HB   | 1:M:51:ASP:HA   | 1.48                     | 0.95              |
| 1:D:32:VAL:HB   | 1:D:51:ASP:HA   | 1.48                     | 0.94              |
| 1:D:57:PHE:HB3  | 1:E:103:GLY:HA3 | 1.44                     | 0.94              |
| 1:A:32:VAL:HB   | 1:A:51:ASP:HA   | 1.47                     | 0.94              |
| 1:N:88:ILE:HD11 | 1:N:107:LYS:HG3 | 1.49                     | 0.94              |
| 1:C:80:VAL:HG22 | 1:C:88:ILE:HG23 | 1.46                     | 0.94              |
| 1:F:32:VAL:HB   | 1:F:51:ASP:HA   | 1.48                     | 0.94              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:32:VAL:HB   | 1:I:51:ASP:HA   | 1.48                     | 0.94              |
| 1:A:14:LYS:HE3  | 1:N:44:TYR:H    | 1.33                     | 0.94              |
| 1:C:44:TYR:H    | 1:D:14:LYS:HE3  | 1.33                     | 0.94              |
| 1:A:98:LYS:HE3  | 1:A:100:ASN:HA  | 1.50                     | 0.94              |
| 1:C:32:VAL:HB   | 1:C:51:ASP:HA   | 1.48                     | 0.94              |
| 1:F:44:TYR:H    | 1:G:14:LYS:HE3  | 1.33                     | 0.94              |
| 1:C:88:ILE:HD11 | 1:C:107:LYS:HG3 | 1.49                     | 0.94              |
| 1:D:98:LYS:HE3  | 1:D:100:ASN:HA  | 1.50                     | 0.94              |
| 1:B:88:ILE:HD11 | 1:B:107:LYS:HG3 | 1.49                     | 0.93              |
| 1:D:46:THR:OG1  | 1:E:13:ILE:HG22 | 1.68                     | 0.93              |
| 1:J:46:THR:OG1  | 1:K:13:ILE:HG22 | 1.69                     | 0.93              |
| 1:M:80:VAL:HG22 | 1:M:88:ILE:HG23 | 1.46                     | 0.93              |
| 1:A:46:THR:OG1  | 1:B:13:ILE:HG22 | 1.68                     | 0.93              |
| 1:E:46:THR:OG1  | 1:F:13:ILE:HG22 | 1.69                     | 0.93              |
| 1:F:98:LYS:HE3  | 1:F:100:ASN:HA  | 1.50                     | 0.93              |
| 1:G:88:ILE:HD11 | 1:G:107:LYS:HG3 | 1.49                     | 0.93              |
| 1:A:13:ILE:HG22 | 1:N:46:THR:OG1  | 1.69                     | 0.93              |
| 1:E:44:TYR:H    | 1:F:14:LYS:HE3  | 1.33                     | 0.93              |
| 1:G:44:TYR:H    | 1:H:14:LYS:HE3  | 1.33                     | 0.93              |
| 1:H:88:ILE:HD11 | 1:H:107:LYS:HG3 | 1.49                     | 0.93              |
| 1:K:46:THR:OG1  | 1:L:13:ILE:HG22 | 1.68                     | 0.93              |
| 1:L:59:HIS:HA   | 1:L:64:PHE:HD2  | 1.34                     | 0.93              |
| 1:M:98:LYS:HE3  | 1:M:100:ASN:HA  | 1.50                     | 0.93              |
| 1:A:49:PHE:HB2  | 1:A:55:ARG:HH22 | 1.34                     | 0.93              |
| 1:D:44:TYR:H    | 1:E:14:LYS:HE3  | 1.33                     | 0.93              |
| 1:I:59:HIS:HA   | 1:I:64:PHE:HD2  | 1.34                     | 0.93              |
| 1:I:88:ILE:HD11 | 1:I:107:LYS:HG3 | 1.49                     | 0.93              |
| 1:K:44:TYR:H    | 1:L:14:LYS:HE3  | 1.33                     | 0.93              |
| 1:L:49:PHE:HB2  | 1:L:55:ARG:HH22 | 1.34                     | 0.93              |
| 1:B:46:THR:OG1  | 1:C:13:ILE:HG22 | 1.69                     | 0.93              |
| 1:H:32:VAL:HB   | 1:H:51:ASP:HA   | 1.47                     | 0.93              |
| 1:I:46:THR:OG1  | 1:J:13:ILE:HG22 | 1.69                     | 0.93              |
| 1:B:32:VAL:HB   | 1:B:51:ASP:HA   | 1.48                     | 0.93              |
| 1:F:88:ILE:HD11 | 1:F:107:LYS:HG3 | 1.49                     | 0.93              |
| 1:G:32:VAL:HB   | 1:G:51:ASP:HA   | 1.48                     | 0.93              |
| 1:J:18:TYR:CE2  | 1:J:23:VAL:HG13 | 2.04                     | 0.93              |
| 1:M:44:TYR:H    | 1:N:14:LYS:HE3  | 1.33                     | 0.93              |
| 1:A:59:HIS:HA   | 1:A:64:PHE:HD2  | 1.34                     | 0.93              |
| 1:C:98:LYS:HE3  | 1:C:100:ASN:HA  | 1.50                     | 0.93              |
| 1:K:18:TYR:CE2  | 1:K:23:VAL:HG13 | 2.04                     | 0.93              |
| 1:L:44:TYR:H    | 1:M:14:LYS:HE3  | 1.33                     | 0.93              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:80:VAL:HG22 | 1:A:88:ILE:HG23 | 1.46                     | 0.92              |
| 1:D:49:PHE:HB2  | 1:D:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:J:88:ILE:HD11 | 1:J:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:L:88:ILE:HD11 | 1:L:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:A:88:ILE:HD11 | 1:A:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:C:46:THR:OG1  | 1:D:13:ILE:HG22 | 1.69                     | 0.92              |
| 1:F:46:THR:OG1  | 1:G:13:ILE:HG22 | 1.68                     | 0.92              |
| 1:J:44:TYR:H    | 1:K:14:LYS:HE3  | 1.33                     | 0.92              |
| 1:M:18:TYR:CE2  | 1:M:23:VAL:HG13 | 2.04                     | 0.92              |
| 1:B:98:LYS:HE3  | 1:B:100:ASN:HA  | 1.50                     | 0.92              |
| 1:I:18:TYR:CE2  | 1:I:23:VAL:HG13 | 2.04                     | 0.92              |
| 1:L:18:TYR:CE2  | 1:L:23:VAL:HG13 | 2.04                     | 0.92              |
| 1:M:46:THR:OG1  | 1:N:13:ILE:HG22 | 1.68                     | 0.92              |
| 1:F:59:HIS:HA   | 1:F:64:PHE:HD2  | 1.34                     | 0.92              |
| 1:H:59:HIS:HA   | 1:H:64:PHE:HD2  | 1.34                     | 0.92              |
| 1:K:49:PHE:HB2  | 1:K:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:B:59:HIS:HA   | 1:B:64:PHE:HD2  | 1.34                     | 0.92              |
| 1:E:59:HIS:HA   | 1:E:64:PHE:HD2  | 1.34                     | 0.92              |
| 1:H:44:TYR:H    | 1:I:14:LYS:HE3  | 1.33                     | 0.92              |
| 1:H:98:LYS:HE3  | 1:H:100:ASN:HA  | 1.50                     | 0.92              |
| 1:M:88:ILE:HD11 | 1:M:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:I:49:PHE:HB2  | 1:I:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:L:98:LYS:HE3  | 1:L:100:ASN:HA  | 1.50                     | 0.92              |
| 1:M:59:HIS:HA   | 1:M:64:PHE:HD2  | 1.34                     | 0.92              |
| 1:B:49:PHE:HB2  | 1:B:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:E:88:ILE:HD11 | 1:E:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:H:49:PHE:HB2  | 1:H:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:E:49:PHE:HB2  | 1:E:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:H:18:TYR:CE2  | 1:H:23:VAL:HG13 | 2.04                     | 0.92              |
| 1:H:46:THR:OG1  | 1:I:13:ILE:HG22 | 1.68                     | 0.92              |
| 1:K:98:LYS:HE3  | 1:K:100:ASN:HA  | 1.50                     | 0.92              |
| 1:L:46:THR:OG1  | 1:M:13:ILE:HG22 | 1.69                     | 0.92              |
| 1:J:98:LYS:HE3  | 1:J:100:ASN:HA  | 1.50                     | 0.92              |
| 1:K:88:ILE:HD11 | 1:K:107:LYS:HG3 | 1.49                     | 0.92              |
| 1:N:49:PHE:HB2  | 1:N:55:ARG:HH22 | 1.34                     | 0.92              |
| 1:G:98:LYS:HE3  | 1:G:100:ASN:HA  | 1.50                     | 0.91              |
| 1:I:98:LYS:HE3  | 1:I:100:ASN:HA  | 1.50                     | 0.91              |
| 1:J:59:HIS:HA   | 1:J:64:PHE:HD2  | 1.34                     | 0.91              |
| 1:K:59:HIS:HA   | 1:K:64:PHE:HD2  | 1.34                     | 0.91              |
| 1:M:49:PHE:HB2  | 1:M:55:ARG:HH22 | 1.34                     | 0.91              |
| 1:B:44:TYR:H    | 1:C:14:LYS:HE3  | 1.33                     | 0.91              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:98:LYS:HE3  | 1:N:100:ASN:HA   | 1.50                     | 0.91              |
| 1:A:44:TYR:H    | 1:B:14:LYS:HE3   | 1.33                     | 0.91              |
| 1:E:18:TYR:CE2  | 1:E:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:F:18:TYR:CE2  | 1:F:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:I:44:TYR:H    | 1:J:14:LYS:HE3   | 1.33                     | 0.91              |
| 1:N:18:TYR:CE2  | 1:N:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:E:98:LYS:HE3  | 1:E:100:ASN:HA   | 1.50                     | 0.91              |
| 1:G:46:THR:OG1  | 1:H:13:ILE:HG22  | 1.69                     | 0.91              |
| 1:C:49:PHE:HB2  | 1:C:55:ARG:HH22  | 1.34                     | 0.91              |
| 1:C:18:TYR:CE2  | 1:C:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:E:5:ARG:H     | 1:E:36:ILE:HB    | 1.36                     | 0.91              |
| 1:G:18:TYR:CE2  | 1:G:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:H:91:HIS:HB3  | 1:H:104:THR:HG21 | 1.53                     | 0.91              |
| 1:I:91:HIS:HB3  | 1:I:104:THR:HG21 | 1.53                     | 0.91              |
| 1:K:5:ARG:H     | 1:K:36:ILE:HB    | 1.36                     | 0.91              |
| 1:D:18:TYR:CE2  | 1:D:23:VAL:HG13  | 2.04                     | 0.91              |
| 1:D:88:ILE:HD11 | 1:D:107:LYS:HG3  | 1.49                     | 0.91              |
| 1:N:59:HIS:HA   | 1:N:64:PHE:HD2   | 1.34                     | 0.91              |
| 1:B:18:TYR:CE2  | 1:B:23:VAL:HG13  | 2.04                     | 0.90              |
| 1:G:91:HIS:HB3  | 1:G:104:THR:HG21 | 1.53                     | 0.90              |
| 1:J:5:ARG:H     | 1:J:36:ILE:HB    | 1.36                     | 0.90              |
| 1:A:18:TYR:CE2  | 1:A:23:VAL:HG13  | 2.04                     | 0.90              |
| 1:D:5:ARG:H     | 1:D:36:ILE:HB    | 1.36                     | 0.90              |
| 1:D:59:HIS:HA   | 1:D:64:PHE:HD2   | 1.34                     | 0.90              |
| 1:F:5:ARG:H     | 1:F:36:ILE:HB    | 1.36                     | 0.90              |
| 1:F:91:HIS:HB3  | 1:F:104:THR:HG21 | 1.53                     | 0.90              |
| 1:G:49:PHE:HB2  | 1:G:55:ARG:HH22  | 1.34                     | 0.90              |
| 1:J:91:HIS:HB3  | 1:J:104:THR:HG21 | 1.53                     | 0.90              |
| 1:G:59:HIS:HA   | 1:G:64:PHE:HD2   | 1.34                     | 0.90              |
| 1:L:98:LYS:H    | 1:L:98:LYS:HD3   | 1.37                     | 0.90              |
| 1:C:59:HIS:HA   | 1:C:64:PHE:HD2   | 1.34                     | 0.90              |
| 1:J:49:PHE:HB2  | 1:J:55:ARG:HH22  | 1.34                     | 0.90              |
| 1:K:98:LYS:HD3  | 1:K:98:LYS:H     | 1.37                     | 0.90              |
| 1:L:5:ARG:H     | 1:L:36:ILE:HB    | 1.36                     | 0.90              |
| 1:C:5:ARG:H     | 1:C:36:ILE:HB    | 1.36                     | 0.90              |
| 1:F:49:PHE:HB2  | 1:F:55:ARG:HH22  | 1.34                     | 0.90              |
| 1:G:5:ARG:H     | 1:G:36:ILE:HB    | 1.36                     | 0.90              |
| 1:K:91:HIS:HB3  | 1:K:104:THR:HG21 | 1.53                     | 0.90              |
| 1:E:91:HIS:HB3  | 1:E:104:THR:HG21 | 1.53                     | 0.89              |
| 1:B:98:LYS:H    | 1:B:98:LYS:HD3   | 1.37                     | 0.89              |
| 1:B:5:ARG:H     | 1:B:36:ILE:HB    | 1.36                     | 0.89              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:E:98:LYS:HD3 | 1:E:98:LYS:H     | 1.37                     | 0.89              |
| 1:I:5:ARG:H    | 1:I:36:ILE:HB    | 1.36                     | 0.89              |
| 1:G:98:LYS:H   | 1:G:98:LYS:HD3   | 1.37                     | 0.89              |
| 1:A:5:ARG:H    | 1:A:36:ILE:HB    | 1.36                     | 0.89              |
| 1:D:91:HIS:HB3 | 1:D:104:THR:HG21 | 1.53                     | 0.89              |
| 1:D:98:LYS:H   | 1:D:98:LYS:HD3   | 1.37                     | 0.89              |
| 1:L:2:GLU:HG2  | 1:L:3:VAL:H      | 1.38                     | 0.89              |
| 1:L:91:HIS:HB3 | 1:L:104:THR:HG21 | 1.53                     | 0.89              |
| 1:D:91:HIS:HA  | 1:D:104:THR:CB   | 2.03                     | 0.89              |
| 1:J:98:LYS:H   | 1:J:98:LYS:HD3   | 1.37                     | 0.89              |
| 1:C:91:HIS:HA  | 1:C:104:THR:CB   | 2.03                     | 0.88              |
| 1:E:91:HIS:HA  | 1:E:104:THR:CB   | 2.03                     | 0.88              |
| 1:K:2:GLU:HG2  | 1:K:3:VAL:H      | 1.38                     | 0.88              |
| 1:A:98:LYS:H   | 1:A:98:LYS:HD3   | 1.37                     | 0.88              |
| 1:B:91:HIS:HB3 | 1:B:104:THR:HG21 | 1.53                     | 0.88              |
| 1:N:5:ARG:H    | 1:N:36:ILE:HB    | 1.36                     | 0.88              |
| 1:F:91:HIS:HA  | 1:F:104:THR:CB   | 2.04                     | 0.88              |
| 1:N:91:HIS:HB3 | 1:N:104:THR:HG21 | 1.53                     | 0.88              |
| 1:B:46:THR:HB  | 1:C:14:LYS:NZ    | 1.89                     | 0.88              |
| 1:B:91:HIS:HA  | 1:B:104:THR:CB   | 2.04                     | 0.88              |
| 1:G:46:THR:HB  | 1:H:14:LYS:NZ    | 1.89                     | 0.88              |
| 1:G:91:HIS:HA  | 1:G:104:THR:CB   | 2.03                     | 0.88              |
| 1:J:91:HIS:HA  | 1:J:104:THR:CB   | 2.03                     | 0.88              |
| 1:K:91:HIS:HA  | 1:K:104:THR:CB   | 2.03                     | 0.88              |
| 1:M:98:LYS:H   | 1:M:98:LYS:HD3   | 1.37                     | 0.88              |
| 1:H:5:ARG:H    | 1:H:36:ILE:HB    | 1.36                     | 0.88              |
| 1:H:91:HIS:HA  | 1:H:104:THR:CB   | 2.03                     | 0.88              |
| 1:I:91:HIS:HA  | 1:I:104:THR:CB   | 2.04                     | 0.88              |
| 1:L:46:THR:HB  | 1:M:14:LYS:NZ    | 1.89                     | 0.88              |
| 1:M:5:ARG:H    | 1:M:36:ILE:HB    | 1.36                     | 0.88              |
| 1:M:46:THR:HB  | 1:N:14:LYS:NZ    | 1.89                     | 0.88              |
| 1:A:91:HIS:HA  | 1:A:104:THR:CB   | 2.03                     | 0.88              |
| 1:C:91:HIS:HB3 | 1:C:104:THR:HG21 | 1.53                     | 0.88              |
| 1:L:91:HIS:HA  | 1:L:104:THR:CB   | 2.03                     | 0.88              |
| 1:M:91:HIS:HB3 | 1:M:104:THR:HG21 | 1.53                     | 0.88              |
| 1:A:14:LYS:NZ  | 1:N:46:THR:HB    | 1.89                     | 0.88              |
| 1:A:91:HIS:HB3 | 1:A:104:THR:HG21 | 1.53                     | 0.88              |
| 1:H:2:GLU:HG2  | 1:H:3:VAL:H      | 1.38                     | 0.88              |
| 1:K:46:THR:HB  | 1:L:14:LYS:NZ    | 1.89                     | 0.88              |
| 1:N:91:HIS:HA  | 1:N:104:THR:CB   | 2.03                     | 0.88              |
| 1:M:91:HIS:HA  | 1:M:104:THR:CB   | 2.04                     | 0.88              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:56:THR:H    | 1:A:67:LYS:H    | 1.21                     | 0.88              |
| 1:F:98:LYS:HD3  | 1:F:98:LYS:H    | 1.37                     | 0.88              |
| 1:G:2:GLU:HG2   | 1:G:3:VAL:H     | 1.38                     | 0.88              |
| 1:C:46:THR:HB   | 1:D:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:F:46:THR:HB   | 1:G:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:H:98:LYS:HD3  | 1:H:98:LYS:H    | 1.37                     | 0.87              |
| 1:J:46:THR:HB   | 1:K:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:H:46:THR:HB   | 1:I:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:A:46:THR:HB   | 1:B:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:C:98:LYS:HD3  | 1:C:98:LYS:H    | 1.37                     | 0.87              |
| 1:M:2:GLU:HG2   | 1:M:3:VAL:H     | 1.38                     | 0.87              |
| 1:E:46:THR:HB   | 1:F:13:ILE:HG22 | 1.57                     | 0.87              |
| 1:M:46:THR:HB   | 1:N:13:ILE:HG22 | 1.57                     | 0.87              |
| 1:A:13:ILE:HG22 | 1:N:46:THR:HB   | 1.57                     | 0.87              |
| 1:F:46:THR:HB   | 1:G:13:ILE:HG22 | 1.57                     | 0.87              |
| 1:I:2:GLU:HG2   | 1:I:3:VAL:H     | 1.38                     | 0.87              |
| 1:I:46:THR:HB   | 1:J:14:LYS:NZ   | 1.89                     | 0.87              |
| 1:I:98:LYS:H    | 1:I:98:LYS:HD3  | 1.37                     | 0.87              |
| 1:J:2:GLU:HG2   | 1:J:3:VAL:H     | 1.38                     | 0.87              |
| 1:B:2:GLU:HG2   | 1:B:3:VAL:H     | 1.38                     | 0.86              |
| 1:H:50:GLY:HA2  | 1:H:77:LEU:HD13 | 1.58                     | 0.86              |
| 1:I:46:THR:HB   | 1:J:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:I:50:GLY:HA2  | 1:I:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:G:50:GLY:HA2  | 1:G:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:L:56:THR:H    | 1:L:67:LYS:H    | 1.21                     | 0.86              |
| 1:N:56:THR:H    | 1:N:67:LYS:H    | 1.21                     | 0.86              |
| 1:N:98:LYS:HD3  | 1:N:98:LYS:H    | 1.37                     | 0.86              |
| 1:D:46:THR:HB   | 1:E:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:J:46:THR:HB   | 1:K:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:A:2:GLU:HG2   | 1:A:3:VAL:H     | 1.38                     | 0.86              |
| 1:E:46:THR:HB   | 1:F:14:LYS:NZ   | 1.89                     | 0.86              |
| 1:J:50:GLY:HA2  | 1:J:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:N:63:HIS:CA   | 1:N:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:C:2:GLU:HG2   | 1:C:3:VAL:H     | 1.38                     | 0.86              |
| 1:L:63:HIS:CA   | 1:L:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:M:63:HIS:CA   | 1:M:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:N:50:GLY:HA2  | 1:N:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:A:50:GLY:HA2  | 1:A:77:LEU:HD13 | 1.58                     | 0.86              |
| 1:A:63:HIS:CA   | 1:A:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:F:2:GLU:HG2   | 1:F:3:VAL:H     | 1.38                     | 0.86              |
| 1:K:50:GLY:HA2  | 1:K:77:LEU:HD13 | 1.58                     | 0.86              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:F:50:GLY:HA2 | 1:F:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:M:50:GLY:HA2 | 1:M:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:A:46:THR:HB  | 1:B:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:B:50:GLY:HA2 | 1:B:77:LEU:HD13 | 1.57                     | 0.86              |
| 1:K:63:HIS:CA  | 1:K:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:L:46:THR:HB  | 1:M:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:D:46:THR:HB  | 1:E:14:LYS:NZ   | 1.89                     | 0.86              |
| 1:L:50:GLY:HA2 | 1:L:77:LEU:HD13 | 1.58                     | 0.86              |
| 1:B:63:HIS:CA  | 1:B:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:H:46:THR:HB  | 1:I:13:ILE:HG22 | 1.57                     | 0.86              |
| 1:J:63:HIS:CA  | 1:J:82:ASP:HB2  | 2.04                     | 0.86              |
| 1:C:50:GLY:HA2 | 1:C:77:LEU:HD13 | 1.57                     | 0.85              |
| 1:N:2:GLU:HG2  | 1:N:3:VAL:H     | 1.38                     | 0.85              |
| 1:D:56:THR:H   | 1:D:67:LYS:H    | 1.21                     | 0.85              |
| 1:F:24:VAL:CG1 | 1:F:26:ILE:HD12 | 2.07                     | 0.85              |
| 1:I:63:HIS:CA  | 1:I:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:L:67:LYS:HE3 | 1:L:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:C:46:THR:HB  | 1:D:13:ILE:HG22 | 1.57                     | 0.85              |
| 1:D:50:GLY:HA2 | 1:D:77:LEU:HD13 | 1.58                     | 0.85              |
| 1:C:63:HIS:CA  | 1:C:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:E:2:GLU:HG2  | 1:E:3:VAL:H     | 1.38                     | 0.85              |
| 1:E:50:GLY:HA2 | 1:E:77:LEU:HD13 | 1.58                     | 0.85              |
| 1:I:67:LYS:HE3 | 1:I:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:K:56:THR:H   | 1:K:67:LYS:H    | 1.21                     | 0.85              |
| 1:K:67:LYS:HE3 | 1:K:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:B:24:VAL:CG1 | 1:B:26:ILE:HD12 | 2.07                     | 0.85              |
| 1:D:2:GLU:HG2  | 1:D:3:VAL:H     | 1.38                     | 0.85              |
| 1:H:63:HIS:CA  | 1:H:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:H:67:LYS:HE3 | 1:H:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:C:56:THR:H   | 1:C:67:LYS:H    | 1.21                     | 0.85              |
| 1:M:67:LYS:HE3 | 1:M:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:D:63:HIS:CA  | 1:D:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:G:63:HIS:CA  | 1:G:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:B:56:THR:H   | 1:B:67:LYS:H    | 1.21                     | 0.85              |
| 1:C:24:VAL:CG1 | 1:C:26:ILE:HD12 | 2.07                     | 0.85              |
| 1:G:46:THR:HB  | 1:H:13:ILE:HG22 | 1.57                     | 0.85              |
| 1:G:56:THR:H   | 1:G:67:LYS:H    | 1.21                     | 0.85              |
| 1:N:67:LYS:HE3 | 1:N:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:E:24:VAL:CG1 | 1:E:26:ILE:HD12 | 2.07                     | 0.85              |
| 1:E:63:HIS:CA  | 1:E:82:ASP:HB2  | 2.04                     | 0.85              |
| 1:G:24:VAL:CG1 | 1:G:26:ILE:HD12 | 2.07                     | 0.85              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:29:VAL:CG1  | 1:H:77:LEU:HD21 | 2.07                     | 0.85              |
| 1:J:67:LYS:HE3  | 1:J:78:VAL:HG13 | 1.59                     | 0.85              |
| 1:L:29:VAL:CG1  | 1:L:77:LEU:HD21 | 2.07                     | 0.85              |
| 1:B:75:THR:HG22 | 1:B:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:F:63:HIS:CA   | 1:F:82:ASP:HB2  | 2.04                     | 0.84              |
| 1:H:56:THR:H    | 1:H:67:LYS:H    | 1.21                     | 0.84              |
| 1:N:66:VAL:HG13 | 1:N:79:ILE:O    | 1.77                     | 0.84              |
| 1:A:67:LYS:HE3  | 1:A:78:VAL:HG13 | 1.59                     | 0.84              |
| 1:G:66:VAL:HG13 | 1:G:79:ILE:O    | 1.77                     | 0.84              |
| 1:L:24:VAL:CG1  | 1:L:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:A:75:THR:HG22 | 1:A:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:D:24:VAL:CG1  | 1:D:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:F:56:THR:H    | 1:F:67:LYS:H    | 1.21                     | 0.84              |
| 1:I:29:VAL:CG1  | 1:I:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:K:24:VAL:CG1  | 1:K:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:K:29:VAL:CG1  | 1:K:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:K:46:THR:HB   | 1:L:13:ILE:HG22 | 1.57                     | 0.84              |
| 1:M:46:THR:HB   | 1:N:14:LYS:HZ1  | 1.41                     | 0.84              |
| 1:C:29:VAL:CG1  | 1:C:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:G:67:LYS:HE3  | 1:G:78:VAL:HG13 | 1.59                     | 0.84              |
| 1:B:29:VAL:CG1  | 1:B:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:G:29:VAL:CG1  | 1:G:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:K:75:THR:HG22 | 1:K:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:M:56:THR:H    | 1:M:67:LYS:H    | 1.21                     | 0.84              |
| 1:N:75:THR:HG22 | 1:N:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:A:24:VAL:CG1  | 1:A:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:D:66:VAL:HG13 | 1:D:79:ILE:O    | 1.77                     | 0.84              |
| 1:D:75:THR:HG22 | 1:D:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:I:24:VAL:CG1  | 1:I:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:J:24:VAL:CG1  | 1:J:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:M:75:THR:HG22 | 1:M:92:PHE:CZ   | 2.12                     | 0.84              |
| 1:B:46:THR:HB   | 1:C:13:ILE:HG22 | 1.57                     | 0.84              |
| 1:C:66:VAL:HG13 | 1:C:79:ILE:O    | 1.77                     | 0.84              |
| 1:D:29:VAL:CG1  | 1:D:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:E:66:VAL:HG13 | 1:E:79:ILE:O    | 1.77                     | 0.84              |
| 1:F:66:VAL:HG13 | 1:F:79:ILE:O    | 1.77                     | 0.84              |
| 1:F:67:LYS:HE3  | 1:F:78:VAL:HG13 | 1.59                     | 0.84              |
| 1:I:56:THR:H    | 1:I:67:LYS:H    | 1.21                     | 0.84              |
| 1:M:24:VAL:CG1  | 1:M:26:ILE:HD12 | 2.07                     | 0.84              |
| 1:M:29:VAL:CG1  | 1:M:77:LEU:HD21 | 2.07                     | 0.84              |
| 1:A:29:VAL:CG1  | 1:A:77:LEU:HD21 | 2.07                     | 0.84              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:66:VAL:HG13 | 1:M:79:ILE:O    | 1.77                     | 0.84              |
| 1:A:14:LYS:HZ1  | 1:N:46:THR:HB   | 1.42                     | 0.84              |
| 1:A:66:VAL:HG13 | 1:A:79:ILE:O    | 1.77                     | 0.83              |
| 1:E:34:THR:HG23 | 1:E:47:HIS:HB3  | 1.60                     | 0.83              |
| 1:H:46:THR:HB   | 1:I:14:LYS:HZ1  | 1.41                     | 0.83              |
| 1:B:66:VAL:HG13 | 1:B:79:ILE:O    | 1.77                     | 0.83              |
| 1:B:67:LYS:HE3  | 1:B:78:VAL:HG13 | 1.59                     | 0.83              |
| 1:E:29:VAL:CG1  | 1:E:77:LEU:HD21 | 2.07                     | 0.83              |
| 1:I:75:THR:HG22 | 1:I:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:L:34:THR:HG23 | 1:L:47:HIS:HB3  | 1.60                     | 0.83              |
| 1:L:75:THR:HG22 | 1:L:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:C:67:LYS:HE3  | 1:C:78:VAL:HG13 | 1.59                     | 0.83              |
| 1:E:75:THR:HG22 | 1:E:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:F:34:THR:HG23 | 1:F:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:F:75:THR:HG22 | 1:F:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:H:24:VAL:CG1  | 1:H:26:ILE:HD12 | 2.07                     | 0.83              |
| 1:I:46:THR:HB   | 1:J:14:LYS:HZ1  | 1.42                     | 0.83              |
| 1:C:75:THR:HG22 | 1:C:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:D:34:THR:HG23 | 1:D:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:H:66:VAL:HG13 | 1:H:79:ILE:O    | 1.77                     | 0.83              |
| 1:K:34:THR:HG23 | 1:K:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:K:66:VAL:HG13 | 1:K:79:ILE:O    | 1.77                     | 0.83              |
| 1:M:34:THR:HG23 | 1:M:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:D:67:LYS:HE3  | 1:D:78:VAL:HG13 | 1.59                     | 0.83              |
| 1:E:56:THR:H    | 1:E:67:LYS:H    | 1.21                     | 0.83              |
| 1:G:34:THR:HG23 | 1:G:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:A:26:ILE:HD11 | 1:A:37:VAL:HB   | 1.61                     | 0.83              |
| 1:E:67:LYS:HE3  | 1:E:78:VAL:HG13 | 1.59                     | 0.83              |
| 1:J:29:VAL:CG1  | 1:J:77:LEU:HD21 | 2.07                     | 0.83              |
| 1:J:66:VAL:HG13 | 1:J:79:ILE:O    | 1.77                     | 0.83              |
| 1:J:75:THR:HG22 | 1:J:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:K:46:THR:HB   | 1:L:14:LYS:HZ1  | 1.43                     | 0.83              |
| 1:N:29:VAL:CG1  | 1:N:77:LEU:HD21 | 2.07                     | 0.83              |
| 1:F:46:THR:HB   | 1:G:14:LYS:HZ1  | 1.43                     | 0.83              |
| 1:H:34:THR:HG23 | 1:H:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:I:66:VAL:HG13 | 1:I:79:ILE:O    | 1.77                     | 0.83              |
| 1:N:34:THR:HG23 | 1:N:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:N:50:GLY:CA   | 1:N:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:C:26:ILE:HD11 | 1:C:37:VAL:HB   | 1.61                     | 0.83              |
| 1:F:29:VAL:CG1  | 1:F:77:LEU:HD21 | 2.07                     | 0.83              |
| 1:G:75:THR:HG22 | 1:G:92:PHE:CZ   | 2.12                     | 0.83              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:50:GLY:CA   | 1:H:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:H:75:THR:HG22 | 1:H:92:PHE:CZ   | 2.12                     | 0.83              |
| 1:J:34:THR:HG23 | 1:J:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:L:66:VAL:HG13 | 1:L:79:ILE:O    | 1.77                     | 0.83              |
| 1:N:24:VAL:CG1  | 1:N:26:ILE:HD12 | 2.07                     | 0.83              |
| 1:N:26:ILE:HD11 | 1:N:37:VAL:HB   | 1.61                     | 0.83              |
| 1:C:34:THR:HG23 | 1:C:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:E:50:GLY:CA   | 1:E:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:F:50:GLY:CA   | 1:F:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:I:34:THR:HG23 | 1:I:47:HIS:HB3  | 1.61                     | 0.83              |
| 1:M:50:GLY:CA   | 1:M:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:C:46:THR:HB   | 1:D:14:LYS:HZ1  | 1.42                     | 0.83              |
| 1:D:26:ILE:HD11 | 1:D:37:VAL:HB   | 1.61                     | 0.83              |
| 1:D:50:GLY:CA   | 1:D:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:G:50:GLY:CA   | 1:G:77:LEU:HD13 | 2.09                     | 0.83              |
| 1:I:92:PHE:O    | 1:I:93:ILE:HG13 | 1.79                     | 0.83              |
| 1:J:56:THR:H    | 1:J:67:LYS:H    | 1.21                     | 0.83              |
| 1:A:34:THR:HG23 | 1:A:47:HIS:HB3  | 1.61                     | 0.82              |
| 1:C:50:GLY:CA   | 1:C:77:LEU:HD13 | 2.09                     | 0.82              |
| 1:D:46:THR:HB   | 1:E:14:LYS:HZ1  | 1.44                     | 0.82              |
| 1:M:26:ILE:HD11 | 1:M:37:VAL:HB   | 1.61                     | 0.82              |
| 1:A:50:GLY:CA   | 1:A:77:LEU:HD13 | 2.09                     | 0.82              |
| 1:F:92:PHE:O    | 1:F:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:I:50:GLY:CA   | 1:I:77:LEU:HD13 | 2.09                     | 0.82              |
| 1:J:18:TYR:HB3  | 1:J:19:ASN:O    | 1.79                     | 0.82              |
| 1:L:26:ILE:HD11 | 1:L:37:VAL:HB   | 1.61                     | 0.82              |
| 1:L:46:THR:HB   | 1:M:14:LYS:HZ1  | 1.44                     | 0.82              |
| 1:N:92:PHE:O    | 1:N:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:B:26:ILE:HD11 | 1:B:37:VAL:HB   | 1.61                     | 0.82              |
| 1:B:50:GLY:CA   | 1:B:77:LEU:HD13 | 2.09                     | 0.82              |
| 1:B:92:PHE:O    | 1:B:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:I:18:TYR:HB3  | 1:I:19:ASN:O    | 1.79                     | 0.82              |
| 1:K:18:TYR:HB3  | 1:K:19:ASN:O    | 1.79                     | 0.82              |
| 1:B:34:THR:HG23 | 1:B:47:HIS:HB3  | 1.61                     | 0.82              |
| 1:I:32:VAL:HG22 | 1:I:48:ALA:HB3  | 1.61                     | 0.82              |
| 1:K:32:VAL:HG22 | 1:K:48:ALA:HB3  | 1.61                     | 0.82              |
| 1:K:92:PHE:O    | 1:K:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:L:18:TYR:HB3  | 1:L:19:ASN:O    | 1.79                     | 0.82              |
| 1:C:92:PHE:O    | 1:C:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:L:32:VAL:HG22 | 1:L:48:ALA:HB3  | 1.61                     | 0.82              |
| 1:H:1:LEU:CD1   | 1:H:13:ILE:HD11 | 2.10                     | 0.82              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:18:TYR:HB3  | 1:H:19:ASN:O    | 1.79                     | 0.82              |
| 1:H:32:VAL:HG22 | 1:H:48:ALA:HB3  | 1.61                     | 0.82              |
| 1:K:49:PHE:HB2  | 1:K:55:ARG:NH2  | 1.94                     | 0.82              |
| 1:M:1:LEU:CD1   | 1:M:13:ILE:HD11 | 2.10                     | 0.82              |
| 1:M:92:PHE:O    | 1:M:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:B:75:THR:HG22 | 1:B:92:PHE:HZ   | 1.45                     | 0.82              |
| 1:E:26:ILE:HD11 | 1:E:37:VAL:HB   | 1.61                     | 0.82              |
| 1:E:92:PHE:O    | 1:E:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:G:1:LEU:CD1   | 1:G:13:ILE:HD11 | 2.10                     | 0.82              |
| 1:L:49:PHE:HB2  | 1:L:55:ARG:NH2  | 1.94                     | 0.82              |
| 1:G:92:PHE:O    | 1:G:93:ILE:HG13 | 1.79                     | 0.82              |
| 1:L:1:LEU:CD1   | 1:L:13:ILE:HD11 | 2.10                     | 0.82              |
| 1:J:32:VAL:HG22 | 1:J:48:ALA:HB3  | 1.61                     | 0.82              |
| 1:J:49:PHE:HB2  | 1:J:55:ARG:NH2  | 1.94                     | 0.82              |
| 1:M:18:TYR:HB3  | 1:M:19:ASN:O    | 1.79                     | 0.82              |
| 1:M:49:PHE:HB2  | 1:M:55:ARG:NH2  | 1.94                     | 0.82              |
| 1:F:26:ILE:HD11 | 1:F:37:VAL:HB   | 1.61                     | 0.81              |
| 1:G:18:TYR:HB3  | 1:G:19:ASN:O    | 1.79                     | 0.81              |
| 1:C:18:TYR:HB3  | 1:C:19:ASN:O    | 1.79                     | 0.81              |
| 1:F:1:LEU:CD1   | 1:F:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:I:1:LEU:CD1   | 1:I:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:J:26:ILE:HD11 | 1:J:37:VAL:HB   | 1.61                     | 0.81              |
| 1:N:49:PHE:HB2  | 1:N:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:A:49:PHE:HB2  | 1:A:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:B:49:PHE:HB2  | 1:B:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:C:1:LEU:CD1   | 1:C:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:D:92:PHE:O    | 1:D:93:ILE:HG13 | 1.79                     | 0.81              |
| 1:E:75:THR:HG22 | 1:E:92:PHE:HZ   | 1.45                     | 0.81              |
| 1:G:32:VAL:HG22 | 1:G:48:ALA:HB3  | 1.61                     | 0.81              |
| 1:H:92:PHE:O    | 1:H:93:ILE:HG13 | 1.79                     | 0.81              |
| 1:I:49:PHE:HB2  | 1:I:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:K:26:ILE:HD11 | 1:K:37:VAL:HB   | 1.61                     | 0.81              |
| 1:L:92:PHE:O    | 1:L:93:ILE:HG13 | 1.79                     | 0.81              |
| 1:M:32:VAL:HG22 | 1:M:48:ALA:HB3  | 1.62                     | 0.81              |
| 1:M:75:THR:HG22 | 1:M:92:PHE:HZ   | 1.45                     | 0.81              |
| 1:N:32:VAL:HG22 | 1:N:48:ALA:HB3  | 1.61                     | 0.81              |
| 1:C:49:PHE:HB2  | 1:C:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:D:49:PHE:HB2  | 1:D:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:I:66:VAL:HG23 | 1:I:68:PRO:HD3  | 1.63                     | 0.81              |
| 1:J:50:GLY:CA   | 1:J:77:LEU:HD13 | 2.09                     | 0.81              |
| 1:N:75:THR:HG22 | 1:N:92:PHE:HZ   | 1.45                     | 0.81              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:13:ILE:HD12 | 1:H:14:LYS:HG3  | 1.62                     | 0.81              |
| 1:H:49:PHE:HB2  | 1:H:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:L:50:GLY:CA   | 1:L:77:LEU:HD13 | 2.09                     | 0.81              |
| 1:N:1:LEU:CD1   | 1:N:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:A:92:PHE:O    | 1:A:93:ILE:HG13 | 1.79                     | 0.81              |
| 1:B:1:LEU:CD1   | 1:B:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:D:1:LEU:CD1   | 1:D:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:E:49:PHE:HB2  | 1:E:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:F:49:PHE:HB2  | 1:F:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:I:13:ILE:HD12 | 1:I:14:LYS:HG3  | 1.62                     | 0.81              |
| 1:L:66:VAL:HG23 | 1:L:68:PRO:HD3  | 1.63                     | 0.81              |
| 1:G:13:ILE:HD12 | 1:G:14:LYS:HG3  | 1.62                     | 0.81              |
| 1:G:24:VAL:CG1  | 1:G:107:LYS:HD3 | 2.11                     | 0.81              |
| 1:G:49:PHE:HB2  | 1:G:55:ARG:NH2  | 1.94                     | 0.81              |
| 1:H:26:ILE:HD11 | 1:H:37:VAL:HB   | 1.61                     | 0.81              |
| 1:M:24:VAL:CG1  | 1:M:107:LYS:HD3 | 2.11                     | 0.81              |
| 1:N:18:TYR:HB3  | 1:N:19:ASN:O    | 1.79                     | 0.81              |
| 1:F:18:TYR:HB3  | 1:F:19:ASN:O    | 1.79                     | 0.81              |
| 1:F:32:VAL:HG22 | 1:F:48:ALA:HB3  | 1.62                     | 0.81              |
| 1:F:66:VAL:HG23 | 1:F:68:PRO:HD3  | 1.63                     | 0.81              |
| 1:G:75:THR:HG22 | 1:G:92:PHE:HZ   | 1.45                     | 0.81              |
| 1:I:24:VAL:CG1  | 1:I:107:LYS:HD3 | 2.11                     | 0.81              |
| 1:K:24:VAL:CG1  | 1:K:107:LYS:HD3 | 2.11                     | 0.81              |
| 1:K:50:GLY:CA   | 1:K:77:LEU:HD13 | 2.09                     | 0.81              |
| 1:K:75:THR:HG22 | 1:K:92:PHE:HZ   | 1.45                     | 0.81              |
| 1:G:66:VAL:HG23 | 1:G:68:PRO:HD3  | 1.63                     | 0.81              |
| 1:I:26:ILE:HD11 | 1:I:37:VAL:HB   | 1.61                     | 0.81              |
| 1:J:13:ILE:HD12 | 1:J:14:LYS:HG3  | 1.62                     | 0.81              |
| 1:K:66:VAL:HG23 | 1:K:68:PRO:HD3  | 1.63                     | 0.81              |
| 1:D:75:THR:HG22 | 1:D:92:PHE:HZ   | 1.45                     | 0.81              |
| 1:J:1:LEU:CD1   | 1:J:13:ILE:HD11 | 2.10                     | 0.81              |
| 1:B:13:ILE:HD12 | 1:B:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:B:24:VAL:CG1  | 1:B:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:C:24:VAL:CG1  | 1:C:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:E:24:VAL:CG1  | 1:E:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:F:13:ILE:HD12 | 1:F:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:I:75:THR:HG22 | 1:I:92:PHE:HZ   | 1.45                     | 0.80              |
| 1:J:24:VAL:CG1  | 1:J:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:J:92:PHE:O    | 1:J:93:ILE:HG13 | 1.79                     | 0.80              |
| 1:N:66:VAL:HG23 | 1:N:68:PRO:HD3  | 1.63                     | 0.80              |
| 1:A:13:ILE:HD12 | 1:A:14:LYS:HG3  | 1.62                     | 0.80              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:18:TYR:HB3  | 1:A:19:ASN:O    | 1.79                     | 0.80              |
| 1:C:75:THR:HG22 | 1:C:92:PHE:HZ   | 1.45                     | 0.80              |
| 1:G:26:ILE:HD11 | 1:G:37:VAL:HB   | 1.61                     | 0.80              |
| 1:G:86:TYR:CB   | 1:G:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:K:13:ILE:HD12 | 1:K:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:N:24:VAL:CG1  | 1:N:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:D:24:VAL:CG1  | 1:D:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:D:66:VAL:HG23 | 1:D:68:PRO:HD3  | 1.63                     | 0.80              |
| 1:F:86:TYR:CB   | 1:F:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:H:86:TYR:CB   | 1:H:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:B:18:TYR:HB3  | 1:B:19:ASN:O    | 1.79                     | 0.80              |
| 1:B:46:THR:HB   | 1:C:14:LYS:HZ1  | 1.46                     | 0.80              |
| 1:C:13:ILE:HD12 | 1:C:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:E:18:TYR:HB3  | 1:E:19:ASN:O    | 1.79                     | 0.80              |
| 1:E:86:TYR:CB   | 1:E:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:I:86:TYR:CB   | 1:I:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:K:86:TYR:CB   | 1:K:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:A:24:VAL:CG1  | 1:A:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:A:32:VAL:HG22 | 1:A:48:ALA:HB3  | 1.61                     | 0.80              |
| 1:E:1:LEU:CD1   | 1:E:13:ILE:HD11 | 2.10                     | 0.80              |
| 1:H:66:VAL:HG23 | 1:H:68:PRO:HD3  | 1.63                     | 0.80              |
| 1:J:86:TYR:CB   | 1:J:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:A:75:THR:HG22 | 1:A:92:PHE:HZ   | 1.45                     | 0.80              |
| 1:B:32:VAL:HG22 | 1:B:48:ALA:HB3  | 1.61                     | 0.80              |
| 1:D:86:TYR:CB   | 1:D:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:G:46:THR:HB   | 1:H:14:LYS:HZ1  | 1.42                     | 0.80              |
| 1:L:24:VAL:CG1  | 1:L:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:L:86:TYR:CB   | 1:L:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:B:66:VAL:HG23 | 1:B:68:PRO:HD3  | 1.63                     | 0.80              |
| 1:D:32:VAL:HG22 | 1:D:48:ALA:HB3  | 1.61                     | 0.80              |
| 1:E:13:ILE:HD12 | 1:E:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:F:24:VAL:CG1  | 1:F:107:LYS:HD3 | 2.11                     | 0.80              |
| 1:J:66:VAL:HG23 | 1:J:68:PRO:HD3  | 1.63                     | 0.80              |
| 1:N:13:ILE:HD12 | 1:N:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:D:18:TYR:HB3  | 1:D:19:ASN:O    | 1.79                     | 0.80              |
| 1:E:32:VAL:HG22 | 1:E:48:ALA:HB3  | 1.61                     | 0.80              |
| 1:L:13:ILE:HD12 | 1:L:14:LYS:HG3  | 1.62                     | 0.80              |
| 1:A:1:LEU:CD1   | 1:A:13:ILE:HD11 | 2.10                     | 0.80              |
| 1:M:86:TYR:CB   | 1:M:109:PHE:HB3 | 2.12                     | 0.80              |
| 1:A:46:THR:HB   | 1:B:14:LYS:HZ1  | 1.45                     | 0.79              |
| 1:D:13:ILE:HD12 | 1:D:14:LYS:HG3  | 1.62                     | 0.79              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:24:VAL:CG1  | 1:H:107:LYS:HD3  | 2.11                     | 0.79              |
| 1:N:86:TYR:CB   | 1:N:109:PHE:HB3  | 2.12                     | 0.79              |
| 1:C:86:TYR:CB   | 1:C:109:PHE:HB3  | 2.12                     | 0.79              |
| 1:A:86:TYR:CB   | 1:A:109:PHE:HB3  | 2.12                     | 0.79              |
| 1:B:86:TYR:CB   | 1:B:109:PHE:HB3  | 2.12                     | 0.79              |
| 1:K:1:LEU:CD1   | 1:K:13:ILE:HD11  | 2.10                     | 0.79              |
| 1:C:32:VAL:HG22 | 1:C:48:ALA:HB3   | 1.61                     | 0.79              |
| 1:E:66:VAL:HG23 | 1:E:68:PRO:HD3   | 1.63                     | 0.79              |
| 1:L:75:THR:HG22 | 1:L:92:PHE:HZ    | 1.45                     | 0.79              |
| 1:M:66:VAL:HG23 | 1:M:68:PRO:HD3   | 1.63                     | 0.79              |
| 1:M:13:ILE:HD12 | 1:M:14:LYS:HG3   | 1.62                     | 0.79              |
| 1:N:90:LEU:HB2  | 1:N:105:VAL:HG23 | 1.65                     | 0.79              |
| 1:E:46:THR:HB   | 1:F:14:LYS:HZ1   | 1.45                     | 0.79              |
| 1:K:90:LEU:HB2  | 1:K:105:VAL:HG23 | 1.65                     | 0.79              |
| 1:C:90:LEU:HB2  | 1:C:105:VAL:HG23 | 1.65                     | 0.79              |
| 1:B:90:LEU:HB2  | 1:B:105:VAL:HG23 | 1.65                     | 0.79              |
| 1:E:90:LEU:HB2  | 1:E:105:VAL:HG23 | 1.65                     | 0.79              |
| 1:E:29:VAL:HG12 | 1:E:77:LEU:HD21  | 1.65                     | 0.78              |
| 1:F:29:VAL:HG12 | 1:F:77:LEU:HD21  | 1.65                     | 0.78              |
| 1:I:90:LEU:HB2  | 1:I:105:VAL:HG23 | 1.65                     | 0.78              |
| 1:J:46:THR:HB   | 1:K:14:LYS:HZ1   | 1.43                     | 0.78              |
| 1:L:90:LEU:HB2  | 1:L:105:VAL:HG23 | 1.65                     | 0.78              |
| 1:G:29:VAL:HG12 | 1:G:77:LEU:HD21  | 1.65                     | 0.78              |
| 1:G:90:LEU:HB2  | 1:G:105:VAL:HG23 | 1.65                     | 0.78              |
| 1:F:75:THR:HG22 | 1:F:92:PHE:HZ    | 1.45                     | 0.78              |
| 1:M:90:LEU:HB2  | 1:M:105:VAL:HG23 | 1.65                     | 0.78              |
| 1:H:29:VAL:HG12 | 1:H:77:LEU:HD21  | 1.65                     | 0.78              |
| 1:C:66:VAL:HG23 | 1:C:68:PRO:HD3   | 1.63                     | 0.78              |
| 1:J:13:ILE:HB   | 1:J:14:LYS:HG3   | 1.66                     | 0.78              |
| 1:J:59:HIS:HA   | 1:J:64:PHE:CD2   | 2.19                     | 0.78              |
| 1:N:13:ILE:HB   | 1:N:14:LYS:HG3   | 1.66                     | 0.78              |
| 1:A:66:VAL:HG23 | 1:A:68:PRO:HD3   | 1.63                     | 0.78              |
| 1:I:29:VAL:HG12 | 1:I:77:LEU:HD21  | 1.65                     | 0.78              |
| 1:L:13:ILE:HB   | 1:L:14:LYS:HG3   | 1.66                     | 0.78              |
| 1:N:59:HIS:HA   | 1:N:64:PHE:CD2   | 2.19                     | 0.78              |
| 1:B:13:ILE:HB   | 1:B:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:D:29:VAL:HG12 | 1:D:77:LEU:HD21  | 1.65                     | 0.77              |
| 1:D:90:LEU:HB2  | 1:D:105:VAL:HG23 | 1.65                     | 0.77              |
| 1:A:90:LEU:HB2  | 1:A:105:VAL:HG23 | 1.65                     | 0.77              |
| 1:C:13:ILE:HB   | 1:C:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:E:56:THR:HG22 | 1:E:57:PHE:H     | 1.50                     | 0.77              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:13:ILE:HB   | 1:E:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:F:59:HIS:HA   | 1:F:64:PHE:CD2   | 2.19                     | 0.77              |
| 1:H:13:ILE:HB   | 1:H:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:H:56:THR:HG22 | 1:H:57:PHE:H     | 1.50                     | 0.77              |
| 1:M:29:VAL:HG12 | 1:M:77:LEU:HD21  | 1.65                     | 0.77              |
| 1:A:13:ILE:HB   | 1:A:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:I:49:PHE:HB3  | 1:I:68:PRO:HG2   | 1.67                     | 0.77              |
| 1:K:13:ILE:HB   | 1:K:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:M:13:ILE:HB   | 1:M:14:LYS:HG3   | 1.66                     | 0.77              |
| 1:N:29:VAL:HG12 | 1:N:77:LEU:HD21  | 1.65                     | 0.77              |
| 1:D:56:THR:HG22 | 1:D:57:PHE:H     | 1.50                     | 0.77              |
| 1:G:49:PHE:HB3  | 1:G:68:PRO:HG2   | 1.67                     | 0.77              |
| 1:H:25:LYS:HD2  | 1:H:25:LYS:N     | 1.99                     | 0.77              |
| 1:I:25:LYS:HD2  | 1:I:25:LYS:N     | 2.00                     | 0.77              |
| 1:J:29:VAL:HG12 | 1:J:77:LEU:HD21  | 1.65                     | 0.77              |
| 1:J:90:LEU:HB2  | 1:J:105:VAL:HG23 | 1.65                     | 0.77              |
| 1:A:59:HIS:HA   | 1:A:64:PHE:CD2   | 2.19                     | 0.77              |
| 1:D:25:LYS:N    | 1:D:25:LYS:HD2   | 1.99                     | 0.77              |
| 1:F:25:LYS:HD2  | 1:F:25:LYS:N     | 2.00                     | 0.77              |
| 1:G:25:LYS:N    | 1:G:25:LYS:HD2   | 1.99                     | 0.77              |
| 1:J:25:LYS:N    | 1:J:25:LYS:HD2   | 1.99                     | 0.77              |
| 1:J:75:THR:HG22 | 1:J:92:PHE:HZ    | 1.45                     | 0.77              |
| 1:K:49:PHE:HB3  | 1:K:68:PRO:HG2   | 1.67                     | 0.77              |
| 1:K:59:HIS:HA   | 1:K:64:PHE:CD2   | 2.19                     | 0.77              |
| 1:L:29:VAL:HG12 | 1:L:77:LEU:HD21  | 1.65                     | 0.77              |
| 1:G:59:HIS:HA   | 1:G:64:PHE:CD2   | 2.19                     | 0.77              |
| 1:I:56:THR:HG22 | 1:I:57:PHE:H     | 1.50                     | 0.77              |
| 1:F:18:TYR:CD2  | 1:F:23:VAL:HG22  | 2.20                     | 0.77              |
| 1:I:18:TYR:CD2  | 1:I:23:VAL:HG22  | 2.20                     | 0.77              |
| 1:K:25:LYS:HD2  | 1:K:25:LYS:N     | 1.99                     | 0.77              |
| 1:L:18:TYR:CD2  | 1:L:23:VAL:HG22  | 2.20                     | 0.77              |
| 1:N:25:LYS:HD2  | 1:N:25:LYS:N     | 1.99                     | 0.77              |
| 1:L:25:LYS:N    | 1:L:25:LYS:HD2   | 2.00                     | 0.76              |
| 1:N:18:TYR:CD2  | 1:N:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:F:44:TYR:H    | 1:G:14:LYS:CE    | 1.98                     | 0.76              |
| 1:I:44:TYR:H    | 1:J:14:LYS:CE    | 1.98                     | 0.76              |
| 1:L:80:VAL:CG1  | 1:L:88:ILE:HG22  | 2.14                     | 0.76              |
| 1:A:25:LYS:HD2  | 1:A:25:LYS:N     | 1.99                     | 0.76              |
| 1:A:29:VAL:HG12 | 1:A:77:LEU:HD21  | 1.65                     | 0.76              |
| 1:F:90:LEU:HB2  | 1:F:105:VAL:HG23 | 1.65                     | 0.76              |
| 1:G:44:TYR:H    | 1:H:14:LYS:CE    | 1.98                     | 0.76              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:75:THR:HG22 | 1:H:92:PHE:HZ    | 1.45                     | 0.76              |
| 1:K:18:TYR:CD2  | 1:K:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:M:49:PHE:HB3  | 1:M:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:A:56:THR:HG22 | 1:A:57:PHE:H     | 1.50                     | 0.76              |
| 1:B:25:LYS:N    | 1:B:25:LYS:HD2   | 2.00                     | 0.76              |
| 1:C:25:LYS:HD2  | 1:C:25:LYS:N     | 1.99                     | 0.76              |
| 1:F:56:THR:HG22 | 1:F:57:PHE:H     | 1.50                     | 0.76              |
| 1:H:18:TYR:CD2  | 1:H:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:J:44:TYR:H    | 1:K:14:LYS:CE    | 1.98                     | 0.76              |
| 1:F:49:PHE:HB3  | 1:F:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:G:13:ILE:HB   | 1:G:14:LYS:HG3   | 1.66                     | 0.76              |
| 1:G:56:THR:HG22 | 1:G:57:PHE:H     | 1.50                     | 0.76              |
| 1:K:29:VAL:HG12 | 1:K:77:LEU:HD21  | 1.65                     | 0.76              |
| 1:L:56:THR:HG22 | 1:L:57:PHE:H     | 1.50                     | 0.76              |
| 1:M:25:LYS:N    | 1:M:25:LYS:HD2   | 2.00                     | 0.76              |
| 1:A:44:TYR:H    | 1:B:14:LYS:CE    | 1.98                     | 0.76              |
| 1:C:29:VAL:HG12 | 1:C:77:LEU:HD21  | 1.65                     | 0.76              |
| 1:D:18:TYR:CD2  | 1:D:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:E:49:PHE:HB3  | 1:E:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:H:49:PHE:HB3  | 1:H:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:A:18:TYR:CD2  | 1:A:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:B:56:THR:HG22 | 1:B:57:PHE:H     | 1.50                     | 0.76              |
| 1:H:90:LEU:HB2  | 1:H:105:VAL:HG23 | 1.65                     | 0.76              |
| 1:I:9:TYR:HB2   | 1:I:10:ASP:C     | 2.11                     | 0.76              |
| 1:J:18:TYR:CD2  | 1:J:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:L:9:TYR:HB2   | 1:L:10:ASP:C     | 2.11                     | 0.76              |
| 1:M:44:TYR:H    | 1:N:14:LYS:CE    | 1.98                     | 0.76              |
| 1:M:80:VAL:CG1  | 1:M:88:ILE:HG22  | 2.14                     | 0.76              |
| 1:B:18:TYR:CD2  | 1:B:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:B:59:HIS:HA   | 1:B:64:PHE:CD2   | 2.19                     | 0.76              |
| 1:C:9:TYR:HB2   | 1:C:10:ASP:C     | 2.11                     | 0.76              |
| 1:F:9:TYR:HB2   | 1:F:10:ASP:C     | 2.11                     | 0.76              |
| 1:G:18:TYR:CD2  | 1:G:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:J:49:PHE:HB3  | 1:J:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:B:9:TYR:HB2   | 1:B:10:ASP:C     | 2.11                     | 0.76              |
| 1:D:13:ILE:HB   | 1:D:14:LYS:HG3   | 1.66                     | 0.76              |
| 1:D:49:PHE:HB3  | 1:D:68:PRO:HG2   | 1.67                     | 0.76              |
| 1:K:9:TYR:HB2   | 1:K:10:ASP:C     | 2.11                     | 0.76              |
| 1:K:56:THR:HG22 | 1:K:57:PHE:H     | 1.50                     | 0.76              |
| 1:M:18:TYR:CD2  | 1:M:23:VAL:HG22  | 2.20                     | 0.76              |
| 1:B:29:VAL:HG12 | 1:B:77:LEU:HD21  | 1.65                     | 0.75              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:59:HIS:HA   | 1:H:64:PHE:CD2  | 2.19                     | 0.75              |
| 1:N:9:TYR:HB2   | 1:N:10:ASP:C    | 2.11                     | 0.75              |
| 1:C:18:TYR:CD2  | 1:C:23:VAL:HG22 | 2.20                     | 0.75              |
| 1:C:44:TYR:H    | 1:D:14:LYS:CE   | 1.98                     | 0.75              |
| 1:E:25:LYS:N    | 1:E:25:LYS:HD2  | 2.00                     | 0.75              |
| 1:F:13:ILE:HB   | 1:F:14:LYS:HG3  | 1.66                     | 0.75              |
| 1:J:56:THR:HG22 | 1:J:57:PHE:H    | 1.50                     | 0.75              |
| 1:L:59:HIS:HA   | 1:L:64:PHE:CD2  | 2.19                     | 0.75              |
| 1:B:44:TYR:H    | 1:C:14:LYS:CE   | 1.98                     | 0.75              |
| 1:D:44:TYR:H    | 1:E:14:LYS:CE   | 1.98                     | 0.75              |
| 1:H:44:TYR:H    | 1:I:14:LYS:CE   | 1.98                     | 0.75              |
| 1:A:44:TYR:N    | 1:A:45:ILE:HA   | 2.02                     | 0.75              |
| 1:B:49:PHE:HB3  | 1:B:68:PRO:HG2  | 1.67                     | 0.75              |
| 1:E:9:TYR:HB2   | 1:E:10:ASP:C    | 2.11                     | 0.75              |
| 1:E:59:HIS:HA   | 1:E:64:PHE:CD2  | 2.19                     | 0.75              |
| 1:I:13:ILE:HB   | 1:I:14:LYS:HG3  | 1.66                     | 0.75              |
| 1:N:80:VAL:CG1  | 1:N:88:ILE:HG22 | 2.14                     | 0.75              |
| 1:C:59:HIS:HA   | 1:C:64:PHE:CD2  | 2.19                     | 0.75              |
| 1:E:44:TYR:H    | 1:F:14:LYS:CE   | 1.98                     | 0.75              |
| 1:G:9:TYR:HB2   | 1:G:10:ASP:C    | 2.11                     | 0.75              |
| 1:G:44:TYR:N    | 1:G:45:ILE:HA   | 2.02                     | 0.75              |
| 1:I:98:LYS:HD3  | 1:I:98:LYS:N    | 2.02                     | 0.75              |
| 1:K:36:ILE:HG22 | 1:K:44:TYR:HB3  | 1.69                     | 0.75              |
| 1:L:44:TYR:H    | 1:M:14:LYS:CE   | 1.98                     | 0.75              |
| 1:N:98:LYS:HD3  | 1:N:98:LYS:N    | 2.02                     | 0.75              |
| 1:A:14:LYS:CE   | 1:N:44:TYR:H    | 1.98                     | 0.75              |
| 1:B:44:TYR:N    | 1:B:45:ILE:HA   | 2.02                     | 0.75              |
| 1:C:56:THR:HG22 | 1:C:57:PHE:H    | 1.50                     | 0.75              |
| 1:E:18:TYR:CD2  | 1:E:23:VAL:HG22 | 2.20                     | 0.75              |
| 1:L:36:ILE:HG22 | 1:L:44:TYR:HB3  | 1.69                     | 0.75              |
| 1:H:44:TYR:N    | 1:H:45:ILE:HA   | 2.02                     | 0.75              |
| 1:H:98:LYS:HD3  | 1:H:98:LYS:N    | 2.02                     | 0.75              |
| 1:J:9:TYR:HB2   | 1:J:10:ASP:C    | 2.11                     | 0.75              |
| 1:J:36:ILE:HG22 | 1:J:44:TYR:HB3  | 1.69                     | 0.75              |
| 1:M:24:VAL:HG11 | 1:M:107:LYS:HD3 | 1.69                     | 0.75              |
| 1:F:44:TYR:N    | 1:F:45:ILE:HA   | 2.02                     | 0.75              |
| 1:I:36:ILE:HG22 | 1:I:44:TYR:HB3  | 1.69                     | 0.75              |
| 1:J:98:LYS:HD3  | 1:J:98:LYS:N    | 2.02                     | 0.75              |
| 1:K:24:VAL:HG11 | 1:K:107:LYS:HD3 | 1.69                     | 0.75              |
| 1:L:49:PHE:HB3  | 1:L:68:PRO:HG2  | 1.67                     | 0.75              |
| 1:M:36:ILE:HG22 | 1:M:44:TYR:HB3  | 1.69                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:TYR:HB2    | 1:A:10:ASP:C     | 2.11                     | 0.74              |
| 1:A:49:PHE:HB3   | 1:A:68:PRO:HG2   | 1.67                     | 0.74              |
| 1:A:98:LYS:HD3   | 1:A:98:LYS:N     | 2.02                     | 0.74              |
| 1:D:9:TYR:HB2    | 1:D:10:ASP:C     | 2.11                     | 0.74              |
| 1:K:44:TYR:H     | 1:L:14:LYS:CE    | 1.98                     | 0.74              |
| 1:K:44:TYR:N     | 1:K:45:ILE:HA    | 2.02                     | 0.74              |
| 1:M:98:LYS:HD3   | 1:M:98:LYS:N     | 2.02                     | 0.74              |
| 1:N:49:PHE:HB3   | 1:N:68:PRO:HG2   | 1.67                     | 0.74              |
| 1:N:56:THR:HG22  | 1:N:57:PHE:H     | 1.50                     | 0.74              |
| 1:A:24:VAL:HG11  | 1:A:107:LYS:HD3  | 1.69                     | 0.74              |
| 1:A:80:VAL:CG1   | 1:A:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:D:59:HIS:HA    | 1:D:64:PHE:CD2   | 2.19                     | 0.74              |
| 1:E:44:TYR:N     | 1:E:45:ILE:HA    | 2.02                     | 0.74              |
| 1:H:36:ILE:HG22  | 1:H:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:I:24:VAL:HG11  | 1:I:107:LYS:HD3  | 1.69                     | 0.74              |
| 1:M:56:THR:HG22  | 1:M:57:PHE:H     | 1.50                     | 0.74              |
| 1:D:36:ILE:HG22  | 1:D:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:E:36:ILE:HG22  | 1:E:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:F:36:ILE:HG22  | 1:F:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:F:57:PHE:HE1   | 1:G:105:VAL:HG13 | 1.53                     | 0.74              |
| 1:H:9:TYR:HB2    | 1:H:10:ASP:C     | 2.11                     | 0.74              |
| 1:B:36:ILE:HG22  | 1:B:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:H:80:VAL:CG1   | 1:H:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:I:65:PHE:HD1   | 1:I:80:VAL:HG12  | 1.53                     | 0.74              |
| 1:I:80:VAL:CG1   | 1:I:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:K:57:PHE:HE1   | 1:L:105:VAL:HG13 | 1.53                     | 0.74              |
| 1:L:44:TYR:N     | 1:L:45:ILE:HA    | 2.02                     | 0.74              |
| 1:N:36:ILE:HG22  | 1:N:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:A:36:ILE:HG22  | 1:A:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:C:36:ILE:HG22  | 1:C:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:G:36:ILE:HG22  | 1:G:44:TYR:HB3   | 1.69                     | 0.74              |
| 1:M:9:TYR:HB2    | 1:M:10:ASP:C     | 2.11                     | 0.74              |
| 1:N:44:TYR:N     | 1:N:45:ILE:HA    | 2.02                     | 0.74              |
| 1:D:98:LYS:HD3   | 1:D:98:LYS:N     | 2.02                     | 0.74              |
| 1:A:105:VAL:HG13 | 1:N:57:PHE:HE1   | 1.53                     | 0.74              |
| 1:E:98:LYS:HD3   | 1:E:98:LYS:N     | 2.02                     | 0.74              |
| 1:J:65:PHE:HD1   | 1:J:80:VAL:HG12  | 1.53                     | 0.74              |
| 1:K:98:LYS:HD3   | 1:K:98:LYS:N     | 2.02                     | 0.74              |
| 1:B:80:VAL:CG1   | 1:B:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:G:80:VAL:CG1   | 1:G:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:H:57:PHE:HE1   | 1:I:105:VAL:HG13 | 1.53                     | 0.74              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:80:VAL:CG1  | 1:J:88:ILE:HG22  | 2.14                     | 0.74              |
| 1:C:49:PHE:HB3  | 1:C:68:PRO:HG2   | 1.67                     | 0.74              |
| 1:E:65:PHE:HD1  | 1:E:80:VAL:HG12  | 1.53                     | 0.74              |
| 1:G:98:LYS:HD3  | 1:G:98:LYS:N     | 2.02                     | 0.74              |
| 1:M:80:VAL:HG22 | 1:M:88:ILE:CG2   | 2.18                     | 0.74              |
| 1:C:44:TYR:N    | 1:C:45:ILE:HA    | 2.02                     | 0.74              |
| 1:D:65:PHE:HD1  | 1:D:80:VAL:HG12  | 1.53                     | 0.74              |
| 1:I:44:TYR:N    | 1:I:45:ILE:HA    | 2.02                     | 0.74              |
| 1:J:44:TYR:N    | 1:J:45:ILE:HA    | 2.02                     | 0.74              |
| 1:B:57:PHE:HE1  | 1:C:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:D:57:PHE:HE1  | 1:E:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:F:24:VAL:HG11 | 1:F:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:H:24:VAL:HG11 | 1:H:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:I:57:PHE:HE1  | 1:J:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:M:57:PHE:HE1  | 1:N:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:N:80:VAL:HG22 | 1:N:88:ILE:CG2   | 2.18                     | 0.73              |
| 1:J:24:VAL:HG11 | 1:J:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:L:27:ASP:OD1  | 1:L:105:VAL:HG11 | 1.88                     | 0.73              |
| 1:B:98:LYS:HD3  | 1:B:98:LYS:N     | 2.02                     | 0.73              |
| 1:C:80:VAL:CG1  | 1:C:88:ILE:HG22  | 2.14                     | 0.73              |
| 1:C:98:LYS:HD3  | 1:C:98:LYS:N     | 2.02                     | 0.73              |
| 1:F:65:PHE:HD1  | 1:F:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:G:24:VAL:HG11 | 1:G:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:I:59:HIS:HA   | 1:I:64:PHE:CD2   | 2.19                     | 0.73              |
| 1:A:80:VAL:HG22 | 1:A:88:ILE:CG2   | 2.18                     | 0.73              |
| 1:C:24:VAL:HG11 | 1:C:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:C:65:PHE:HD1  | 1:C:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:F:80:VAL:CG1  | 1:F:88:ILE:HG22  | 2.14                     | 0.73              |
| 1:F:98:LYS:HD3  | 1:F:98:LYS:N     | 2.02                     | 0.73              |
| 1:H:65:PHE:HD1  | 1:H:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:I:49:PHE:H    | 1:I:55:ARG:HH12  | 1.37                     | 0.73              |
| 1:K:27:ASP:OD1  | 1:K:105:VAL:HG11 | 1.89                     | 0.73              |
| 1:K:80:VAL:CG1  | 1:K:88:ILE:HG22  | 2.14                     | 0.73              |
| 1:L:24:VAL:HG11 | 1:L:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:M:27:ASP:OD1  | 1:M:105:VAL:HG11 | 1.89                     | 0.73              |
| 1:M:59:HIS:HA   | 1:M:64:PHE:CD2   | 2.19                     | 0.73              |
| 1:J:57:PHE:HE1  | 1:K:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:N:65:PHE:HD1  | 1:N:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:D:24:VAL:HG11 | 1:D:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:F:49:PHE:H    | 1:F:55:ARG:HH12  | 1.37                     | 0.73              |
| 1:J:27:ASP:OD1  | 1:J:105:VAL:HG11 | 1.89                     | 0.73              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:27:ASP:OD1  | 1:N:105:VAL:HG11 | 1.88                     | 0.73              |
| 1:A:65:PHE:HD1  | 1:A:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:B:65:PHE:HD1  | 1:B:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:L:57:PHE:HE1  | 1:M:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:M:65:PHE:HD1  | 1:M:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:C:57:PHE:HE1  | 1:D:105:VAL:HG13 | 1.53                     | 0.73              |
| 1:K:65:PHE:HD1  | 1:K:80:VAL:HG12  | 1.53                     | 0.73              |
| 1:M:44:TYR:N    | 1:M:45:ILE:HA    | 2.02                     | 0.73              |
| 1:D:80:VAL:CG1  | 1:D:88:ILE:HG22  | 2.14                     | 0.73              |
| 1:E:5:ARG:HH22  | 1:E:24:VAL:H     | 1.37                     | 0.73              |
| 1:E:27:ASP:OD1  | 1:E:105:VAL:HG11 | 1.88                     | 0.73              |
| 1:N:24:VAL:HG11 | 1:N:107:LYS:HD3  | 1.69                     | 0.73              |
| 1:A:57:PHE:HE1  | 1:B:105:VAL:HG13 | 1.53                     | 0.72              |
| 1:B:80:VAL:HG22 | 1:B:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:D:44:TYR:N    | 1:D:45:ILE:HA    | 2.02                     | 0.72              |
| 1:H:80:VAL:HG22 | 1:H:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:J:49:PHE:H    | 1:J:55:ARG:HH12  | 1.37                     | 0.72              |
| 1:A:27:ASP:OD1  | 1:A:105:VAL:HG11 | 1.88                     | 0.72              |
| 1:B:24:VAL:HG11 | 1:B:107:LYS:HD3  | 1.69                     | 0.72              |
| 1:C:5:ARG:HH22  | 1:C:24:VAL:H     | 1.37                     | 0.72              |
| 1:E:49:PHE:H    | 1:E:55:ARG:HH12  | 1.37                     | 0.72              |
| 1:F:80:VAL:HG22 | 1:F:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:G:80:VAL:HG22 | 1:G:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:I:27:ASP:OD1  | 1:I:105:VAL:HG11 | 1.89                     | 0.72              |
| 1:I:80:VAL:HG22 | 1:I:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:D:27:ASP:OD1  | 1:D:105:VAL:HG11 | 1.89                     | 0.72              |
| 1:D:5:ARG:HH22  | 1:D:24:VAL:H     | 1.37                     | 0.72              |
| 1:G:5:ARG:HH22  | 1:G:24:VAL:H     | 1.37                     | 0.72              |
| 1:E:80:VAL:CG1  | 1:E:88:ILE:HG22  | 2.14                     | 0.72              |
| 1:M:44:TYR:HB2  | 1:M:45:ILE:C     | 2.15                     | 0.72              |
| 1:A:38:VAL:HA   | 1:A:109:PHE:HE2  | 1.55                     | 0.72              |
| 1:B:27:ASP:OD1  | 1:B:105:VAL:HG11 | 1.89                     | 0.72              |
| 1:D:38:VAL:HA   | 1:D:109:PHE:HE2  | 1.55                     | 0.72              |
| 1:L:44:TYR:HB2  | 1:L:45:ILE:C     | 2.15                     | 0.72              |
| 1:N:44:TYR:HB2  | 1:N:45:ILE:C     | 2.15                     | 0.72              |
| 1:B:5:ARG:HH22  | 1:B:24:VAL:H     | 1.37                     | 0.72              |
| 1:C:67:LYS:HA   | 1:C:77:LEU:O     | 1.90                     | 0.72              |
| 1:G:57:PHE:HE1  | 1:H:105:VAL:HG13 | 1.53                     | 0.72              |
| 1:G:65:PHE:HD1  | 1:G:80:VAL:HG12  | 1.53                     | 0.72              |
| 1:A:67:LYS:HA   | 1:A:77:LEU:O     | 1.90                     | 0.72              |
| 1:E:60:LYS:N    | 1:E:64:PHE:HB2   | 2.04                     | 0.72              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:27:ASP:OD1  | 1:G:105:VAL:HG11 | 1.88                     | 0.72              |
| 1:H:27:ASP:OD1  | 1:H:105:VAL:HG11 | 1.88                     | 0.72              |
| 1:K:44:TYR:HB2  | 1:K:45:ILE:C     | 2.15                     | 0.72              |
| 1:L:67:LYS:HA   | 1:L:77:LEU:O     | 1.90                     | 0.72              |
| 1:B:49:PHE:HE2  | 1:B:79:ILE:HD11  | 1.55                     | 0.72              |
| 1:C:27:ASP:OD1  | 1:C:105:VAL:HG11 | 1.89                     | 0.72              |
| 1:E:38:VAL:HA   | 1:E:109:PHE:HE2  | 1.55                     | 0.72              |
| 1:E:57:PHE:HE1  | 1:F:105:VAL:HG13 | 1.53                     | 0.72              |
| 1:H:49:PHE:HE2  | 1:H:79:ILE:HD11  | 1.55                     | 0.72              |
| 1:J:80:VAL:HG22 | 1:J:88:ILE:CG2   | 2.18                     | 0.72              |
| 1:A:29:VAL:CG1  | 1:A:77:LEU:HD11  | 2.20                     | 0.72              |
| 1:A:44:TYR:HB2  | 1:A:45:ILE:C     | 2.15                     | 0.72              |
| 1:A:57:PHE:HB3  | 1:B:103:GLY:CA   | 2.20                     | 0.72              |
| 1:B:38:VAL:HA   | 1:B:109:PHE:HE2  | 1.55                     | 0.72              |
| 1:D:67:LYS:HA   | 1:D:77:LEU:O     | 1.90                     | 0.72              |
| 1:F:5:ARG:HH22  | 1:F:24:VAL:H     | 1.37                     | 0.72              |
| 1:G:44:TYR:HB2  | 1:G:45:ILE:C     | 2.15                     | 0.72              |
| 1:J:44:TYR:HB2  | 1:J:45:ILE:C     | 2.15                     | 0.72              |
| 1:L:65:PHE:HD1  | 1:L:80:VAL:HG12  | 1.53                     | 0.72              |
| 1:B:29:VAL:CG1  | 1:B:77:LEU:HD11  | 2.20                     | 0.71              |
| 1:C:80:VAL:HG22 | 1:C:88:ILE:CG2   | 2.18                     | 0.71              |
| 1:E:49:PHE:HE2  | 1:E:79:ILE:HD11  | 1.55                     | 0.71              |
| 1:E:67:LYS:HA   | 1:E:77:LEU:O     | 1.90                     | 0.71              |
| 1:F:27:ASP:OD1  | 1:F:105:VAL:HG11 | 1.89                     | 0.71              |
| 1:G:49:PHE:H    | 1:G:55:ARG:HH12  | 1.37                     | 0.71              |
| 1:H:49:PHE:H    | 1:H:55:ARG:HH12  | 1.37                     | 0.71              |
| 1:I:49:PHE:HE2  | 1:I:79:ILE:HD11  | 1.55                     | 0.71              |
| 1:L:49:PHE:HE2  | 1:L:79:ILE:HD11  | 1.55                     | 0.71              |
| 1:N:29:VAL:CG1  | 1:N:77:LEU:HD11  | 2.20                     | 0.71              |
| 1:A:5:ARG:HH22  | 1:A:24:VAL:H     | 1.37                     | 0.71              |
| 1:B:67:LYS:HA   | 1:B:77:LEU:O     | 1.90                     | 0.71              |
| 1:C:29:VAL:CG1  | 1:C:77:LEU:HD11  | 2.20                     | 0.71              |
| 1:D:57:PHE:HB3  | 1:E:103:GLY:CA   | 2.20                     | 0.71              |
| 1:F:49:PHE:HE2  | 1:F:79:ILE:HD11  | 1.55                     | 0.71              |
| 1:H:44:TYR:HB2  | 1:H:45:ILE:C     | 2.15                     | 0.71              |
| 1:I:38:VAL:HA   | 1:I:109:PHE:HE2  | 1.55                     | 0.71              |
| 1:L:92:PHE:C    | 1:L:93:ILE:HG13  | 2.15                     | 0.71              |
| 1:B:44:TYR:HB2  | 1:B:45:ILE:C     | 2.15                     | 0.71              |
| 1:E:24:VAL:HG11 | 1:E:107:LYS:HD3  | 1.69                     | 0.71              |
| 1:F:67:LYS:HA   | 1:F:77:LEU:O     | 1.90                     | 0.71              |
| 1:H:5:ARG:HH22  | 1:H:24:VAL:H     | 1.37                     | 0.71              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:38:VAL:HA   | 1:H:109:PHE:HE2 | 1.55                     | 0.71              |
| 1:J:67:LYS:HA   | 1:J:77:LEU:O    | 1.90                     | 0.71              |
| 1:M:49:PHE:HE2  | 1:M:79:ILE:HD11 | 1.55                     | 0.71              |
| 1:M:57:PHE:HB3  | 1:N:103:GLY:CA  | 2.20                     | 0.71              |
| 1:M:92:PHE:C    | 1:M:93:ILE:HG13 | 2.15                     | 0.71              |
| 1:A:49:PHE:HE2  | 1:A:79:ILE:HD11 | 1.55                     | 0.71              |
| 1:C:44:TYR:HB2  | 1:C:45:ILE:C    | 2.15                     | 0.71              |
| 1:D:29:VAL:CG1  | 1:D:77:LEU:HD11 | 2.20                     | 0.71              |
| 1:E:44:TYR:HB2  | 1:E:45:ILE:C    | 2.15                     | 0.71              |
| 1:G:49:PHE:HE2  | 1:G:79:ILE:HD11 | 1.55                     | 0.71              |
| 1:G:67:LYS:HA   | 1:G:77:LEU:O    | 1.90                     | 0.71              |
| 1:I:44:TYR:HB2  | 1:I:45:ILE:C    | 2.15                     | 0.71              |
| 1:M:49:PHE:H    | 1:M:55:ARG:HH12 | 1.37                     | 0.71              |
| 1:N:67:LYS:HA   | 1:N:77:LEU:O    | 1.90                     | 0.71              |
| 1:C:49:PHE:HE2  | 1:C:79:ILE:HD11 | 1.55                     | 0.71              |
| 1:D:44:TYR:HB2  | 1:D:45:ILE:C    | 2.15                     | 0.71              |
| 1:F:44:TYR:HB2  | 1:F:45:ILE:C    | 2.15                     | 0.71              |
| 1:H:67:LYS:HA   | 1:H:77:LEU:O    | 1.90                     | 0.71              |
| 1:I:5:ARG:HH22  | 1:I:24:VAL:H    | 1.37                     | 0.71              |
| 1:I:67:LYS:HA   | 1:I:77:LEU:O    | 1.90                     | 0.71              |
| 1:L:49:PHE:H    | 1:L:55:ARG:HH12 | 1.37                     | 0.71              |
| 1:M:29:VAL:CG1  | 1:M:77:LEU:HD11 | 2.20                     | 0.71              |
| 1:N:60:LYS:N    | 1:N:64:PHE:HB2  | 2.04                     | 0.71              |
| 1:N:92:PHE:C    | 1:N:93:ILE:HG13 | 2.15                     | 0.71              |
| 1:D:49:PHE:HE2  | 1:D:79:ILE:HD11 | 1.55                     | 0.71              |
| 1:M:67:LYS:HA   | 1:M:77:LEU:O    | 1.90                     | 0.71              |
| 1:B:49:PHE:H    | 1:B:55:ARG:HH12 | 1.37                     | 0.71              |
| 1:E:29:VAL:CG1  | 1:E:77:LEU:HD11 | 2.20                     | 0.71              |
| 1:I:9:TYR:HB2   | 1:I:11:TYR:N    | 2.06                     | 0.71              |
| 1:N:5:ARG:HH22  | 1:N:24:VAL:H    | 1.37                     | 0.71              |
| 1:E:80:VAL:HG22 | 1:E:88:ILE:CG2  | 2.18                     | 0.71              |
| 1:H:83:LYS:HE2  | 1:H:109:PHE:HZ  | 1.56                     | 0.71              |
| 1:J:92:PHE:C    | 1:J:93:ILE:HG13 | 2.15                     | 0.71              |
| 1:K:57:PHE:HB3  | 1:L:103:GLY:CA  | 2.20                     | 0.71              |
| 1:K:80:VAL:HG22 | 1:K:88:ILE:CG2  | 2.18                     | 0.71              |
| 1:L:29:VAL:CG1  | 1:L:77:LEU:HD11 | 2.20                     | 0.71              |
| 1:L:38:VAL:HA   | 1:L:109:PHE:HE2 | 1.55                     | 0.71              |
| 1:C:49:PHE:H    | 1:C:55:ARG:HH12 | 1.37                     | 0.71              |
| 1:I:57:PHE:HB3  | 1:J:103:GLY:CA  | 2.20                     | 0.71              |
| 1:J:38:VAL:HA   | 1:J:109:PHE:HE2 | 1.55                     | 0.71              |
| 1:J:83:LYS:HE2  | 1:J:109:PHE:HZ  | 1.56                     | 0.71              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:92:PHE:C    | 1:A:93:ILE:HG13 | 2.15                     | 0.71              |
| 1:K:67:LYS:HA   | 1:K:77:LEU:O    | 1.90                     | 0.71              |
| 1:K:92:PHE:C    | 1:K:93:ILE:HG13 | 2.15                     | 0.71              |
| 1:F:60:LYS:N    | 1:F:64:PHE:HB2  | 2.04                     | 0.70              |
| 1:F:92:PHE:C    | 1:F:93:ILE:HG13 | 2.15                     | 0.70              |
| 1:G:9:TYR:HB2   | 1:G:11:TYR:N    | 2.06                     | 0.70              |
| 1:G:38:VAL:HA   | 1:G:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:G:57:PHE:HB3  | 1:H:103:GLY:CA  | 2.20                     | 0.70              |
| 1:K:49:PHE:HE2  | 1:K:79:ILE:HD11 | 1.55                     | 0.70              |
| 1:L:9:TYR:HB2   | 1:L:11:TYR:N    | 2.06                     | 0.70              |
| 1:M:83:LYS:HE2  | 1:M:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:F:83:LYS:HE2  | 1:F:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:L:83:LYS:HE2  | 1:L:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:M:38:VAL:HA   | 1:M:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:B:57:PHE:HB3  | 1:C:103:GLY:CA  | 2.20                     | 0.70              |
| 1:C:9:TYR:HB2   | 1:C:11:TYR:N    | 2.06                     | 0.70              |
| 1:D:9:TYR:HB2   | 1:D:11:TYR:N    | 2.06                     | 0.70              |
| 1:D:83:LYS:HE2  | 1:D:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:K:9:TYR:HB2   | 1:K:11:TYR:N    | 2.06                     | 0.70              |
| 1:K:29:VAL:CG1  | 1:K:77:LEU:HD11 | 2.20                     | 0.70              |
| 1:N:38:VAL:HA   | 1:N:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:B:83:LYS:HE2  | 1:B:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:F:29:VAL:CG1  | 1:F:77:LEU:HD11 | 2.20                     | 0.70              |
| 1:J:5:ARG:HH22  | 1:J:24:VAL:H    | 1.37                     | 0.70              |
| 1:J:9:TYR:HB2   | 1:J:11:TYR:N    | 2.06                     | 0.70              |
| 1:N:83:LYS:HE2  | 1:N:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:C:38:VAL:HA   | 1:C:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:C:83:LYS:HE2  | 1:C:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:F:9:TYR:HB2   | 1:F:11:TYR:N    | 2.06                     | 0.70              |
| 1:H:9:TYR:HB2   | 1:H:11:TYR:N    | 2.06                     | 0.70              |
| 1:J:49:PHE:HE2  | 1:J:79:ILE:HD11 | 1.55                     | 0.70              |
| 1:D:80:VAL:HG22 | 1:D:88:ILE:CG2  | 2.18                     | 0.70              |
| 1:J:56:THR:N    | 1:J:67:LYS:H    | 1.90                     | 0.70              |
| 1:K:38:VAL:HA   | 1:K:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:K:49:PHE:H    | 1:K:55:ARG:HH12 | 1.37                     | 0.70              |
| 1:L:5:ARG:HH22  | 1:L:24:VAL:H    | 1.37                     | 0.70              |
| 1:A:83:LYS:HE2  | 1:A:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:E:56:THR:N    | 1:E:67:LYS:H    | 1.90                     | 0.70              |
| 1:J:60:LYS:N    | 1:J:64:PHE:HB2  | 2.04                     | 0.70              |
| 1:B:9:TYR:HB2   | 1:B:11:TYR:N    | 2.06                     | 0.70              |
| 1:D:92:PHE:C    | 1:D:93:ILE:HG13 | 2.15                     | 0.70              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:29:VAL:CG1  | 1:H:77:LEU:HD11 | 2.20                     | 0.70              |
| 1:M:5:ARG:HH22  | 1:M:24:VAL:H    | 1.37                     | 0.70              |
| 1:A:56:THR:N    | 1:A:67:LYS:H    | 1.90                     | 0.70              |
| 1:A:80:VAL:HG13 | 1:A:88:ILE:CG2  | 2.18                     | 0.70              |
| 1:E:57:PHE:HB3  | 1:F:103:GLY:CA  | 2.20                     | 0.70              |
| 1:F:56:THR:N    | 1:F:67:LYS:H    | 1.90                     | 0.70              |
| 1:N:9:TYR:HB2   | 1:N:11:TYR:N    | 2.06                     | 0.70              |
| 1:N:49:PHE:HE2  | 1:N:79:ILE:HD11 | 1.55                     | 0.70              |
| 1:A:9:TYR:HB2   | 1:A:11:TYR:N    | 2.06                     | 0.70              |
| 1:D:49:PHE:H    | 1:D:55:ARG:HH12 | 1.37                     | 0.70              |
| 1:D:56:THR:N    | 1:D:67:LYS:H    | 1.90                     | 0.70              |
| 1:E:83:LYS:HE2  | 1:E:109:PHE:HZ  | 1.56                     | 0.70              |
| 1:F:38:VAL:HA   | 1:F:109:PHE:HE2 | 1.55                     | 0.70              |
| 1:G:29:VAL:CG1  | 1:G:77:LEU:HD11 | 2.20                     | 0.70              |
| 1:I:56:THR:N    | 1:I:67:LYS:H    | 1.90                     | 0.70              |
| 1:J:29:VAL:CG1  | 1:J:77:LEU:HD11 | 2.20                     | 0.70              |
| 1:K:5:ARG:HH22  | 1:K:24:VAL:H    | 1.37                     | 0.70              |
| 1:K:56:THR:N    | 1:K:67:LYS:H    | 1.90                     | 0.70              |
| 1:N:56:THR:N    | 1:N:67:LYS:H    | 1.90                     | 0.70              |
| 1:A:49:PHE:H    | 1:A:55:ARG:HH12 | 1.37                     | 0.69              |
| 1:E:9:TYR:HB2   | 1:E:11:TYR:N    | 2.06                     | 0.69              |
| 1:A:60:LYS:N    | 1:A:64:PHE:HB2  | 2.04                     | 0.69              |
| 1:H:82:ASP:O    | 1:H:83:LYS:HB2  | 1.93                     | 0.69              |
| 1:I:29:VAL:CG1  | 1:I:77:LEU:HD11 | 2.20                     | 0.69              |
| 1:N:49:PHE:H    | 1:N:55:ARG:HH12 | 1.37                     | 0.69              |
| 1:H:92:PHE:C    | 1:H:93:ILE:HG13 | 2.15                     | 0.69              |
| 1:I:83:LYS:HE2  | 1:I:109:PHE:HZ  | 1.56                     | 0.69              |
| 1:L:80:VAL:HG22 | 1:L:88:ILE:CG2  | 2.18                     | 0.69              |
| 1:G:82:ASP:O    | 1:G:83:LYS:HB2  | 1.93                     | 0.69              |
| 1:G:92:PHE:C    | 1:G:93:ILE:HG13 | 2.15                     | 0.69              |
| 1:M:55:ARG:HD2  | 1:N:11:TYR:CD2  | 2.27                     | 0.69              |
| 1:B:55:ARG:HD2  | 1:C:11:TYR:CD2  | 2.27                     | 0.69              |
| 1:K:55:ARG:HD2  | 1:L:11:TYR:CD2  | 2.28                     | 0.69              |
| 1:A:55:ARG:HD2  | 1:B:11:TYR:CD2  | 2.28                     | 0.69              |
| 1:B:56:THR:N    | 1:B:67:LYS:H    | 1.90                     | 0.69              |
| 1:G:83:LYS:HE2  | 1:G:109:PHE:HZ  | 1.56                     | 0.69              |
| 1:J:55:ARG:HD2  | 1:K:11:TYR:CD2  | 2.27                     | 0.69              |
| 1:M:56:THR:N    | 1:M:67:LYS:H    | 1.90                     | 0.69              |
| 1:M:9:TYR:HB2   | 1:M:11:TYR:N    | 2.06                     | 0.69              |
| 1:A:103:GLY:CA  | 1:N:57:PHE:HB3  | 2.20                     | 0.69              |
| 1:E:55:ARG:HD2  | 1:F:11:TYR:CD2  | 2.27                     | 0.69              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:56:THR:N    | 1:G:67:LYS:H    | 1.90                     | 0.69              |
| 1:H:56:THR:N    | 1:H:67:LYS:H    | 1.90                     | 0.69              |
| 1:I:92:PHE:C    | 1:I:93:ILE:HG13 | 2.15                     | 0.69              |
| 1:K:83:LYS:HE2  | 1:K:109:PHE:HZ  | 1.56                     | 0.69              |
| 1:L:55:ARG:HD2  | 1:M:11:TYR:CD2  | 2.27                     | 0.69              |
| 1:L:82:ASP:O    | 1:L:83:LYS:HB2  | 1.93                     | 0.69              |
| 1:L:98:LYS:HD3  | 1:L:98:LYS:N    | 2.02                     | 0.69              |
| 1:N:38:VAL:HG12 | 1:N:109:PHE:HD2 | 1.58                     | 0.69              |
| 1:A:11:TYR:CD2  | 1:N:55:ARG:HD2  | 2.27                     | 0.69              |
| 1:C:56:THR:N    | 1:C:67:LYS:H    | 1.90                     | 0.69              |
| 1:D:2:GLU:HG2   | 1:D:3:VAL:N     | 2.08                     | 0.69              |
| 1:E:92:PHE:C    | 1:E:93:ILE:HG13 | 2.15                     | 0.69              |
| 1:G:44:TYR:HB2  | 1:G:45:ILE:O    | 1.93                     | 0.69              |
| 1:I:82:ASP:O    | 1:I:83:LYS:HB2  | 1.93                     | 0.69              |
| 1:K:82:ASP:O    | 1:K:83:LYS:HB2  | 1.93                     | 0.69              |
| 1:C:44:TYR:HB2  | 1:C:45:ILE:O    | 1.93                     | 0.69              |
| 1:E:2:GLU:HG2   | 1:E:3:VAL:N     | 2.08                     | 0.69              |
| 1:H:38:VAL:HG12 | 1:H:109:PHE:HD2 | 1.58                     | 0.69              |
| 1:C:55:ARG:HD2  | 1:D:11:TYR:CD2  | 2.27                     | 0.68              |
| 1:C:92:PHE:C    | 1:C:93:ILE:HG13 | 2.15                     | 0.68              |
| 1:D:38:VAL:HG12 | 1:D:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:D:55:ARG:HD2  | 1:E:11:TYR:CD2  | 2.28                     | 0.68              |
| 1:J:38:VAL:HG12 | 1:J:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:C:2:GLU:HG2   | 1:C:3:VAL:N     | 2.08                     | 0.68              |
| 1:L:56:THR:N    | 1:L:67:LYS:H    | 1.90                     | 0.68              |
| 1:A:84:ARG:NH1  | 1:A:84:ARG:HA   | 2.09                     | 0.68              |
| 1:F:44:TYR:HB2  | 1:F:45:ILE:O    | 1.93                     | 0.68              |
| 1:F:55:ARG:HD2  | 1:G:11:TYR:CD2  | 2.27                     | 0.68              |
| 1:L:88:ILE:HG12 | 1:L:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:M:44:TYR:HB2  | 1:M:45:ILE:O    | 1.93                     | 0.68              |
| 1:M:82:ASP:O    | 1:M:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:N:80:VAL:HG13 | 1:N:88:ILE:CG2  | 2.18                     | 0.68              |
| 1:D:44:TYR:HB2  | 1:D:45:ILE:O    | 1.93                     | 0.68              |
| 1:D:82:ASP:O    | 1:D:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:F:82:ASP:O    | 1:F:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:H:44:TYR:HB2  | 1:H:45:ILE:O    | 1.93                     | 0.68              |
| 1:M:38:VAL:HG12 | 1:M:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:B:44:TYR:HB2  | 1:B:45:ILE:O    | 1.93                     | 0.68              |
| 1:C:38:VAL:HG12 | 1:C:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:E:84:ARG:NH1  | 1:E:84:ARG:HA   | 2.09                     | 0.68              |
| 1:G:60:LYS:N    | 1:G:64:PHE:HB2  | 2.04                     | 0.68              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:55:ARG:HD2  | 1:I:11:TYR:CD2  | 2.28                     | 0.68              |
| 1:I:55:ARG:HD2  | 1:J:11:TYR:CD2  | 2.27                     | 0.68              |
| 1:N:2:GLU:HG2   | 1:N:3:VAL:N     | 2.08                     | 0.68              |
| 1:B:84:ARG:NH1  | 1:B:84:ARG:HA   | 2.09                     | 0.68              |
| 1:C:82:ASP:O    | 1:C:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:C:88:ILE:HG12 | 1:C:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:F:2:GLU:HG2   | 1:F:3:VAL:N     | 2.08                     | 0.68              |
| 1:L:38:VAL:HG12 | 1:L:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:L:44:TYR:HB2  | 1:L:45:ILE:O    | 1.93                     | 0.68              |
| 1:M:2:GLU:HG2   | 1:M:3:VAL:N     | 2.08                     | 0.68              |
| 1:E:44:TYR:HB2  | 1:E:45:ILE:O    | 1.93                     | 0.68              |
| 1:F:38:VAL:HG12 | 1:F:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:F:84:ARG:NH1  | 1:F:84:ARG:HA   | 2.09                     | 0.68              |
| 1:F:88:ILE:HG12 | 1:F:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:I:2:GLU:HG2   | 1:I:3:VAL:N     | 2.08                     | 0.68              |
| 1:J:84:ARG:NH1  | 1:J:84:ARG:HA   | 2.09                     | 0.68              |
| 1:J:88:ILE:HG12 | 1:J:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:C:57:PHE:HB3  | 1:D:103:GLY:CA  | 2.20                     | 0.68              |
| 1:E:82:ASP:O    | 1:E:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:E:88:ILE:HG12 | 1:E:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:G:38:VAL:HG12 | 1:G:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:G:46:THR:HB   | 1:H:13:ILE:CG2  | 2.24                     | 0.68              |
| 1:G:55:ARG:HD2  | 1:H:11:TYR:CD2  | 2.27                     | 0.68              |
| 1:H:46:THR:HB   | 1:I:13:ILE:CG2  | 2.24                     | 0.68              |
| 1:H:84:ARG:HA   | 1:H:84:ARG:NH1  | 2.09                     | 0.68              |
| 1:H:88:ILE:HG12 | 1:H:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:N:44:TYR:HB2  | 1:N:45:ILE:O    | 1.93                     | 0.68              |
| 1:A:38:VAL:HG12 | 1:A:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:F:46:THR:HB   | 1:G:13:ILE:CG2  | 2.24                     | 0.68              |
| 1:H:2:GLU:HG2   | 1:H:3:VAL:N     | 2.08                     | 0.68              |
| 1:I:38:VAL:HG12 | 1:I:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:J:82:ASP:O    | 1:J:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:K:80:VAL:HG13 | 1:K:88:ILE:CG2  | 2.18                     | 0.68              |
| 1:L:57:PHE:HB3  | 1:M:103:GLY:CA  | 2.20                     | 0.68              |
| 1:N:82:ASP:O    | 1:N:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:N:84:ARG:NH1  | 1:N:84:ARG:HA   | 2.09                     | 0.68              |
| 1:N:88:ILE:HG12 | 1:N:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:A:88:ILE:HG12 | 1:A:107:LYS:HB2 | 1.76                     | 0.68              |
| 1:B:60:LYS:N    | 1:B:64:PHE:HB2  | 2.04                     | 0.68              |
| 1:B:82:ASP:O    | 1:B:83:LYS:HB2  | 1.93                     | 0.68              |
| 1:C:80:VAL:H    | 1:C:88:ILE:HG21 | 1.59                     | 0.68              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:38:VAL:HG12 | 1:E:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:K:38:VAL:HG12 | 1:K:109:PHE:HD2 | 1.58                     | 0.68              |
| 1:K:60:LYS:N    | 1:K:64:PHE:HB2  | 2.04                     | 0.68              |
| 1:N:80:VAL:H    | 1:N:88:ILE:HG21 | 1.59                     | 0.68              |
| 1:A:2:GLU:HG2   | 1:A:3:VAL:N     | 2.08                     | 0.67              |
| 1:D:84:ARG:NH1  | 1:D:84:ARG:HA   | 2.09                     | 0.67              |
| 1:I:46:THR:HB   | 1:J:13:ILE:CG2  | 2.24                     | 0.67              |
| 1:J:2:GLU:HG2   | 1:J:3:VAL:N     | 2.08                     | 0.67              |
| 1:K:43:THR:HG22 | 1:K:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:K:44:TYR:HB2  | 1:K:45:ILE:O    | 1.93                     | 0.67              |
| 1:A:82:ASP:O    | 1:A:83:LYS:HB2  | 1.93                     | 0.67              |
| 1:B:2:GLU:HG2   | 1:B:3:VAL:N     | 2.08                     | 0.67              |
| 1:J:80:VAL:H    | 1:J:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:K:80:VAL:H    | 1:K:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:D:88:ILE:HG12 | 1:D:107:LYS:HB2 | 1.76                     | 0.67              |
| 1:E:46:THR:HB   | 1:F:13:ILE:CG2  | 2.24                     | 0.67              |
| 1:H:43:THR:HG22 | 1:H:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:J:44:TYR:HB2  | 1:J:45:ILE:O    | 1.93                     | 0.67              |
| 1:J:46:THR:HB   | 1:K:13:ILE:CG2  | 2.24                     | 0.67              |
| 1:M:80:VAL:H    | 1:M:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:B:80:VAL:H    | 1:B:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:B:92:PHE:C    | 1:B:93:ILE:HG13 | 2.15                     | 0.67              |
| 1:F:43:THR:HG22 | 1:F:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:I:43:THR:HG22 | 1:I:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:J:80:VAL:HG13 | 1:J:88:ILE:CG2  | 2.18                     | 0.67              |
| 1:L:2:GLU:HG2   | 1:L:3:VAL:N     | 2.08                     | 0.67              |
| 1:C:60:LYS:N    | 1:C:64:PHE:HB2  | 2.04                     | 0.67              |
| 1:D:60:LYS:N    | 1:D:64:PHE:HB2  | 2.04                     | 0.67              |
| 1:G:84:ARG:NH1  | 1:G:84:ARG:HA   | 2.09                     | 0.67              |
| 1:I:44:TYR:HB2  | 1:I:45:ILE:O    | 1.93                     | 0.67              |
| 1:I:84:ARG:NH1  | 1:I:84:ARG:HA   | 2.09                     | 0.67              |
| 1:L:43:THR:HG22 | 1:L:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:L:84:ARG:NH1  | 1:L:84:ARG:HA   | 2.09                     | 0.67              |
| 1:A:44:TYR:HB2  | 1:A:45:ILE:O    | 1.93                     | 0.67              |
| 1:A:80:VAL:H    | 1:A:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:G:88:ILE:HG12 | 1:G:107:LYS:HB2 | 1.76                     | 0.67              |
| 1:I:80:VAL:HG13 | 1:I:88:ILE:CG2  | 2.18                     | 0.67              |
| 1:J:57:PHE:HB3  | 1:K:103:GLY:CA  | 2.20                     | 0.67              |
| 1:L:80:VAL:H    | 1:L:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:B:38:VAL:HG12 | 1:B:109:PHE:HD2 | 1.58                     | 0.67              |
| 1:C:29:VAL:HG13 | 1:C:77:LEU:HD21 | 1.77                     | 0.67              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:80:VAL:HG13 | 1:F:88:ILE:CG2  | 2.18                     | 0.67              |
| 1:G:80:VAL:HG13 | 1:G:88:ILE:CG2  | 2.18                     | 0.67              |
| 1:H:36:ILE:CG2  | 1:H:44:TYR:HB3  | 2.25                     | 0.67              |
| 1:I:36:ILE:CG2  | 1:I:44:TYR:HB3  | 2.25                     | 0.67              |
| 1:J:43:THR:HG22 | 1:J:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:K:84:ARG:NH1  | 1:K:84:ARG:HA   | 2.09                     | 0.67              |
| 1:M:43:THR:HG22 | 1:M:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:N:43:THR:HG22 | 1:N:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:D:43:THR:HG22 | 1:D:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:D:46:THR:HB   | 1:E:13:ILE:CG2  | 2.24                     | 0.67              |
| 1:G:43:THR:HG22 | 1:G:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:I:88:ILE:HG12 | 1:I:107:LYS:HB2 | 1.76                     | 0.67              |
| 1:E:43:THR:HG22 | 1:E:45:ILE:HG23 | 1.77                     | 0.67              |
| 1:F:36:ILE:CG2  | 1:F:44:TYR:HB3  | 2.25                     | 0.67              |
| 1:F:80:VAL:H    | 1:F:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:G:2:GLU:HG2   | 1:G:3:VAL:N     | 2.08                     | 0.67              |
| 1:G:36:ILE:CG2  | 1:G:44:TYR:HB3  | 2.25                     | 0.67              |
| 1:G:80:VAL:H    | 1:G:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:H:57:PHE:HB3  | 1:I:103:GLY:CA  | 2.20                     | 0.67              |
| 1:K:46:THR:HB   | 1:L:13:ILE:CG2  | 2.24                     | 0.67              |
| 1:L:38:VAL:HA   | 1:L:109:PHE:CE2 | 2.30                     | 0.67              |
| 1:M:88:ILE:HG12 | 1:M:107:LYS:HB2 | 1.76                     | 0.67              |
| 1:C:84:ARG:NH1  | 1:C:84:ARG:HA   | 2.09                     | 0.67              |
| 1:D:80:VAL:H    | 1:D:88:ILE:HG21 | 1.59                     | 0.67              |
| 1:G:29:VAL:HG13 | 1:G:77:LEU:HD21 | 1.77                     | 0.67              |
| 1:G:38:VAL:HA   | 1:G:109:PHE:CE2 | 2.30                     | 0.67              |
| 1:H:80:VAL:HG13 | 1:H:88:ILE:CG2  | 2.18                     | 0.67              |
| 1:K:88:ILE:HG12 | 1:K:107:LYS:HB2 | 1.76                     | 0.67              |
| 1:M:38:VAL:HA   | 1:M:109:PHE:CE2 | 2.30                     | 0.67              |
| 1:M:84:ARG:NH1  | 1:M:84:ARG:HA   | 2.09                     | 0.67              |
| 1:N:56:THR:H    | 1:N:67:LYS:N    | 1.93                     | 0.67              |
| 1:C:46:THR:HB   | 1:D:13:ILE:CG2  | 2.24                     | 0.66              |
| 1:H:38:VAL:HA   | 1:H:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:J:36:ILE:CG2  | 1:J:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:A:43:THR:HG22 | 1:A:45:ILE:HG23 | 1.77                     | 0.66              |
| 1:B:43:THR:HG22 | 1:B:45:ILE:HG23 | 1.77                     | 0.66              |
| 1:D:29:VAL:HG13 | 1:D:77:LEU:HD21 | 1.77                     | 0.66              |
| 1:E:80:VAL:HG13 | 1:E:88:ILE:CG2  | 2.18                     | 0.66              |
| 1:F:57:PHE:HB3  | 1:G:103:GLY:CA  | 2.20                     | 0.66              |
| 1:A:43:THR:HA   | 1:B:14:LYS:CD   | 2.26                     | 0.66              |
| 1:B:88:ILE:HG12 | 1:B:107:LYS:HB2 | 1.76                     | 0.66              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:56:THR:H    | 1:D:67:LYS:N    | 1.93                     | 0.66              |
| 1:E:36:ILE:CG2  | 1:E:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:E:43:THR:HA   | 1:F:14:LYS:CD   | 2.26                     | 0.66              |
| 1:K:2:GLU:HG2   | 1:K:3:VAL:N     | 2.08                     | 0.66              |
| 1:K:38:VAL:HA   | 1:K:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:L:46:THR:HB   | 1:M:13:ILE:CG2  | 2.24                     | 0.66              |
| 1:M:46:THR:HB   | 1:N:13:ILE:CG2  | 2.24                     | 0.66              |
| 1:A:13:ILE:CG2  | 1:N:46:THR:HB   | 2.24                     | 0.66              |
| 1:B:36:ILE:CG2  | 1:B:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:E:6:ASN:HA    | 1:E:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:K:36:ILE:CG2  | 1:K:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:K:98:LYS:HZ1  | 1:K:102:ASP:HB2 | 1.61                     | 0.66              |
| 1:M:50:GLY:HA2  | 1:M:77:LEU:CD1  | 2.24                     | 0.66              |
| 1:N:50:GLY:HA2  | 1:N:77:LEU:CD1  | 2.24                     | 0.66              |
| 1:A:46:THR:HB   | 1:B:13:ILE:CG2  | 2.24                     | 0.66              |
| 1:A:56:THR:H    | 1:A:67:LYS:N    | 1.93                     | 0.66              |
| 1:B:46:THR:HB   | 1:C:13:ILE:CG2  | 2.24                     | 0.66              |
| 1:C:6:ASN:HA    | 1:C:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:C:38:VAL:HA   | 1:C:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:C:43:THR:HG22 | 1:C:45:ILE:HG23 | 1.77                     | 0.66              |
| 1:C:56:THR:H    | 1:C:67:LYS:N    | 1.93                     | 0.66              |
| 1:D:6:ASN:HA    | 1:D:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:F:29:VAL:HG13 | 1:F:77:LEU:HD21 | 1.77                     | 0.66              |
| 1:F:38:VAL:HA   | 1:F:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:I:80:VAL:H    | 1:I:88:ILE:HG21 | 1.59                     | 0.66              |
| 1:J:56:THR:H    | 1:J:67:LYS:N    | 1.93                     | 0.66              |
| 1:J:98:LYS:HZ1  | 1:J:102:ASP:HB2 | 1.61                     | 0.66              |
| 1:A:26:ILE:HG12 | 1:A:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:B:16:VAL:HG12 | 1:B:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:B:29:VAL:HG13 | 1:B:77:LEU:HD21 | 1.77                     | 0.66              |
| 1:D:43:THR:HA   | 1:E:14:LYS:CD   | 2.26                     | 0.66              |
| 1:E:80:VAL:H    | 1:E:88:ILE:HG21 | 1.59                     | 0.66              |
| 1:I:60:LYS:N    | 1:I:64:PHE:HB2  | 2.04                     | 0.66              |
| 1:L:50:GLY:HA2  | 1:L:77:LEU:CD1  | 2.25                     | 0.66              |
| 1:L:60:LYS:H    | 1:L:64:PHE:CB   | 2.06                     | 0.66              |
| 1:N:26:ILE:HG12 | 1:N:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:N:38:VAL:HA   | 1:N:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:A:14:LYS:CD   | 1:N:43:THR:HA   | 2.26                     | 0.66              |
| 1:A:36:ILE:CG2  | 1:A:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:A:50:GLY:HA2  | 1:A:77:LEU:CD1  | 2.25                     | 0.66              |
| 1:B:38:VAL:HA   | 1:B:109:PHE:CE2 | 2.30                     | 0.66              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:43:THR:HA   | 1:C:14:LYS:CD   | 2.26                     | 0.66              |
| 1:B:98:LYS:HZ1  | 1:B:102:ASP:HB2 | 1.60                     | 0.66              |
| 1:C:16:VAL:HG12 | 1:C:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:D:36:ILE:CG2  | 1:D:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:F:6:ASN:HA    | 1:F:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:I:43:THR:HA   | 1:J:14:LYS:CD   | 2.26                     | 0.66              |
| 1:I:56:THR:H    | 1:I:67:LYS:N    | 1.93                     | 0.66              |
| 1:J:43:THR:HA   | 1:K:14:LYS:CD   | 2.26                     | 0.66              |
| 1:L:98:LYS:HZ1  | 1:L:102:ASP:HB2 | 1.61                     | 0.66              |
| 1:A:16:VAL:HG12 | 1:A:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:B:6:ASN:HA    | 1:B:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:C:36:ILE:CG2  | 1:C:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:E:16:VAL:HG12 | 1:E:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:E:56:THR:H    | 1:E:67:LYS:N    | 1.94                     | 0.66              |
| 1:K:50:GLY:HA2  | 1:K:77:LEU:CD1  | 2.24                     | 0.66              |
| 1:L:16:VAL:HG12 | 1:L:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:L:36:ILE:CG2  | 1:L:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:M:16:VAL:HG12 | 1:M:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:M:26:ILE:HG12 | 1:M:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:M:36:ILE:CG2  | 1:M:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:M:80:VAL:HG13 | 1:M:88:ILE:CG2  | 2.18                     | 0.66              |
| 1:N:16:VAL:HG12 | 1:N:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:A:6:ASN:HA    | 1:A:35:HIS:HB3  | 1.77                     | 0.66              |
| 1:B:50:GLY:HA2  | 1:B:77:LEU:CD1  | 2.24                     | 0.66              |
| 1:D:16:VAL:HG12 | 1:D:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:F:16:VAL:HG12 | 1:F:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:F:26:ILE:HG12 | 1:F:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:F:43:THR:HA   | 1:G:14:LYS:CD   | 2.26                     | 0.66              |
| 1:G:16:VAL:HG12 | 1:G:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:G:26:ILE:HG12 | 1:G:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:H:29:VAL:HG13 | 1:H:77:LEU:HD21 | 1.77                     | 0.66              |
| 1:H:43:THR:HA   | 1:I:14:LYS:CD   | 2.26                     | 0.66              |
| 1:H:60:LYS:N    | 1:H:64:PHE:HB2  | 2.04                     | 0.66              |
| 1:H:80:VAL:H    | 1:H:88:ILE:HG21 | 1.59                     | 0.66              |
| 1:I:38:VAL:HA   | 1:I:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:K:16:VAL:HG12 | 1:K:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:K:43:THR:HA   | 1:L:14:LYS:CD   | 2.26                     | 0.66              |
| 1:B:26:ILE:HG12 | 1:B:37:VAL:HG23 | 1.77                     | 0.66              |
| 1:D:38:VAL:HA   | 1:D:109:PHE:CE2 | 2.30                     | 0.66              |
| 1:H:16:VAL:HG12 | 1:H:18:TYR:CE1  | 2.30                     | 0.66              |
| 1:J:50:GLY:HA2  | 1:J:77:LEU:CD1  | 2.24                     | 0.66              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:N:36:ILE:CG2  | 1:N:44:TYR:HB3  | 2.25                     | 0.66              |
| 1:E:50:GLY:HA2  | 1:E:77:LEU:CD1  | 2.25                     | 0.65              |
| 1:H:26:ILE:HG12 | 1:H:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:I:16:VAL:HG12 | 1:I:18:TYR:CE1  | 2.30                     | 0.65              |
| 1:I:50:GLY:HA2  | 1:I:77:LEU:CD1  | 2.24                     | 0.65              |
| 1:J:16:VAL:HG12 | 1:J:18:TYR:CE1  | 2.30                     | 0.65              |
| 1:J:38:VAL:HA   | 1:J:109:PHE:CE2 | 2.30                     | 0.65              |
| 1:M:98:LYS:HZ1  | 1:M:102:ASP:HB2 | 1.61                     | 0.65              |
| 1:F:50:GLY:HA2  | 1:F:77:LEU:CD1  | 2.24                     | 0.65              |
| 1:G:6:ASN:HA    | 1:G:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:I:26:ILE:HG12 | 1:I:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:K:56:THR:H    | 1:K:67:LYS:N    | 1.93                     | 0.65              |
| 1:L:43:THR:HA   | 1:M:14:LYS:CD   | 2.26                     | 0.65              |
| 1:C:26:ILE:HG12 | 1:C:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:D:80:VAL:HG13 | 1:D:88:ILE:CG2  | 2.18                     | 0.65              |
| 1:H:56:THR:H    | 1:H:67:LYS:N    | 1.93                     | 0.65              |
| 1:I:98:LYS:HZ1  | 1:I:102:ASP:HB2 | 1.60                     | 0.65              |
| 1:J:26:ILE:HG12 | 1:J:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:N:6:ASN:HA    | 1:N:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:C:50:GLY:HA2  | 1:C:77:LEU:CD1  | 2.24                     | 0.65              |
| 1:E:26:ILE:HG12 | 1:E:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:M:6:ASN:HA    | 1:M:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:N:29:VAL:HG13 | 1:N:77:LEU:HD21 | 1.77                     | 0.65              |
| 1:A:38:VAL:HA   | 1:A:109:PHE:CE2 | 2.30                     | 0.65              |
| 1:G:43:THR:HA   | 1:H:14:LYS:CD   | 2.26                     | 0.65              |
| 1:H:6:ASN:HA    | 1:H:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:H:50:GLY:HA2  | 1:H:77:LEU:CD1  | 2.25                     | 0.65              |
| 1:L:6:ASN:HA    | 1:L:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:L:26:ILE:HG12 | 1:L:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:M:29:VAL:HG13 | 1:M:77:LEU:HD21 | 1.77                     | 0.65              |
| 1:A:98:LYS:HZ1  | 1:A:102:ASP:HB2 | 1.61                     | 0.65              |
| 1:D:50:GLY:HA2  | 1:D:77:LEU:CD1  | 2.24                     | 0.65              |
| 1:G:50:GLY:HA2  | 1:G:77:LEU:CD1  | 2.24                     | 0.65              |
| 1:K:29:VAL:HG13 | 1:K:77:LEU:HD21 | 1.77                     | 0.65              |
| 1:C:43:THR:HA   | 1:D:14:LYS:CD   | 2.26                     | 0.65              |
| 1:C:98:LYS:HZ1  | 1:C:102:ASP:HB2 | 1.60                     | 0.65              |
| 1:E:38:VAL:HA   | 1:E:109:PHE:CE2 | 2.30                     | 0.65              |
| 1:F:5:ARG:HB2   | 1:F:36:ILE:HB   | 1.79                     | 0.65              |
| 1:F:56:THR:H    | 1:F:67:LYS:N    | 1.93                     | 0.65              |
| 1:B:56:THR:H    | 1:B:67:LYS:N    | 1.93                     | 0.65              |
| 1:F:35:HIS:HB2  | 1:F:45:ILE:O    | 1.97                     | 0.65              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:5:ARG:HB2   | 1:H:36:ILE:HB   | 1.79                     | 0.65              |
| 1:J:6:ASN:HA    | 1:J:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:K:6:ASN:HA    | 1:K:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:M:43:THR:HA   | 1:N:14:LYS:CD   | 2.26                     | 0.65              |
| 1:C:46:THR:HG1  | 1:D:13:ILE:HG22 | 1.59                     | 0.65              |
| 1:E:5:ARG:HB2   | 1:E:36:ILE:HB   | 1.79                     | 0.65              |
| 1:F:98:LYS:HZ1  | 1:F:102:ASP:HB2 | 1.62                     | 0.65              |
| 1:G:5:ARG:HB2   | 1:G:36:ILE:HB   | 1.79                     | 0.65              |
| 1:G:98:LYS:HZ1  | 1:G:102:ASP:HB2 | 1.61                     | 0.65              |
| 1:I:6:ASN:HA    | 1:I:35:HIS:HB3  | 1.77                     | 0.65              |
| 1:J:35:HIS:HB2  | 1:J:45:ILE:O    | 1.97                     | 0.65              |
| 1:L:29:VAL:HG13 | 1:L:77:LEU:HD21 | 1.77                     | 0.65              |
| 1:D:26:ILE:HG12 | 1:D:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:F:80:VAL:CG2  | 1:F:88:ILE:HG23 | 2.26                     | 0.65              |
| 1:H:35:HIS:HB2  | 1:H:45:ILE:O    | 1.97                     | 0.65              |
| 1:I:5:ARG:HB2   | 1:I:36:ILE:HB   | 1.79                     | 0.65              |
| 1:K:26:ILE:HG12 | 1:K:37:VAL:HG23 | 1.77                     | 0.65              |
| 1:K:35:HIS:HB2  | 1:K:45:ILE:O    | 1.97                     | 0.65              |
| 1:E:29:VAL:HG13 | 1:E:77:LEU:HD21 | 1.77                     | 0.64              |
| 1:E:98:LYS:HZ1  | 1:E:102:ASP:HB2 | 1.61                     | 0.64              |
| 1:L:60:LYS:N    | 1:L:64:PHE:HB2  | 2.04                     | 0.64              |
| 1:A:80:VAL:CG2  | 1:A:88:ILE:HG23 | 2.26                     | 0.64              |
| 1:I:35:HIS:HB2  | 1:I:45:ILE:O    | 1.97                     | 0.64              |
| 1:J:5:ARG:HB2   | 1:J:36:ILE:HB   | 1.79                     | 0.64              |
| 1:A:29:VAL:HG13 | 1:A:77:LEU:HD21 | 1.77                     | 0.64              |
| 1:G:56:THR:H    | 1:G:67:LYS:N    | 1.93                     | 0.64              |
| 1:L:35:HIS:HB2  | 1:L:45:ILE:O    | 1.97                     | 0.64              |
| 1:K:60:LYS:H    | 1:K:64:PHE:CB   | 2.06                     | 0.64              |
| 1:K:80:VAL:CG2  | 1:K:88:ILE:HG23 | 2.26                     | 0.64              |
| 1:D:5:ARG:HB2   | 1:D:36:ILE:HB   | 1.79                     | 0.64              |
| 1:D:35:HIS:HB2  | 1:D:45:ILE:O    | 1.97                     | 0.64              |
| 1:E:12:ARG:HG2  | 1:E:13:ILE:N    | 2.12                     | 0.64              |
| 1:I:29:VAL:HG13 | 1:I:77:LEU:HD21 | 1.77                     | 0.64              |
| 1:M:35:HIS:HB2  | 1:M:45:ILE:O    | 1.97                     | 0.64              |
| 1:J:24:VAL:CG2  | 1:J:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:K:5:ARG:HB2   | 1:K:36:ILE:HB   | 1.79                     | 0.64              |
| 1:L:56:THR:H    | 1:L:67:LYS:N    | 1.94                     | 0.64              |
| 1:A:24:VAL:CG2  | 1:A:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:L:12:ARG:HG2  | 1:L:13:ILE:N    | 2.12                     | 0.64              |
| 1:C:24:VAL:CG2  | 1:C:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:E:24:VAL:CG2  | 1:E:107:LYS:HD3 | 2.28                     | 0.64              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:80:VAL:CG2  | 1:E:88:ILE:HG23 | 2.26                     | 0.64              |
| 1:F:12:ARG:HG2  | 1:F:13:ILE:N    | 2.13                     | 0.64              |
| 1:H:98:LYS:HZ1  | 1:H:102:ASP:HB2 | 1.61                     | 0.64              |
| 1:J:29:VAL:HG13 | 1:J:77:LEU:HD21 | 1.77                     | 0.64              |
| 1:K:12:ARG:HG2  | 1:K:13:ILE:N    | 2.13                     | 0.64              |
| 1:L:24:VAL:CG2  | 1:L:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:M:60:LYS:N    | 1:M:64:PHE:HB2  | 2.04                     | 0.64              |
| 1:D:24:VAL:CG2  | 1:D:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:E:60:LYS:H    | 1:E:64:PHE:CB   | 2.06                     | 0.64              |
| 1:G:35:HIS:HB2  | 1:G:45:ILE:O    | 1.97                     | 0.64              |
| 1:H:46:THR:CB   | 1:I:14:LYS:HZ1  | 2.11                     | 0.64              |
| 1:L:5:ARG:HB2   | 1:L:36:ILE:HB   | 1.79                     | 0.64              |
| 1:N:98:LYS:HZ1  | 1:N:102:ASP:HB2 | 1.61                     | 0.64              |
| 1:C:5:ARG:HB2   | 1:C:36:ILE:HB   | 1.79                     | 0.64              |
| 1:C:80:VAL:HG13 | 1:C:88:ILE:CG2  | 2.18                     | 0.64              |
| 1:D:60:LYS:H    | 1:D:64:PHE:CB   | 2.06                     | 0.64              |
| 1:E:61:MET:HG2  | 1:E:62:ASN:H    | 1.63                     | 0.64              |
| 1:H:24:VAL:CG2  | 1:H:107:LYS:HD3 | 2.28                     | 0.64              |
| 1:N:35:HIS:HB2  | 1:N:45:ILE:O    | 1.97                     | 0.64              |
| 1:A:79:ILE:HG22 | 1:A:81:THR:HG22 | 1.80                     | 0.63              |
| 1:F:60:LYS:H    | 1:F:64:PHE:CB   | 2.05                     | 0.63              |
| 1:N:24:VAL:HG11 | 1:N:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:B:79:ILE:HG22 | 1:B:81:THR:HG22 | 1.80                     | 0.63              |
| 1:C:24:VAL:HG11 | 1:C:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:D:98:LYS:HZ1  | 1:D:102:ASP:HB2 | 1.61                     | 0.63              |
| 1:F:13:ILE:HB   | 1:F:14:LYS:CG   | 2.29                     | 0.63              |
| 1:G:24:VAL:CG2  | 1:G:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:M:24:VAL:CG2  | 1:M:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:M:79:ILE:HG22 | 1:M:81:THR:HG22 | 1.80                     | 0.63              |
| 1:N:12:ARG:HG2  | 1:N:13:ILE:N    | 2.13                     | 0.63              |
| 1:N:79:ILE:HG22 | 1:N:81:THR:HG22 | 1.81                     | 0.63              |
| 1:A:5:ARG:HB2   | 1:A:36:ILE:HB   | 1.79                     | 0.63              |
| 1:A:61:MET:HG2  | 1:A:62:ASN:H    | 1.64                     | 0.63              |
| 1:B:61:MET:HG2  | 1:B:62:ASN:H    | 1.64                     | 0.63              |
| 1:F:24:VAL:CG2  | 1:F:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:I:24:VAL:CG2  | 1:I:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:M:61:MET:HG2  | 1:M:62:ASN:H    | 1.63                     | 0.63              |
| 1:N:61:MET:HG2  | 1:N:62:ASN:H    | 1.64                     | 0.63              |
| 1:A:35:HIS:HB2  | 1:A:45:ILE:O    | 1.97                     | 0.63              |
| 1:B:12:ARG:HG2  | 1:B:13:ILE:N    | 2.13                     | 0.63              |
| 1:C:35:HIS:HB2  | 1:C:45:ILE:O    | 1.97                     | 0.63              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:61:MET:HG2  | 1:F:62:ASN:H    | 1.63                     | 0.63              |
| 1:G:13:ILE:HB   | 1:G:14:LYS:CG   | 2.29                     | 0.63              |
| 1:I:12:ARG:HG2  | 1:I:13:ILE:N    | 2.13                     | 0.63              |
| 1:L:79:ILE:HG22 | 1:L:81:THR:HG22 | 1.80                     | 0.63              |
| 1:M:5:ARG:HB2   | 1:M:36:ILE:HB   | 1.79                     | 0.63              |
| 1:M:24:VAL:HG11 | 1:M:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:B:24:VAL:CG2  | 1:B:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:B:35:HIS:HB2  | 1:B:45:ILE:O    | 1.97                     | 0.63              |
| 1:D:24:VAL:HG11 | 1:D:38:VAL:CG1  | 2.29                     | 0.63              |
| 1:E:13:ILE:HB   | 1:E:14:LYS:CG   | 2.29                     | 0.63              |
| 1:I:61:MET:HG2  | 1:I:62:ASN:H    | 1.64                     | 0.63              |
| 1:L:61:MET:HG2  | 1:L:62:ASN:H    | 1.63                     | 0.63              |
| 1:N:5:ARG:HB2   | 1:N:36:ILE:HB   | 1.79                     | 0.63              |
| 1:B:5:ARG:HB2   | 1:B:36:ILE:HB   | 1.79                     | 0.63              |
| 1:C:60:LYS:H    | 1:C:64:PHE:CB   | 2.05                     | 0.63              |
| 1:E:35:HIS:HB2  | 1:E:45:ILE:O    | 1.97                     | 0.63              |
| 1:K:61:MET:HG2  | 1:K:62:ASN:H    | 1.63                     | 0.63              |
| 1:N:24:VAL:CG2  | 1:N:107:LYS:HD3 | 2.28                     | 0.63              |
| 1:C:79:ILE:HG22 | 1:C:81:THR:HG22 | 1.80                     | 0.63              |
| 1:H:61:MET:HG2  | 1:H:62:ASN:H    | 1.64                     | 0.63              |
| 1:J:24:VAL:HG11 | 1:J:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:M:88:ILE:O    | 1:M:88:ILE:HG13 | 1.99                     | 0.63              |
| 1:B:24:VAL:HG11 | 1:B:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:C:12:ARG:HG2  | 1:C:13:ILE:N    | 2.13                     | 0.63              |
| 1:D:12:ARG:HG2  | 1:D:13:ILE:N    | 2.13                     | 0.63              |
| 1:D:61:MET:HG2  | 1:D:62:ASN:H    | 1.63                     | 0.63              |
| 1:H:13:ILE:HB   | 1:H:14:LYS:CG   | 2.29                     | 0.63              |
| 1:J:61:MET:HG2  | 1:J:62:ASN:H    | 1.64                     | 0.63              |
| 1:A:24:VAL:HG11 | 1:A:38:VAL:CG1  | 2.29                     | 0.63              |
| 1:F:24:VAL:HG11 | 1:F:38:VAL:CG1  | 2.28                     | 0.63              |
| 1:K:13:ILE:HB   | 1:K:14:LYS:CG   | 2.29                     | 0.63              |
| 1:L:13:ILE:HB   | 1:L:14:LYS:CG   | 2.29                     | 0.63              |
| 1:C:61:MET:HG2  | 1:C:62:ASN:H    | 1.64                     | 0.62              |
| 1:G:60:LYS:H    | 1:G:64:PHE:CB   | 2.05                     | 0.62              |
| 1:G:61:MET:HG2  | 1:G:62:ASN:H    | 1.64                     | 0.62              |
| 1:J:80:VAL:CG2  | 1:J:88:ILE:HG23 | 2.26                     | 0.62              |
| 1:K:24:VAL:HG11 | 1:K:38:VAL:CG1  | 2.29                     | 0.62              |
| 1:K:24:VAL:CG2  | 1:K:107:LYS:HD3 | 2.28                     | 0.62              |
| 1:G:24:VAL:HG11 | 1:G:38:VAL:CG1  | 2.28                     | 0.62              |
| 1:H:24:VAL:HG11 | 1:H:38:VAL:CG1  | 2.29                     | 0.62              |
| 1:I:24:VAL:HG11 | 1:I:38:VAL:CG1  | 2.28                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:79:ILE:HG22 | 1:K:81:THR:HG22 | 1.80                     | 0.62              |
| 1:J:88:ILE:HG13 | 1:J:88:ILE:O    | 1.99                     | 0.62              |
| 1:K:88:ILE:O    | 1:K:88:ILE:HG13 | 1.99                     | 0.62              |
| 1:L:80:VAL:HG13 | 1:L:88:ILE:CG2  | 2.18                     | 0.62              |
| 1:M:12:ARG:HG2  | 1:M:13:ILE:N    | 2.13                     | 0.62              |
| 1:N:80:VAL:CG2  | 1:N:88:ILE:HG23 | 2.26                     | 0.62              |
| 1:A:12:ARG:HG2  | 1:A:13:ILE:N    | 2.13                     | 0.62              |
| 1:A:88:ILE:HG13 | 1:A:88:ILE:O    | 1.99                     | 0.62              |
| 1:D:13:ILE:HB   | 1:D:14:LYS:CG   | 2.29                     | 0.62              |
| 1:D:80:VAL:CG2  | 1:D:88:ILE:HG23 | 2.26                     | 0.62              |
| 1:E:24:VAL:HG11 | 1:E:38:VAL:CG1  | 2.29                     | 0.62              |
| 1:J:5:ARG:N     | 1:J:36:ILE:HB   | 2.13                     | 0.62              |
| 1:J:12:ARG:HG2  | 1:J:13:ILE:N    | 2.13                     | 0.62              |
| 1:J:13:ILE:HB   | 1:J:14:LYS:CG   | 2.29                     | 0.62              |
| 1:J:60:LYS:H    | 1:J:64:PHE:CB   | 2.05                     | 0.62              |
| 1:A:60:LYS:H    | 1:A:64:PHE:CB   | 2.06                     | 0.62              |
| 1:B:13:ILE:HB   | 1:B:14:LYS:CG   | 2.29                     | 0.62              |
| 1:B:60:LYS:H    | 1:B:64:PHE:CB   | 2.06                     | 0.62              |
| 1:D:79:ILE:HG22 | 1:D:81:THR:HG22 | 1.80                     | 0.62              |
| 1:G:12:ARG:HG2  | 1:G:13:ILE:N    | 2.13                     | 0.62              |
| 1:J:79:ILE:HG22 | 1:J:81:THR:HG22 | 1.80                     | 0.62              |
| 1:I:13:ILE:HB   | 1:I:14:LYS:CG   | 2.29                     | 0.62              |
| 1:M:67:LYS:HE3  | 1:M:78:VAL:CG1  | 2.30                     | 0.62              |
| 1:N:67:LYS:HE3  | 1:N:78:VAL:CG1  | 2.30                     | 0.62              |
| 1:A:13:ILE:HB   | 1:A:14:LYS:CG   | 2.29                     | 0.62              |
| 1:A:67:LYS:HE3  | 1:A:78:VAL:CG1  | 2.30                     | 0.62              |
| 1:M:56:THR:H    | 1:M:67:LYS:N    | 1.93                     | 0.62              |
| 1:N:60:LYS:H    | 1:N:64:PHE:CB   | 2.05                     | 0.62              |
| 1:H:88:ILE:O    | 1:H:88:ILE:HG13 | 1.99                     | 0.62              |
| 1:I:79:ILE:HG22 | 1:I:81:THR:HG22 | 1.80                     | 0.62              |
| 1:L:88:ILE:HG13 | 1:L:88:ILE:O    | 1.99                     | 0.62              |
| 1:M:13:ILE:HB   | 1:M:14:LYS:CG   | 2.29                     | 0.62              |
| 1:B:67:LYS:HE3  | 1:B:78:VAL:CG1  | 2.30                     | 0.62              |
| 1:H:5:ARG:N     | 1:H:36:ILE:HB   | 2.13                     | 0.62              |
| 1:I:5:ARG:N     | 1:I:36:ILE:HB   | 2.13                     | 0.62              |
| 1:K:5:ARG:N     | 1:K:36:ILE:HB   | 2.13                     | 0.62              |
| 1:L:24:VAL:HG11 | 1:L:38:VAL:CG1  | 2.29                     | 0.62              |
| 1:E:54:SER:C    | 1:E:55:ARG:HG2  | 2.25                     | 0.62              |
| 1:I:54:SER:C    | 1:I:55:ARG:HG2  | 2.25                     | 0.62              |
| 1:L:5:ARG:N     | 1:L:36:ILE:HB   | 2.13                     | 0.62              |
| 1:B:32:VAL:CG2  | 1:B:48:ALA:HB3  | 2.30                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:13:ILE:HB   | 1:C:14:LYS:CG   | 2.29                     | 0.61              |
| 1:C:54:SER:C    | 1:C:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:D:32:VAL:CG2  | 1:D:48:ALA:HB3  | 2.30                     | 0.61              |
| 1:E:79:ILE:HG22 | 1:E:81:THR:HG22 | 1.80                     | 0.61              |
| 1:G:17:VAL:O    | 1:G:18:TYR:HD1  | 1.83                     | 0.61              |
| 1:G:54:SER:C    | 1:G:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:H:12:ARG:HG2  | 1:H:13:ILE:N    | 2.13                     | 0.61              |
| 1:H:79:ILE:HG22 | 1:H:81:THR:HG22 | 1.80                     | 0.61              |
| 1:B:80:VAL:HG13 | 1:B:88:ILE:CG2  | 2.18                     | 0.61              |
| 1:C:67:LYS:HE3  | 1:C:78:VAL:CG1  | 2.30                     | 0.61              |
| 1:D:88:ILE:HG13 | 1:D:88:ILE:O    | 1.99                     | 0.61              |
| 1:F:79:ILE:HG22 | 1:F:81:THR:HG22 | 1.80                     | 0.61              |
| 1:H:67:LYS:HE3  | 1:H:78:VAL:CG1  | 2.30                     | 0.61              |
| 1:D:98:LYS:HE3  | 1:D:101:ALA:H   | 1.66                     | 0.61              |
| 1:F:17:VAL:O    | 1:F:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:K:17:VAL:O    | 1:K:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:K:54:SER:C    | 1:K:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:L:17:VAL:O    | 1:L:18:TYR:HD1  | 1.83                     | 0.61              |
| 1:M:60:LYS:H    | 1:M:64:PHE:CB   | 2.05                     | 0.61              |
| 1:N:54:SER:C    | 1:N:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:D:17:VAL:O    | 1:D:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:G:79:ILE:HG22 | 1:G:81:THR:HG22 | 1.81                     | 0.61              |
| 1:H:17:VAL:O    | 1:H:18:TYR:HD1  | 1.83                     | 0.61              |
| 1:H:60:LYS:H    | 1:H:64:PHE:CB   | 2.06                     | 0.61              |
| 1:I:88:ILE:HG13 | 1:I:88:ILE:O    | 1.99                     | 0.61              |
| 1:J:17:VAL:O    | 1:J:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:M:54:SER:C    | 1:M:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:N:13:ILE:HB   | 1:N:14:LYS:CG   | 2.29                     | 0.61              |
| 1:B:17:VAL:O    | 1:B:18:TYR:HD1  | 1.83                     | 0.61              |
| 1:B:98:LYS:HE3  | 1:B:101:ALA:H   | 1.66                     | 0.61              |
| 1:C:17:VAL:O    | 1:C:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:J:26:ILE:CG1  | 1:J:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:K:46:THR:HG1  | 1:L:13:ILE:HG22 | 1.62                     | 0.61              |
| 1:L:98:LYS:HE3  | 1:L:101:ALA:H   | 1.66                     | 0.61              |
| 1:M:17:VAL:O    | 1:M:18:TYR:HD1  | 1.84                     | 0.61              |
| 1:M:46:THR:CB   | 1:N:14:LYS:HZ1  | 2.12                     | 0.61              |
| 1:A:17:VAL:O    | 1:A:18:TYR:HD1  | 1.83                     | 0.61              |
| 1:A:26:ILE:CG1  | 1:A:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:B:26:ILE:CG1  | 1:B:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:C:26:ILE:CG1  | 1:C:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:D:67:LYS:HE3  | 1:D:78:VAL:CG1  | 2.30                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:5:ARG:N     | 1:G:36:ILE:HB   | 2.13                     | 0.61              |
| 1:K:26:ILE:CG1  | 1:K:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:L:26:ILE:CG1  | 1:L:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:M:26:ILE:CG1  | 1:M:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:N:26:ILE:CG1  | 1:N:37:VAL:HG23 | 2.30                     | 0.61              |
| 1:N:98:LYS:HE3  | 1:N:101:ALA:H   | 1.66                     | 0.61              |
| 1:B:88:ILE:O    | 1:B:88:ILE:HG13 | 1.99                     | 0.61              |
| 1:F:88:ILE:HG13 | 1:F:88:ILE:O    | 1.99                     | 0.61              |
| 1:H:26:ILE:CG1  | 1:H:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:I:26:ILE:CG1  | 1:I:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:I:46:THR:HG1  | 1:J:13:ILE:HG22 | 1.64                     | 0.61              |
| 1:D:26:ILE:CG1  | 1:D:37:VAL:HG23 | 2.31                     | 0.61              |
| 1:I:80:VAL:CG2  | 1:I:88:ILE:HG23 | 2.26                     | 0.61              |
| 1:J:54:SER:C    | 1:J:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:M:73:SER:HB2  | 1:M:94:GLY:HA2  | 1.83                     | 0.61              |
| 1:N:88:ILE:O    | 1:N:88:ILE:HG13 | 1.99                     | 0.61              |
| 1:A:73:SER:HB2  | 1:A:94:GLY:HA2  | 1.83                     | 0.61              |
| 1:G:88:ILE:HG13 | 1:G:88:ILE:O    | 1.99                     | 0.61              |
| 1:I:67:LYS:HE3  | 1:I:78:VAL:CG1  | 2.30                     | 0.61              |
| 1:I:98:LYS:HE3  | 1:I:101:ALA:H   | 1.66                     | 0.61              |
| 1:L:54:SER:C    | 1:L:55:ARG:HG2  | 2.25                     | 0.61              |
| 1:N:73:SER:HB2  | 1:N:94:GLY:HA2  | 1.83                     | 0.61              |
| 1:C:88:ILE:O    | 1:C:88:ILE:HG13 | 1.99                     | 0.60              |
| 1:F:98:LYS:HE3  | 1:F:101:ALA:H   | 1.66                     | 0.60              |
| 1:G:26:ILE:CG1  | 1:G:37:VAL:HG23 | 2.30                     | 0.60              |
| 1:I:43:THR:CG2  | 1:I:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:A:54:SER:C    | 1:A:55:ARG:HG2  | 2.25                     | 0.60              |
| 1:E:26:ILE:CG1  | 1:E:37:VAL:HG23 | 2.31                     | 0.60              |
| 1:E:32:VAL:CG2  | 1:E:48:ALA:HB3  | 2.30                     | 0.60              |
| 1:M:5:ARG:N     | 1:M:36:ILE:HB   | 2.13                     | 0.60              |
| 1:C:32:VAL:CG2  | 1:C:48:ALA:HB3  | 2.30                     | 0.60              |
| 1:E:17:VAL:O    | 1:E:18:TYR:HD1  | 1.83                     | 0.60              |
| 1:E:88:ILE:O    | 1:E:88:ILE:HG13 | 1.99                     | 0.60              |
| 1:F:54:SER:C    | 1:F:55:ARG:HG2  | 2.25                     | 0.60              |
| 1:G:98:LYS:HE3  | 1:G:101:ALA:H   | 1.66                     | 0.60              |
| 1:K:98:LYS:HE3  | 1:K:101:ALA:H   | 1.66                     | 0.60              |
| 1:L:73:SER:HB2  | 1:L:94:GLY:HA2  | 1.83                     | 0.60              |
| 1:A:32:VAL:CG2  | 1:A:48:ALA:HB3  | 2.30                     | 0.60              |
| 1:B:73:SER:HB2  | 1:B:94:GLY:HA2  | 1.83                     | 0.60              |
| 1:D:2:GLU:HG2   | 1:D:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:F:5:ARG:N     | 1:F:36:ILE:HB   | 2.13                     | 0.60              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:17:VAL:O    | 1:I:18:TYR:HD1  | 1.83                     | 0.60              |
| 1:N:5:ARG:N     | 1:N:36:ILE:HB   | 2.13                     | 0.60              |
| 1:C:2:GLU:HG2   | 1:C:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:E:2:GLU:HG2   | 1:E:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:F:26:ILE:CG1  | 1:F:37:VAL:HG23 | 2.31                     | 0.60              |
| 1:G:67:LYS:HE3  | 1:G:78:VAL:CG1  | 2.30                     | 0.60              |
| 1:I:60:LYS:H    | 1:I:64:PHE:CB   | 2.06                     | 0.60              |
| 1:J:43:THR:CG2  | 1:J:45:ILE:HG23 | 2.32                     | 0.60              |
| 1:L:2:GLU:HG2   | 1:L:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:M:2:GLU:HG2   | 1:M:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:N:2:GLU:HG2   | 1:N:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:A:2:GLU:HG2   | 1:A:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:B:2:GLU:HG2   | 1:B:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:E:29:VAL:HG12 | 1:E:92:PHE:CE2  | 2.37                     | 0.60              |
| 1:E:67:LYS:HE3  | 1:E:78:VAL:CG1  | 2.30                     | 0.60              |
| 1:F:43:THR:CG2  | 1:F:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:G:2:GLU:HG2   | 1:G:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:J:98:LYS:HE3  | 1:J:101:ALA:H   | 1.66                     | 0.60              |
| 1:M:43:THR:CG2  | 1:M:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:C:73:SER:HB2  | 1:C:94:GLY:HA2  | 1.83                     | 0.60              |
| 1:E:43:THR:CG2  | 1:E:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:E:98:LYS:HE3  | 1:E:101:ALA:H   | 1.66                     | 0.60              |
| 1:K:32:VAL:CG2  | 1:K:48:ALA:HB3  | 2.30                     | 0.60              |
| 1:K:73:SER:HB2  | 1:K:94:GLY:HA2  | 1.83                     | 0.60              |
| 1:L:43:THR:CG2  | 1:L:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:D:29:VAL:HG12 | 1:D:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:F:2:GLU:HG2   | 1:F:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:H:43:THR:CG2  | 1:H:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:H:98:LYS:HE3  | 1:H:101:ALA:H   | 1.66                     | 0.60              |
| 1:J:29:VAL:HG12 | 1:J:92:PHE:CE2  | 2.37                     | 0.60              |
| 1:J:32:VAL:CG2  | 1:J:48:ALA:HB3  | 2.30                     | 0.60              |
| 1:K:29:VAL:HG12 | 1:K:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:A:29:VAL:HG12 | 1:A:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:A:98:LYS:HE3  | 1:A:101:ALA:H   | 1.66                     | 0.60              |
| 1:B:29:VAL:HG12 | 1:B:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:C:80:VAL:CG2  | 1:C:88:ILE:HG23 | 2.26                     | 0.60              |
| 1:D:54:SER:C    | 1:D:55:ARG:HG2  | 2.25                     | 0.60              |
| 1:D:73:SER:HB2  | 1:D:94:GLY:HA2  | 1.83                     | 0.60              |
| 1:E:5:ARG:N     | 1:E:36:ILE:HB   | 2.13                     | 0.60              |
| 1:H:29:VAL:HG12 | 1:H:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:J:2:GLU:HG2   | 1:J:3:VAL:HG22  | 1.84                     | 0.60              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:29:VAL:HG12 | 1:M:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:A:43:THR:CG2  | 1:A:45:ILE:HG23 | 2.31                     | 0.60              |
| 1:C:29:VAL:HG12 | 1:C:92:PHE:CE2  | 2.37                     | 0.60              |
| 1:I:2:GLU:HG2   | 1:I:3:VAL:HG22  | 1.84                     | 0.60              |
| 1:N:29:VAL:HG12 | 1:N:92:PHE:CE2  | 2.36                     | 0.60              |
| 1:N:43:THR:CG2  | 1:N:45:ILE:HG23 | 2.32                     | 0.60              |
| 1:C:98:LYS:HE3  | 1:C:101:ALA:H   | 1.66                     | 0.59              |
| 1:G:46:THR:CB   | 1:H:14:LYS:HZ1  | 2.13                     | 0.59              |
| 1:H:2:GLU:HG2   | 1:H:3:VAL:HG22  | 1.84                     | 0.59              |
| 1:K:2:GLU:HG2   | 1:K:3:VAL:HG22  | 1.84                     | 0.59              |
| 1:L:29:VAL:HG12 | 1:L:92:PHE:CE2  | 2.37                     | 0.59              |
| 1:L:67:LYS:HE3  | 1:L:78:VAL:CG1  | 2.30                     | 0.59              |
| 1:B:92:PHE:HB3  | 1:B:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:D:43:THR:CG2  | 1:D:45:ILE:HG23 | 2.31                     | 0.59              |
| 1:H:54:SER:C    | 1:H:55:ARG:HG2  | 2.25                     | 0.59              |
| 1:I:29:VAL:HG12 | 1:I:92:PHE:CE2  | 2.36                     | 0.59              |
| 1:J:67:LYS:HE3  | 1:J:78:VAL:CG1  | 2.30                     | 0.59              |
| 1:K:67:LYS:HE3  | 1:K:78:VAL:CG1  | 2.30                     | 0.59              |
| 1:M:80:VAL:CG2  | 1:M:88:ILE:HG23 | 2.26                     | 0.59              |
| 1:B:43:THR:CG2  | 1:B:45:ILE:HG23 | 2.31                     | 0.59              |
| 1:F:29:VAL:HG12 | 1:F:92:PHE:CE2  | 2.36                     | 0.59              |
| 1:F:67:LYS:HE3  | 1:F:78:VAL:CG1  | 2.30                     | 0.59              |
| 1:G:43:THR:CG2  | 1:G:45:ILE:HG23 | 2.32                     | 0.59              |
| 1:M:98:LYS:HE3  | 1:M:101:ALA:H   | 1.66                     | 0.59              |
| 1:C:92:PHE:HB3  | 1:C:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:E:73:SER:HB2  | 1:E:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:G:29:VAL:HG12 | 1:G:92:PHE:CE2  | 2.36                     | 0.59              |
| 1:J:73:SER:HB2  | 1:J:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:M:32:VAL:CG2  | 1:M:48:ALA:HB3  | 2.31                     | 0.59              |
| 1:A:13:ILE:CD1  | 1:A:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:A:92:PHE:HB3  | 1:A:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:B:13:ILE:CD1  | 1:B:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:C:13:ILE:CD1  | 1:C:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:D:92:PHE:HB3  | 1:D:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:G:73:SER:HB2  | 1:G:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:H:73:SER:HB2  | 1:H:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:D:13:ILE:CD1  | 1:D:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:E:92:PHE:HB3  | 1:E:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:F:73:SER:HB2  | 1:F:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:F:92:PHE:HB3  | 1:F:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:G:32:VAL:CG2  | 1:G:48:ALA:HB3  | 2.30                     | 0.59              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:32:VAL:CG2  | 1:H:48:ALA:HB3  | 2.30                     | 0.59              |
| 1:H:80:VAL:CG2  | 1:H:88:ILE:HG23 | 2.26                     | 0.59              |
| 1:K:43:THR:CG2  | 1:K:45:ILE:HG23 | 2.31                     | 0.59              |
| 1:N:17:VAL:O    | 1:N:18:TYR:HD1  | 1.83                     | 0.59              |
| 1:B:54:SER:C    | 1:B:55:ARG:HG2  | 2.25                     | 0.59              |
| 1:C:46:THR:CB   | 1:D:14:LYS:HZ1  | 2.15                     | 0.59              |
| 1:E:80:VAL:H    | 1:E:88:ILE:CG2  | 2.16                     | 0.59              |
| 1:N:13:ILE:CD1  | 1:N:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:N:92:PHE:HB3  | 1:N:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:G:92:PHE:HB3  | 1:G:101:ALA:HB1 | 1.84                     | 0.59              |
| 1:A:14:LYS:HZ1  | 1:N:46:THR:CB   | 2.15                     | 0.59              |
| 1:E:13:ILE:CD1  | 1:E:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:E:32:VAL:HG13 | 1:E:32:VAL:O    | 2.03                     | 0.59              |
| 1:I:73:SER:HB2  | 1:I:94:GLY:HA2  | 1.83                     | 0.59              |
| 1:J:32:VAL:HG13 | 1:J:32:VAL:O    | 2.03                     | 0.59              |
| 1:L:32:VAL:CG2  | 1:L:48:ALA:HB3  | 2.30                     | 0.59              |
| 1:B:5:ARG:N     | 1:B:36:ILE:HB   | 2.13                     | 0.59              |
| 1:C:5:ARG:N     | 1:C:36:ILE:HB   | 2.13                     | 0.59              |
| 1:C:43:THR:CG2  | 1:C:45:ILE:HG23 | 2.32                     | 0.59              |
| 1:F:80:VAL:H    | 1:F:88:ILE:CG2  | 2.16                     | 0.59              |
| 1:I:32:VAL:CG2  | 1:I:48:ALA:HB3  | 2.30                     | 0.59              |
| 1:L:32:VAL:HG13 | 1:L:32:VAL:O    | 2.03                     | 0.59              |
| 1:M:13:ILE:CD1  | 1:M:14:LYS:HG3  | 2.33                     | 0.59              |
| 1:I:46:THR:CB   | 1:J:14:LYS:HZ1  | 2.13                     | 0.58              |
| 1:I:80:VAL:H    | 1:I:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:A:32:VAL:O    | 1:A:32:VAL:HG13 | 2.03                     | 0.58              |
| 1:F:32:VAL:O    | 1:F:32:VAL:HG13 | 2.03                     | 0.58              |
| 1:G:39:ALA:HB1  | 1:G:40:PRO:HA   | 1.85                     | 0.58              |
| 1:A:5:ARG:N     | 1:A:36:ILE:HB   | 2.13                     | 0.58              |
| 1:F:13:ILE:CD1  | 1:F:14:LYS:HG3  | 2.33                     | 0.58              |
| 1:F:56:THR:HG22 | 1:F:57:PHE:N    | 2.18                     | 0.58              |
| 1:H:92:PHE:HB3  | 1:H:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:M:92:PHE:HB3  | 1:M:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:B:46:THR:CB   | 1:C:14:LYS:NZ   | 2.66                     | 0.58              |
| 1:F:39:ALA:HB1  | 1:F:40:PRO:HA   | 1.85                     | 0.58              |
| 1:H:80:VAL:H    | 1:H:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:B:80:VAL:H    | 1:B:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:E:56:THR:HG22 | 1:E:57:PHE:N    | 2.18                     | 0.58              |
| 1:F:32:VAL:CG2  | 1:F:48:ALA:HB3  | 2.31                     | 0.58              |
| 1:G:32:VAL:HG13 | 1:G:32:VAL:O    | 2.03                     | 0.58              |
| 1:H:32:VAL:O    | 1:H:32:VAL:HG13 | 2.03                     | 0.58              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:95:GLU:HG2  | 1:J:95:GLU:O    | 2.04                     | 0.58              |
| 1:L:56:THR:HG22 | 1:L:57:PHE:N    | 2.18                     | 0.58              |
| 1:M:56:THR:HG22 | 1:M:57:PHE:N    | 2.18                     | 0.58              |
| 1:H:39:ALA:HB1  | 1:H:40:PRO:HA   | 1.85                     | 0.58              |
| 1:I:32:VAL:O    | 1:I:32:VAL:HG13 | 2.03                     | 0.58              |
| 1:I:39:ALA:HB1  | 1:I:40:PRO:HA   | 1.85                     | 0.58              |
| 1:I:92:PHE:HB3  | 1:I:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:L:13:ILE:CD1  | 1:L:14:LYS:HG3  | 2.33                     | 0.58              |
| 1:L:80:VAL:CG2  | 1:L:88:ILE:HG23 | 2.26                     | 0.58              |
| 1:L:95:GLU:HG2  | 1:L:95:GLU:O    | 2.04                     | 0.58              |
| 1:D:37:VAL:HG12 | 1:D:38:VAL:N    | 2.19                     | 0.58              |
| 1:D:80:VAL:H    | 1:D:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:G:46:THR:CB   | 1:H:14:LYS:NZ   | 2.66                     | 0.58              |
| 1:K:56:THR:HG22 | 1:K:57:PHE:N    | 2.18                     | 0.58              |
| 1:N:32:VAL:CG2  | 1:N:48:ALA:HB3  | 2.30                     | 0.58              |
| 1:A:80:VAL:H    | 1:A:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:A:95:GLU:HG2  | 1:A:95:GLU:O    | 2.04                     | 0.58              |
| 1:D:5:ARG:N     | 1:D:36:ILE:HB   | 2.13                     | 0.58              |
| 1:E:37:VAL:HG12 | 1:E:38:VAL:N    | 2.19                     | 0.58              |
| 1:G:56:THR:HG22 | 1:G:57:PHE:N    | 2.18                     | 0.58              |
| 1:H:46:THR:CB   | 1:I:14:LYS:NZ   | 2.66                     | 0.58              |
| 1:J:80:VAL:H    | 1:J:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:N:56:THR:HG22 | 1:N:57:PHE:N    | 2.18                     | 0.58              |
| 1:C:80:VAL:H    | 1:C:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:D:32:VAL:HG13 | 1:D:32:VAL:O    | 2.03                     | 0.58              |
| 1:G:13:ILE:CD1  | 1:G:14:LYS:HG3  | 2.33                     | 0.58              |
| 1:I:46:THR:CB   | 1:J:14:LYS:NZ   | 2.66                     | 0.58              |
| 1:J:92:PHE:HB3  | 1:J:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:K:92:PHE:HB3  | 1:K:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:L:92:PHE:HB3  | 1:L:101:ALA:HB1 | 1.84                     | 0.58              |
| 1:M:54:SER:OG   | 1:M:68:PRO:HA   | 2.04                     | 0.58              |
| 1:N:37:VAL:HG12 | 1:N:38:VAL:N    | 2.19                     | 0.58              |
| 1:N:54:SER:OG   | 1:N:68:PRO:HA   | 2.04                     | 0.58              |
| 1:G:80:VAL:H    | 1:G:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:J:37:VAL:HG12 | 1:J:38:VAL:N    | 2.19                     | 0.58              |
| 1:J:56:THR:HG22 | 1:J:57:PHE:N    | 2.18                     | 0.58              |
| 1:K:16:VAL:HG12 | 1:K:18:TYR:HE1  | 1.69                     | 0.58              |
| 1:M:80:VAL:H    | 1:M:88:ILE:CG2  | 2.16                     | 0.58              |
| 1:A:38:VAL:HG23 | 1:A:39:ALA:N    | 2.19                     | 0.57              |
| 1:C:79:ILE:HG22 | 1:C:81:THR:CG2  | 2.34                     | 0.57              |
| 1:F:16:VAL:HG12 | 1:F:18:TYR:HE1  | 1.69                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:37:VAL:HG12 | 1:G:38:VAL:N    | 2.19                     | 0.57              |
| 1:H:9:TYR:HB2   | 1:H:11:TYR:CA   | 2.34                     | 0.57              |
| 1:I:95:GLU:HG2  | 1:I:95:GLU:O    | 2.04                     | 0.57              |
| 1:J:46:THR:CB   | 1:K:14:LYS:NZ   | 2.66                     | 0.57              |
| 1:J:54:SER:OG   | 1:J:68:PRO:HA   | 2.04                     | 0.57              |
| 1:J:79:ILE:HG22 | 1:J:81:THR:CG2  | 2.34                     | 0.57              |
| 1:K:13:ILE:CD1  | 1:K:14:LYS:HG3  | 2.33                     | 0.57              |
| 1:K:32:VAL:O    | 1:K:32:VAL:HG13 | 2.03                     | 0.57              |
| 1:K:79:ILE:HG22 | 1:K:81:THR:CG2  | 2.34                     | 0.57              |
| 1:L:37:VAL:HG12 | 1:L:38:VAL:N    | 2.19                     | 0.57              |
| 1:L:80:VAL:H    | 1:L:88:ILE:CG2  | 2.16                     | 0.57              |
| 1:M:95:GLU:O    | 1:M:95:GLU:HG2  | 2.04                     | 0.57              |
| 1:N:79:ILE:HG22 | 1:N:81:THR:CG2  | 2.34                     | 0.57              |
| 1:A:37:VAL:HG12 | 1:A:38:VAL:N    | 2.19                     | 0.57              |
| 1:B:38:VAL:HG23 | 1:B:39:ALA:N    | 2.19                     | 0.57              |
| 1:C:37:VAL:HG12 | 1:C:38:VAL:N    | 2.19                     | 0.57              |
| 1:D:39:ALA:HB1  | 1:D:40:PRO:HA   | 1.85                     | 0.57              |
| 1:D:79:ILE:HG22 | 1:D:81:THR:CG2  | 2.34                     | 0.57              |
| 1:E:39:ALA:HB1  | 1:E:40:PRO:HA   | 1.85                     | 0.57              |
| 1:F:9:TYR:HB2   | 1:F:11:TYR:CA   | 2.34                     | 0.57              |
| 1:F:54:SER:OG   | 1:F:68:PRO:HA   | 2.04                     | 0.57              |
| 1:H:13:ILE:CD1  | 1:H:14:LYS:HG3  | 2.33                     | 0.57              |
| 1:I:9:TYR:HB2   | 1:I:11:TYR:CA   | 2.35                     | 0.57              |
| 1:I:66:VAL:HG23 | 1:I:67:LYS:N    | 2.19                     | 0.57              |
| 1:J:9:TYR:HB2   | 1:J:11:TYR:CA   | 2.35                     | 0.57              |
| 1:M:32:VAL:HG13 | 1:M:32:VAL:O    | 2.03                     | 0.57              |
| 1:N:80:VAL:H    | 1:N:88:ILE:CG2  | 2.16                     | 0.57              |
| 1:A:56:THR:HG22 | 1:A:57:PHE:N    | 2.18                     | 0.57              |
| 1:A:62:ASN:HB2  | 1:A:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:A:79:ILE:HG22 | 1:A:81:THR:CG2  | 2.34                     | 0.57              |
| 1:C:62:ASN:CB   | 1:C:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:E:24:VAL:HG12 | 1:E:26:ILE:HD12 | 1.86                     | 0.57              |
| 1:E:54:SER:OG   | 1:E:68:PRO:HA   | 2.04                     | 0.57              |
| 1:E:79:ILE:HG22 | 1:E:81:THR:CG2  | 2.34                     | 0.57              |
| 1:G:9:TYR:HB2   | 1:G:11:TYR:CA   | 2.35                     | 0.57              |
| 1:G:24:VAL:HG12 | 1:G:26:ILE:HD12 | 1.86                     | 0.57              |
| 1:G:95:GLU:HG2  | 1:G:95:GLU:O    | 2.04                     | 0.57              |
| 1:I:37:VAL:HG12 | 1:I:38:VAL:N    | 2.19                     | 0.57              |
| 1:J:39:ALA:HB1  | 1:J:40:PRO:HA   | 1.85                     | 0.57              |
| 1:L:16:VAL:HG12 | 1:L:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:M:39:ALA:HB1  | 1:M:40:PRO:HA   | 1.85                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:N:39:ALA:HB1  | 1:N:40:PRO:HA   | 1.85                     | 0.57              |
| 1:A:9:TYR:HB2   | 1:A:11:TYR:CA   | 2.34                     | 0.57              |
| 1:B:62:ASN:HB2  | 1:B:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:D:54:SER:OG   | 1:D:68:PRO:HA   | 2.04                     | 0.57              |
| 1:E:9:TYR:HB2   | 1:E:11:TYR:CA   | 2.34                     | 0.57              |
| 1:E:16:VAL:HG12 | 1:E:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:G:54:SER:OG   | 1:G:68:PRO:HA   | 2.04                     | 0.57              |
| 1:G:80:VAL:CG2  | 1:G:88:ILE:HG23 | 2.26                     | 0.57              |
| 1:H:37:VAL:HG12 | 1:H:38:VAL:N    | 2.19                     | 0.57              |
| 1:K:46:THR:CB   | 1:L:14:LYS:NZ   | 2.66                     | 0.57              |
| 1:M:62:ASN:CB   | 1:M:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:N:24:VAL:HG11 | 1:N:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:N:32:VAL:O    | 1:N:32:VAL:HG13 | 2.03                     | 0.57              |
| 1:N:38:VAL:HG23 | 1:N:39:ALA:N    | 2.19                     | 0.57              |
| 1:A:46:THR:CB   | 1:B:14:LYS:NZ   | 2.66                     | 0.57              |
| 1:B:62:ASN:CB   | 1:B:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:B:80:VAL:CG2  | 1:B:88:ILE:HG23 | 2.26                     | 0.57              |
| 1:C:62:ASN:HB2  | 1:C:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:F:24:VAL:HG11 | 1:F:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:H:66:VAL:HG23 | 1:H:67:LYS:N    | 2.19                     | 0.57              |
| 1:I:54:SER:OG   | 1:I:68:PRO:HA   | 2.04                     | 0.57              |
| 1:I:79:ILE:HG22 | 1:I:81:THR:CG2  | 2.34                     | 0.57              |
| 1:L:39:ALA:HB1  | 1:L:40:PRO:HA   | 1.85                     | 0.57              |
| 1:M:37:VAL:HG12 | 1:M:38:VAL:N    | 2.19                     | 0.57              |
| 1:N:62:ASN:CB   | 1:N:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:A:39:ALA:HB1  | 1:A:40:PRO:HA   | 1.85                     | 0.57              |
| 1:B:9:TYR:HB2   | 1:B:11:TYR:CA   | 2.35                     | 0.57              |
| 1:B:24:VAL:HG11 | 1:B:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:C:38:VAL:HG23 | 1:C:39:ALA:N    | 2.20                     | 0.57              |
| 1:C:54:SER:OG   | 1:C:68:PRO:HA   | 2.04                     | 0.57              |
| 1:D:24:VAL:HG11 | 1:D:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:E:62:ASN:HB2  | 1:E:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:I:13:ILE:CD1  | 1:I:14:LYS:HG3  | 2.33                     | 0.57              |
| 1:J:16:VAL:HG12 | 1:J:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:J:61:MET:CG   | 1:J:62:ASN:H    | 2.18                     | 0.57              |
| 1:L:62:ASN:HB2  | 1:L:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:M:79:ILE:HG22 | 1:M:81:THR:CG2  | 2.34                     | 0.57              |
| 1:N:9:TYR:HB2   | 1:N:11:TYR:CA   | 2.35                     | 0.57              |
| 1:N:62:ASN:HB2  | 1:N:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:N:95:GLU:O    | 1:N:95:GLU:HG2  | 2.04                     | 0.57              |
| 1:B:37:VAL:HG12 | 1:B:38:VAL:N    | 2.19                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:61:MET:CG   | 1:B:62:ASN:H    | 2.18                     | 0.57              |
| 1:D:9:TYR:HB2   | 1:D:11:TYR:CA   | 2.34                     | 0.57              |
| 1:D:79:ILE:HD12 | 1:D:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:E:79:ILE:HD12 | 1:E:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:G:16:VAL:HG12 | 1:G:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:K:39:ALA:HB1  | 1:K:40:PRO:HA   | 1.85                     | 0.57              |
| 1:K:54:SER:OG   | 1:K:68:PRO:HA   | 2.04                     | 0.57              |
| 1:L:24:VAL:HG11 | 1:L:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:L:79:ILE:HD12 | 1:L:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:M:61:MET:CG   | 1:M:62:ASN:H    | 2.18                     | 0.57              |
| 1:M:62:ASN:HB2  | 1:M:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:N:79:ILE:HD12 | 1:N:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:D:62:ASN:CB   | 1:D:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:D:62:ASN:HB2  | 1:D:84:ARG:HG3  | 1.86                     | 0.57              |
| 1:E:24:VAL:HG11 | 1:E:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:F:38:VAL:HG23 | 1:F:39:ALA:N    | 2.19                     | 0.57              |
| 1:F:46:THR:CB   | 1:G:14:LYS:NZ   | 2.66                     | 0.57              |
| 1:F:79:ILE:HG22 | 1:F:81:THR:CG2  | 2.34                     | 0.57              |
| 1:H:54:SER:OG   | 1:H:68:PRO:HA   | 2.04                     | 0.57              |
| 1:I:61:MET:CG   | 1:I:62:ASN:H    | 2.18                     | 0.57              |
| 1:J:13:ILE:CD1  | 1:J:14:LYS:HG3  | 2.33                     | 0.57              |
| 1:K:9:TYR:HB2   | 1:K:11:TYR:CA   | 2.34                     | 0.57              |
| 1:K:38:VAL:HG23 | 1:K:39:ALA:N    | 2.19                     | 0.57              |
| 1:L:54:SER:OG   | 1:L:68:PRO:HA   | 2.04                     | 0.57              |
| 1:A:16:VAL:HG12 | 1:A:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:B:16:VAL:HG12 | 1:B:18:TYR:HE1  | 1.69                     | 0.57              |
| 1:B:56:THR:HG22 | 1:B:57:PHE:N    | 2.18                     | 0.57              |
| 1:C:79:ILE:HD12 | 1:C:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:D:95:GLU:HG2  | 1:D:95:GLU:O    | 2.04                     | 0.57              |
| 1:F:37:VAL:HG12 | 1:F:38:VAL:N    | 2.19                     | 0.57              |
| 1:F:46:THR:CB   | 1:G:14:LYS:HZ1  | 2.17                     | 0.57              |
| 1:G:66:VAL:HG23 | 1:G:67:LYS:N    | 2.19                     | 0.57              |
| 1:J:79:ILE:HD12 | 1:J:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:K:80:VAL:H    | 1:K:88:ILE:CG2  | 2.16                     | 0.57              |
| 1:L:62:ASN:CB   | 1:L:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:M:9:TYR:HB2   | 1:M:11:TYR:CA   | 2.34                     | 0.57              |
| 1:A:24:VAL:HG11 | 1:A:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:A:79:ILE:HD12 | 1:A:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:B:79:ILE:HD12 | 1:B:107:LYS:NZ  | 2.20                     | 0.57              |
| 1:C:9:TYR:HB2   | 1:C:11:TYR:CA   | 2.35                     | 0.57              |
| 1:C:61:MET:CG   | 1:C:62:ASN:H    | 2.18                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:24:VAL:HG11 | 1:G:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:H:38:VAL:HG23 | 1:H:39:ALA:N    | 2.19                     | 0.57              |
| 1:H:62:ASN:CB   | 1:H:84:ARG:HG3  | 2.35                     | 0.57              |
| 1:H:80:VAL:HG23 | 1:H:86:TYR:CD2  | 2.40                     | 0.57              |
| 1:H:95:GLU:O    | 1:H:95:GLU:HG2  | 2.04                     | 0.57              |
| 1:I:24:VAL:HG11 | 1:I:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:I:80:VAL:HG23 | 1:I:86:TYR:CD2  | 2.40                     | 0.57              |
| 1:J:80:VAL:HG23 | 1:J:86:TYR:CD2  | 2.40                     | 0.57              |
| 1:K:24:VAL:HG11 | 1:K:38:VAL:HG11 | 1.87                     | 0.57              |
| 1:L:46:THR:CB   | 1:M:14:LYS:NZ   | 2.66                     | 0.57              |
| 1:A:54:SER:OG   | 1:A:68:PRO:HA   | 2.04                     | 0.56              |
| 1:A:66:VAL:HG23 | 1:A:67:LYS:N    | 2.19                     | 0.56              |
| 1:B:32:VAL:HG13 | 1:B:32:VAL:O    | 2.03                     | 0.56              |
| 1:F:61:MET:CG   | 1:F:62:ASN:H    | 2.18                     | 0.56              |
| 1:G:62:ASN:CB   | 1:G:84:ARG:HG3  | 2.35                     | 0.56              |
| 1:H:24:VAL:HG11 | 1:H:38:VAL:HG11 | 1.87                     | 0.56              |
| 1:H:79:ILE:HG22 | 1:H:81:THR:CG2  | 2.34                     | 0.56              |
| 1:I:62:ASN:CB   | 1:I:84:ARG:HG3  | 2.35                     | 0.56              |
| 1:J:38:VAL:HG23 | 1:J:39:ALA:N    | 2.20                     | 0.56              |
| 1:J:81:THR:HG23 | 1:J:81:THR:O    | 2.06                     | 0.56              |
| 1:K:80:VAL:HG23 | 1:K:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:L:79:ILE:HG22 | 1:L:81:THR:CG2  | 2.34                     | 0.56              |
| 1:M:38:VAL:HG23 | 1:M:39:ALA:N    | 2.19                     | 0.56              |
| 1:A:80:VAL:HG23 | 1:A:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:B:39:ALA:HB1  | 1:B:40:PRO:HA   | 1.85                     | 0.56              |
| 1:B:54:SER:OG   | 1:B:68:PRO:HA   | 2.04                     | 0.56              |
| 1:B:79:ILE:HG22 | 1:B:81:THR:CG2  | 2.34                     | 0.56              |
| 1:B:95:GLU:HG2  | 1:B:95:GLU:O    | 2.04                     | 0.56              |
| 1:C:95:GLU:O    | 1:C:95:GLU:HG2  | 2.04                     | 0.56              |
| 1:D:80:VAL:HG23 | 1:D:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:E:38:VAL:HG23 | 1:E:39:ALA:N    | 2.20                     | 0.56              |
| 1:G:38:VAL:HG23 | 1:G:39:ALA:N    | 2.19                     | 0.56              |
| 1:G:80:VAL:HG23 | 1:G:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:J:62:ASN:HB2  | 1:J:84:ARG:HG3  | 1.86                     | 0.56              |
| 1:L:80:VAL:HG23 | 1:L:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:M:24:VAL:HG11 | 1:M:38:VAL:HG11 | 1.87                     | 0.56              |
| 1:M:79:ILE:HD12 | 1:M:107:LYS:NZ  | 2.20                     | 0.56              |
| 1:B:66:VAL:HG23 | 1:B:67:LYS:N    | 2.19                     | 0.56              |
| 1:C:24:VAL:HG11 | 1:C:38:VAL:HG11 | 1.87                     | 0.56              |
| 1:C:32:VAL:O    | 1:C:32:VAL:HG13 | 2.03                     | 0.56              |
| 1:C:39:ALA:HB1  | 1:C:40:PRO:HA   | 1.85                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:56:THR:HG22 | 1:C:57:PHE:N    | 2.18                     | 0.56              |
| 1:D:38:VAL:HG12 | 1:D:109:PHE:CD2 | 2.41                     | 0.56              |
| 1:D:38:VAL:HG23 | 1:D:39:ALA:N    | 2.19                     | 0.56              |
| 1:E:80:VAL:HG23 | 1:E:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:F:62:ASN:CB   | 1:F:84:ARG:HG3  | 2.35                     | 0.56              |
| 1:F:66:VAL:HG23 | 1:F:67:LYS:N    | 2.19                     | 0.56              |
| 1:F:95:GLU:O    | 1:F:95:GLU:HG2  | 2.04                     | 0.56              |
| 1:G:56:THR:OG1  | 1:G:67:LYS:HB2  | 2.06                     | 0.56              |
| 1:G:61:MET:CG   | 1:G:62:ASN:H    | 2.18                     | 0.56              |
| 1:G:62:ASN:HB2  | 1:G:84:ARG:HG3  | 1.86                     | 0.56              |
| 1:G:79:ILE:HD12 | 1:G:107:LYS:NZ  | 2.20                     | 0.56              |
| 1:G:81:THR:HG23 | 1:G:81:THR:O    | 2.05                     | 0.56              |
| 1:I:79:ILE:HD12 | 1:I:107:LYS:NZ  | 2.20                     | 0.56              |
| 1:J:24:VAL:HG11 | 1:J:38:VAL:HG11 | 1.87                     | 0.56              |
| 1:J:46:THR:CB   | 1:K:14:LYS:HZ1  | 2.16                     | 0.56              |
| 1:K:37:VAL:HG12 | 1:K:38:VAL:N    | 2.19                     | 0.56              |
| 1:K:79:ILE:HD12 | 1:K:107:LYS:NZ  | 2.20                     | 0.56              |
| 1:K:95:GLU:O    | 1:K:95:GLU:HG2  | 2.04                     | 0.56              |
| 1:N:38:VAL:HG12 | 1:N:109:PHE:CD2 | 2.41                     | 0.56              |
| 1:N:61:MET:CG   | 1:N:62:ASN:H    | 2.18                     | 0.56              |
| 1:A:62:ASN:CB   | 1:A:84:ARG:HG3  | 2.35                     | 0.56              |
| 1:D:56:THR:OG1  | 1:D:67:LYS:HB2  | 2.06                     | 0.56              |
| 1:E:61:MET:CG   | 1:E:62:ASN:H    | 2.18                     | 0.56              |
| 1:E:66:VAL:HG23 | 1:E:67:LYS:N    | 2.19                     | 0.56              |
| 1:H:81:THR:HG23 | 1:H:81:THR:O    | 2.05                     | 0.56              |
| 1:I:56:THR:OG1  | 1:I:67:LYS:HB2  | 2.06                     | 0.56              |
| 1:J:62:ASN:CB   | 1:J:84:ARG:HG3  | 2.35                     | 0.56              |
| 1:K:61:MET:CG   | 1:K:62:ASN:H    | 2.18                     | 0.56              |
| 1:L:9:TYR:HB2   | 1:L:11:TYR:CA   | 2.34                     | 0.56              |
| 1:M:80:VAL:HG23 | 1:M:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:M:81:THR:HG23 | 1:M:81:THR:O    | 2.06                     | 0.56              |
| 1:N:80:VAL:HG23 | 1:N:86:TYR:CD2  | 2.40                     | 0.56              |
| 1:B:38:VAL:HG12 | 1:B:109:PHE:CD2 | 2.41                     | 0.56              |
| 1:C:66:VAL:HG23 | 1:C:67:LYS:N    | 2.19                     | 0.56              |
| 1:D:66:VAL:HG23 | 1:D:67:LYS:N    | 2.19                     | 0.56              |
| 1:G:79:ILE:HG22 | 1:G:81:THR:CG2  | 2.34                     | 0.56              |
| 1:L:24:VAL:HG12 | 1:L:26:ILE:HD12 | 1.86                     | 0.56              |
| 1:L:38:VAL:HG23 | 1:L:39:ALA:N    | 2.20                     | 0.56              |
| 1:L:81:THR:O    | 1:L:81:THR:HG23 | 2.06                     | 0.56              |
| 1:C:16:VAL:HG12 | 1:C:18:TYR:HE1  | 1.69                     | 0.56              |
| 1:E:46:THR:CB   | 1:F:14:LYS:NZ   | 2.66                     | 0.56              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:80:VAL:HG23 | 1:F:86:TYR:CD2   | 2.40                     | 0.56              |
| 1:G:91:HIS:CB   | 1:G:104:THR:HG21 | 2.33                     | 0.56              |
| 1:H:79:ILE:HD12 | 1:H:107:LYS:NZ   | 2.20                     | 0.56              |
| 1:I:16:VAL:HG12 | 1:I:18:TYR:HE1   | 1.69                     | 0.56              |
| 1:J:56:THR:OG1  | 1:J:67:LYS:HB2   | 2.06                     | 0.56              |
| 1:L:56:THR:OG1  | 1:L:67:LYS:HB2   | 2.06                     | 0.56              |
| 1:M:16:VAL:HG12 | 1:M:18:TYR:HE1   | 1.69                     | 0.56              |
| 1:C:80:VAL:HG23 | 1:C:86:TYR:CD2   | 2.40                     | 0.56              |
| 1:H:91:HIS:CB   | 1:H:104:THR:HG21 | 2.32                     | 0.56              |
| 1:K:46:THR:CB   | 1:L:14:LYS:HZ1   | 2.16                     | 0.56              |
| 1:B:80:VAL:HG23 | 1:B:86:TYR:CD2   | 2.40                     | 0.56              |
| 1:D:16:VAL:HG12 | 1:D:18:TYR:HE1   | 1.69                     | 0.56              |
| 1:D:56:THR:HG22 | 1:D:57:PHE:N     | 2.18                     | 0.56              |
| 1:E:95:GLU:O    | 1:E:95:GLU:HG2   | 2.04                     | 0.56              |
| 1:F:70:GLN:H    | 1:F:75:THR:HB    | 1.70                     | 0.56              |
| 1:F:91:HIS:CB   | 1:F:104:THR:HG21 | 2.32                     | 0.56              |
| 1:H:24:VAL:HG21 | 1:H:107:LYS:HB3  | 1.88                     | 0.56              |
| 1:C:46:THR:CB   | 1:D:14:LYS:NZ    | 2.66                     | 0.56              |
| 1:D:61:MET:CG   | 1:D:62:ASN:H     | 2.18                     | 0.56              |
| 1:E:62:ASN:CB   | 1:E:84:ARG:HG3   | 2.35                     | 0.56              |
| 1:F:79:ILE:HD12 | 1:F:107:LYS:NZ   | 2.20                     | 0.56              |
| 1:H:16:VAL:HG12 | 1:H:18:TYR:HE1   | 1.69                     | 0.56              |
| 1:J:24:VAL:HG21 | 1:J:107:LYS:HB3  | 1.88                     | 0.56              |
| 1:L:38:VAL:HG12 | 1:L:109:PHE:CD2  | 2.41                     | 0.56              |
| 1:L:70:GLN:H    | 1:L:75:THR:HB    | 1.70                     | 0.56              |
| 1:N:16:VAL:HG12 | 1:N:18:TYR:HE1   | 1.69                     | 0.56              |
| 1:F:24:VAL:HG21 | 1:F:107:LYS:HB3  | 1.88                     | 0.56              |
| 1:F:56:THR:OG1  | 1:F:67:LYS:HB2   | 2.06                     | 0.56              |
| 1:I:38:VAL:HG23 | 1:I:39:ALA:N     | 2.19                     | 0.56              |
| 1:I:81:THR:HG23 | 1:I:81:THR:O     | 2.05                     | 0.56              |
| 1:K:62:ASN:CB   | 1:K:84:ARG:HG3   | 2.35                     | 0.56              |
| 1:L:24:VAL:HG21 | 1:L:107:LYS:HB3  | 1.88                     | 0.56              |
| 1:M:46:THR:CB   | 1:N:14:LYS:NZ    | 2.66                     | 0.56              |
| 1:N:66:VAL:HG23 | 1:N:67:LYS:N     | 2.19                     | 0.56              |
| 1:A:81:THR:O    | 1:A:81:THR:HG23  | 2.05                     | 0.55              |
| 1:E:56:THR:OG1  | 1:E:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:F:84:ARG:HA   | 1:F:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:G:70:GLN:H    | 1:G:75:THR:HB    | 1.71                     | 0.55              |
| 1:H:61:MET:CG   | 1:H:62:ASN:H     | 2.18                     | 0.55              |
| 1:I:91:HIS:CB   | 1:I:104:THR:HG21 | 2.32                     | 0.55              |
| 1:K:70:GLN:H    | 1:K:75:THR:HB    | 1.70                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:M:24:VAL:HG12 | 1:M:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:M:24:VAL:HG21 | 1:M:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:M:70:GLN:H    | 1:M:75:THR:HB    | 1.70                     | 0.55              |
| 1:A:14:LYS:NZ   | 1:N:46:THR:CB    | 2.66                     | 0.55              |
| 1:A:24:VAL:HG21 | 1:A:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:A:56:THR:OG1  | 1:A:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:D:84:ARG:HA   | 1:D:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:E:81:THR:HG23 | 1:E:81:THR:O     | 2.06                     | 0.55              |
| 1:K:24:VAL:HG21 | 1:K:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:K:81:THR:HG23 | 1:K:81:THR:O     | 2.06                     | 0.55              |
| 1:A:24:VAL:HG12 | 1:A:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:B:84:ARG:HA   | 1:B:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:C:81:THR:HG23 | 1:C:81:THR:O     | 2.06                     | 0.55              |
| 1:H:62:ASN:HB2  | 1:H:84:ARG:HG3   | 1.86                     | 0.55              |
| 1:H:84:ARG:HA   | 1:H:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:I:24:VAL:HG21 | 1:I:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:B:81:THR:HG23 | 1:B:81:THR:O     | 2.05                     | 0.55              |
| 1:E:70:GLN:H    | 1:E:75:THR:HB    | 1.70                     | 0.55              |
| 1:G:38:VAL:HG12 | 1:G:109:PHE:CD2  | 2.41                     | 0.55              |
| 1:G:84:ARG:HA   | 1:G:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:H:56:THR:OG1  | 1:H:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:I:6:ASN:HA    | 1:I:35:HIS:CB    | 2.37                     | 0.55              |
| 1:I:62:ASN:HB2  | 1:I:84:ARG:HG3   | 1.86                     | 0.55              |
| 1:I:84:ARG:HA   | 1:I:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:K:24:VAL:HG12 | 1:K:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:B:56:THR:OG1  | 1:B:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:D:81:THR:O    | 1:D:81:THR:HG23  | 2.06                     | 0.55              |
| 1:E:91:HIS:CB   | 1:E:104:THR:HG21 | 2.32                     | 0.55              |
| 1:H:6:ASN:HA    | 1:H:35:HIS:CB    | 2.37                     | 0.55              |
| 1:N:24:VAL:HG21 | 1:N:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:A:70:GLN:H    | 1:A:75:THR:HB    | 1.70                     | 0.55              |
| 1:E:2:GLU:HG2   | 1:E:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:K:26:ILE:HD11 | 1:K:37:VAL:CB    | 2.34                     | 0.55              |
| 1:K:56:THR:OG1  | 1:K:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:L:2:GLU:HG2   | 1:L:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:M:56:THR:OG1  | 1:M:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:N:70:GLN:H    | 1:N:75:THR:HB    | 1.71                     | 0.55              |
| 1:N:84:ARG:HA   | 1:N:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:A:84:ARG:HA   | 1:A:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:B:24:VAL:HG12 | 1:B:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:B:70:GLN:H    | 1:B:75:THR:HB    | 1.70                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:56:THR:OG1  | 1:C:67:LYS:HB2   | 2.06                     | 0.55              |
| 1:F:24:VAL:HG12 | 1:F:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:F:62:ASN:HB2  | 1:F:84:ARG:HG3   | 1.86                     | 0.55              |
| 1:G:24:VAL:HG21 | 1:G:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:L:6:ASN:HA    | 1:L:35:HIS:CB    | 2.37                     | 0.55              |
| 1:A:61:MET:CG   | 1:A:62:ASN:H     | 2.18                     | 0.55              |
| 1:C:24:VAL:HG21 | 1:C:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:C:26:ILE:HD11 | 1:C:37:VAL:CB    | 2.34                     | 0.55              |
| 1:D:2:GLU:HG2   | 1:D:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:D:24:VAL:HG21 | 1:D:107:LYS:HB3  | 1.88                     | 0.55              |
| 1:D:24:VAL:HG12 | 1:D:26:ILE:HD12  | 1.86                     | 0.55              |
| 1:E:6:ASN:HA    | 1:E:35:HIS:CB    | 2.37                     | 0.55              |
| 1:H:70:GLN:H    | 1:H:75:THR:HB    | 1.70                     | 0.55              |
| 1:J:70:GLN:H    | 1:J:75:THR:HB    | 1.70                     | 0.55              |
| 1:K:62:ASN:HB2  | 1:K:84:ARG:HG3   | 1.86                     | 0.55              |
| 1:D:46:THR:CB   | 1:E:14:LYS:NZ    | 2.66                     | 0.55              |
| 1:I:2:GLU:HG2   | 1:I:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:J:66:VAL:HG23 | 1:J:67:LYS:N     | 2.19                     | 0.55              |
| 1:K:2:GLU:HG2   | 1:K:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:K:66:VAL:HG23 | 1:K:67:LYS:N     | 2.19                     | 0.55              |
| 1:K:84:ARG:HA   | 1:K:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:L:46:THR:CB   | 1:M:14:LYS:HZ1   | 2.19                     | 0.55              |
| 1:L:84:ARG:HA   | 1:L:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:M:2:GLU:HG2   | 1:M:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:M:84:ARG:HA   | 1:M:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:C:84:ARG:HA   | 1:C:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:E:84:ARG:HA   | 1:E:84:ARG:CZ    | 2.36                     | 0.55              |
| 1:G:2:GLU:HG2   | 1:G:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:H:2:GLU:HG2   | 1:H:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:I:70:GLN:H    | 1:I:75:THR:HB    | 1.70                     | 0.55              |
| 1:J:2:GLU:HG2   | 1:J:3:VAL:CG2    | 2.37                     | 0.55              |
| 1:J:91:HIS:CB   | 1:J:104:THR:HG21 | 2.32                     | 0.55              |
| 1:C:70:GLN:H    | 1:C:75:THR:HB    | 1.70                     | 0.54              |
| 1:D:6:ASN:HA    | 1:D:35:HIS:CB    | 2.37                     | 0.54              |
| 1:M:6:ASN:HA    | 1:M:35:HIS:CB    | 2.37                     | 0.54              |
| 1:N:24:VAL:HG12 | 1:N:26:ILE:HD12  | 1.86                     | 0.54              |
| 1:N:56:THR:OG1  | 1:N:67:LYS:HB2   | 2.06                     | 0.54              |
| 1:E:38:VAL:HG12 | 1:E:109:PHE:CD2  | 2.41                     | 0.54              |
| 1:F:26:ILE:HD11 | 1:F:37:VAL:CB    | 2.34                     | 0.54              |
| 1:F:81:THR:HG23 | 1:F:81:THR:O     | 2.06                     | 0.54              |
| 1:H:24:VAL:HG12 | 1:H:26:ILE:HD12  | 1.86                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:6:ASN:HA    | 1:J:35:HIS:CB    | 2.37                     | 0.54              |
| 1:K:6:ASN:HA    | 1:K:35:HIS:CB    | 2.37                     | 0.54              |
| 1:L:26:ILE:HD11 | 1:L:37:VAL:CB    | 2.34                     | 0.54              |
| 1:M:66:VAL:HG23 | 1:M:67:LYS:N     | 2.19                     | 0.54              |
| 1:N:81:THR:HG23 | 1:N:81:THR:O     | 2.05                     | 0.54              |
| 1:A:24:VAL:HG21 | 1:A:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:D:91:HIS:CB   | 1:D:104:THR:HG21 | 2.32                     | 0.54              |
| 1:E:26:ILE:HD11 | 1:E:37:VAL:CB    | 2.34                     | 0.54              |
| 1:F:6:ASN:HA    | 1:F:35:HIS:CB    | 2.37                     | 0.54              |
| 1:J:38:VAL:HG12 | 1:J:109:PHE:CD2  | 2.41                     | 0.54              |
| 1:L:66:VAL:HB   | 1:M:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:A:66:VAL:HB   | 1:B:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:C:2:GLU:HG2   | 1:C:3:VAL:CG2    | 2.37                     | 0.54              |
| 1:F:2:GLU:HG2   | 1:F:3:VAL:CG2    | 2.37                     | 0.54              |
| 1:G:6:ASN:HA    | 1:G:35:HIS:CB    | 2.37                     | 0.54              |
| 1:D:26:ILE:HD11 | 1:D:37:VAL:CB    | 2.34                     | 0.54              |
| 1:G:26:ILE:HD11 | 1:G:37:VAL:CB    | 2.35                     | 0.54              |
| 1:H:24:VAL:HG21 | 1:H:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:J:24:VAL:HG21 | 1:J:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:N:2:GLU:HG2   | 1:N:3:VAL:CG2    | 2.37                     | 0.54              |
| 1:D:66:VAL:HB   | 1:E:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:E:24:VAL:HG21 | 1:E:107:LYS:HB3  | 1.88                     | 0.54              |
| 1:K:91:HIS:CB   | 1:K:104:THR:HG21 | 2.32                     | 0.54              |
| 1:L:66:VAL:HG23 | 1:L:67:LYS:N     | 2.19                     | 0.54              |
| 1:M:24:VAL:HG21 | 1:M:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:B:2:GLU:HG2   | 1:B:3:VAL:CG2    | 2.37                     | 0.54              |
| 1:C:24:VAL:HG21 | 1:C:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:C:38:VAL:HG12 | 1:C:109:PHE:CD2  | 2.41                     | 0.54              |
| 1:G:24:VAL:HG21 | 1:G:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:H:26:ILE:HD11 | 1:H:37:VAL:CB    | 2.34                     | 0.54              |
| 1:B:6:ASN:HA    | 1:B:35:HIS:CB    | 2.37                     | 0.54              |
| 1:E:24:VAL:HG21 | 1:E:107:LYS:HD3  | 1.90                     | 0.54              |
| 1:J:84:ARG:HA   | 1:J:84:ARG:CZ    | 2.36                     | 0.54              |
| 1:K:66:VAL:HB   | 1:L:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:N:6:ASN:HA    | 1:N:35:HIS:CB    | 2.37                     | 0.54              |
| 1:A:2:GLU:HG2   | 1:A:3:VAL:CG2    | 2.37                     | 0.54              |
| 1:A:38:VAL:HG12 | 1:A:109:PHE:CD2  | 2.41                     | 0.54              |
| 1:B:24:VAL:HG21 | 1:B:107:LYS:HB3  | 1.88                     | 0.54              |
| 1:E:66:VAL:HB   | 1:F:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:H:66:VAL:HB   | 1:I:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:L:24:VAL:HG21 | 1:L:107:LYS:HD3  | 1.90                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:46:THR:CB   | 1:F:14:LYS:HZ1   | 2.20                     | 0.54              |
| 1:E:90:LEU:HB2  | 1:E:105:VAL:CG2  | 2.38                     | 0.54              |
| 1:F:50:GLY:HA3  | 1:F:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:F:78:VAL:O    | 1:F:79:ILE:HD13  | 2.08                     | 0.54              |
| 1:I:66:VAL:HB   | 1:J:12:ARG:HH12  | 1.73                     | 0.54              |
| 1:B:66:VAL:HB   | 1:C:12:ARG:HH12  | 1.73                     | 0.53              |
| 1:D:26:ILE:CD1  | 1:D:37:VAL:HB    | 2.37                     | 0.53              |
| 1:D:70:GLN:H    | 1:D:75:THR:HB    | 1.70                     | 0.53              |
| 1:D:78:VAL:O    | 1:D:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:E:78:VAL:O    | 1:E:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:F:24:VAL:HG21 | 1:F:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:G:50:GLY:HA3  | 1:G:77:LEU:HD13  | 1.90                     | 0.53              |
| 1:I:26:ILE:HD11 | 1:I:37:VAL:CB    | 2.34                     | 0.53              |
| 1:A:12:ARG:HH12 | 1:N:66:VAL:HB    | 1.73                     | 0.53              |
| 1:B:24:VAL:HG21 | 1:B:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:C:91:HIS:CB   | 1:C:104:THR:HG21 | 2.32                     | 0.53              |
| 1:D:24:VAL:HG21 | 1:D:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:D:79:ILE:C    | 1:D:81:THR:H     | 2.17                     | 0.53              |
| 1:H:90:LEU:HB2  | 1:H:105:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:29:VAL:HG13 | 1:A:77:LEU:HD11  | 1.90                     | 0.53              |
| 1:C:24:VAL:HG12 | 1:C:26:ILE:HD12  | 1.86                     | 0.53              |
| 1:E:79:ILE:C    | 1:E:81:THR:H     | 2.17                     | 0.53              |
| 1:I:24:VAL:HG21 | 1:I:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:L:91:HIS:CB   | 1:L:104:THR:HG21 | 2.32                     | 0.53              |
| 1:M:26:ILE:HD11 | 1:M:37:VAL:CB    | 2.34                     | 0.53              |
| 1:M:79:ILE:C    | 1:M:81:THR:H     | 2.17                     | 0.53              |
| 1:B:26:ILE:HD11 | 1:B:37:VAL:CB    | 2.34                     | 0.53              |
| 1:H:50:GLY:HA3  | 1:H:77:LEU:HD13  | 1.91                     | 0.53              |
| 1:I:79:ILE:C    | 1:I:81:THR:H     | 2.17                     | 0.53              |
| 1:J:26:ILE:HD11 | 1:J:37:VAL:CB    | 2.34                     | 0.53              |
| 1:M:38:VAL:HG12 | 1:M:109:PHE:CD2  | 2.41                     | 0.53              |
| 1:C:66:VAL:HB   | 1:D:12:ARG:HH12  | 1.73                     | 0.53              |
| 1:C:78:VAL:O    | 1:C:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:C:79:ILE:C    | 1:C:81:THR:H     | 2.17                     | 0.53              |
| 1:F:79:ILE:C    | 1:F:81:THR:H     | 2.17                     | 0.53              |
| 1:G:78:VAL:O    | 1:G:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:K:24:VAL:HG21 | 1:K:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:L:79:ILE:C    | 1:L:81:THR:H     | 2.17                     | 0.53              |
| 1:M:66:VAL:HB   | 1:N:12:ARG:HH12  | 1.73                     | 0.53              |
| 1:N:79:ILE:C    | 1:N:81:THR:H     | 2.17                     | 0.53              |
| 1:A:6:ASN:HA    | 1:A:35:HIS:CB    | 2.37                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:49:PHE:N    | 1:B:55:ARG:HH12  | 2.06                     | 0.53              |
| 1:C:80:VAL:HG22 | 1:C:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:E:80:VAL:HG22 | 1:E:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:I:24:VAL:HG12 | 1:I:26:ILE:HD12  | 1.86                     | 0.53              |
| 1:J:24:VAL:HG12 | 1:J:26:ILE:HD12  | 1.86                     | 0.53              |
| 1:J:78:VAL:O    | 1:J:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:K:78:VAL:O    | 1:K:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:L:78:VAL:O    | 1:L:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:N:29:VAL:HG13 | 1:N:77:LEU:HD11  | 1.90                     | 0.53              |
| 1:N:80:VAL:HG22 | 1:N:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:B:29:VAL:HG13 | 1:B:77:LEU:HD11  | 1.90                     | 0.53              |
| 1:B:65:PHE:CD1  | 1:B:80:VAL:HG12  | 2.41                     | 0.53              |
| 1:B:78:VAL:O    | 1:B:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:C:6:ASN:HA    | 1:C:35:HIS:CB    | 2.37                     | 0.53              |
| 1:C:49:PHE:N    | 1:C:55:ARG:HH12  | 2.06                     | 0.53              |
| 1:G:79:ILE:C    | 1:G:81:THR:H     | 2.17                     | 0.53              |
| 1:I:50:GLY:HA3  | 1:I:77:LEU:HD13  | 1.90                     | 0.53              |
| 1:K:38:VAL:HG12 | 1:K:109:PHE:CD2  | 2.41                     | 0.53              |
| 1:M:86:TYR:CG   | 1:M:109:PHE:HB3  | 2.44                     | 0.53              |
| 1:A:80:VAL:HG22 | 1:A:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:D:80:VAL:HG22 | 1:D:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:F:80:VAL:HG22 | 1:F:86:TYR:CZ    | 2.44                     | 0.53              |
| 1:H:79:ILE:C    | 1:H:81:THR:H     | 2.17                     | 0.53              |
| 1:M:49:PHE:N    | 1:M:55:ARG:HH12  | 2.06                     | 0.53              |
| 1:M:78:VAL:O    | 1:M:79:ILE:HD13  | 2.08                     | 0.53              |
| 1:M:90:LEU:HB2  | 1:M:105:VAL:CG2  | 2.38                     | 0.53              |
| 1:M:91:HIS:CB   | 1:M:104:THR:HG21 | 2.32                     | 0.53              |
| 1:B:91:HIS:CB   | 1:B:104:THR:HG21 | 2.32                     | 0.53              |
| 1:C:26:ILE:CD1  | 1:C:37:VAL:HB    | 2.37                     | 0.53              |
| 1:D:90:LEU:HB2  | 1:D:105:VAL:CG2  | 2.38                     | 0.53              |
| 1:G:66:VAL:HB   | 1:H:12:ARG:HH12  | 1.73                     | 0.53              |
| 1:H:42:GLU:HG2  | 1:H:43:THR:H     | 1.74                     | 0.53              |
| 1:L:49:PHE:N    | 1:L:55:ARG:HH12  | 2.06                     | 0.53              |
| 1:N:86:TYR:CG   | 1:N:109:PHE:HB3  | 2.44                     | 0.53              |
| 1:A:26:ILE:HD11 | 1:A:37:VAL:CB    | 2.34                     | 0.53              |
| 1:B:86:TYR:CG   | 1:B:109:PHE:HB3  | 2.44                     | 0.53              |
| 1:G:42:GLU:HG2  | 1:G:43:THR:H     | 1.74                     | 0.53              |
| 1:G:86:TYR:CG   | 1:G:109:PHE:HB3  | 2.44                     | 0.53              |
| 1:I:38:VAL:HG12 | 1:I:109:PHE:CD2  | 2.41                     | 0.53              |
| 1:I:42:GLU:HG2  | 1:I:43:THR:H     | 1.74                     | 0.53              |
| 1:K:66:VAL:CG2  | 1:K:68:PRO:HD3   | 2.37                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:90:LEU:HB2  | 1:L:105:VAL:CG2  | 2.38                     | 0.53              |
| 1:N:24:VAL:HG21 | 1:N:107:LYS:HD3  | 1.90                     | 0.53              |
| 1:N:90:LEU:HB2  | 1:N:105:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:78:VAL:O    | 1:A:79:ILE:HD13  | 2.08                     | 0.52              |
| 1:C:86:TYR:CG   | 1:C:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:I:78:VAL:O    | 1:I:79:ILE:HD13  | 2.08                     | 0.52              |
| 1:K:79:ILE:C    | 1:K:81:THR:H     | 2.17                     | 0.52              |
| 1:L:66:VAL:CG2  | 1:L:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:M:80:VAL:HG22 | 1:M:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:B:79:ILE:C    | 1:B:81:THR:H     | 2.17                     | 0.52              |
| 1:D:38:VAL:HG13 | 1:D:107:LYS:HZ3  | 1.74                     | 0.52              |
| 1:F:42:GLU:HG2  | 1:F:43:THR:H     | 1.74                     | 0.52              |
| 1:H:38:VAL:HG12 | 1:H:109:PHE:CD2  | 2.41                     | 0.52              |
| 1:I:86:TYR:CG   | 1:I:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:J:42:GLU:HG2  | 1:J:43:THR:H     | 1.74                     | 0.52              |
| 1:J:50:GLY:HA3  | 1:J:77:LEU:HD13  | 1.91                     | 0.52              |
| 1:J:66:VAL:CG2  | 1:J:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:J:66:VAL:HB   | 1:K:12:ARG:HH12  | 1.73                     | 0.52              |
| 1:J:79:ILE:C    | 1:J:81:THR:H     | 2.17                     | 0.52              |
| 1:A:79:ILE:C    | 1:A:81:THR:H     | 2.17                     | 0.52              |
| 1:A:91:HIS:CB   | 1:A:104:THR:HG21 | 2.32                     | 0.52              |
| 1:D:49:PHE:N    | 1:D:55:ARG:HH12  | 2.06                     | 0.52              |
| 1:J:80:VAL:HG22 | 1:J:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:N:49:PHE:N    | 1:N:55:ARG:HH12  | 2.06                     | 0.52              |
| 1:N:91:HIS:CB   | 1:N:104:THR:HG21 | 2.33                     | 0.52              |
| 1:E:86:TYR:CG   | 1:E:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:F:66:VAL:HB   | 1:G:12:ARG:HH12  | 1.73                     | 0.52              |
| 1:L:86:TYR:CG   | 1:L:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:N:26:ILE:HD11 | 1:N:37:VAL:CB    | 2.35                     | 0.52              |
| 1:N:78:VAL:O    | 1:N:79:ILE:HD13  | 2.08                     | 0.52              |
| 1:A:49:PHE:N    | 1:A:55:ARG:HH12  | 2.06                     | 0.52              |
| 1:B:80:VAL:HG22 | 1:B:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:E:57:PHE:CE1  | 1:F:105:VAL:HG13 | 2.41                     | 0.52              |
| 1:G:80:VAL:HG22 | 1:G:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:H:78:VAL:O    | 1:H:79:ILE:HD13  | 2.08                     | 0.52              |
| 1:I:80:VAL:HG22 | 1:I:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:K:42:GLU:HG2  | 1:K:43:THR:H     | 1.74                     | 0.52              |
| 1:M:66:VAL:CG2  | 1:M:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:C:30:ALA:HB2  | 1:C:49:PHE:HE1   | 1.75                     | 0.52              |
| 1:E:42:GLU:HG2  | 1:E:43:THR:H     | 1.74                     | 0.52              |
| 1:H:86:TYR:CG   | 1:H:109:PHE:HB3  | 2.44                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:30:ALA:HB2  | 1:I:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:I:66:VAL:CG2  | 1:I:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:B:26:ILE:CD1  | 1:B:37:VAL:HB    | 2.37                     | 0.52              |
| 1:B:30:ALA:HB2  | 1:B:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:D:86:TYR:CG   | 1:D:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:E:29:VAL:HG13 | 1:E:77:LEU:HD11  | 1.90                     | 0.52              |
| 1:F:86:TYR:CG   | 1:F:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:G:30:ALA:HB2  | 1:G:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:G:90:LEU:HB2  | 1:G:105:VAL:CG2  | 2.38                     | 0.52              |
| 1:H:30:ALA:HB2  | 1:H:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:M:30:ALA:HB2  | 1:M:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:G:66:VAL:CG2  | 1:G:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:J:57:PHE:CE1  | 1:K:105:VAL:HG13 | 2.41                     | 0.52              |
| 1:K:80:VAL:HG22 | 1:K:86:TYR:CZ    | 2.44                     | 0.52              |
| 1:K:86:TYR:CG   | 1:K:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:K:90:LEU:HB2  | 1:K:105:VAL:CG2  | 2.38                     | 0.52              |
| 1:L:42:GLU:HG2  | 1:L:43:THR:H     | 1.74                     | 0.52              |
| 1:C:29:VAL:HG13 | 1:C:77:LEU:HD11  | 1.90                     | 0.52              |
| 1:D:29:VAL:HG13 | 1:D:77:LEU:HD11  | 1.90                     | 0.52              |
| 1:D:30:ALA:HB2  | 1:D:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:D:42:GLU:HG2  | 1:D:43:THR:H     | 1.74                     | 0.52              |
| 1:F:66:VAL:CG2  | 1:F:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:H:66:VAL:CG2  | 1:H:68:PRO:HD3   | 2.37                     | 0.52              |
| 1:J:29:VAL:HG13 | 1:J:77:LEU:HD11  | 1.90                     | 0.52              |
| 1:K:49:PHE:N    | 1:K:55:ARG:HH12  | 2.06                     | 0.52              |
| 1:K:50:GLY:HA3  | 1:K:77:LEU:HD13  | 1.91                     | 0.52              |
| 1:L:83:LYS:CE   | 1:L:109:PHE:HZ   | 2.23                     | 0.52              |
| 1:N:30:ALA:HB2  | 1:N:49:PHE:HE1   | 1.74                     | 0.52              |
| 1:A:86:TYR:CG   | 1:A:109:PHE:HB3  | 2.44                     | 0.52              |
| 1:F:38:VAL:HG12 | 1:F:109:PHE:CD2  | 2.41                     | 0.52              |
| 1:L:61:MET:CG   | 1:L:62:ASN:H     | 2.18                     | 0.52              |
| 1:M:29:VAL:HG13 | 1:M:77:LEU:HD11  | 1.90                     | 0.52              |
| 1:A:30:ALA:HB2  | 1:A:49:PHE:HE1   | 1.74                     | 0.51              |
| 1:C:57:PHE:CE1  | 1:D:105:VAL:HG13 | 2.41                     | 0.51              |
| 1:H:80:VAL:HG22 | 1:H:86:TYR:CZ    | 2.44                     | 0.51              |
| 1:L:13:ILE:HG13 | 1:L:15:SER:N     | 2.26                     | 0.51              |
| 1:L:80:VAL:HG22 | 1:L:86:TYR:CZ    | 2.44                     | 0.51              |
| 1:M:42:GLU:HG2  | 1:M:43:THR:H     | 1.74                     | 0.51              |
| 1:C:42:GLU:HG2  | 1:C:43:THR:H     | 1.74                     | 0.51              |
| 1:D:56:THR:CG2  | 1:D:57:PHE:H     | 2.23                     | 0.51              |
| 1:F:30:ALA:HB2  | 1:F:49:PHE:HE1   | 1.74                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:30:ALA:HB2  | 1:J:49:PHE:HE1   | 1.75                     | 0.51              |
| 1:N:13:ILE:HG13 | 1:N:15:SER:N     | 2.26                     | 0.51              |
| 1:C:65:PHE:CD1  | 1:C:80:VAL:HG12  | 2.41                     | 0.51              |
| 1:C:90:LEU:HB2  | 1:C:105:VAL:CG2  | 2.38                     | 0.51              |
| 1:D:83:LYS:CE   | 1:D:109:PHE:HZ   | 2.23                     | 0.51              |
| 1:E:66:VAL:CG2  | 1:E:68:PRO:HD3   | 2.37                     | 0.51              |
| 1:F:29:VAL:HG13 | 1:F:77:LEU:HD11  | 1.90                     | 0.51              |
| 1:F:56:THR:CG2  | 1:F:57:PHE:H     | 2.23                     | 0.51              |
| 1:J:13:ILE:HG13 | 1:J:15:SER:N     | 2.26                     | 0.51              |
| 1:J:86:TYR:CG   | 1:J:109:PHE:HB3  | 2.44                     | 0.51              |
| 1:K:29:VAL:CG1  | 1:K:92:PHE:CE2   | 2.94                     | 0.51              |
| 1:K:29:VAL:HG13 | 1:K:77:LEU:HD11  | 1.90                     | 0.51              |
| 1:N:42:GLU:HG2  | 1:N:43:THR:H     | 1.74                     | 0.51              |
| 1:N:66:VAL:CG2  | 1:N:68:PRO:HD3   | 2.37                     | 0.51              |
| 1:A:26:ILE:CD1  | 1:A:37:VAL:HB    | 2.37                     | 0.51              |
| 1:A:42:GLU:HG2  | 1:A:43:THR:H     | 1.74                     | 0.51              |
| 1:A:57:PHE:CE1  | 1:B:105:VAL:HG13 | 2.41                     | 0.51              |
| 1:B:42:GLU:HG2  | 1:B:43:THR:H     | 1.74                     | 0.51              |
| 1:G:57:PHE:CE1  | 1:H:105:VAL:HG13 | 2.41                     | 0.51              |
| 1:I:29:VAL:HG13 | 1:I:77:LEU:HD11  | 1.90                     | 0.51              |
| 1:J:29:VAL:CG1  | 1:J:92:PHE:CE2   | 2.94                     | 0.51              |
| 1:J:45:ILE:HG22 | 1:J:46:THR:H     | 1.75                     | 0.51              |
| 1:K:45:ILE:HG22 | 1:K:46:THR:H     | 1.75                     | 0.51              |
| 1:M:29:VAL:CG1  | 1:M:92:PHE:CE2   | 2.94                     | 0.51              |
| 1:M:83:LYS:CE   | 1:M:109:PHE:HZ   | 2.23                     | 0.51              |
| 1:A:29:VAL:CG1  | 1:A:92:PHE:CE2   | 2.94                     | 0.51              |
| 1:G:49:PHE:N    | 1:G:55:ARG:HH12  | 2.06                     | 0.51              |
| 1:H:49:PHE:N    | 1:H:55:ARG:HH12  | 2.06                     | 0.51              |
| 1:K:30:ALA:HB2  | 1:K:49:PHE:HE1   | 1.74                     | 0.51              |
| 1:L:30:ALA:HB2  | 1:L:49:PHE:HE1   | 1.75                     | 0.51              |
| 1:L:50:GLY:HA3  | 1:L:77:LEU:HD13  | 1.91                     | 0.51              |
| 1:B:38:VAL:HG13 | 1:B:107:LYS:HZ3  | 1.75                     | 0.51              |
| 1:C:45:ILE:HG22 | 1:C:46:THR:H     | 1.75                     | 0.51              |
| 1:L:29:VAL:CG1  | 1:L:92:PHE:CE2   | 2.94                     | 0.51              |
| 1:N:65:PHE:CD1  | 1:N:80:VAL:HG12  | 2.41                     | 0.51              |
| 1:D:45:ILE:HG22 | 1:D:46:THR:H     | 1.75                     | 0.51              |
| 1:E:49:PHE:N    | 1:E:55:ARG:HH12  | 2.06                     | 0.51              |
| 1:H:83:LYS:CE   | 1:H:109:PHE:HZ   | 2.23                     | 0.51              |
| 1:L:45:ILE:HG22 | 1:L:46:THR:H     | 1.75                     | 0.51              |
| 1:B:45:ILE:HG22 | 1:B:46:THR:H     | 1.75                     | 0.51              |
| 1:B:56:THR:CG2  | 1:B:57:PHE:H     | 2.23                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:49:PHE:N    | 1:F:55:ARG:HH12  | 2.06                     | 0.51              |
| 1:H:29:VAL:HG13 | 1:H:77:LEU:HD11  | 1.90                     | 0.51              |
| 1:H:56:THR:CG2  | 1:H:57:PHE:H     | 2.23                     | 0.51              |
| 1:I:45:ILE:HG22 | 1:I:46:THR:H     | 1.75                     | 0.51              |
| 1:I:49:PHE:N    | 1:I:55:ARG:HH12  | 2.06                     | 0.51              |
| 1:L:29:VAL:HG13 | 1:L:77:LEU:HD11  | 1.90                     | 0.51              |
| 1:N:25:LYS:HD2  | 1:N:25:LYS:H     | 1.75                     | 0.51              |
| 1:B:13:ILE:HG13 | 1:B:15:SER:N     | 2.26                     | 0.51              |
| 1:E:30:ALA:HB2  | 1:E:49:PHE:HE1   | 1.75                     | 0.51              |
| 1:J:18:TYR:CD2  | 1:J:23:VAL:HG13  | 2.46                     | 0.51              |
| 1:K:18:TYR:CD2  | 1:K:23:VAL:HG13  | 2.46                     | 0.51              |
| 1:L:25:LYS:HD2  | 1:L:25:LYS:H     | 1.75                     | 0.51              |
| 1:M:25:LYS:HD2  | 1:M:25:LYS:H     | 1.75                     | 0.51              |
| 1:M:50:GLY:HA3  | 1:M:77:LEU:HD13  | 1.90                     | 0.51              |
| 1:D:13:ILE:HG13 | 1:D:15:SER:N     | 2.26                     | 0.51              |
| 1:E:45:ILE:HG22 | 1:E:46:THR:H     | 1.75                     | 0.51              |
| 1:A:45:ILE:HG22 | 1:A:46:THR:H     | 1.75                     | 0.50              |
| 1:C:13:ILE:HG13 | 1:C:15:SER:N     | 2.26                     | 0.50              |
| 1:D:66:VAL:CG2  | 1:D:68:PRO:HD3   | 2.37                     | 0.50              |
| 1:E:13:ILE:HG13 | 1:E:15:SER:N     | 2.26                     | 0.50              |
| 1:F:29:VAL:CG1  | 1:F:92:PHE:CE2   | 2.94                     | 0.50              |
| 1:H:13:ILE:HG13 | 1:H:15:SER:N     | 2.26                     | 0.50              |
| 1:M:57:PHE:CE1  | 1:N:105:VAL:HG13 | 2.41                     | 0.50              |
| 1:N:26:ILE:CD1  | 1:N:37:VAL:HB    | 2.37                     | 0.50              |
| 1:N:29:VAL:CG1  | 1:N:92:PHE:CE2   | 2.94                     | 0.50              |
| 1:N:83:LYS:CE   | 1:N:109:PHE:HZ   | 2.23                     | 0.50              |
| 1:A:25:LYS:HD2  | 1:A:25:LYS:H     | 1.75                     | 0.50              |
| 1:E:29:VAL:CG1  | 1:E:92:PHE:CE2   | 2.94                     | 0.50              |
| 1:H:29:VAL:CG1  | 1:H:92:PHE:CE2   | 2.94                     | 0.50              |
| 1:H:45:ILE:HG22 | 1:H:46:THR:H     | 1.75                     | 0.50              |
| 1:I:18:TYR:CD2  | 1:I:23:VAL:HG13  | 2.46                     | 0.50              |
| 1:I:49:PHE:CB   | 1:I:55:ARG:HH22  | 2.17                     | 0.50              |
| 1:K:25:LYS:HD2  | 1:K:25:LYS:H     | 1.75                     | 0.50              |
| 1:L:18:TYR:CD2  | 1:L:23:VAL:HG13  | 2.46                     | 0.50              |
| 1:D:29:VAL:CG1  | 1:D:92:PHE:CE2   | 2.94                     | 0.50              |
| 1:F:13:ILE:HG13 | 1:F:15:SER:N     | 2.26                     | 0.50              |
| 1:G:29:VAL:HG13 | 1:G:77:LEU:HD11  | 1.90                     | 0.50              |
| 1:J:56:THR:CG2  | 1:J:57:PHE:H     | 2.23                     | 0.50              |
| 1:N:50:GLY:HA3  | 1:N:77:LEU:HD13  | 1.90                     | 0.50              |
| 1:A:13:ILE:HG13 | 1:A:15:SER:N     | 2.26                     | 0.50              |
| 1:A:66:VAL:CG2  | 1:A:68:PRO:HD3   | 2.37                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:13:ILE:HG13 | 1:I:15:SER:N    | 2.26                     | 0.50              |
| 1:M:26:ILE:CD1  | 1:M:37:VAL:HB   | 2.37                     | 0.50              |
| 1:N:56:THR:CG2  | 1:N:57:PHE:H    | 2.23                     | 0.50              |
| 1:B:25:LYS:HD2  | 1:B:25:LYS:H    | 1.75                     | 0.50              |
| 1:B:29:VAL:CG1  | 1:B:92:PHE:CE2  | 2.94                     | 0.50              |
| 1:E:83:LYS:CE   | 1:E:109:PHE:HZ  | 2.23                     | 0.50              |
| 1:F:45:ILE:HG22 | 1:F:46:THR:H    | 1.75                     | 0.50              |
| 1:G:13:ILE:HG13 | 1:G:15:SER:N    | 2.26                     | 0.50              |
| 1:G:29:VAL:CG1  | 1:G:92:PHE:CE2  | 2.94                     | 0.50              |
| 1:J:49:PHE:N    | 1:J:55:ARG:HH12 | 2.06                     | 0.50              |
| 1:M:45:ILE:HG22 | 1:M:46:THR:H    | 1.75                     | 0.50              |
| 1:B:90:LEU:HB2  | 1:B:105:VAL:CG2 | 2.38                     | 0.50              |
| 1:C:29:VAL:CG1  | 1:C:92:PHE:CE2  | 2.94                     | 0.50              |
| 1:I:29:VAL:CG1  | 1:I:92:PHE:CE2  | 2.94                     | 0.50              |
| 1:J:25:LYS:HD2  | 1:J:25:LYS:H    | 1.75                     | 0.50              |
| 1:J:90:LEU:HB2  | 1:J:105:VAL:CG2 | 2.38                     | 0.50              |
| 1:L:56:THR:CG2  | 1:L:57:PHE:H    | 2.23                     | 0.50              |
| 1:A:49:PHE:CB   | 1:A:55:ARG:HH22 | 2.17                     | 0.50              |
| 1:B:91:HIS:HA   | 1:B:104:THR:CG2 | 2.42                     | 0.50              |
| 1:C:91:HIS:HA   | 1:C:104:THR:CG2 | 2.42                     | 0.50              |
| 1:G:45:ILE:HG22 | 1:G:46:THR:H    | 1.75                     | 0.50              |
| 1:K:13:ILE:HG13 | 1:K:15:SER:N    | 2.26                     | 0.50              |
| 1:M:13:ILE:HG13 | 1:M:15:SER:N    | 2.26                     | 0.50              |
| 1:N:18:TYR:CD2  | 1:N:23:VAL:HG13 | 2.46                     | 0.50              |
| 1:A:91:HIS:HA   | 1:A:104:THR:CG2 | 2.42                     | 0.50              |
| 1:C:25:LYS:HD2  | 1:C:25:LYS:H    | 1.75                     | 0.50              |
| 1:D:91:HIS:HA   | 1:D:104:THR:CG2 | 2.42                     | 0.50              |
| 1:I:83:LYS:CE   | 1:I:109:PHE:HZ  | 2.23                     | 0.50              |
| 1:K:54:SER:O    | 1:K:55:ARG:HG2  | 2.12                     | 0.50              |
| 1:L:26:ILE:CD1  | 1:L:37:VAL:HB   | 2.37                     | 0.50              |
| 1:L:53:GLU:OE2  | 1:M:11:TYR:HB2  | 2.12                     | 0.50              |
| 1:N:45:ILE:HG22 | 1:N:46:THR:H    | 1.75                     | 0.50              |
| 1:N:91:HIS:HA   | 1:N:104:THR:CG2 | 2.42                     | 0.50              |
| 1:A:5:ARG:CB    | 1:A:36:ILE:HB   | 2.42                     | 0.50              |
| 1:A:50:GLY:HA3  | 1:A:77:LEU:HD13 | 1.91                     | 0.50              |
| 1:B:5:ARG:CB    | 1:B:36:ILE:HB   | 2.42                     | 0.50              |
| 1:B:54:SER:O    | 1:B:55:ARG:HG2  | 2.12                     | 0.50              |
| 1:C:5:ARG:CB    | 1:C:36:ILE:HB   | 2.42                     | 0.50              |
| 1:D:53:GLU:OE2  | 1:E:11:TYR:HB2  | 2.12                     | 0.50              |
| 1:D:54:SER:O    | 1:D:55:ARG:HG2  | 2.12                     | 0.50              |
| 1:I:53:GLU:OE2  | 1:J:11:TYR:HB2  | 2.12                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:91:HIS:HA   | 1:L:104:THR:CG2 | 2.42                     | 0.50              |
| 1:M:91:HIS:HA   | 1:M:104:THR:CG2 | 2.42                     | 0.50              |
| 1:E:53:GLU:OE2  | 1:F:11:TYR:HB2  | 2.12                     | 0.49              |
| 1:E:91:HIS:HA   | 1:E:104:THR:CG2 | 2.42                     | 0.49              |
| 1:F:53:GLU:OE2  | 1:G:11:TYR:HB2  | 2.12                     | 0.49              |
| 1:F:90:LEU:HB2  | 1:F:105:VAL:CG2 | 2.38                     | 0.49              |
| 1:K:26:ILE:CD1  | 1:K:37:VAL:HB   | 2.37                     | 0.49              |
| 1:K:91:HIS:HA   | 1:K:104:THR:CG2 | 2.42                     | 0.49              |
| 1:M:38:VAL:HG13 | 1:M:107:LYS:HZ3 | 1.77                     | 0.49              |
| 1:M:53:GLU:OE2  | 1:N:11:TYR:HB2  | 2.12                     | 0.49              |
| 1:N:5:ARG:CB    | 1:N:36:ILE:HB   | 2.42                     | 0.49              |
| 1:A:83:LYS:CE   | 1:A:109:PHE:HZ  | 2.23                     | 0.49              |
| 1:C:66:VAL:CG2  | 1:C:68:PRO:HD3  | 2.37                     | 0.49              |
| 1:D:5:ARG:CB    | 1:D:36:ILE:HB   | 2.42                     | 0.49              |
| 1:K:32:VAL:HG13 | 1:K:48:ALA:C    | 2.38                     | 0.49              |
| 1:K:49:PHE:CB   | 1:K:55:ARG:HH22 | 2.17                     | 0.49              |
| 1:M:54:SER:O    | 1:M:55:ARG:HG2  | 2.12                     | 0.49              |
| 1:E:68:PRO:O    | 1:E:77:LEU:HB2  | 2.13                     | 0.49              |
| 1:F:32:VAL:HG13 | 1:F:48:ALA:C    | 2.38                     | 0.49              |
| 1:G:68:PRO:O    | 1:G:77:LEU:HB2  | 2.13                     | 0.49              |
| 1:H:24:VAL:HG22 | 1:H:25:LYS:H    | 1.77                     | 0.49              |
| 1:I:55:ARG:CD   | 1:J:11:TYR:CD2  | 2.96                     | 0.49              |
| 1:I:68:PRO:O    | 1:I:77:LEU:HB2  | 2.12                     | 0.49              |
| 1:J:91:HIS:HA   | 1:J:104:THR:CG2 | 2.42                     | 0.49              |
| 1:M:5:ARG:CB    | 1:M:36:ILE:HB   | 2.42                     | 0.49              |
| 1:B:32:VAL:HG13 | 1:B:48:ALA:C    | 2.38                     | 0.49              |
| 1:C:53:GLU:OE2  | 1:D:11:TYR:HB2  | 2.12                     | 0.49              |
| 1:C:55:ARG:CD   | 1:D:11:TYR:CD2  | 2.95                     | 0.49              |
| 1:D:32:VAL:HG13 | 1:D:48:ALA:C    | 2.38                     | 0.49              |
| 1:E:5:ARG:CB    | 1:E:36:ILE:HB   | 2.42                     | 0.49              |
| 1:E:54:SER:O    | 1:E:55:ARG:HG2  | 2.12                     | 0.49              |
| 1:F:54:SER:O    | 1:F:55:ARG:HG2  | 2.12                     | 0.49              |
| 1:F:91:HIS:HA   | 1:F:104:THR:CG2 | 2.42                     | 0.49              |
| 1:H:55:ARG:CD   | 1:I:11:TYR:CD2  | 2.96                     | 0.49              |
| 1:J:32:VAL:HG13 | 1:J:48:ALA:C    | 2.38                     | 0.49              |
| 1:J:55:ARG:CD   | 1:K:11:TYR:CD2  | 2.95                     | 0.49              |
| 1:K:53:GLU:OE2  | 1:L:11:TYR:HB2  | 2.12                     | 0.49              |
| 1:M:49:PHE:CB   | 1:M:55:ARG:HH22 | 2.17                     | 0.49              |
| 1:A:11:TYR:HB2  | 1:N:53:GLU:OE2  | 2.12                     | 0.49              |
| 1:A:49:PHE:CD2  | 1:A:79:ILE:HG13 | 2.48                     | 0.49              |
| 1:B:50:GLY:HA3  | 1:B:77:LEU:HD13 | 1.90                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:65:PHE:CD1  | 1:D:80:VAL:HG12  | 2.41                     | 0.49              |
| 1:E:32:VAL:HG13 | 1:E:48:ALA:C     | 2.38                     | 0.49              |
| 1:I:25:LYS:HD2  | 1:I:25:LYS:H     | 1.75                     | 0.49              |
| 1:I:54:SER:O    | 1:I:55:ARG:HG2   | 2.12                     | 0.49              |
| 1:I:91:HIS:HA   | 1:I:104:THR:CG2  | 2.42                     | 0.49              |
| 1:J:68:PRO:O    | 1:J:77:LEU:HB2   | 2.13                     | 0.49              |
| 1:K:24:VAL:HG22 | 1:K:25:LYS:H     | 1.77                     | 0.49              |
| 1:L:32:VAL:HG13 | 1:L:48:ALA:C     | 2.38                     | 0.49              |
| 1:N:54:SER:O    | 1:N:55:ARG:HG2   | 2.12                     | 0.49              |
| 1:A:32:VAL:HG13 | 1:A:48:ALA:C     | 2.38                     | 0.49              |
| 1:A:32:VAL:HG11 | 1:A:49:PHE:O     | 2.13                     | 0.49              |
| 1:A:68:PRO:O    | 1:A:77:LEU:HB2   | 2.13                     | 0.49              |
| 1:B:68:PRO:O    | 1:B:77:LEU:HB2   | 2.12                     | 0.49              |
| 1:C:49:PHE:CD2  | 1:C:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:D:25:LYS:HD2  | 1:D:25:LYS:H     | 1.75                     | 0.49              |
| 1:E:32:VAL:HG11 | 1:E:49:PHE:O     | 2.13                     | 0.49              |
| 1:E:49:PHE:CD2  | 1:E:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:F:32:VAL:HG11 | 1:F:49:PHE:O     | 2.13                     | 0.49              |
| 1:G:24:VAL:HG22 | 1:G:25:LYS:H     | 1.78                     | 0.49              |
| 1:G:53:GLU:OE2  | 1:H:11:TYR:HB2   | 2.12                     | 0.49              |
| 1:G:91:HIS:HA   | 1:G:104:THR:CG2  | 2.42                     | 0.49              |
| 1:H:53:GLU:OE2  | 1:I:11:TYR:HB2   | 2.12                     | 0.49              |
| 1:H:57:PHE:CE1  | 1:I:105:VAL:HG13 | 2.41                     | 0.49              |
| 1:H:91:HIS:HA   | 1:H:104:THR:CG2  | 2.42                     | 0.49              |
| 1:J:26:ILE:CD1  | 1:J:37:VAL:HB    | 2.37                     | 0.49              |
| 1:K:32:VAL:HG11 | 1:K:49:PHE:O     | 2.13                     | 0.49              |
| 1:N:32:VAL:HG13 | 1:N:48:ALA:C     | 2.38                     | 0.49              |
| 1:A:54:SER:O    | 1:A:55:ARG:HG2   | 2.12                     | 0.49              |
| 1:B:57:PHE:HZ   | 1:C:28:ALA:N     | 2.11                     | 0.49              |
| 1:C:57:PHE:HZ   | 1:D:28:ALA:N     | 2.11                     | 0.49              |
| 1:D:57:PHE:HZ   | 1:E:28:ALA:N     | 2.11                     | 0.49              |
| 1:D:68:PRO:O    | 1:D:77:LEU:HB2   | 2.13                     | 0.49              |
| 1:D:88:ILE:HD11 | 1:D:107:LYS:CG   | 2.34                     | 0.49              |
| 1:G:32:VAL:HG13 | 1:G:48:ALA:C     | 2.38                     | 0.49              |
| 1:G:57:PHE:HZ   | 1:H:28:ALA:N     | 2.11                     | 0.49              |
| 1:J:24:VAL:HG22 | 1:J:25:LYS:H     | 1.78                     | 0.49              |
| 1:L:5:ARG:CB    | 1:L:36:ILE:HB    | 2.42                     | 0.49              |
| 1:L:24:VAL:HG22 | 1:L:25:LYS:H     | 1.78                     | 0.49              |
| 1:L:68:PRO:O    | 1:L:77:LEU:HB2   | 2.13                     | 0.49              |
| 1:M:32:VAL:HG13 | 1:M:48:ALA:C     | 2.38                     | 0.49              |
| 1:M:49:PHE:CD2  | 1:M:79:ILE:HG13  | 2.48                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:49:PHE:HE2  | 1:A:79:ILE:CD1   | 2.26                     | 0.49              |
| 1:B:32:VAL:HG11 | 1:B:49:PHE:O     | 2.13                     | 0.49              |
| 1:C:32:VAL:HG13 | 1:C:48:ALA:C     | 2.38                     | 0.49              |
| 1:D:32:VAL:HG11 | 1:D:49:PHE:O     | 2.13                     | 0.49              |
| 1:E:57:PHE:HZ   | 1:F:28:ALA:N     | 2.11                     | 0.49              |
| 1:G:49:PHE:CD2  | 1:G:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:H:57:PHE:HZ   | 1:I:28:ALA:N     | 2.11                     | 0.49              |
| 1:J:32:VAL:HG11 | 1:J:49:PHE:O     | 2.13                     | 0.49              |
| 1:K:49:PHE:CD2  | 1:K:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:M:18:TYR:CD2  | 1:M:23:VAL:HG13  | 2.46                     | 0.49              |
| 1:N:32:VAL:HG11 | 1:N:49:PHE:O     | 2.13                     | 0.49              |
| 1:B:57:PHE:CE1  | 1:C:105:VAL:HG13 | 2.41                     | 0.49              |
| 1:B:66:VAL:CG2  | 1:B:68:PRO:HD3   | 2.37                     | 0.49              |
| 1:F:5:ARG:CB    | 1:F:36:ILE:HB    | 2.42                     | 0.49              |
| 1:H:49:PHE:CD2  | 1:H:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:I:24:VAL:HG22 | 1:I:25:LYS:H     | 1.78                     | 0.49              |
| 1:I:32:VAL:HG13 | 1:I:48:ALA:C     | 2.38                     | 0.49              |
| 1:J:49:PHE:CD2  | 1:J:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:J:54:SER:O    | 1:J:55:ARG:HG2   | 2.12                     | 0.49              |
| 1:K:55:ARG:CD   | 1:L:11:TYR:CD2   | 2.96                     | 0.49              |
| 1:N:38:VAL:HG13 | 1:N:107:LYS:HZ3  | 1.78                     | 0.49              |
| 1:H:109:PHE:CD1 | 1:H:109:PHE:C    | 2.91                     | 0.49              |
| 1:L:32:VAL:HG11 | 1:L:49:PHE:O     | 2.13                     | 0.49              |
| 1:L:49:PHE:CD2  | 1:L:79:ILE:HG13  | 2.48                     | 0.49              |
| 1:L:54:SER:O    | 1:L:55:ARG:HG2   | 2.12                     | 0.49              |
| 1:M:24:VAL:HG22 | 1:M:25:LYS:H     | 1.78                     | 0.49              |
| 1:M:68:PRO:O    | 1:M:77:LEU:HB2   | 2.12                     | 0.49              |
| 1:A:90:LEU:HB2  | 1:A:105:VAL:CG2  | 2.38                     | 0.48              |
| 1:B:49:PHE:CD2  | 1:B:79:ILE:HG13  | 2.48                     | 0.48              |
| 1:C:83:LYS:HZ2  | 1:C:111:GLU:HB3  | 1.78                     | 0.48              |
| 1:D:55:ARG:CD   | 1:E:11:TYR:CD2   | 2.96                     | 0.48              |
| 1:E:25:LYS:HD2  | 1:E:25:LYS:H     | 1.75                     | 0.48              |
| 1:F:49:PHE:CD2  | 1:F:79:ILE:HG13  | 2.48                     | 0.48              |
| 1:G:54:SER:O    | 1:G:55:ARG:HG2   | 2.12                     | 0.48              |
| 1:H:25:LYS:HD2  | 1:H:25:LYS:H     | 1.75                     | 0.48              |
| 1:I:26:ILE:CD1  | 1:I:37:VAL:HB    | 2.37                     | 0.48              |
| 1:I:109:PHE:C   | 1:I:109:PHE:CD1  | 2.91                     | 0.48              |
| 1:A:43:THR:HG22 | 1:B:14:LYS:HE2   | 1.95                     | 0.48              |
| 1:B:53:GLU:OE2  | 1:C:11:TYR:HB2   | 2.12                     | 0.48              |
| 1:C:43:THR:HG22 | 1:D:14:LYS:HE2   | 1.96                     | 0.48              |
| 1:D:24:VAL:HG22 | 1:D:25:LYS:H     | 1.77                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:109:PHE:CD1 | 1:E:109:PHE:C    | 2.91                     | 0.48              |
| 1:F:24:VAL:HG22 | 1:F:25:LYS:H     | 1.78                     | 0.48              |
| 1:F:57:PHE:CE1  | 1:G:105:VAL:HG13 | 2.41                     | 0.48              |
| 1:G:32:VAL:HG11 | 1:G:49:PHE:O     | 2.13                     | 0.48              |
| 1:H:29:VAL:HG13 | 1:H:29:VAL:O     | 2.13                     | 0.48              |
| 1:H:54:SER:O    | 1:H:55:ARG:HG2   | 2.12                     | 0.48              |
| 1:I:32:VAL:HG11 | 1:I:49:PHE:O     | 2.13                     | 0.48              |
| 1:I:57:PHE:HZ   | 1:J:28:ALA:N     | 2.11                     | 0.48              |
| 1:J:53:GLU:OE2  | 1:K:11:TYR:HB2   | 2.12                     | 0.48              |
| 1:M:29:VAL:HG13 | 1:M:29:VAL:O     | 2.13                     | 0.48              |
| 1:A:53:GLU:OE2  | 1:B:11:TYR:HB2   | 2.12                     | 0.48              |
| 1:C:50:GLY:HA3  | 1:C:77:LEU:HD13  | 1.91                     | 0.48              |
| 1:C:68:PRO:O    | 1:C:77:LEU:HB2   | 2.13                     | 0.48              |
| 1:D:49:PHE:CD2  | 1:D:79:ILE:HG13  | 2.48                     | 0.48              |
| 1:E:24:VAL:HG22 | 1:E:25:LYS:H     | 1.78                     | 0.48              |
| 1:G:25:LYS:HD2  | 1:G:25:LYS:H     | 1.75                     | 0.48              |
| 1:H:43:THR:HG22 | 1:I:14:LYS:HE2   | 1.95                     | 0.48              |
| 1:J:57:PHE:HZ   | 1:K:28:ALA:N     | 2.11                     | 0.48              |
| 1:J:83:LYS:CE   | 1:J:109:PHE:HZ   | 2.23                     | 0.48              |
| 1:L:55:ARG:CD   | 1:M:11:TYR:CD2   | 2.95                     | 0.48              |
| 1:D:109:PHE:CD1 | 1:D:109:PHE:C    | 2.91                     | 0.48              |
| 1:H:68:PRO:O    | 1:H:77:LEU:HB2   | 2.13                     | 0.48              |
| 1:I:29:VAL:HG13 | 1:I:29:VAL:O     | 2.14                     | 0.48              |
| 1:J:109:PHE:CD1 | 1:J:109:PHE:C    | 2.91                     | 0.48              |
| 1:K:43:THR:HG22 | 1:L:14:LYS:HE2   | 1.96                     | 0.48              |
| 1:K:68:PRO:O    | 1:K:77:LEU:HB2   | 2.13                     | 0.48              |
| 1:L:29:VAL:HG13 | 1:L:29:VAL:O     | 2.13                     | 0.48              |
| 1:N:29:VAL:HG13 | 1:N:29:VAL:O     | 2.13                     | 0.48              |
| 1:A:65:PHE:CD1  | 1:A:80:VAL:HG12  | 2.41                     | 0.48              |
| 1:E:89:VAL:HG13 | 1:E:89:VAL:O     | 2.14                     | 0.48              |
| 1:F:25:LYS:HD2  | 1:F:25:LYS:H     | 1.75                     | 0.48              |
| 1:F:68:PRO:O    | 1:F:77:LEU:HB2   | 2.12                     | 0.48              |
| 1:F:83:LYS:CE   | 1:F:109:PHE:HZ   | 2.23                     | 0.48              |
| 1:H:32:VAL:HG13 | 1:H:48:ALA:C     | 2.38                     | 0.48              |
| 1:I:86:TYR:C    | 1:I:87:ASN:HD22  | 2.22                     | 0.48              |
| 1:L:110:ILE:H   | 1:L:110:ILE:HG12 | 1.51                     | 0.48              |
| 1:M:32:VAL:HG11 | 1:M:49:PHE:O     | 2.13                     | 0.48              |
| 1:M:43:THR:HG22 | 1:N:14:LYS:HE2   | 1.96                     | 0.48              |
| 1:N:24:VAL:HG22 | 1:N:25:LYS:H     | 1.78                     | 0.48              |
| 1:A:24:VAL:HG22 | 1:A:25:LYS:H     | 1.77                     | 0.48              |
| 1:B:24:VAL:HG23 | 1:B:108:SER:O    | 2.14                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:83:LYS:CE   | 1:B:109:PHE:HZ   | 2.23                     | 0.48              |
| 1:C:54:SER:O    | 1:C:55:ARG:HG2   | 2.12                     | 0.48              |
| 1:C:109:PHE:C   | 1:C:109:PHE:CD1  | 2.91                     | 0.48              |
| 1:E:24:VAL:HG23 | 1:E:108:SER:O    | 2.14                     | 0.48              |
| 1:G:5:ARG:CB    | 1:G:36:ILE:HB    | 2.42                     | 0.48              |
| 1:G:24:VAL:HG23 | 1:G:108:SER:O    | 2.14                     | 0.48              |
| 1:H:86:TYR:C    | 1:H:87:ASN:HD22  | 2.22                     | 0.48              |
| 1:I:43:THR:HG22 | 1:J:14:LYS:HE2   | 1.95                     | 0.48              |
| 1:J:24:VAL:HG23 | 1:J:108:SER:O    | 2.14                     | 0.48              |
| 1:K:24:VAL:HG23 | 1:K:108:SER:O    | 2.14                     | 0.48              |
| 1:K:57:PHE:CE1  | 1:L:105:VAL:HG13 | 2.41                     | 0.48              |
| 1:L:24:VAL:HG23 | 1:L:108:SER:O    | 2.14                     | 0.48              |
| 1:M:24:VAL:HG23 | 1:M:108:SER:O    | 2.14                     | 0.48              |
| 1:A:57:PHE:HZ   | 1:B:28:ALA:N     | 2.11                     | 0.48              |
| 1:B:83:LYS:HA   | 1:B:83:LYS:HD3   | 1.57                     | 0.48              |
| 1:B:89:VAL:HG13 | 1:B:89:VAL:O     | 2.14                     | 0.48              |
| 1:C:32:VAL:HG11 | 1:C:49:PHE:O     | 2.13                     | 0.48              |
| 1:F:24:VAL:HG23 | 1:F:108:SER:O    | 2.14                     | 0.48              |
| 1:F:43:THR:HG22 | 1:G:14:LYS:HE2   | 1.96                     | 0.48              |
| 1:F:55:ARG:CD   | 1:G:11:TYR:CD2   | 2.95                     | 0.48              |
| 1:H:24:VAL:HG23 | 1:H:108:SER:O    | 2.14                     | 0.48              |
| 1:H:26:ILE:CD1  | 1:H:37:VAL:HB    | 2.37                     | 0.48              |
| 1:I:24:VAL:HG23 | 1:I:108:SER:O    | 2.14                     | 0.48              |
| 1:I:90:LEU:HB2  | 1:I:105:VAL:CG2  | 2.38                     | 0.48              |
| 1:J:86:TYR:C    | 1:J:87:ASN:HD22  | 2.22                     | 0.48              |
| 1:M:55:ARG:CD   | 1:N:11:TYR:CD2   | 2.95                     | 0.48              |
| 1:N:24:VAL:HG23 | 1:N:108:SER:O    | 2.14                     | 0.48              |
| 1:A:26:ILE:CG1  | 1:A:37:VAL:CG2   | 2.92                     | 0.48              |
| 1:A:29:VAL:HG13 | 1:A:29:VAL:O     | 2.13                     | 0.48              |
| 1:A:86:TYR:C    | 1:A:87:ASN:HD22  | 2.22                     | 0.48              |
| 1:B:26:ILE:CG1  | 1:B:37:VAL:CG2   | 2.92                     | 0.48              |
| 1:C:24:VAL:HG22 | 1:C:25:LYS:H     | 1.78                     | 0.48              |
| 1:E:43:THR:HG22 | 1:F:14:LYS:HE2   | 1.96                     | 0.48              |
| 1:F:57:PHE:HZ   | 1:G:28:ALA:N     | 2.11                     | 0.48              |
| 1:G:29:VAL:HG13 | 1:G:29:VAL:O     | 2.13                     | 0.48              |
| 1:G:89:VAL:HG13 | 1:G:89:VAL:O     | 2.14                     | 0.48              |
| 1:H:49:PHE:HE2  | 1:H:79:ILE:CD1   | 2.26                     | 0.48              |
| 1:I:26:ILE:HG13 | 1:I:37:VAL:CG2   | 2.44                     | 0.48              |
| 1:I:49:PHE:CD2  | 1:I:79:ILE:HG13  | 2.48                     | 0.48              |
| 1:I:65:PHE:CD1  | 1:I:80:VAL:HG12  | 2.41                     | 0.48              |
| 1:J:43:THR:HG22 | 1:K:14:LYS:HE2   | 1.96                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:109:PHE:C   | 1:K:109:PHE:CD1 | 2.91                     | 0.48              |
| 1:L:86:TYR:C    | 1:L:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:M:9:TYR:H     | 1:M:9:TYR:HD1   | 1.62                     | 0.48              |
| 1:M:86:TYR:C    | 1:M:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:N:68:PRO:O    | 1:N:77:LEU:HB2  | 2.13                     | 0.48              |
| 1:N:86:TYR:C    | 1:N:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:A:24:VAL:HG23 | 1:A:108:SER:O   | 2.14                     | 0.48              |
| 1:C:89:VAL:O    | 1:C:89:VAL:HG13 | 2.14                     | 0.48              |
| 1:D:24:VAL:HG11 | 1:D:26:ILE:HD12 | 1.92                     | 0.48              |
| 1:D:24:VAL:HG23 | 1:D:108:SER:O   | 2.14                     | 0.48              |
| 1:D:29:VAL:HG13 | 1:D:29:VAL:O    | 2.13                     | 0.48              |
| 1:E:24:VAL:HG11 | 1:E:26:ILE:HD12 | 1.92                     | 0.48              |
| 1:E:49:PHE:HE2  | 1:E:79:ILE:CD1  | 2.26                     | 0.48              |
| 1:E:55:ARG:CD   | 1:F:11:TYR:CD2  | 2.95                     | 0.48              |
| 1:H:26:ILE:HG13 | 1:H:37:VAL:CG2  | 2.44                     | 0.48              |
| 1:H:32:VAL:HG11 | 1:H:49:PHE:O    | 2.13                     | 0.48              |
| 1:J:26:ILE:HG13 | 1:J:37:VAL:CG2  | 2.44                     | 0.48              |
| 1:L:57:PHE:HZ   | 1:M:28:ALA:N    | 2.11                     | 0.48              |
| 1:M:57:PHE:HZ   | 1:N:28:ALA:N    | 2.11                     | 0.48              |
| 1:N:49:PHE:CD2  | 1:N:79:ILE:HG13 | 2.48                     | 0.48              |
| 1:B:24:VAL:HG22 | 1:B:25:LYS:H    | 1.78                     | 0.48              |
| 1:B:29:VAL:HG13 | 1:B:29:VAL:O    | 2.14                     | 0.48              |
| 1:B:86:TYR:C    | 1:B:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:B:109:PHE:CD1 | 1:B:109:PHE:C   | 2.91                     | 0.48              |
| 1:C:24:VAL:HG23 | 1:C:108:SER:O   | 2.14                     | 0.48              |
| 1:C:29:VAL:HG13 | 1:C:29:VAL:O    | 2.14                     | 0.48              |
| 1:D:86:TYR:C    | 1:D:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:D:89:VAL:HG13 | 1:D:89:VAL:O    | 2.14                     | 0.48              |
| 1:E:29:VAL:HG13 | 1:E:29:VAL:O    | 2.13                     | 0.48              |
| 1:G:55:ARG:CD   | 1:H:11:TYR:CD2  | 2.95                     | 0.48              |
| 1:G:86:TYR:C    | 1:G:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:K:65:PHE:CD1  | 1:K:80:VAL:HG12 | 2.41                     | 0.48              |
| 1:K:86:TYR:C    | 1:K:87:ASN:HD22 | 2.22                     | 0.48              |
| 1:L:9:TYR:H     | 1:L:9:TYR:HD1   | 1.62                     | 0.48              |
| 1:N:26:ILE:CG1  | 1:N:37:VAL:CG2  | 2.92                     | 0.48              |
| 1:A:28:ALA:N    | 1:N:57:PHE:HZ   | 2.11                     | 0.47              |
| 1:A:89:VAL:O    | 1:A:89:VAL:HG13 | 2.14                     | 0.47              |
| 1:C:26:ILE:CG1  | 1:C:37:VAL:CG2  | 2.92                     | 0.47              |
| 1:D:38:VAL:CA   | 1:D:109:PHE:CE2 | 2.97                     | 0.47              |
| 1:E:56:THR:CG2  | 1:E:57:PHE:H    | 2.23                     | 0.47              |
| 1:G:26:ILE:HG13 | 1:G:37:VAL:CG2  | 2.44                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:26:ILE:CD1  | 1:G:37:VAL:HB    | 2.37                     | 0.47              |
| 1:H:5:ARG:CB    | 1:H:36:ILE:HB    | 2.42                     | 0.47              |
| 1:K:26:ILE:HG13 | 1:K:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:A:109:PHE:C   | 1:A:109:PHE:CD1  | 2.91                     | 0.47              |
| 1:C:26:ILE:HG13 | 1:C:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:C:38:VAL:CA   | 1:C:109:PHE:CE2  | 2.98                     | 0.47              |
| 1:C:86:TYR:C    | 1:C:87:ASN:HD22  | 2.22                     | 0.47              |
| 1:D:84:ARG:HB3  | 1:D:85:THR:H     | 1.34                     | 0.47              |
| 1:D:110:ILE:H   | 1:D:110:ILE:HG12 | 1.51                     | 0.47              |
| 1:F:24:VAL:HG11 | 1:F:26:ILE:HD12  | 1.92                     | 0.47              |
| 1:G:83:LYS:CE   | 1:G:109:PHE:HZ   | 2.23                     | 0.47              |
| 1:J:38:VAL:HG13 | 1:J:107:LYS:HZ3  | 1.78                     | 0.47              |
| 1:K:38:VAL:HG23 | 1:K:39:ALA:H     | 1.79                     | 0.47              |
| 1:L:49:PHE:HE2  | 1:L:79:ILE:CD1   | 2.26                     | 0.47              |
| 1:L:109:PHE:CD1 | 1:L:109:PHE:C    | 2.91                     | 0.47              |
| 1:A:11:TYR:CD2  | 1:N:55:ARG:CD    | 2.95                     | 0.47              |
| 1:B:49:PHE:HE2  | 1:B:79:ILE:CD1   | 2.26                     | 0.47              |
| 1:C:83:LYS:CE   | 1:C:109:PHE:HZ   | 2.23                     | 0.47              |
| 1:D:43:THR:HG22 | 1:E:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:D:50:GLY:HA3  | 1:D:77:LEU:HD13  | 1.91                     | 0.47              |
| 1:E:38:VAL:CA   | 1:E:109:PHE:CE2  | 2.97                     | 0.47              |
| 1:J:29:VAL:HG13 | 1:J:29:VAL:O     | 2.14                     | 0.47              |
| 1:K:29:VAL:HG13 | 1:K:29:VAL:O     | 2.13                     | 0.47              |
| 1:K:89:VAL:O    | 1:K:89:VAL:HG13  | 2.14                     | 0.47              |
| 1:L:43:THR:HG22 | 1:M:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:L:83:LYS:HD3  | 1:L:83:LYS:HA    | 1.57                     | 0.47              |
| 1:N:9:TYR:H     | 1:N:9:TYR:HD1    | 1.62                     | 0.47              |
| 1:N:89:VAL:O    | 1:N:89:VAL:HG13  | 2.14                     | 0.47              |
| 1:B:26:ILE:HG13 | 1:B:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:B:38:VAL:CA   | 1:B:109:PHE:CE2  | 2.98                     | 0.47              |
| 1:C:24:VAL:HG11 | 1:C:26:ILE:HD12  | 1.92                     | 0.47              |
| 1:C:56:THR:CG2  | 1:C:57:PHE:H     | 2.23                     | 0.47              |
| 1:D:18:TYR:CD2  | 1:D:23:VAL:HG13  | 2.46                     | 0.47              |
| 1:D:26:ILE:HG13 | 1:D:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:E:64:PHE:N    | 1:E:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:F:23:VAL:HG23 | 1:F:23:VAL:O     | 2.15                     | 0.47              |
| 1:F:26:ILE:HG13 | 1:F:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:H:23:VAL:O    | 1:H:23:VAL:HG23  | 2.15                     | 0.47              |
| 1:H:38:VAL:HG23 | 1:H:39:ALA:H     | 1.79                     | 0.47              |
| 1:H:64:PHE:N    | 1:H:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:I:38:VAL:HG23 | 1:I:39:ALA:H     | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:57:PHE:CE1   | 1:J:105:VAL:HG13 | 2.41                     | 0.47              |
| 1:K:57:PHE:HZ    | 1:L:28:ALA:N     | 2.11                     | 0.47              |
| 1:L:26:ILE:HG13  | 1:L:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:L:88:ILE:HD11  | 1:L:107:LYS:CG   | 2.34                     | 0.47              |
| 1:L:89:VAL:HG13  | 1:L:89:VAL:O     | 2.14                     | 0.47              |
| 1:M:26:ILE:CG1   | 1:M:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:M:109:PHE:CD1  | 1:M:109:PHE:C    | 2.91                     | 0.47              |
| 1:N:109:PHE:C    | 1:N:109:PHE:CD1  | 2.91                     | 0.47              |
| 1:A:14:LYS:HE2   | 1:N:43:THR:HG22  | 1.96                     | 0.47              |
| 1:E:18:TYR:CD2   | 1:E:23:VAL:HG13  | 2.46                     | 0.47              |
| 1:E:86:TYR:C     | 1:E:87:ASN:HD22  | 2.22                     | 0.47              |
| 1:J:65:PHE:CD1   | 1:J:80:VAL:HG12  | 2.41                     | 0.47              |
| 1:J:89:VAL:HG13  | 1:J:89:VAL:O     | 2.14                     | 0.47              |
| 1:K:9:TYR:H      | 1:K:9:TYR:HD1    | 1.62                     | 0.47              |
| 1:K:88:ILE:HD11  | 1:K:107:LYS:CG   | 2.34                     | 0.47              |
| 1:M:88:ILE:HD11  | 1:M:107:LYS:CG   | 2.34                     | 0.47              |
| 1:A:26:ILE:HG13  | 1:A:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:B:43:THR:HG22  | 1:C:14:LYS:HE2   | 1.95                     | 0.47              |
| 1:C:18:TYR:CD2   | 1:C:23:VAL:HG13  | 2.46                     | 0.47              |
| 1:C:45:ILE:HG23  | 1:D:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:C:64:PHE:N     | 1:C:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:C:83:LYS:HA    | 1:C:83:LYS:HD3   | 1.57                     | 0.47              |
| 1:D:45:ILE:HG23  | 1:E:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:E:26:ILE:HG13  | 1:E:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:E:88:ILE:HD11  | 1:E:107:LYS:CG   | 2.34                     | 0.47              |
| 1:F:38:VAL:HG23  | 1:F:39:ALA:H     | 1.79                     | 0.47              |
| 1:F:86:TYR:C     | 1:F:87:ASN:HD22  | 2.22                     | 0.47              |
| 1:F:92:PHE:H     | 1:F:104:THR:HG22 | 1.80                     | 0.47              |
| 1:G:24:VAL:HG21  | 1:G:107:LYS:CD   | 2.45                     | 0.47              |
| 1:G:38:VAL:HG13  | 1:G:107:LYS:HZ3  | 1.79                     | 0.47              |
| 1:H:65:PHE:CD1   | 1:H:80:VAL:HG12  | 2.41                     | 0.47              |
| 1:I:5:ARG:CB     | 1:I:36:ILE:HB    | 2.42                     | 0.47              |
| 1:J:23:VAL:HG23  | 1:J:23:VAL:O     | 2.15                     | 0.47              |
| 1:A:24:VAL:HG21  | 1:A:107:LYS:CD   | 2.45                     | 0.47              |
| 1:A:38:VAL:CA    | 1:A:109:PHE:CE2  | 2.98                     | 0.47              |
| 1:A:105:VAL:HG13 | 1:N:57:PHE:CE1   | 2.41                     | 0.47              |
| 1:B:24:VAL:HG21  | 1:B:107:LYS:CD   | 2.45                     | 0.47              |
| 1:B:45:ILE:HG23  | 1:C:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:B:64:PHE:N     | 1:B:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:D:92:PHE:H     | 1:D:104:THR:HG22 | 1.80                     | 0.47              |
| 1:E:45:ILE:HG23  | 1:F:14:LYS:HE2   | 1.96                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:26:ILE:CD1  | 1:F:37:VAL:HB    | 2.37                     | 0.47              |
| 1:F:29:VAL:HG13 | 1:F:29:VAL:O     | 2.13                     | 0.47              |
| 1:F:38:VAL:CA   | 1:F:109:PHE:CE2  | 2.98                     | 0.47              |
| 1:G:36:ILE:HG12 | 1:G:37:VAL:N     | 2.30                     | 0.47              |
| 1:H:24:VAL:HG21 | 1:H:107:LYS:CD   | 2.45                     | 0.47              |
| 1:H:26:ILE:CG1  | 1:H:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:H:36:ILE:HG12 | 1:H:37:VAL:N     | 2.30                     | 0.47              |
| 1:H:56:THR:HG22 | 1:H:57:PHE:N     | 2.18                     | 0.47              |
| 1:H:92:PHE:H    | 1:H:104:THR:HG22 | 1.80                     | 0.47              |
| 1:I:26:ILE:CG1  | 1:I:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:I:79:ILE:HG22 | 1:I:81:THR:CB    | 2.45                     | 0.47              |
| 1:J:26:ILE:CG1  | 1:J:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:J:79:ILE:HG22 | 1:J:81:THR:CB    | 2.45                     | 0.47              |
| 1:J:88:ILE:HD11 | 1:J:107:LYS:CG   | 2.34                     | 0.47              |
| 1:K:23:VAL:O    | 1:K:23:VAL:HG23  | 2.15                     | 0.47              |
| 1:M:23:VAL:O    | 1:M:23:VAL:HG23  | 2.15                     | 0.47              |
| 1:M:26:ILE:HG13 | 1:M:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:N:26:ILE:HG13 | 1:N:37:VAL:CG2   | 2.44                     | 0.47              |
| 1:C:70:GLN:HE21 | 1:C:70:GLN:HB3   | 1.50                     | 0.47              |
| 1:D:26:ILE:CG1  | 1:D:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:E:23:VAL:HG23 | 1:E:23:VAL:O     | 2.15                     | 0.47              |
| 1:E:65:PHE:CD1  | 1:E:80:VAL:HG12  | 2.41                     | 0.47              |
| 1:F:18:TYR:CD2  | 1:F:23:VAL:HG13  | 2.46                     | 0.47              |
| 1:F:24:VAL:HG21 | 1:F:107:LYS:CD   | 2.45                     | 0.47              |
| 1:F:45:ILE:HG23 | 1:G:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:F:89:VAL:O    | 1:F:89:VAL:HG13  | 2.14                     | 0.47              |
| 1:G:56:THR:CG2  | 1:G:57:PHE:H     | 2.23                     | 0.47              |
| 1:G:79:ILE:HG22 | 1:G:81:THR:CB    | 2.45                     | 0.47              |
| 1:H:79:ILE:HG22 | 1:H:81:THR:CB    | 2.45                     | 0.47              |
| 1:I:89:VAL:O    | 1:I:89:VAL:HG13  | 2.14                     | 0.47              |
| 1:J:5:ARG:CB    | 1:J:36:ILE:HB    | 2.42                     | 0.47              |
| 1:K:26:ILE:CG1  | 1:K:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:L:79:ILE:HG22 | 1:L:81:THR:CB    | 2.45                     | 0.47              |
| 1:L:92:PHE:H    | 1:L:104:THR:HG22 | 1.80                     | 0.47              |
| 1:M:89:VAL:HG13 | 1:M:89:VAL:O     | 2.14                     | 0.47              |
| 1:N:88:ILE:HD11 | 1:N:107:LYS:CG   | 2.34                     | 0.47              |
| 1:A:55:ARG:CD   | 1:B:11:TYR:CD2   | 2.96                     | 0.47              |
| 1:C:23:VAL:O    | 1:C:23:VAL:HG23  | 2.15                     | 0.47              |
| 1:D:24:VAL:HG21 | 1:D:107:LYS:CD   | 2.45                     | 0.47              |
| 1:E:26:ILE:CG1  | 1:E:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:F:64:PHE:N    | 1:F:64:PHE:CD1   | 2.83                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:79:ILE:HG22 | 1:F:81:THR:CB    | 2.45                     | 0.47              |
| 1:G:24:VAL:HG11 | 1:G:26:ILE:HD12  | 1.92                     | 0.47              |
| 1:G:26:ILE:CG1  | 1:G:37:VAL:CG2   | 2.92                     | 0.47              |
| 1:G:43:THR:HG22 | 1:H:14:LYS:HE2   | 1.96                     | 0.47              |
| 1:G:65:PHE:CD1  | 1:G:80:VAL:HG12  | 2.41                     | 0.47              |
| 1:H:34:THR:HG23 | 1:H:47:HIS:CB    | 2.41                     | 0.47              |
| 1:I:24:VAL:HG21 | 1:I:107:LYS:CD   | 2.45                     | 0.47              |
| 1:I:36:ILE:HG12 | 1:I:37:VAL:N     | 2.30                     | 0.47              |
| 1:J:64:PHE:N    | 1:J:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:K:24:VAL:HG21 | 1:K:107:LYS:CD   | 2.45                     | 0.47              |
| 1:K:44:TYR:N    | 1:K:44:TYR:CD1   | 2.81                     | 0.47              |
| 1:K:64:PHE:N    | 1:K:64:PHE:CD1   | 2.83                     | 0.47              |
| 1:N:38:VAL:HG23 | 1:N:39:ALA:H     | 1.79                     | 0.47              |
| 1:A:12:ARG:HH11 | 1:N:66:VAL:CG1   | 2.28                     | 0.47              |
| 1:A:23:VAL:O    | 1:A:23:VAL:HG23  | 2.15                     | 0.47              |
| 1:A:92:PHE:H    | 1:A:104:THR:HG22 | 1.80                     | 0.47              |
| 1:B:18:TYR:CD2  | 1:B:23:VAL:HG13  | 2.46                     | 0.47              |
| 1:C:79:ILE:HG22 | 1:C:81:THR:CB    | 2.45                     | 0.47              |
| 1:D:23:VAL:HG23 | 1:D:23:VAL:O     | 2.15                     | 0.47              |
| 1:K:79:ILE:HG22 | 1:K:81:THR:CB    | 2.45                     | 0.47              |
| 1:M:44:TYR:N    | 1:M:44:TYR:CD1   | 2.81                     | 0.47              |
| 1:A:9:TYR:H     | 1:A:9:TYR:HD1    | 1.62                     | 0.46              |
| 1:A:45:ILE:HG23 | 1:B:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:B:64:PHE:N    | 1:B:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:B:92:PHE:H    | 1:B:104:THR:HG22 | 1.80                     | 0.46              |
| 1:C:36:ILE:HG12 | 1:C:37:VAL:N     | 2.30                     | 0.46              |
| 1:D:64:PHE:N    | 1:D:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:E:24:VAL:HG21 | 1:E:107:LYS:CD   | 2.45                     | 0.46              |
| 1:E:36:ILE:HG12 | 1:E:37:VAL:N     | 2.30                     | 0.46              |
| 1:F:36:ILE:HG12 | 1:F:37:VAL:N     | 2.30                     | 0.46              |
| 1:G:45:ILE:HG23 | 1:H:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:I:56:THR:HG22 | 1:I:57:PHE:N     | 2.18                     | 0.46              |
| 1:I:83:LYS:HD3  | 1:I:83:LYS:HA    | 1.57                     | 0.46              |
| 1:J:92:PHE:H    | 1:J:104:THR:HG22 | 1.80                     | 0.46              |
| 1:K:5:ARG:CB    | 1:K:36:ILE:HB    | 2.42                     | 0.46              |
| 1:K:45:ILE:HG23 | 1:L:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:L:23:VAL:HG23 | 1:L:23:VAL:O     | 2.15                     | 0.46              |
| 1:L:24:VAL:HG21 | 1:L:107:LYS:CD   | 2.45                     | 0.46              |
| 1:L:26:ILE:CG1  | 1:L:37:VAL:CG2   | 2.92                     | 0.46              |
| 1:M:38:VAL:HG23 | 1:M:39:ALA:H     | 1.79                     | 0.46              |
| 1:N:38:VAL:CA   | 1:N:109:PHE:CE2  | 2.98                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:64:PHE:N    | 1:N:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:N:92:PHE:H    | 1:N:104:THR:HG22 | 1.80                     | 0.46              |
| 1:B:36:ILE:HG12 | 1:B:37:VAL:N     | 2.30                     | 0.46              |
| 1:B:38:VAL:HG23 | 1:B:39:ALA:H     | 1.79                     | 0.46              |
| 1:D:79:ILE:HG22 | 1:D:81:THR:CB    | 2.45                     | 0.46              |
| 1:F:109:PHE:C   | 1:F:109:PHE:CD1  | 2.91                     | 0.46              |
| 1:G:38:VAL:CA   | 1:G:109:PHE:CE2  | 2.98                     | 0.46              |
| 1:I:9:TYR:H     | 1:I:9:TYR:HD1    | 1.62                     | 0.46              |
| 1:I:64:PHE:N    | 1:I:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:I:64:PHE:N    | 1:I:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:J:64:PHE:N    | 1:J:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:K:83:LYS:CE   | 1:K:109:PHE:HZ   | 2.23                     | 0.46              |
| 1:L:45:ILE:HG23 | 1:M:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:M:36:ILE:HG12 | 1:M:37:VAL:N     | 2.30                     | 0.46              |
| 1:N:36:ILE:HG12 | 1:N:37:VAL:N     | 2.30                     | 0.46              |
| 1:A:56:THR:CG2  | 1:A:57:PHE:H     | 2.23                     | 0.46              |
| 1:A:66:VAL:CG1  | 1:B:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:A:88:ILE:CG1  | 1:A:107:LYS:HB2  | 2.45                     | 0.46              |
| 1:B:24:VAL:HG11 | 1:B:26:ILE:HD12  | 1.92                     | 0.46              |
| 1:C:24:VAL:HG21 | 1:C:107:LYS:CD   | 2.45                     | 0.46              |
| 1:E:50:GLY:HA3  | 1:E:77:LEU:HD13  | 1.91                     | 0.46              |
| 1:E:64:PHE:N    | 1:E:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:G:86:TYR:HE1  | 1:G:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:H:86:TYR:HE1  | 1:H:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:I:23:VAL:HG23 | 1:I:23:VAL:O     | 2.15                     | 0.46              |
| 1:I:88:ILE:HD11 | 1:I:107:LYS:CG   | 2.34                     | 0.46              |
| 1:J:45:ILE:HG23 | 1:K:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:L:44:TYR:N    | 1:L:44:TYR:CD1   | 2.81                     | 0.46              |
| 1:M:88:ILE:CG1  | 1:M:107:LYS:HB2  | 2.45                     | 0.46              |
| 1:C:64:PHE:N    | 1:C:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:F:86:TYR:HE1  | 1:F:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:G:109:PHE:CD1 | 1:G:109:PHE:C    | 2.91                     | 0.46              |
| 1:H:3:VAL:HB    | 1:H:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:H:64:PHE:N    | 1:H:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:H:70:GLN:HE21 | 1:H:70:GLN:HB3   | 1.50                     | 0.46              |
| 1:I:92:PHE:H    | 1:I:104:THR:HG22 | 1.80                     | 0.46              |
| 1:L:38:VAL:HG23 | 1:L:39:ALA:H     | 1.80                     | 0.46              |
| 1:M:64:PHE:N    | 1:M:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:M:79:ILE:HG22 | 1:M:81:THR:CB    | 2.45                     | 0.46              |
| 1:N:86:TYR:HE1  | 1:N:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:N:88:ILE:CG1  | 1:N:107:LYS:HB2  | 2.45                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:14:LYS:HE2  | 1:N:45:ILE:HG23  | 1.96                     | 0.46              |
| 1:A:79:ILE:HG22 | 1:A:81:THR:CB    | 2.45                     | 0.46              |
| 1:B:79:ILE:HG22 | 1:B:81:THR:CB    | 2.45                     | 0.46              |
| 1:C:92:PHE:H    | 1:C:104:THR:HG22 | 1.80                     | 0.46              |
| 1:E:79:ILE:HG22 | 1:E:81:THR:CB    | 2.45                     | 0.46              |
| 1:F:26:ILE:CG1  | 1:F:37:VAL:CG2   | 2.92                     | 0.46              |
| 1:G:18:TYR:CD2  | 1:G:23:VAL:HG13  | 2.46                     | 0.46              |
| 1:G:23:VAL:HG23 | 1:G:23:VAL:O     | 2.15                     | 0.46              |
| 1:H:89:VAL:O    | 1:H:89:VAL:HG13  | 2.14                     | 0.46              |
| 1:I:66:VAL:CG1  | 1:J:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:I:86:TYR:HE1  | 1:I:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:J:3:VAL:HB    | 1:J:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:J:66:VAL:CG1  | 1:K:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:K:1:LEU:CD1   | 1:K:16:VAL:H     | 2.29                     | 0.46              |
| 1:K:66:VAL:CG1  | 1:L:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:L:1:LEU:CD1   | 1:L:16:VAL:H     | 2.29                     | 0.46              |
| 1:M:49:PHE:HE2  | 1:M:79:ILE:CD1   | 2.26                     | 0.46              |
| 1:M:64:PHE:N    | 1:M:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:N:64:PHE:N    | 1:N:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:B:88:ILE:CG1  | 1:B:107:LYS:HB2  | 2.45                     | 0.46              |
| 1:C:1:LEU:CD1   | 1:C:16:VAL:H     | 2.29                     | 0.46              |
| 1:E:86:TYR:HE1  | 1:E:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:H:66:VAL:CG1  | 1:I:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:I:49:PHE:HE2  | 1:I:79:ILE:CD1   | 2.26                     | 0.46              |
| 1:J:1:LEU:CD1   | 1:J:16:VAL:H     | 2.29                     | 0.46              |
| 1:J:36:ILE:HG12 | 1:J:37:VAL:N     | 2.30                     | 0.46              |
| 1:J:44:TYR:N    | 1:J:44:TYR:CD1   | 2.81                     | 0.46              |
| 1:K:64:PHE:N    | 1:K:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:K:83:LYS:HD3  | 1:K:83:LYS:HA    | 1.57                     | 0.46              |
| 1:L:36:ILE:HG12 | 1:L:37:VAL:N     | 2.30                     | 0.46              |
| 1:M:45:ILE:HG23 | 1:N:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:N:24:VAL:HG21 | 1:N:107:LYS:CD   | 2.45                     | 0.46              |
| 1:A:86:TYR:HE1  | 1:A:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:D:36:ILE:HG12 | 1:D:37:VAL:N     | 2.30                     | 0.46              |
| 1:D:38:VAL:HG23 | 1:D:39:ALA:H     | 1.79                     | 0.46              |
| 1:D:66:VAL:CG1  | 1:E:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:E:49:PHE:CB   | 1:E:55:ARG:HH22  | 2.17                     | 0.46              |
| 1:E:81:THR:HA   | 1:E:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:E:83:LYS:HZ2  | 1:E:111:GLU:HB3  | 1.81                     | 0.46              |
| 1:F:81:THR:HA   | 1:F:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:G:81:THR:HA   | 1:G:86:TYR:CE2   | 2.51                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:45:ILE:HG23 | 1:I:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:H:98:LYS:HE3  | 1:H:100:ASN:CA   | 2.36                     | 0.46              |
| 1:I:38:VAL:HG13 | 1:I:107:LYS:HZ3  | 1.80                     | 0.46              |
| 1:J:38:VAL:HG23 | 1:J:39:ALA:H     | 1.79                     | 0.46              |
| 1:J:81:THR:HA   | 1:J:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:K:29:VAL:HG12 | 1:K:92:PHE:HE2   | 1.81                     | 0.46              |
| 1:K:36:ILE:HG12 | 1:K:37:VAL:N     | 2.30                     | 0.46              |
| 1:L:38:VAL:HG13 | 1:L:107:LYS:HZ3  | 1.81                     | 0.46              |
| 1:M:66:VAL:CG1  | 1:N:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:M:86:TYR:HE1  | 1:M:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:A:18:TYR:CD2  | 1:A:23:VAL:HG13  | 2.46                     | 0.46              |
| 1:C:81:THR:HA   | 1:C:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:C:91:HIS:HB3  | 1:C:104:THR:CG2  | 2.37                     | 0.46              |
| 1:D:1:LEU:CD1   | 1:D:16:VAL:H     | 2.29                     | 0.46              |
| 1:D:46:THR:CB   | 1:E:14:LYS:HZ1   | 2.19                     | 0.46              |
| 1:D:57:PHE:CE1  | 1:E:105:VAL:HG13 | 2.41                     | 0.46              |
| 1:D:81:THR:HA   | 1:D:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:D:83:LYS:HZ2  | 1:D:111:GLU:HB3  | 1.81                     | 0.46              |
| 1:G:1:LEU:CD1   | 1:G:16:VAL:H     | 2.29                     | 0.46              |
| 1:G:92:PHE:H    | 1:G:104:THR:HG22 | 1.80                     | 0.46              |
| 1:H:81:THR:HA   | 1:H:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:H:88:ILE:HD11 | 1:H:107:LYS:CG   | 2.34                     | 0.46              |
| 1:I:34:THR:HG23 | 1:I:47:HIS:CB    | 2.41                     | 0.46              |
| 1:I:45:ILE:HG23 | 1:J:14:LYS:HE2   | 1.96                     | 0.46              |
| 1:I:56:THR:CG2  | 1:I:57:PHE:H     | 2.23                     | 0.46              |
| 1:I:81:THR:HA   | 1:I:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:J:49:PHE:HE2  | 1:J:79:ILE:CD1   | 2.25                     | 0.46              |
| 1:L:88:ILE:CG1  | 1:L:107:LYS:HB2  | 2.45                     | 0.46              |
| 1:M:1:LEU:CD1   | 1:M:16:VAL:H     | 2.29                     | 0.46              |
| 1:M:81:THR:HA   | 1:M:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:N:110:ILE:H   | 1:N:110:ILE:HG12 | 1.51                     | 0.46              |
| 1:A:36:ILE:HG12 | 1:A:37:VAL:N     | 2.30                     | 0.46              |
| 1:A:64:PHE:N    | 1:A:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:A:88:ILE:HD11 | 1:A:107:LYS:CG   | 2.34                     | 0.46              |
| 1:C:66:VAL:CG1  | 1:D:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:D:64:PHE:N    | 1:D:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:D:86:TYR:HE1  | 1:D:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:E:66:VAL:CG1  | 1:F:12:ARG:HH11  | 2.29                     | 0.46              |
| 1:H:1:LEU:CD1   | 1:H:16:VAL:H     | 2.29                     | 0.46              |
| 1:H:24:VAL:HG11 | 1:H:26:ILE:HD12  | 1.92                     | 0.46              |
| 1:H:38:VAL:CA   | 1:H:109:PHE:CE2  | 2.98                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:3:VAL:HB    | 1:I:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:J:24:VAL:HG21 | 1:J:107:LYS:CD   | 2.45                     | 0.46              |
| 1:J:86:TYR:HE1  | 1:J:88:ILE:HG12  | 1.81                     | 0.46              |
| 1:M:29:VAL:HG12 | 1:M:92:PHE:HE2   | 1.81                     | 0.46              |
| 1:M:38:VAL:CA   | 1:M:109:PHE:CE2  | 2.98                     | 0.46              |
| 1:N:79:ILE:HG22 | 1:N:81:THR:CB    | 2.45                     | 0.46              |
| 1:N:81:THR:HA   | 1:N:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:A:64:PHE:N    | 1:A:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:B:110:ILE:H   | 1:B:110:ILE:HG12 | 1.51                     | 0.46              |
| 1:C:81:THR:CA   | 1:C:86:TYR:HE2   | 2.29                     | 0.46              |
| 1:E:26:ILE:CD1  | 1:E:37:VAL:HB    | 2.37                     | 0.46              |
| 1:F:3:VAL:HB    | 1:F:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:F:64:PHE:N    | 1:F:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:G:3:VAL:HB    | 1:G:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:G:64:PHE:N    | 1:G:64:PHE:HD1   | 2.14                     | 0.46              |
| 1:K:3:VAL:HB    | 1:K:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:K:38:VAL:HG13 | 1:K:107:LYS:HZ3  | 1.81                     | 0.46              |
| 1:K:81:THR:HA   | 1:K:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:K:92:PHE:H    | 1:K:104:THR:HG22 | 1.80                     | 0.46              |
| 1:L:3:VAL:HB    | 1:L:40:PRO:HG3   | 1.98                     | 0.46              |
| 1:L:57:PHE:CE1  | 1:M:105:VAL:HG13 | 2.41                     | 0.46              |
| 1:L:64:PHE:N    | 1:L:64:PHE:CD1   | 2.83                     | 0.46              |
| 1:L:65:PHE:CD1  | 1:L:80:VAL:HG12  | 2.41                     | 0.46              |
| 1:L:81:THR:HA   | 1:L:86:TYR:CE2   | 2.51                     | 0.46              |
| 1:M:24:VAL:HG21 | 1:M:107:LYS:CD   | 2.45                     | 0.46              |
| 1:N:81:THR:CA   | 1:N:86:TYR:HE2   | 2.29                     | 0.46              |
| 1:A:81:THR:CA   | 1:A:86:TYR:HE2   | 2.30                     | 0.45              |
| 1:B:23:VAL:HG23 | 1:B:23:VAL:O     | 2.15                     | 0.45              |
| 1:B:55:ARG:CD   | 1:C:11:TYR:CD2   | 2.96                     | 0.45              |
| 1:B:66:VAL:CG1  | 1:C:12:ARG:HH11  | 2.29                     | 0.45              |
| 1:B:81:THR:HA   | 1:B:86:TYR:CE2   | 2.51                     | 0.45              |
| 1:C:88:ILE:CG1  | 1:C:107:LYS:HB2  | 2.45                     | 0.45              |
| 1:D:38:VAL:CG2  | 1:D:39:ALA:N     | 2.79                     | 0.45              |
| 1:G:66:VAL:CG1  | 1:H:12:ARG:HH11  | 2.28                     | 0.45              |
| 1:G:81:THR:CA   | 1:G:86:TYR:HE2   | 2.29                     | 0.45              |
| 1:H:81:THR:CA   | 1:H:86:TYR:HE2   | 2.30                     | 0.45              |
| 1:I:29:VAL:HG12 | 1:I:92:PHE:HE2   | 1.81                     | 0.45              |
| 1:I:44:TYR:N    | 1:I:44:TYR:CD1   | 2.81                     | 0.45              |
| 1:M:81:THR:CA   | 1:M:86:TYR:HE2   | 2.29                     | 0.45              |
| 1:M:92:PHE:H    | 1:M:104:THR:HG22 | 1.80                     | 0.45              |
| 1:A:3:VAL:HB    | 1:A:40:PRO:HG3   | 1.98                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:44:TYR:N    | 1:A:44:TYR:CD1   | 2.81                     | 0.45              |
| 1:A:81:THR:HA   | 1:A:86:TYR:CE2   | 2.51                     | 0.45              |
| 1:B:81:THR:CA   | 1:B:86:TYR:HE2   | 2.29                     | 0.45              |
| 1:C:38:VAL:CG2  | 1:C:39:ALA:N     | 2.79                     | 0.45              |
| 1:F:91:HIS:HB3  | 1:F:104:THR:CG2  | 2.37                     | 0.45              |
| 1:G:88:ILE:HD11 | 1:G:107:LYS:CG   | 2.34                     | 0.45              |
| 1:H:18:TYR:CD2  | 1:H:23:VAL:HG13  | 2.46                     | 0.45              |
| 1:L:81:THR:CA   | 1:L:86:TYR:HE2   | 2.30                     | 0.45              |
| 1:M:56:THR:CG2  | 1:M:57:PHE:H     | 2.23                     | 0.45              |
| 1:M:109:PHE:C   | 1:M:109:PHE:HD1  | 2.25                     | 0.45              |
| 1:N:44:TYR:N    | 1:N:44:TYR:CD1   | 2.81                     | 0.45              |
| 1:N:109:PHE:C   | 1:N:109:PHE:HD1  | 2.25                     | 0.45              |
| 1:B:1:LEU:CD1   | 1:B:16:VAL:H     | 2.29                     | 0.45              |
| 1:C:3:VAL:HB    | 1:C:40:PRO:HG3   | 1.98                     | 0.45              |
| 1:E:92:PHE:H    | 1:E:104:THR:HG22 | 1.80                     | 0.45              |
| 1:F:1:LEU:CD1   | 1:F:16:VAL:H     | 2.29                     | 0.45              |
| 1:F:49:PHE:HE2  | 1:F:79:ILE:CD1   | 2.26                     | 0.45              |
| 1:F:66:VAL:CG1  | 1:G:12:ARG:HH11  | 2.29                     | 0.45              |
| 1:H:38:VAL:HG13 | 1:H:107:LYS:HZ3  | 1.81                     | 0.45              |
| 1:H:46:THR:CA   | 1:I:14:LYS:HZ1   | 2.29                     | 0.45              |
| 1:K:56:THR:CG2  | 1:K:57:PHE:H     | 2.23                     | 0.45              |
| 1:L:64:PHE:N    | 1:L:64:PHE:HD1   | 2.14                     | 0.45              |
| 1:M:50:GLY:O    | 1:M:70:GLN:HG3   | 2.17                     | 0.45              |
| 1:M:86:TYR:C    | 1:M:86:TYR:CD1   | 2.94                     | 0.45              |
| 1:N:1:LEU:CD1   | 1:N:16:VAL:H     | 2.29                     | 0.45              |
| 1:N:23:VAL:O    | 1:N:23:VAL:HG23  | 2.15                     | 0.45              |
| 1:A:38:VAL:HG13 | 1:A:107:LYS:HZ3  | 1.82                     | 0.45              |
| 1:D:81:THR:CA   | 1:D:86:TYR:HE2   | 2.29                     | 0.45              |
| 1:F:65:PHE:CD1  | 1:F:80:VAL:HG12  | 2.41                     | 0.45              |
| 1:H:34:THR:OG1  | 1:H:47:HIS:HB2   | 2.17                     | 0.45              |
| 1:H:86:TYR:C    | 1:H:86:TYR:CD1   | 2.94                     | 0.45              |
| 1:I:1:LEU:CD1   | 1:I:16:VAL:H     | 2.29                     | 0.45              |
| 1:I:109:PHE:C   | 1:I:109:PHE:HD1  | 2.25                     | 0.45              |
| 1:J:109:PHE:C   | 1:J:109:PHE:HD1  | 2.25                     | 0.45              |
| 1:L:66:VAL:CG1  | 1:M:12:ARG:HH11  | 2.29                     | 0.45              |
| 1:L:86:TYR:C    | 1:L:86:TYR:CD1   | 2.94                     | 0.45              |
| 1:L:109:PHE:C   | 1:L:109:PHE:HD1  | 2.25                     | 0.45              |
| 1:N:86:TYR:C    | 1:N:86:TYR:CD1   | 2.94                     | 0.45              |
| 1:A:50:GLY:O    | 1:A:70:GLN:HG3   | 2.17                     | 0.45              |
| 1:B:38:VAL:CG2  | 1:B:39:ALA:N     | 2.79                     | 0.45              |
| 1:C:86:TYR:C    | 1:C:86:TYR:CD1   | 2.94                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:86:TYR:HE1  | 1:C:88:ILE:HG12 | 1.81                     | 0.45              |
| 1:D:50:GLY:O    | 1:D:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:D:86:TYR:C    | 1:D:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:E:44:TYR:N    | 1:E:44:TYR:CD1  | 2.81                     | 0.45              |
| 1:G:64:PHE:N    | 1:G:64:PHE:CD1  | 2.83                     | 0.45              |
| 1:G:86:TYR:C    | 1:G:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:I:38:VAL:CA   | 1:I:109:PHE:CE2 | 2.98                     | 0.45              |
| 1:I:86:TYR:C    | 1:I:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:J:91:HIS:HB3  | 1:J:104:THR:CG2 | 2.37                     | 0.45              |
| 1:K:81:THR:CA   | 1:K:86:TYR:HE2  | 2.29                     | 0.45              |
| 1:K:86:TYR:C    | 1:K:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:K:109:PHE:C   | 1:K:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:L:38:VAL:CA   | 1:L:109:PHE:CE2 | 2.97                     | 0.45              |
| 1:L:86:TYR:HE1  | 1:L:88:ILE:HG12 | 1.81                     | 0.45              |
| 1:A:86:TYR:C    | 1:A:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:B:86:TYR:HE1  | 1:B:88:ILE:HG12 | 1.81                     | 0.45              |
| 1:C:109:PHE:C   | 1:C:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:D:109:PHE:C   | 1:D:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:E:1:LEU:CD1   | 1:E:16:VAL:H    | 2.29                     | 0.45              |
| 1:E:79:ILE:HD12 | 1:E:107:LYS:HZ1 | 1.82                     | 0.45              |
| 1:F:81:THR:CA   | 1:F:86:TYR:HE2  | 2.29                     | 0.45              |
| 1:I:81:THR:CA   | 1:I:86:TYR:HE2  | 2.29                     | 0.45              |
| 1:J:9:TYR:H     | 1:J:9:TYR:HD1   | 1.62                     | 0.45              |
| 1:K:86:TYR:HE1  | 1:K:88:ILE:HG12 | 1.81                     | 0.45              |
| 1:K:88:ILE:CG1  | 1:K:107:LYS:HB2 | 2.45                     | 0.45              |
| 1:A:24:VAL:HG11 | 1:A:26:ILE:HD12 | 1.92                     | 0.45              |
| 1:A:38:VAL:HG23 | 1:A:39:ALA:H    | 1.79                     | 0.45              |
| 1:A:46:THR:CB   | 1:B:14:LYS:HZ1  | 2.21                     | 0.45              |
| 1:A:109:PHE:C   | 1:A:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:C:38:VAL:HG23 | 1:C:39:ALA:H    | 1.79                     | 0.45              |
| 1:C:49:PHE:HE2  | 1:C:79:ILE:CD1  | 2.25                     | 0.45              |
| 1:F:50:GLY:O    | 1:F:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:F:88:ILE:HD11 | 1:F:107:LYS:CG  | 2.34                     | 0.45              |
| 1:F:88:ILE:CG1  | 1:F:107:LYS:HB2 | 2.45                     | 0.45              |
| 1:G:98:LYS:HE3  | 1:G:100:ASN:CA  | 2.36                     | 0.45              |
| 1:H:1:LEU:CG    | 1:H:13:ILE:HD11 | 2.47                     | 0.45              |
| 1:H:79:ILE:HG22 | 1:H:81:THR:HB   | 1.99                     | 0.45              |
| 1:H:83:LYS:HA   | 1:H:83:LYS:HD3  | 1.57                     | 0.45              |
| 1:H:84:ARG:HB3  | 1:H:85:THR:H    | 1.34                     | 0.45              |
| 1:I:29:VAL:HG11 | 1:I:77:LEU:HD11 | 1.98                     | 0.45              |
| 1:I:79:ILE:HG22 | 1:I:81:THR:HB   | 1.99                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:79:ILE:HG22 | 1:J:81:THR:HB   | 1.99                     | 0.45              |
| 1:J:86:TYR:C    | 1:J:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:K:38:VAL:CA   | 1:K:109:PHE:CE2 | 2.97                     | 0.45              |
| 1:M:65:PHE:CD1  | 1:M:80:VAL:HG12 | 2.41                     | 0.45              |
| 1:A:13:ILE:HG22 | 1:N:46:THR:HG1  | 1.76                     | 0.45              |
| 1:A:29:VAL:HG12 | 1:A:92:PHE:HE2  | 1.81                     | 0.45              |
| 1:B:34:THR:OG1  | 1:B:47:HIS:HB2  | 2.17                     | 0.45              |
| 1:B:86:TYR:C    | 1:B:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:E:109:PHE:C   | 1:E:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:F:49:PHE:CB   | 1:F:55:ARG:HH22 | 2.17                     | 0.45              |
| 1:F:86:TYR:C    | 1:F:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:G:83:LYS:HZ2  | 1:G:111:GLU:HB3 | 1.82                     | 0.45              |
| 1:I:24:VAL:HG11 | 1:I:26:ILE:HD12 | 1.92                     | 0.45              |
| 1:I:34:THR:OG1  | 1:I:47:HIS:HB2  | 2.17                     | 0.45              |
| 1:J:24:VAL:HG11 | 1:J:38:VAL:HG13 | 1.99                     | 0.45              |
| 1:J:38:VAL:CA   | 1:J:109:PHE:CE2 | 2.98                     | 0.45              |
| 1:K:24:VAL:HG11 | 1:K:38:VAL:HG13 | 1.99                     | 0.45              |
| 1:M:84:ARG:HB3  | 1:M:85:THR:H    | 1.34                     | 0.45              |
| 1:N:49:PHE:HE2  | 1:N:79:ILE:CD1  | 2.26                     | 0.45              |
| 1:A:34:THR:OG1  | 1:A:47:HIS:HB2  | 2.17                     | 0.45              |
| 1:C:34:THR:OG1  | 1:C:47:HIS:HB2  | 2.17                     | 0.45              |
| 1:C:50:GLY:O    | 1:C:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:D:49:PHE:CB   | 1:D:55:ARG:HH22 | 2.17                     | 0.45              |
| 1:E:3:VAL:HB    | 1:E:40:PRO:HG3  | 1.98                     | 0.45              |
| 1:E:38:VAL:HG23 | 1:E:39:ALA:H    | 1.80                     | 0.45              |
| 1:E:86:TYR:C    | 1:E:86:TYR:CD1  | 2.94                     | 0.45              |
| 1:E:88:ILE:CG1  | 1:E:107:LYS:HB2 | 2.45                     | 0.45              |
| 1:F:13:ILE:HD12 | 1:F:14:LYS:O    | 2.17                     | 0.45              |
| 1:G:1:LEU:CG    | 1:G:13:ILE:HD11 | 2.47                     | 0.45              |
| 1:G:13:ILE:HD12 | 1:G:14:LYS:O    | 2.17                     | 0.45              |
| 1:H:109:PHE:C   | 1:H:109:PHE:HD1 | 2.25                     | 0.45              |
| 1:I:50:GLY:O    | 1:I:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:J:50:GLY:O    | 1:J:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:K:50:GLY:O    | 1:K:70:GLN:HG3  | 2.17                     | 0.45              |
| 1:L:24:VAL:HG11 | 1:L:38:VAL:HG13 | 1.99                     | 0.45              |
| 1:A:1:LEU:CD1   | 1:A:16:VAL:H    | 2.29                     | 0.45              |
| 1:A:38:VAL:CG2  | 1:A:39:ALA:N    | 2.79                     | 0.45              |
| 1:B:9:TYR:H     | 1:B:9:TYR:HD1   | 1.62                     | 0.45              |
| 1:D:3:VAL:HB    | 1:D:40:PRO:HG3  | 1.98                     | 0.45              |
| 1:D:34:THR:OG1  | 1:D:47:HIS:HB2  | 2.17                     | 0.45              |
| 1:G:34:THR:OG1  | 1:G:47:HIS:HB2  | 2.17                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:79:ILE:HG22 | 1:G:81:THR:HB   | 1.99                     | 0.45              |
| 1:G:88:ILE:CG1  | 1:G:107:LYS:HB2 | 2.45                     | 0.45              |
| 1:H:29:VAL:HG11 | 1:H:77:LEU:HD11 | 1.98                     | 0.45              |
| 1:H:44:TYR:N    | 1:H:44:TYR:CD1  | 2.81                     | 0.45              |
| 1:I:24:VAL:HG11 | 1:I:38:VAL:HG13 | 1.99                     | 0.45              |
| 1:K:79:ILE:HG22 | 1:K:81:THR:HB   | 1.99                     | 0.45              |
| 1:M:3:VAL:HB    | 1:M:40:PRO:HG3  | 1.98                     | 0.45              |
| 1:M:83:LYS:HD3  | 1:M:83:LYS:HA   | 1.57                     | 0.45              |
| 1:N:3:VAL:HB    | 1:N:40:PRO:HG3  | 1.98                     | 0.45              |
| 1:N:24:VAL:HG11 | 1:N:26:ILE:HD12 | 1.92                     | 0.45              |
| 1:A:5:ARG:HB2   | 1:A:36:ILE:CB   | 2.47                     | 0.44              |
| 1:B:50:GLY:O    | 1:B:70:GLN:HG3  | 2.17                     | 0.44              |
| 1:C:13:ILE:HD12 | 1:C:14:LYS:O    | 2.17                     | 0.44              |
| 1:D:13:ILE:HD12 | 1:D:14:LYS:O    | 2.17                     | 0.44              |
| 1:D:88:ILE:CG1  | 1:D:107:LYS:HB2 | 2.45                     | 0.44              |
| 1:E:13:ILE:HD12 | 1:E:14:LYS:O    | 2.17                     | 0.44              |
| 1:E:84:ARG:HB3  | 1:E:85:THR:H    | 1.34                     | 0.44              |
| 1:F:109:PHE:C   | 1:F:109:PHE:HD1 | 2.25                     | 0.44              |
| 1:G:38:VAL:HG23 | 1:G:39:ALA:H    | 1.79                     | 0.44              |
| 1:G:50:GLY:O    | 1:G:70:GLN:HG3  | 2.17                     | 0.44              |
| 1:H:13:ILE:HD12 | 1:H:14:LYS:O    | 2.17                     | 0.44              |
| 1:J:81:THR:CA   | 1:J:86:TYR:HE2  | 2.29                     | 0.44              |
| 1:M:5:ARG:HB2   | 1:M:36:ILE:CB   | 2.47                     | 0.44              |
| 1:M:24:VAL:HG11 | 1:M:26:ILE:HD12 | 1.92                     | 0.44              |
| 1:N:5:ARG:HB2   | 1:N:36:ILE:CB   | 2.47                     | 0.44              |
| 1:N:34:THR:OG1  | 1:N:47:HIS:HB2  | 2.17                     | 0.44              |
| 1:A:83:LYS:HD3  | 1:A:83:LYS:HA   | 1.57                     | 0.44              |
| 1:B:13:ILE:HD12 | 1:B:14:LYS:O    | 2.17                     | 0.44              |
| 1:B:109:PHE:C   | 1:B:109:PHE:HD1 | 2.25                     | 0.44              |
| 1:F:1:LEU:CG    | 1:F:13:ILE:HD11 | 2.47                     | 0.44              |
| 1:I:1:LEU:CG    | 1:I:13:ILE:HD11 | 2.47                     | 0.44              |
| 1:I:13:ILE:HD12 | 1:I:14:LYS:O    | 2.17                     | 0.44              |
| 1:J:29:VAL:HG11 | 1:J:77:LEU:HD11 | 1.98                     | 0.44              |
| 1:C:38:VAL:HG13 | 1:C:107:LYS:HZ3 | 1.81                     | 0.44              |
| 1:D:38:VAL:CG2  | 1:D:39:ALA:H    | 2.31                     | 0.44              |
| 1:E:18:TYR:HD2  | 1:E:23:VAL:HG22 | 1.80                     | 0.44              |
| 1:E:34:THR:OG1  | 1:E:47:HIS:HB2  | 2.17                     | 0.44              |
| 1:F:79:ILE:HD12 | 1:F:107:LYS:HZ1 | 1.82                     | 0.44              |
| 1:G:29:VAL:HG12 | 1:G:92:PHE:HE2  | 1.81                     | 0.44              |
| 1:G:109:PHE:C   | 1:G:109:PHE:HD1 | 2.25                     | 0.44              |
| 1:H:24:VAL:HG11 | 1:H:38:VAL:HG13 | 1.99                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:88:ILE:CG1  | 1:H:107:LYS:HB2  | 2.45                     | 0.44              |
| 1:L:34:THR:OG1  | 1:L:47:HIS:HB2   | 2.17                     | 0.44              |
| 1:N:38:VAL:CG2  | 1:N:39:ALA:N     | 2.79                     | 0.44              |
| 1:A:1:LEU:CG    | 1:A:13:ILE:HD11  | 2.47                     | 0.44              |
| 1:A:37:VAL:HG11 | 1:A:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:B:5:ARG:HB2   | 1:B:36:ILE:CB    | 2.47                     | 0.44              |
| 1:B:38:VAL:CG2  | 1:B:39:ALA:H     | 2.31                     | 0.44              |
| 1:C:25:LYS:HB3  | 1:C:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:37:VAL:HG11 | 1:C:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:E:50:GLY:O    | 1:E:70:GLN:HG3   | 2.17                     | 0.44              |
| 1:E:76:ASN:HD22 | 1:E:76:ASN:HA    | 1.65                     | 0.44              |
| 1:E:81:THR:CA   | 1:E:86:TYR:HE2   | 2.30                     | 0.44              |
| 1:F:79:ILE:HG22 | 1:F:81:THR:HB    | 1.99                     | 0.44              |
| 1:F:98:LYS:HE3  | 1:F:100:ASN:CA   | 2.36                     | 0.44              |
| 1:G:83:LYS:HD3  | 1:G:83:LYS:HA    | 1.57                     | 0.44              |
| 1:H:16:VAL:CG1  | 1:H:18:TYR:HE1   | 2.31                     | 0.44              |
| 1:K:34:THR:OG1  | 1:K:47:HIS:HB2   | 2.17                     | 0.44              |
| 1:L:5:ARG:HB2   | 1:L:36:ILE:CB    | 2.47                     | 0.44              |
| 1:L:16:VAL:CG1  | 1:L:18:TYR:HE1   | 2.31                     | 0.44              |
| 1:L:50:GLY:O    | 1:L:70:GLN:HG3   | 2.17                     | 0.44              |
| 1:L:79:ILE:HG22 | 1:L:81:THR:HB    | 1.99                     | 0.44              |
| 1:M:1:LEU:CG    | 1:M:13:ILE:HD11  | 2.47                     | 0.44              |
| 1:M:34:THR:OG1  | 1:M:47:HIS:HB2   | 2.17                     | 0.44              |
| 1:A:13:ILE:HD12 | 1:A:14:LYS:O     | 2.17                     | 0.44              |
| 1:B:46:THR:CB   | 1:C:14:LYS:HZ1   | 2.22                     | 0.44              |
| 1:C:84:ARG:HB3  | 1:C:85:THR:H     | 1.34                     | 0.44              |
| 1:D:25:LYS:HB3  | 1:D:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:37:VAL:HG11 | 1:D:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:G:24:VAL:HG11 | 1:G:38:VAL:HG13  | 1.99                     | 0.44              |
| 1:H:32:VAL:HG11 | 1:H:49:PHE:C     | 2.43                     | 0.44              |
| 1:J:13:ILE:HD12 | 1:J:14:LYS:O     | 2.17                     | 0.44              |
| 1:L:24:VAL:HG11 | 1:L:26:ILE:HD12  | 1.92                     | 0.44              |
| 1:M:37:VAL:CG1  | 1:M:38:VAL:N     | 2.80                     | 0.44              |
| 1:M:38:VAL:CG2  | 1:M:39:ALA:H     | 2.31                     | 0.44              |
| 1:M:70:GLN:HE21 | 1:M:70:GLN:HB3   | 1.50                     | 0.44              |
| 1:N:1:LEU:CG    | 1:N:13:ILE:HD11  | 2.47                     | 0.44              |
| 1:N:37:VAL:HG11 | 1:N:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:B:25:LYS:HB3  | 1:B:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:B:44:TYR:N    | 1:B:44:TYR:CD1   | 2.81                     | 0.44              |
| 1:B:88:ILE:HD11 | 1:B:107:LYS:CG   | 2.34                     | 0.44              |
| 1:F:34:THR:HG23 | 1:F:47:HIS:CB    | 2.41                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:16:VAL:CG1  | 1:K:18:TYR:HE1   | 2.31                     | 0.44              |
| 1:K:32:VAL:HG11 | 1:K:49:PHE:C     | 2.43                     | 0.44              |
| 1:N:13:ILE:HD12 | 1:N:14:LYS:O     | 2.17                     | 0.44              |
| 1:N:18:TYR:HD2  | 1:N:23:VAL:HG22  | 1.80                     | 0.44              |
| 1:N:32:VAL:HG11 | 1:N:49:PHE:C     | 2.43                     | 0.44              |
| 1:N:38:VAL:CG2  | 1:N:39:ALA:H     | 2.31                     | 0.44              |
| 1:A:79:ILE:HG22 | 1:A:81:THR:HB    | 1.99                     | 0.44              |
| 1:B:1:LEU:CG    | 1:B:13:ILE:HD11  | 2.47                     | 0.44              |
| 1:B:3:VAL:HB    | 1:B:40:PRO:HG3   | 1.98                     | 0.44              |
| 1:C:5:ARG:HB2   | 1:C:36:ILE:CB    | 2.47                     | 0.44              |
| 1:C:55:ARG:HD2  | 1:D:11:TYR:CG    | 2.53                     | 0.44              |
| 1:D:79:ILE:HG22 | 1:D:81:THR:HB    | 1.99                     | 0.44              |
| 1:H:55:ARG:HD2  | 1:I:11:TYR:CG    | 2.53                     | 0.44              |
| 1:H:66:VAL:HB   | 1:I:12:ARG:NH1   | 2.33                     | 0.44              |
| 1:I:43:THR:HA   | 1:J:14:LYS:HD2   | 2.00                     | 0.44              |
| 1:I:55:ARG:HD2  | 1:J:11:TYR:CG    | 2.53                     | 0.44              |
| 1:J:55:ARG:HD2  | 1:K:11:TYR:CG    | 2.53                     | 0.44              |
| 1:L:32:VAL:HG11 | 1:L:49:PHE:C     | 2.43                     | 0.44              |
| 1:L:91:HIS:HB3  | 1:L:104:THR:CG2  | 2.37                     | 0.44              |
| 1:M:13:ILE:HD12 | 1:M:14:LYS:O     | 2.17                     | 0.44              |
| 1:M:32:VAL:HG11 | 1:M:49:PHE:C     | 2.43                     | 0.44              |
| 1:N:50:GLY:O    | 1:N:70:GLN:HG3   | 2.17                     | 0.44              |
| 1:A:16:VAL:CG1  | 1:A:18:TYR:HE1   | 2.31                     | 0.44              |
| 1:A:32:VAL:HG11 | 1:A:49:PHE:C     | 2.43                     | 0.44              |
| 1:B:29:VAL:HG12 | 1:B:92:PHE:HE2   | 1.81                     | 0.44              |
| 1:B:37:VAL:HG11 | 1:B:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:B:83:LYS:HZ2  | 1:B:111:GLU:HB3  | 1.83                     | 0.44              |
| 1:B:84:ARG:HB3  | 1:B:85:THR:H     | 1.34                     | 0.44              |
| 1:C:79:ILE:HG22 | 1:C:81:THR:HB    | 1.99                     | 0.44              |
| 1:E:25:LYS:HB3  | 1:E:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:F:9:TYR:H     | 1:F:9:TYR:HD1    | 1.62                     | 0.44              |
| 1:F:13:ILE:HG13 | 1:F:14:LYS:C     | 2.43                     | 0.44              |
| 1:F:18:TYR:HD2  | 1:F:23:VAL:HG22  | 1.80                     | 0.44              |
| 1:F:24:VAL:HG11 | 1:F:38:VAL:HG13  | 1.99                     | 0.44              |
| 1:F:34:THR:OG1  | 1:F:47:HIS:HB2   | 2.17                     | 0.44              |
| 1:F:55:ARG:HD2  | 1:G:11:TYR:CG    | 2.53                     | 0.44              |
| 1:F:83:LYS:HZ2  | 1:F:111:GLU:HB3  | 1.83                     | 0.44              |
| 1:G:32:VAL:HG11 | 1:G:49:PHE:C     | 2.43                     | 0.44              |
| 1:G:55:ARG:HD2  | 1:H:11:TYR:CG    | 2.53                     | 0.44              |
| 1:I:25:LYS:HB3  | 1:I:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:J:88:ILE:CG1  | 1:J:107:LYS:HB2  | 2.45                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:13:ILE:HD12 | 1:K:14:LYS:O     | 2.17                     | 0.44              |
| 1:K:25:LYS:HB3  | 1:K:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:L:1:LEU:CG    | 1:L:13:ILE:HD11  | 2.47                     | 0.44              |
| 1:L:25:LYS:HB3  | 1:L:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:M:37:VAL:HG11 | 1:M:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:M:79:ILE:HG22 | 1:M:81:THR:HB    | 1.99                     | 0.44              |
| 1:N:79:ILE:HG22 | 1:N:81:THR:HB    | 1.99                     | 0.44              |
| 1:N:91:HIS:HB3  | 1:N:104:THR:CG2  | 2.37                     | 0.44              |
| 1:A:25:LYS:HB3  | 1:A:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:55:ARG:HD2  | 1:E:11:TYR:CG    | 2.53                     | 0.44              |
| 1:E:16:VAL:CG1  | 1:E:18:TYR:CE1   | 3.01                     | 0.44              |
| 1:E:55:ARG:HD2  | 1:F:11:TYR:CG    | 2.53                     | 0.44              |
| 1:E:66:VAL:HB   | 1:F:12:ARG:NH1   | 2.33                     | 0.44              |
| 1:G:16:VAL:CG1  | 1:G:18:TYR:HE1   | 2.31                     | 0.44              |
| 1:G:29:VAL:HG11 | 1:G:77:LEU:HD11  | 1.98                     | 0.44              |
| 1:H:13:ILE:HG13 | 1:H:14:LYS:C     | 2.43                     | 0.44              |
| 1:H:25:LYS:HB3  | 1:H:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:H:50:GLY:O    | 1:H:70:GLN:HG3   | 2.17                     | 0.44              |
| 1:I:110:ILE:H   | 1:I:110:ILE:HG12 | 1.51                     | 0.44              |
| 1:J:32:VAL:HG11 | 1:J:49:PHE:C     | 2.43                     | 0.44              |
| 1:K:5:ARG:HB2   | 1:K:36:ILE:CB    | 2.47                     | 0.44              |
| 1:K:24:VAL:HG11 | 1:K:26:ILE:HD12  | 1.92                     | 0.44              |
| 1:L:13:ILE:HD12 | 1:L:14:LYS:O     | 2.17                     | 0.44              |
| 1:L:29:VAL:HG12 | 1:L:92:PHE:HE2   | 1.81                     | 0.44              |
| 1:L:37:VAL:HG11 | 1:L:79:ILE:HG21  | 2.00                     | 0.44              |
| 1:N:29:VAL:HG12 | 1:N:92:PHE:HE2   | 1.81                     | 0.44              |
| 1:B:55:ARG:HD2  | 1:C:11:TYR:CG    | 2.53                     | 0.43              |
| 1:C:1:LEU:CG    | 1:C:13:ILE:HD11  | 2.47                     | 0.43              |
| 1:D:13:ILE:HG13 | 1:D:14:LYS:C     | 2.43                     | 0.43              |
| 1:D:16:VAL:CG1  | 1:D:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:D:16:VAL:CG1  | 1:D:18:TYR:HE1   | 2.31                     | 0.43              |
| 1:D:83:LYS:HD3  | 1:D:83:LYS:HA    | 1.57                     | 0.43              |
| 1:E:79:ILE:HG22 | 1:E:81:THR:HB    | 1.99                     | 0.43              |
| 1:F:66:VAL:HB   | 1:G:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:F:80:VAL:HG23 | 1:F:86:TYR:CE2   | 2.53                     | 0.43              |
| 1:G:80:VAL:HG23 | 1:G:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:I:32:VAL:HG11 | 1:I:49:PHE:C     | 2.43                     | 0.43              |
| 1:I:88:ILE:CG1  | 1:I:107:LYS:HB2  | 2.45                     | 0.43              |
| 1:J:29:VAL:HG12 | 1:J:92:PHE:HE2   | 1.81                     | 0.43              |
| 1:J:83:LYS:HZ2  | 1:J:111:GLU:HB3  | 1.82                     | 0.43              |
| 1:K:38:VAL:CG2  | 1:K:39:ALA:H     | 2.31                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:76:ASN:HD22 | 1:L:76:ASN:HA    | 1.65                     | 0.43              |
| 1:M:80:VAL:HG23 | 1:M:86:TYR:CE2   | 2.53                     | 0.43              |
| 1:A:16:VAL:CG1  | 1:A:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:A:38:VAL:CG2  | 1:A:39:ALA:H     | 2.31                     | 0.43              |
| 1:B:16:VAL:CG1  | 1:B:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:C:16:VAL:CG1  | 1:C:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:C:44:TYR:N    | 1:C:44:TYR:CD1   | 2.81                     | 0.43              |
| 1:D:1:LEU:CG    | 1:D:13:ILE:HD11  | 2.47                     | 0.43              |
| 1:E:37:VAL:HG11 | 1:E:79:ILE:HG21  | 2.00                     | 0.43              |
| 1:F:16:VAL:CG1  | 1:F:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:F:32:VAL:HG11 | 1:F:49:PHE:C     | 2.43                     | 0.43              |
| 1:F:37:VAL:HG11 | 1:F:79:ILE:HG21  | 2.00                     | 0.43              |
| 1:F:38:VAL:CG2  | 1:F:39:ALA:H     | 2.31                     | 0.43              |
| 1:G:70:GLN:HE21 | 1:G:70:GLN:HB3   | 1.50                     | 0.43              |
| 1:H:49:PHE:CB   | 1:H:55:ARG:HH22  | 2.17                     | 0.43              |
| 1:H:80:VAL:HG23 | 1:H:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:J:34:THR:OG1  | 1:J:47:HIS:HB2   | 2.17                     | 0.43              |
| 1:J:49:PHE:CB   | 1:J:55:ARG:HH22  | 2.17                     | 0.43              |
| 1:K:56:THR:CG2  | 1:K:57:PHE:N     | 2.82                     | 0.43              |
| 1:L:18:TYR:HD2  | 1:L:23:VAL:HG22  | 1.80                     | 0.43              |
| 1:L:98:LYS:HE3  | 1:L:100:ASN:CA   | 2.36                     | 0.43              |
| 1:A:80:VAL:HG23 | 1:A:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:B:44:TYR:N    | 1:C:14:LYS:HE3   | 2.16                     | 0.43              |
| 1:B:80:VAL:HG23 | 1:B:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:C:66:VAL:HB   | 1:D:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:C:80:VAL:HG23 | 1:C:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:D:5:ARG:HB2   | 1:D:36:ILE:CB    | 2.47                     | 0.43              |
| 1:E:98:LYS:HE3  | 1:E:100:ASN:CA   | 2.36                     | 0.43              |
| 1:F:110:ILE:H   | 1:F:110:ILE:HG12 | 1.51                     | 0.43              |
| 1:I:80:VAL:HG23 | 1:I:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:J:1:LEU:CG    | 1:J:13:ILE:HD11  | 2.47                     | 0.43              |
| 1:J:13:ILE:HG13 | 1:J:14:LYS:C     | 2.43                     | 0.43              |
| 1:J:43:THR:HA   | 1:K:14:LYS:HD2   | 1.99                     | 0.43              |
| 1:J:80:VAL:HG23 | 1:J:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:K:13:ILE:HG13 | 1:K:14:LYS:C     | 2.43                     | 0.43              |
| 1:K:55:ARG:HD2  | 1:L:11:TYR:CG    | 2.53                     | 0.43              |
| 1:K:80:VAL:HG23 | 1:K:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:L:80:VAL:HG23 | 1:L:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:N:16:VAL:CG1  | 1:N:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:N:80:VAL:HG23 | 1:N:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:A:55:ARG:HD2  | 1:B:11:TYR:CG    | 2.53                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:49:PHE:CB   | 1:B:55:ARG:HH22  | 2.17                     | 0.43              |
| 1:C:56:THR:CG2  | 1:C:57:PHE:N     | 2.82                     | 0.43              |
| 1:D:9:TYR:H     | 1:D:9:TYR:HD1    | 1.62                     | 0.43              |
| 1:D:29:VAL:HG12 | 1:D:92:PHE:HE2   | 1.81                     | 0.43              |
| 1:E:24:VAL:HG11 | 1:E:38:VAL:HG13  | 1.99                     | 0.43              |
| 1:E:29:VAL:HG12 | 1:E:92:PHE:HE2   | 1.81                     | 0.43              |
| 1:E:29:VAL:HG11 | 1:E:77:LEU:HD11  | 1.98                     | 0.43              |
| 1:E:80:VAL:HG23 | 1:E:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:F:21:VAL:HG13 | 1:F:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:G:16:VAL:CG1  | 1:G:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:G:21:VAL:HG13 | 1:G:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:G:38:VAL:CG2  | 1:G:39:ALA:H     | 2.31                     | 0.43              |
| 1:H:43:THR:HA   | 1:I:14:LYS:HD2   | 2.00                     | 0.43              |
| 1:I:13:ILE:HG13 | 1:I:14:LYS:C     | 2.43                     | 0.43              |
| 1:J:24:VAL:HG11 | 1:J:26:ILE:HD12  | 1.92                     | 0.43              |
| 1:J:66:VAL:HB   | 1:K:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:K:66:VAL:HB   | 1:L:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:L:56:THR:CG2  | 1:L:57:PHE:N     | 2.82                     | 0.43              |
| 1:M:21:VAL:HG13 | 1:M:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:B:79:ILE:HG22 | 1:B:81:THR:HB    | 1.99                     | 0.43              |
| 1:D:80:VAL:HG23 | 1:D:86:TYR:CE2   | 2.54                     | 0.43              |
| 1:G:7:SER:HB3   | 1:G:8:PRO:O      | 2.19                     | 0.43              |
| 1:H:21:VAL:HG13 | 1:H:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:H:83:LYS:HZ2  | 1:H:111:GLU:HB3  | 1.83                     | 0.43              |
| 1:H:98:LYS:HE3  | 1:H:101:ALA:N    | 2.33                     | 0.43              |
| 1:I:66:VAL:HB   | 1:J:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:K:1:LEU:CG    | 1:K:13:ILE:HD11  | 2.47                     | 0.43              |
| 1:L:55:ARG:HD2  | 1:M:11:TYR:CG    | 2.53                     | 0.43              |
| 1:M:16:VAL:CG1  | 1:M:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:N:16:VAL:CG1  | 1:N:18:TYR:HE1   | 2.31                     | 0.43              |
| 1:N:21:VAL:HG13 | 1:N:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:21:VAL:HG13 | 1:A:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:83:LYS:HZ2  | 1:A:111:GLU:HB3  | 1.83                     | 0.43              |
| 1:B:13:ILE:HG13 | 1:B:14:LYS:C     | 2.43                     | 0.43              |
| 1:B:32:VAL:HG11 | 1:B:49:PHE:C     | 2.43                     | 0.43              |
| 1:C:7:SER:HB3   | 1:C:8:PRO:O      | 2.19                     | 0.43              |
| 1:C:38:VAL:CG2  | 1:C:39:ALA:H     | 2.31                     | 0.43              |
| 1:D:7:SER:HB3   | 1:D:8:PRO:O      | 2.19                     | 0.43              |
| 1:D:29:VAL:HG11 | 1:D:77:LEU:HD11  | 1.98                     | 0.43              |
| 1:F:25:LYS:HB3  | 1:F:105:VAL:HG11 | 1.99                     | 0.43              |
| 1:G:44:TYR:N    | 1:G:44:TYR:CD1   | 2.81                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:98:LYS:HE3  | 1:I:101:ALA:N    | 2.33                     | 0.43              |
| 1:J:5:ARG:HB2   | 1:J:36:ILE:CB    | 2.47                     | 0.43              |
| 1:K:29:VAL:HG11 | 1:K:77:LEU:HD11  | 1.98                     | 0.43              |
| 1:L:21:VAL:HG13 | 1:L:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:M:7:SER:HB3   | 1:M:8:PRO:O      | 2.19                     | 0.43              |
| 1:N:25:LYS:HB3  | 1:N:105:VAL:HG11 | 1.99                     | 0.43              |
| 1:C:62:ASN:HB2  | 1:C:63:HIS:H     | 1.73                     | 0.43              |
| 1:E:9:TYR:H     | 1:E:9:TYR:HD1    | 1.62                     | 0.43              |
| 1:E:21:VAL:HG13 | 1:E:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:G:98:LYS:HE3  | 1:G:101:ALA:N    | 2.33                     | 0.43              |
| 1:H:16:VAL:CG1  | 1:H:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:J:37:VAL:HG11 | 1:J:79:ILE:HG21  | 2.00                     | 0.43              |
| 1:K:21:VAL:HG13 | 1:K:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:L:13:ILE:HG13 | 1:L:14:LYS:C     | 2.43                     | 0.43              |
| 1:L:16:VAL:CG1  | 1:L:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:A:11:TYR:CG   | 1:N:55:ARG:HD2   | 2.53                     | 0.43              |
| 1:B:7:SER:HB3   | 1:B:8:PRO:O      | 2.19                     | 0.43              |
| 1:C:9:TYR:H     | 1:C:9:TYR:HD1    | 1.62                     | 0.43              |
| 1:E:1:LEU:CG    | 1:E:13:ILE:HD11  | 2.47                     | 0.43              |
| 1:E:7:SER:HB3   | 1:E:8:PRO:O      | 2.19                     | 0.43              |
| 1:E:34:THR:HA   | 1:E:47:HIS:HA    | 2.01                     | 0.43              |
| 1:E:38:VAL:CG2  | 1:E:39:ALA:H     | 2.31                     | 0.43              |
| 1:F:38:VAL:HG13 | 1:F:107:LYS:HZ3  | 1.84                     | 0.43              |
| 1:F:44:TYR:N    | 1:F:44:TYR:CD1   | 2.81                     | 0.43              |
| 1:G:18:TYR:HD2  | 1:G:23:VAL:HG22  | 1.80                     | 0.43              |
| 1:J:7:SER:HB3   | 1:J:8:PRO:O      | 2.19                     | 0.43              |
| 1:J:16:VAL:CG1  | 1:J:18:TYR:HE1   | 2.31                     | 0.43              |
| 1:J:25:LYS:HB3  | 1:J:105:VAL:HG11 | 1.99                     | 0.43              |
| 1:L:43:THR:HA   | 1:M:14:LYS:HD2   | 2.00                     | 0.43              |
| 1:M:46:THR:CA   | 1:N:14:LYS:HZ1   | 2.31                     | 0.43              |
| 1:M:55:ARG:HD2  | 1:N:11:TYR:CG    | 2.53                     | 0.43              |
| 1:M:56:THR:CG2  | 1:M:57:PHE:N     | 2.82                     | 0.43              |
| 1:A:66:VAL:HB   | 1:B:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:D:21:VAL:HG13 | 1:D:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:D:24:VAL:HG11 | 1:D:38:VAL:HG13  | 1.99                     | 0.43              |
| 1:D:79:ILE:HD12 | 1:D:107:LYS:HZ2  | 1.84                     | 0.43              |
| 1:E:32:VAL:HG11 | 1:E:49:PHE:C     | 2.43                     | 0.43              |
| 1:F:34:THR:HA   | 1:F:47:HIS:HA    | 2.01                     | 0.43              |
| 1:F:61:MET:CG   | 1:F:62:ASN:N     | 2.82                     | 0.43              |
| 1:G:66:VAL:HB   | 1:H:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:H:5:ARG:O     | 1:H:6:ASN:HB2    | 2.19                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:37:VAL:HG11 | 1:H:79:ILE:HG21  | 2.00                     | 0.43              |
| 1:I:21:VAL:HG13 | 1:I:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:K:18:TYR:HD2  | 1:K:23:VAL:HG22  | 1.80                     | 0.43              |
| 1:K:34:THR:HA   | 1:K:47:HIS:HA    | 2.01                     | 0.43              |
| 1:K:37:VAL:HG11 | 1:K:79:ILE:HG21  | 2.00                     | 0.43              |
| 1:L:7:SER:HB3   | 1:L:8:PRO:O      | 2.19                     | 0.43              |
| 1:L:38:VAL:CG2  | 1:L:39:ALA:H     | 2.31                     | 0.43              |
| 1:M:66:VAL:HB   | 1:N:12:ARG:NH1   | 2.33                     | 0.43              |
| 1:B:21:VAL:HG13 | 1:B:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:B:70:GLN:HE21 | 1:B:70:GLN:HB3   | 1.50                     | 0.43              |
| 1:D:49:PHE:HE2  | 1:D:79:ILE:CD1   | 2.26                     | 0.43              |
| 1:D:56:THR:CG2  | 1:D:57:PHE:N     | 2.82                     | 0.43              |
| 1:E:5:ARG:HB2   | 1:E:36:ILE:CB    | 2.47                     | 0.43              |
| 1:E:5:ARG:O     | 1:E:6:ASN:HB2    | 2.19                     | 0.43              |
| 1:F:7:SER:HB3   | 1:F:8:PRO:O      | 2.19                     | 0.43              |
| 1:G:37:VAL:HG12 | 1:G:38:VAL:H     | 1.84                     | 0.43              |
| 1:H:44:TYR:N    | 1:I:14:LYS:HE3   | 2.16                     | 0.43              |
| 1:I:16:VAL:CG1  | 1:I:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:J:21:VAL:HG13 | 1:J:110:ILE:HG13 | 2.01                     | 0.43              |
| 1:J:98:LYS:HE3  | 1:J:101:ALA:N    | 2.33                     | 0.43              |
| 1:K:16:VAL:CG1  | 1:K:18:TYR:CE1   | 3.01                     | 0.43              |
| 1:L:34:THR:HA   | 1:L:47:HIS:HA    | 2.01                     | 0.43              |
| 1:L:98:LYS:CE   | 1:L:100:ASN:HA   | 2.37                     | 0.43              |
| 1:M:9:TYR:CD1   | 1:M:9:TYR:N      | 2.87                     | 0.43              |
| 1:M:13:ILE:HG13 | 1:M:14:LYS:C     | 2.43                     | 0.43              |
| 1:M:25:LYS:HB3  | 1:M:105:VAL:HG11 | 1.99                     | 0.43              |
| 1:M:44:TYR:N    | 1:N:14:LYS:HE3   | 2.16                     | 0.43              |
| 1:A:13:ILE:HG13 | 1:A:14:LYS:C     | 2.43                     | 0.42              |
| 1:B:11:TYR:HD1  | 1:B:11:TYR:HA    | 1.55                     | 0.42              |
| 1:C:32:VAL:HG11 | 1:C:49:PHE:C     | 2.43                     | 0.42              |
| 1:D:5:ARG:O     | 1:D:6:ASN:HB2    | 2.19                     | 0.42              |
| 1:D:34:THR:HA   | 1:D:47:HIS:HA    | 2.01                     | 0.42              |
| 1:D:66:VAL:HB   | 1:E:12:ARG:NH1   | 2.33                     | 0.42              |
| 1:E:38:VAL:HG13 | 1:E:107:LYS:HZ3  | 1.84                     | 0.42              |
| 1:F:29:VAL:HG11 | 1:F:77:LEU:HD11  | 1.99                     | 0.42              |
| 1:F:43:THR:HA   | 1:G:14:LYS:HD2   | 2.00                     | 0.42              |
| 1:G:13:ILE:HG13 | 1:G:14:LYS:C     | 2.43                     | 0.42              |
| 1:G:25:LYS:HB3  | 1:G:105:VAL:HG11 | 1.99                     | 0.42              |
| 1:G:34:THR:HA   | 1:G:47:HIS:HA    | 2.01                     | 0.42              |
| 1:G:37:VAL:HG11 | 1:G:79:ILE:HG21  | 2.00                     | 0.42              |
| 1:G:56:THR:CG2  | 1:G:57:PHE:N     | 2.82                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:7:SER:HB3   | 1:H:8:PRO:O      | 2.19                     | 0.42              |
| 1:I:5:ARG:HB2   | 1:I:36:ILE:CB    | 2.47                     | 0.42              |
| 1:J:16:VAL:CG1  | 1:J:18:TYR:CE1   | 3.01                     | 0.42              |
| 1:J:34:THR:HA   | 1:J:47:HIS:HA    | 2.01                     | 0.42              |
| 1:M:43:THR:HA   | 1:N:14:LYS:HD2   | 2.00                     | 0.42              |
| 1:N:24:VAL:HG11 | 1:N:107:LYS:CD   | 2.46                     | 0.42              |
| 1:A:30:ALA:CB   | 1:A:49:PHE:HE1   | 2.32                     | 0.42              |
| 1:A:43:THR:HA   | 1:B:14:LYS:HD2   | 2.00                     | 0.42              |
| 1:B:66:VAL:HB   | 1:C:12:ARG:NH1   | 2.33                     | 0.42              |
| 1:C:16:VAL:CG1  | 1:C:18:TYR:HE1   | 2.31                     | 0.42              |
| 1:C:21:VAL:HG13 | 1:C:110:ILE:HG13 | 2.01                     | 0.42              |
| 1:D:44:TYR:N    | 1:D:44:TYR:CD1   | 2.81                     | 0.42              |
| 1:D:98:LYS:HE3  | 1:D:100:ASN:CA   | 2.36                     | 0.42              |
| 1:E:43:THR:HA   | 1:F:14:LYS:HD2   | 2.00                     | 0.42              |
| 1:G:110:ILE:H   | 1:G:110:ILE:HG12 | 1.51                     | 0.42              |
| 1:H:24:VAL:HG11 | 1:H:107:LYS:CD   | 2.46                     | 0.42              |
| 1:H:34:THR:HA   | 1:H:47:HIS:HA    | 2.01                     | 0.42              |
| 1:I:34:THR:HA   | 1:I:47:HIS:HA    | 2.01                     | 0.42              |
| 1:L:61:MET:CG   | 1:L:62:ASN:N     | 2.82                     | 0.42              |
| 1:M:61:MET:CG   | 1:M:62:ASN:N     | 2.82                     | 0.42              |
| 1:C:13:ILE:HG13 | 1:C:14:LYS:C     | 2.43                     | 0.42              |
| 1:D:32:VAL:HG11 | 1:D:49:PHE:C     | 2.43                     | 0.42              |
| 1:E:13:ILE:HG13 | 1:E:14:LYS:C     | 2.43                     | 0.42              |
| 1:F:5:ARG:HB2   | 1:F:36:ILE:CB    | 2.47                     | 0.42              |
| 1:F:37:VAL:HG12 | 1:F:38:VAL:H     | 1.85                     | 0.42              |
| 1:H:5:ARG:HB2   | 1:H:36:ILE:CB    | 2.47                     | 0.42              |
| 1:H:29:VAL:HG12 | 1:H:92:PHE:HE2   | 1.81                     | 0.42              |
| 1:J:32:VAL:CG1  | 1:J:51:ASP:H     | 2.33                     | 0.42              |
| 1:L:5:ARG:O     | 1:L:6:ASN:HB2    | 2.19                     | 0.42              |
| 1:L:30:ALA:CB   | 1:L:49:PHE:HE1   | 2.32                     | 0.42              |
| 1:L:84:ARG:HB3  | 1:L:85:THR:H     | 1.34                     | 0.42              |
| 1:M:34:THR:HA   | 1:M:47:HIS:HA    | 2.01                     | 0.42              |
| 1:N:30:ALA:CB   | 1:N:49:PHE:HE1   | 2.32                     | 0.42              |
| 1:A:5:ARG:O     | 1:A:6:ASN:HB2    | 2.19                     | 0.42              |
| 1:A:7:SER:HB3   | 1:A:8:PRO:O      | 2.19                     | 0.42              |
| 1:A:32:VAL:CG1  | 1:A:51:ASP:H     | 2.33                     | 0.42              |
| 1:B:61:MET:CG   | 1:B:62:ASN:N     | 2.82                     | 0.42              |
| 1:C:32:VAL:CG1  | 1:C:51:ASP:H     | 2.33                     | 0.42              |
| 1:D:30:ALA:CB   | 1:D:49:PHE:HE1   | 2.32                     | 0.42              |
| 1:D:80:VAL:CG2  | 1:D:88:ILE:CG2   | 2.94                     | 0.42              |
| 1:E:30:ALA:CB   | 1:E:49:PHE:HE1   | 2.32                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:16:VAL:CG1  | 1:F:18:TYR:HE1  | 2.31                     | 0.42              |
| 1:F:98:LYS:HE3  | 1:F:101:ALA:N   | 2.33                     | 0.42              |
| 1:G:5:ARG:O     | 1:G:6:ASN:HB2   | 2.19                     | 0.42              |
| 1:H:38:VAL:CG2  | 1:H:39:ALA:H    | 2.31                     | 0.42              |
| 1:H:56:THR:CG2  | 1:H:57:PHE:N    | 2.82                     | 0.42              |
| 1:H:76:ASN:HD22 | 1:H:76:ASN:HA   | 1.65                     | 0.42              |
| 1:I:7:SER:HB3   | 1:I:8:PRO:O     | 2.19                     | 0.42              |
| 1:I:37:VAL:HG11 | 1:I:79:ILE:HG21 | 2.00                     | 0.42              |
| 1:K:17:VAL:C    | 1:K:18:TYR:HD1  | 2.28                     | 0.42              |
| 1:L:66:VAL:HB   | 1:M:12:ARG:NH1  | 2.33                     | 0.42              |
| 1:M:29:VAL:HG11 | 1:M:77:LEU:HD11 | 1.99                     | 0.42              |
| 1:N:56:THR:CG2  | 1:N:57:PHE:N    | 2.82                     | 0.42              |
| 1:B:30:ALA:CB   | 1:B:49:PHE:HE1  | 2.32                     | 0.42              |
| 1:B:36:ILE:CG1  | 1:B:37:VAL:N    | 2.83                     | 0.42              |
| 1:C:24:VAL:HG11 | 1:C:38:VAL:HG13 | 1.99                     | 0.42              |
| 1:C:61:MET:CG   | 1:C:62:ASN:N    | 2.82                     | 0.42              |
| 1:E:36:ILE:CG1  | 1:E:37:VAL:N    | 2.83                     | 0.42              |
| 1:E:91:HIS:HB3  | 1:E:104:THR:CG2 | 2.37                     | 0.42              |
| 1:G:5:ARG:HB2   | 1:G:36:ILE:CB   | 2.47                     | 0.42              |
| 1:G:32:VAL:CG1  | 1:G:51:ASP:H    | 2.33                     | 0.42              |
| 1:H:32:VAL:CG1  | 1:H:51:ASP:H    | 2.33                     | 0.42              |
| 1:I:5:ARG:O     | 1:I:6:ASN:HB2   | 2.19                     | 0.42              |
| 1:J:37:VAL:HG12 | 1:J:38:VAL:H    | 1.85                     | 0.42              |
| 1:K:37:VAL:HG12 | 1:K:38:VAL:H    | 1.84                     | 0.42              |
| 1:K:61:MET:CG   | 1:K:62:ASN:N    | 2.82                     | 0.42              |
| 1:L:29:VAL:HG11 | 1:L:77:LEU:HD11 | 1.98                     | 0.42              |
| 1:L:36:ILE:CG1  | 1:L:37:VAL:N    | 2.83                     | 0.42              |
| 1:M:17:VAL:C    | 1:M:18:TYR:HD1  | 2.28                     | 0.42              |
| 1:M:18:TYR:HD2  | 1:M:23:VAL:HG22 | 1.80                     | 0.42              |
| 1:M:36:ILE:CG1  | 1:M:37:VAL:N    | 2.83                     | 0.42              |
| 1:M:46:THR:HG1  | 1:N:13:ILE:HG22 | 1.78                     | 0.42              |
| 1:N:7:SER:HB3   | 1:N:8:PRO:O     | 2.19                     | 0.42              |
| 1:N:13:ILE:HG13 | 1:N:14:LYS:C    | 2.43                     | 0.42              |
| 1:N:61:MET:CG   | 1:N:62:ASN:N    | 2.82                     | 0.42              |
| 1:A:12:ARG:NH1  | 1:N:66:VAL:HB   | 2.33                     | 0.42              |
| 1:C:34:THR:HA   | 1:C:47:HIS:HA   | 2.01                     | 0.42              |
| 1:C:36:ILE:CG1  | 1:C:37:VAL:N    | 2.83                     | 0.42              |
| 1:D:32:VAL:CG1  | 1:D:51:ASP:H    | 2.33                     | 0.42              |
| 1:D:45:ILE:CG2  | 1:E:14:LYS:HE2  | 2.50                     | 0.42              |
| 1:E:44:TYR:N    | 1:F:14:LYS:HE3  | 2.16                     | 0.42              |
| 1:G:45:ILE:CG2  | 1:H:14:LYS:HE2  | 2.50                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:18:TYR:HD2  | 1:H:23:VAL:HG22  | 1.80                     | 0.42              |
| 1:I:17:VAL:C    | 1:I:18:TYR:HD1   | 2.28                     | 0.42              |
| 1:J:18:TYR:HD2  | 1:J:23:VAL:HG22  | 1.80                     | 0.42              |
| 1:J:36:ILE:CG1  | 1:J:37:VAL:N     | 2.83                     | 0.42              |
| 1:K:66:VAL:CG1  | 1:L:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:L:83:LYS:HZ2  | 1:L:111:GLU:HB3  | 1.84                     | 0.42              |
| 1:N:29:VAL:HG11 | 1:N:77:LEU:HD11  | 1.98                     | 0.42              |
| 1:N:36:ILE:CG1  | 1:N:37:VAL:N     | 2.83                     | 0.42              |
| 1:N:49:PHE:CB   | 1:N:55:ARG:HH22  | 2.17                     | 0.42              |
| 1:A:17:VAL:C    | 1:A:18:TYR:HD1   | 2.28                     | 0.42              |
| 1:B:17:VAL:C    | 1:B:18:TYR:HD1   | 2.28                     | 0.42              |
| 1:C:29:VAL:HG11 | 1:C:77:LEU:HD11  | 1.98                     | 0.42              |
| 1:C:45:ILE:CG2  | 1:D:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:C:66:VAL:CG1  | 1:D:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:E:45:ILE:CG2  | 1:F:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:J:66:VAL:CG1  | 1:K:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:J:70:GLN:HE21 | 1:J:70:GLN:HB3   | 1.50                     | 0.42              |
| 1:N:5:ARG:O     | 1:N:6:ASN:HB2    | 2.19                     | 0.42              |
| 1:N:11:TYR:HD1  | 1:N:11:TYR:HA    | 1.55                     | 0.42              |
| 1:N:34:THR:HA   | 1:N:47:HIS:HA    | 2.01                     | 0.42              |
| 1:A:34:THR:HA   | 1:A:47:HIS:HA    | 2.01                     | 0.42              |
| 1:B:34:THR:HA   | 1:B:47:HIS:HA    | 2.01                     | 0.42              |
| 1:C:17:VAL:C    | 1:C:18:TYR:HD1   | 2.28                     | 0.42              |
| 1:D:17:VAL:C    | 1:D:18:TYR:HD1   | 2.28                     | 0.42              |
| 1:F:45:ILE:CG2  | 1:G:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:F:62:ASN:HB2  | 1:F:63:HIS:H     | 1.73                     | 0.42              |
| 1:G:49:PHE:HE2  | 1:G:79:ILE:CD1   | 2.26                     | 0.42              |
| 1:H:45:ILE:CG2  | 1:I:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:I:9:TYR:CD1   | 1:I:9:TYR:N      | 2.87                     | 0.42              |
| 1:I:45:ILE:CG2  | 1:J:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:I:66:VAL:CG1  | 1:J:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:K:7:SER:HB3   | 1:K:8:PRO:O      | 2.19                     | 0.42              |
| 1:K:49:PHE:CD2  | 1:K:79:ILE:CG1   | 3.03                     | 0.42              |
| 1:K:98:LYS:HE3  | 1:K:101:ALA:N    | 2.33                     | 0.42              |
| 1:K:110:ILE:H   | 1:K:110:ILE:HG12 | 1.51                     | 0.42              |
| 1:L:66:VAL:CG1  | 1:M:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:A:12:ARG:NH1  | 1:N:66:VAL:CG1   | 2.83                     | 0.42              |
| 1:A:66:VAL:CG1  | 1:B:12:ARG:NH1   | 2.83                     | 0.42              |
| 1:B:45:ILE:CG2  | 1:C:14:LYS:HE2   | 2.50                     | 0.42              |
| 1:D:61:MET:CG   | 1:D:62:ASN:N     | 2.82                     | 0.42              |
| 1:E:17:VAL:C    | 1:E:18:TYR:HD1   | 2.28                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:80:VAL:CG2  | 1:E:88:ILE:CG2  | 2.94                     | 0.42              |
| 1:F:5:ARG:O     | 1:F:6:ASN:HB2   | 2.19                     | 0.42              |
| 1:G:17:VAL:C    | 1:G:18:TYR:HD1  | 2.28                     | 0.42              |
| 1:G:43:THR:HA   | 1:H:14:LYS:HD2  | 2.00                     | 0.42              |
| 1:I:18:TYR:HD2  | 1:I:23:VAL:HG22 | 1.80                     | 0.42              |
| 1:K:5:ARG:O     | 1:K:6:ASN:HB2   | 2.19                     | 0.42              |
| 1:L:49:PHE:CD2  | 1:L:79:ILE:CG1  | 3.03                     | 0.42              |
| 1:L:79:ILE:HG23 | 1:L:86:TYR:OH   | 2.20                     | 0.42              |
| 1:B:62:ASN:HB2  | 1:B:63:HIS:H    | 1.73                     | 0.42              |
| 1:C:88:ILE:HD11 | 1:C:107:LYS:CG  | 2.34                     | 0.42              |
| 1:D:66:VAL:CG1  | 1:E:12:ARG:NH1  | 2.83                     | 0.42              |
| 1:F:30:ALA:CB   | 1:F:49:PHE:HE1  | 2.32                     | 0.42              |
| 1:F:66:VAL:CG1  | 1:G:12:ARG:NH1  | 2.83                     | 0.42              |
| 1:H:36:ILE:CG1  | 1:H:37:VAL:N    | 2.83                     | 0.42              |
| 1:H:49:PHE:CD2  | 1:H:79:ILE:CG1  | 3.03                     | 0.42              |
| 1:H:66:VAL:CG1  | 1:I:12:ARG:NH1  | 2.83                     | 0.42              |
| 1:I:49:PHE:CD2  | 1:I:79:ILE:CG1  | 3.03                     | 0.42              |
| 1:K:30:ALA:CB   | 1:K:49:PHE:HE1  | 2.32                     | 0.42              |
| 1:K:32:VAL:CG1  | 1:K:51:ASP:H    | 2.33                     | 0.42              |
| 1:M:5:ARG:O     | 1:M:6:ASN:HB2   | 2.19                     | 0.42              |
| 1:M:30:ALA:CB   | 1:M:49:PHE:HE1  | 2.32                     | 0.42              |
| 1:A:14:LYS:HD2  | 1:N:43:THR:HA   | 2.00                     | 0.41              |
| 1:A:36:ILE:CG1  | 1:A:37:VAL:N    | 2.83                     | 0.41              |
| 1:C:5:ARG:O     | 1:C:6:ASN:HB2   | 2.19                     | 0.41              |
| 1:G:36:ILE:CG1  | 1:G:37:VAL:N    | 2.83                     | 0.41              |
| 1:I:83:LYS:HZ2  | 1:I:111:GLU:HB3 | 1.84                     | 0.41              |
| 1:J:45:ILE:CG2  | 1:K:14:LYS:HE2  | 2.50                     | 0.41              |
| 1:K:43:THR:HA   | 1:L:14:LYS:HD2  | 2.00                     | 0.41              |
| 1:L:32:VAL:CG1  | 1:L:51:ASP:H    | 2.33                     | 0.41              |
| 1:M:16:VAL:CG1  | 1:M:18:TYR:HE1  | 2.31                     | 0.41              |
| 1:M:49:PHE:CD2  | 1:M:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:M:66:VAL:CG1  | 1:N:12:ARG:NH1  | 2.83                     | 0.41              |
| 1:M:79:ILE:HG23 | 1:M:86:TYR:OH   | 2.20                     | 0.41              |
| 1:M:83:LYS:HZ2  | 1:M:111:GLU:HB3 | 1.84                     | 0.41              |
| 1:N:17:VAL:C    | 1:N:18:TYR:HD1  | 2.28                     | 0.41              |
| 1:B:24:VAL:HG11 | 1:B:38:VAL:HG13 | 1.99                     | 0.41              |
| 1:B:91:HIS:HB3  | 1:B:104:THR:CG2 | 2.37                     | 0.41              |
| 1:C:49:PHE:CE2  | 1:C:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:C:98:LYS:HE3  | 1:C:100:ASN:CA  | 2.36                     | 0.41              |
| 1:C:98:LYS:CE   | 1:C:100:ASN:HA  | 2.37                     | 0.41              |
| 1:D:43:THR:HA   | 1:E:14:LYS:HD2  | 2.00                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:17:VAL:C    | 1:F:18:TYR:HD1   | 2.28                     | 0.41              |
| 1:G:30:ALA:CB   | 1:G:49:PHE:HE1   | 2.32                     | 0.41              |
| 1:G:66:VAL:CG1  | 1:H:12:ARG:NH1   | 2.83                     | 0.41              |
| 1:I:37:VAL:HG12 | 1:I:38:VAL:H     | 1.85                     | 0.41              |
| 1:J:30:ALA:CB   | 1:J:49:PHE:HE1   | 2.32                     | 0.41              |
| 1:J:49:PHE:CE2  | 1:J:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:J:61:MET:CG   | 1:J:62:ASN:N     | 2.82                     | 0.41              |
| 1:J:79:ILE:HG23 | 1:J:86:TYR:OH    | 2.20                     | 0.41              |
| 1:L:49:PHE:CB   | 1:L:55:ARG:HH22  | 2.17                     | 0.41              |
| 1:M:32:VAL:CG1  | 1:M:51:ASP:H     | 2.32                     | 0.41              |
| 1:N:32:VAL:CG1  | 1:N:51:ASP:H     | 2.33                     | 0.41              |
| 1:N:49:PHE:CD2  | 1:N:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:N:79:ILE:HG23 | 1:N:86:TYR:OH    | 2.20                     | 0.41              |
| 1:A:49:PHE:CD2  | 1:A:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:A:56:THR:CG2  | 1:A:57:PHE:N     | 2.82                     | 0.41              |
| 1:A:79:ILE:HG23 | 1:A:86:TYR:OH    | 2.20                     | 0.41              |
| 1:B:16:VAL:CG1  | 1:B:18:TYR:HE1   | 2.31                     | 0.41              |
| 1:B:37:VAL:HG12 | 1:B:38:VAL:H     | 1.85                     | 0.41              |
| 1:B:100:ASN:HA  | 1:B:100:ASN:HD22 | 1.53                     | 0.41              |
| 1:C:37:VAL:HG12 | 1:C:38:VAL:H     | 1.85                     | 0.41              |
| 1:E:56:THR:CG2  | 1:E:57:PHE:N     | 2.82                     | 0.41              |
| 1:F:36:ILE:CG1  | 1:F:37:VAL:N     | 2.83                     | 0.41              |
| 1:H:30:ALA:CB   | 1:H:49:PHE:HE1   | 2.32                     | 0.41              |
| 1:H:37:VAL:HG12 | 1:H:38:VAL:H     | 1.84                     | 0.41              |
| 1:I:46:THR:CA   | 1:J:14:LYS:HZ1   | 2.33                     | 0.41              |
| 1:I:56:THR:CG2  | 1:I:57:PHE:N     | 2.82                     | 0.41              |
| 1:K:36:ILE:CG1  | 1:K:37:VAL:N     | 2.83                     | 0.41              |
| 1:K:45:ILE:CG2  | 1:L:14:LYS:HE2   | 2.50                     | 0.41              |
| 1:K:49:PHE:CE2  | 1:K:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:A:49:PHE:CE2  | 1:A:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:A:79:ILE:HD12 | 1:A:107:LYS:HZ1  | 1.85                     | 0.41              |
| 1:B:32:VAL:CG1  | 1:B:51:ASP:H     | 2.33                     | 0.41              |
| 1:B:49:PHE:CE2  | 1:B:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:C:30:ALA:CB   | 1:C:49:PHE:HE1   | 2.32                     | 0.41              |
| 1:D:11:TYR:HD1  | 1:D:11:TYR:HA    | 1.55                     | 0.41              |
| 1:D:36:ILE:CG1  | 1:D:37:VAL:N     | 2.83                     | 0.41              |
| 1:D:49:PHE:CE2  | 1:D:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:E:32:VAL:CG1  | 1:E:51:ASP:H     | 2.33                     | 0.41              |
| 1:E:37:VAL:HG12 | 1:E:38:VAL:H     | 1.85                     | 0.41              |
| 1:E:66:VAL:CG1  | 1:F:12:ARG:NH1   | 2.83                     | 0.41              |
| 1:E:98:LYS:HE3  | 1:E:101:ALA:N    | 2.33                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:49:PHE:CD2  | 1:F:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:G:45:ILE:H    | 1:G:45:ILE:HG13 | 1.76                     | 0.41              |
| 1:G:46:THR:CA   | 1:H:14:LYS:HZ1  | 2.33                     | 0.41              |
| 1:I:36:ILE:CG1  | 1:I:37:VAL:N    | 2.83                     | 0.41              |
| 1:J:49:PHE:CD2  | 1:J:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:K:79:ILE:HG23 | 1:K:86:TYR:OH   | 2.20                     | 0.41              |
| 1:L:1:LEU:N     | 1:L:5:ARG:HH11  | 2.19                     | 0.41              |
| 1:L:12:ARG:CG   | 1:L:13:ILE:N    | 2.83                     | 0.41              |
| 1:L:17:VAL:C    | 1:L:18:TYR:HD1  | 2.28                     | 0.41              |
| 1:M:24:VAL:HG11 | 1:M:38:VAL:HG13 | 1.99                     | 0.41              |
| 1:A:45:ILE:CG2  | 1:B:14:LYS:HE2  | 2.50                     | 0.41              |
| 1:B:66:VAL:CG1  | 1:C:12:ARG:NH1  | 2.83                     | 0.41              |
| 1:E:61:MET:CG   | 1:E:62:ASN:N    | 2.82                     | 0.41              |
| 1:F:32:VAL:CG1  | 1:F:51:ASP:H    | 2.32                     | 0.41              |
| 1:H:9:TYR:H     | 1:H:9:TYR:HD1   | 1.62                     | 0.41              |
| 1:H:17:VAL:C    | 1:H:18:TYR:HD1  | 2.28                     | 0.41              |
| 1:I:16:VAL:CG1  | 1:I:18:TYR:HE1  | 2.31                     | 0.41              |
| 1:I:49:PHE:CE2  | 1:I:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:I:91:HIS:HB3  | 1:I:104:THR:CG2 | 2.37                     | 0.41              |
| 1:L:45:ILE:CG2  | 1:M:14:LYS:HE2  | 2.50                     | 0.41              |
| 1:A:29:VAL:HG11 | 1:A:77:LEU:HD11 | 1.98                     | 0.41              |
| 1:A:44:TYR:N    | 1:B:14:LYS:HE3  | 2.16                     | 0.41              |
| 1:D:37:VAL:HG12 | 1:D:38:VAL:H    | 1.84                     | 0.41              |
| 1:G:34:THR:HG23 | 1:G:47:HIS:CB   | 2.41                     | 0.41              |
| 1:I:32:VAL:CG1  | 1:I:51:ASP:H    | 2.33                     | 0.41              |
| 1:J:1:LEU:N     | 1:J:5:ARG:HH11  | 2.19                     | 0.41              |
| 1:J:17:VAL:C    | 1:J:18:TYR:HD1  | 2.28                     | 0.41              |
| 1:J:79:ILE:CG2  | 1:J:81:THR:HB   | 2.51                     | 0.41              |
| 1:K:49:PHE:HE2  | 1:K:79:ILE:CD1  | 2.26                     | 0.41              |
| 1:L:49:PHE:CE2  | 1:L:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:A:14:LYS:HE2  | 1:N:45:ILE:CG2  | 2.50                     | 0.41              |
| 1:A:37:VAL:HG12 | 1:A:38:VAL:H    | 1.84                     | 0.41              |
| 1:A:79:ILE:C    | 1:A:81:THR:N    | 2.79                     | 0.41              |
| 1:B:49:PHE:CD2  | 1:B:79:ILE:CG1  | 3.03                     | 0.41              |
| 1:B:67:LYS:HG2  | 1:B:77:LEU:O    | 2.21                     | 0.41              |
| 1:B:79:ILE:HG23 | 1:B:86:TYR:OH   | 2.20                     | 0.41              |
| 1:C:9:TYR:CD1   | 1:C:9:TYR:N     | 2.87                     | 0.41              |
| 1:C:67:LYS:HG2  | 1:C:77:LEU:O    | 2.21                     | 0.41              |
| 1:D:67:LYS:HG2  | 1:D:77:LEU:O    | 2.21                     | 0.41              |
| 1:E:67:LYS:HG2  | 1:E:77:LEU:O    | 2.21                     | 0.41              |
| 1:F:37:VAL:CG1  | 1:F:38:VAL:N    | 2.80                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:1:LEU:N     | 1:G:5:ARG:HH11   | 2.19                     | 0.41              |
| 1:G:9:TYR:H     | 1:G:9:TYR:HD1    | 1.62                     | 0.41              |
| 1:G:49:PHE:CB   | 1:G:55:ARG:HH22  | 2.17                     | 0.41              |
| 1:H:37:VAL:CG1  | 1:H:38:VAL:N     | 2.80                     | 0.41              |
| 1:I:30:ALA:CB   | 1:I:49:PHE:HE1   | 2.32                     | 0.41              |
| 1:K:79:ILE:CG2  | 1:K:81:THR:HB    | 2.51                     | 0.41              |
| 1:L:1:LEU:H3    | 1:L:5:ARG:HD3    | 1.86                     | 0.41              |
| 1:L:9:TYR:HB2   | 1:L:11:TYR:C     | 2.46                     | 0.41              |
| 1:M:9:TYR:HB2   | 1:M:11:TYR:C     | 2.46                     | 0.41              |
| 1:M:45:ILE:CG2  | 1:N:14:LYS:HE2   | 2.50                     | 0.41              |
| 1:M:79:ILE:CG2  | 1:M:81:THR:HB    | 2.51                     | 0.41              |
| 1:N:100:ASN:HA  | 1:N:100:ASN:HD22 | 1.52                     | 0.41              |
| 1:A:14:LYS:HE3  | 1:N:44:TYR:N     | 2.16                     | 0.41              |
| 1:A:83:LYS:NZ   | 1:A:111:GLU:HB3  | 2.36                     | 0.41              |
| 1:B:5:ARG:O     | 1:B:6:ASN:HB2    | 2.19                     | 0.41              |
| 1:B:9:TYR:HB2   | 1:B:11:TYR:C     | 2.46                     | 0.41              |
| 1:B:9:TYR:CD1   | 1:B:9:TYR:N      | 2.87                     | 0.41              |
| 1:C:24:VAL:HG11 | 1:C:107:LYS:CD   | 2.46                     | 0.41              |
| 1:D:49:PHE:CD2  | 1:D:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:E:16:VAL:CG1  | 1:E:18:TYR:HE1   | 2.31                     | 0.41              |
| 1:E:79:ILE:C    | 1:E:81:THR:N     | 2.79                     | 0.41              |
| 1:F:67:LYS:HG2  | 1:F:77:LEU:O     | 2.21                     | 0.41              |
| 1:G:24:VAL:HG11 | 1:G:107:LYS:CD   | 2.46                     | 0.41              |
| 1:G:49:PHE:CE2  | 1:G:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:H:46:THR:N    | 1:I:14:LYS:HZ1   | 2.19                     | 0.41              |
| 1:H:49:PHE:CE2  | 1:H:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:H:79:ILE:CG2  | 1:H:81:THR:HB    | 2.51                     | 0.41              |
| 1:I:38:VAL:CG2  | 1:I:39:ALA:H     | 2.31                     | 0.41              |
| 1:I:45:ILE:H    | 1:I:45:ILE:HG13  | 1.76                     | 0.41              |
| 1:I:79:ILE:HG23 | 1:I:86:TYR:OH    | 2.20                     | 0.41              |
| 1:I:79:ILE:CG2  | 1:I:81:THR:HB    | 2.51                     | 0.41              |
| 1:K:1:LEU:N     | 1:K:5:ARG:HH11   | 2.19                     | 0.41              |
| 1:L:37:VAL:HG12 | 1:L:38:VAL:H     | 1.85                     | 0.41              |
| 1:N:9:TYR:HB2   | 1:N:11:TYR:C     | 2.46                     | 0.41              |
| 1:N:67:LYS:HG2  | 1:N:77:LEU:O     | 2.21                     | 0.41              |
| 1:N:79:ILE:C    | 1:N:81:THR:N     | 2.79                     | 0.41              |
| 1:A:9:TYR:HB2   | 1:A:11:TYR:C     | 2.46                     | 0.41              |
| 1:A:24:VAL:HG11 | 1:A:38:VAL:HG13  | 1.99                     | 0.41              |
| 1:A:67:LYS:HG2  | 1:A:77:LEU:O     | 2.21                     | 0.41              |
| 1:A:100:ASN:HA  | 1:A:100:ASN:HD22 | 1.53                     | 0.41              |
| 1:B:79:ILE:C    | 1:B:81:THR:N     | 2.79                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:43:THR:HA   | 1:D:14:LYS:HD2   | 1.99                     | 0.41              |
| 1:C:49:PHE:CD2  | 1:C:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:C:79:ILE:HD12 | 1:C:107:LYS:HZ1  | 1.86                     | 0.41              |
| 1:C:82:ASP:HB3  | 1:C:84:ARG:H     | 1.86                     | 0.41              |
| 1:D:79:ILE:CG2  | 1:D:81:THR:HB    | 2.51                     | 0.41              |
| 1:E:49:PHE:CE2  | 1:E:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:F:83:LYS:NZ   | 1:F:111:GLU:HB3  | 2.36                     | 0.41              |
| 1:G:49:PHE:CD2  | 1:G:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:G:67:LYS:HG2  | 1:G:77:LEU:O     | 2.21                     | 0.41              |
| 1:G:79:ILE:CG2  | 1:G:81:THR:HB    | 2.51                     | 0.41              |
| 1:I:1:LEU:N     | 1:I:5:ARG:HH11   | 2.19                     | 0.41              |
| 1:J:5:ARG:O     | 1:J:6:ASN:HB2    | 2.19                     | 0.41              |
| 1:J:9:TYR:HB2   | 1:J:11:TYR:C     | 2.46                     | 0.41              |
| 1:J:38:VAL:CG2  | 1:J:39:ALA:H     | 2.31                     | 0.41              |
| 1:J:110:ILE:H   | 1:J:110:ILE:HG12 | 1.51                     | 0.41              |
| 1:K:9:TYR:HB2   | 1:K:11:TYR:C     | 2.46                     | 0.41              |
| 1:K:12:ARG:CG   | 1:K:13:ILE:N     | 2.83                     | 0.41              |
| 1:K:79:ILE:C    | 1:K:81:THR:N     | 2.79                     | 0.41              |
| 1:K:80:VAL:CG2  | 1:K:88:ILE:CG2   | 2.94                     | 0.41              |
| 1:L:32:VAL:CB   | 1:L:51:ASP:HA    | 2.35                     | 0.41              |
| 1:L:79:ILE:CG2  | 1:L:81:THR:HB    | 2.51                     | 0.41              |
| 1:M:24:VAL:HG11 | 1:M:107:LYS:CD   | 2.46                     | 0.41              |
| 1:M:83:LYS:NZ   | 1:M:111:GLU:HB3  | 2.36                     | 0.41              |
| 1:M:91:HIS:HB3  | 1:M:104:THR:CG2  | 2.37                     | 0.41              |
| 1:N:24:VAL:HG11 | 1:N:38:VAL:HG13  | 1.99                     | 0.41              |
| 1:N:49:PHE:CE2  | 1:N:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:C:79:ILE:HG23 | 1:C:86:TYR:OH    | 2.20                     | 0.41              |
| 1:E:49:PHE:CD2  | 1:E:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:E:79:ILE:CG2  | 1:E:81:THR:HB    | 2.51                     | 0.41              |
| 1:E:82:ASP:HB3  | 1:E:84:ARG:H     | 1.86                     | 0.41              |
| 1:F:49:PHE:CE2  | 1:F:79:ILE:CG1   | 3.03                     | 0.41              |
| 1:F:79:ILE:C    | 1:F:81:THR:N     | 2.79                     | 0.41              |
| 1:F:80:VAL:CG2  | 1:F:88:ILE:CG2   | 2.94                     | 0.41              |
| 1:H:1:LEU:N     | 1:H:5:ARG:HH11   | 2.19                     | 0.41              |
| 1:H:83:LYS:NZ   | 1:H:111:GLU:HB3  | 2.36                     | 0.41              |
| 1:I:61:MET:CG   | 1:I:62:ASN:N     | 2.82                     | 0.41              |
| 1:L:1:LEU:H3    | 1:L:5:ARG:CD     | 2.33                     | 0.41              |
| 1:L:98:LYS:HE3  | 1:L:101:ALA:N    | 2.33                     | 0.41              |
| 1:A:62:ASN:HB2  | 1:A:63:HIS:H     | 1.73                     | 0.40              |
| 1:C:1:LEU:N     | 1:C:5:ARG:HH11   | 2.19                     | 0.40              |
| 1:C:100:ASN:HA  | 1:C:100:ASN:HD22 | 1.52                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:1:LEU:N     | 1:D:5:ARG:HH11  | 2.19                     | 0.40              |
| 1:D:37:VAL:CG1  | 1:D:38:VAL:H    | 2.34                     | 0.40              |
| 1:E:37:VAL:CG1  | 1:E:38:VAL:H    | 2.34                     | 0.40              |
| 1:F:57:PHE:CZ   | 1:G:27:ASP:HB2  | 2.57                     | 0.40              |
| 1:L:44:TYR:N    | 1:M:14:LYS:HE3  | 2.16                     | 0.40              |
| 1:L:61:MET:HG2  | 1:L:62:ASN:N    | 2.34                     | 0.40              |
| 1:L:67:LYS:HG2  | 1:L:77:LEU:O    | 2.21                     | 0.40              |
| 1:M:17:VAL:HG12 | 1:M:18:TYR:H    | 1.86                     | 0.40              |
| 1:M:82:ASP:HB3  | 1:M:84:ARG:H    | 1.86                     | 0.40              |
| 1:N:37:VAL:HG12 | 1:N:38:VAL:H    | 1.84                     | 0.40              |
| 1:N:83:LYS:HD3  | 1:N:83:LYS:HA   | 1.57                     | 0.40              |
| 1:A:9:TYR:CD1   | 1:A:9:TYR:N     | 2.87                     | 0.40              |
| 1:B:29:VAL:HG11 | 1:B:77:LEU:HD11 | 1.98                     | 0.40              |
| 1:B:98:LYS:HE3  | 1:B:101:ALA:N   | 2.33                     | 0.40              |
| 1:C:9:TYR:HB2   | 1:C:11:TYR:C    | 2.46                     | 0.40              |
| 1:C:79:ILE:CG2  | 1:C:81:THR:HB   | 2.51                     | 0.40              |
| 1:D:9:TYR:CD1   | 1:D:9:TYR:N     | 2.87                     | 0.40              |
| 1:F:70:GLN:HE21 | 1:F:70:GLN:HB3  | 1.50                     | 0.40              |
| 1:G:57:PHE:CZ   | 1:H:27:ASP:HB2  | 2.57                     | 0.40              |
| 1:G:79:ILE:HG23 | 1:G:86:TYR:OH   | 2.20                     | 0.40              |
| 1:G:82:ASP:HB3  | 1:G:84:ARG:H    | 1.86                     | 0.40              |
| 1:H:79:ILE:HG23 | 1:H:86:TYR:OH   | 2.20                     | 0.40              |
| 1:I:9:TYR:HB2   | 1:I:11:TYR:C    | 2.46                     | 0.40              |
| 1:J:82:ASP:HB3  | 1:J:84:ARG:H    | 1.86                     | 0.40              |
| 1:M:49:PHE:CE2  | 1:M:79:ILE:CG1  | 3.03                     | 0.40              |
| 1:N:1:LEU:N     | 1:N:5:ARG:HH11  | 2.19                     | 0.40              |
| 1:A:57:PHE:CZ   | 1:B:27:ASP:HB2  | 2.57                     | 0.40              |
| 1:B:79:ILE:CG2  | 1:B:81:THR:HB   | 2.51                     | 0.40              |
| 1:C:98:LYS:HE3  | 1:C:101:ALA:N   | 2.33                     | 0.40              |
| 1:D:83:LYS:NZ   | 1:D:111:GLU:HB3 | 2.36                     | 0.40              |
| 1:F:79:ILE:CG2  | 1:F:81:THR:HB   | 2.51                     | 0.40              |
| 1:I:82:ASP:HB3  | 1:I:84:ARG:H    | 1.86                     | 0.40              |
| 1:I:83:LYS:NZ   | 1:I:111:GLU:HB3 | 2.36                     | 0.40              |
| 1:K:83:LYS:NZ   | 1:K:111:GLU:HB3 | 2.36                     | 0.40              |
| 1:L:14:LYS:H    | 1:L:14:LYS:HG2  | 1.48                     | 0.40              |
| 1:L:79:ILE:C    | 1:L:81:THR:N    | 2.79                     | 0.40              |
| 1:M:98:LYS:CE   | 1:M:101:ALA:H   | 2.34                     | 0.40              |
| 1:N:17:VAL:HG12 | 1:N:18:TYR:H    | 1.86                     | 0.40              |
| 1:N:79:ILE:CG2  | 1:N:81:THR:HB   | 2.51                     | 0.40              |
| 1:A:27:ASP:HB2  | 1:N:57:PHE:CZ   | 2.57                     | 0.40              |
| 1:A:98:LYS:HE3  | 1:A:101:ALA:N   | 2.33                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:1:LEU:N     | 1:B:5:ARG:HH11   | 2.19                     | 0.40              |
| 1:C:79:ILE:C    | 1:C:81:THR:N     | 2.79                     | 0.40              |
| 1:D:9:TYR:HB2   | 1:D:11:TYR:C     | 2.46                     | 0.40              |
| 1:E:79:ILE:HG23 | 1:E:86:TYR:OH    | 2.20                     | 0.40              |
| 1:F:17:VAL:HG12 | 1:F:18:TYR:H     | 1.86                     | 0.40              |
| 1:F:37:VAL:CG1  | 1:F:38:VAL:H     | 2.34                     | 0.40              |
| 1:H:9:TYR:HB2   | 1:H:11:TYR:C     | 2.46                     | 0.40              |
| 1:H:57:PHE:CZ   | 1:I:27:ASP:HB2   | 2.57                     | 0.40              |
| 1:H:79:ILE:C    | 1:H:81:THR:N     | 2.79                     | 0.40              |
| 1:J:79:ILE:C    | 1:J:81:THR:N     | 2.79                     | 0.40              |
| 1:K:38:VAL:O    | 1:K:44:TYR:CE1   | 2.75                     | 0.40              |
| 1:K:61:MET:HG2  | 1:K:62:ASN:N     | 2.34                     | 0.40              |
| 1:L:82:ASP:HB3  | 1:L:84:ARG:H     | 1.86                     | 0.40              |
| 1:M:61:MET:HG2  | 1:M:62:ASN:N     | 2.34                     | 0.40              |
| 1:N:83:LYS:HZ2  | 1:N:111:GLU:HB3  | 1.85                     | 0.40              |
| 1:A:34:THR:HG23 | 1:A:47:HIS:CB    | 2.41                     | 0.40              |
| 1:B:56:THR:CG2  | 1:B:57:PHE:N     | 2.82                     | 0.40              |
| 1:B:82:ASP:HB3  | 1:B:84:ARG:H     | 1.86                     | 0.40              |
| 1:C:29:VAL:HG12 | 1:C:92:PHE:HE2   | 1.81                     | 0.40              |
| 1:C:83:LYS:NZ   | 1:C:111:GLU:HB3  | 2.36                     | 0.40              |
| 1:D:98:LYS:HE3  | 1:D:101:ALA:N    | 2.33                     | 0.40              |
| 1:E:1:LEU:N     | 1:E:5:ARG:HH11   | 2.19                     | 0.40              |
| 1:E:9:TYR:HB2   | 1:E:11:TYR:C     | 2.46                     | 0.40              |
| 1:E:45:ILE:H    | 1:E:45:ILE:HG13  | 1.76                     | 0.40              |
| 1:E:57:PHE:CZ   | 1:F:27:ASP:HB2   | 2.57                     | 0.40              |
| 1:G:83:LYS:NZ   | 1:G:111:GLU:HB3  | 2.36                     | 0.40              |
| 1:G:98:LYS:CE   | 1:G:101:ALA:H    | 2.34                     | 0.40              |
| 1:H:82:ASP:HB3  | 1:H:84:ARG:H     | 1.86                     | 0.40              |
| 1:J:56:THR:CG2  | 1:J:57:PHE:N     | 2.82                     | 0.40              |
| 1:J:67:LYS:HG2  | 1:J:77:LEU:O     | 2.21                     | 0.40              |
| 1:K:57:PHE:CZ   | 1:L:27:ASP:HB2   | 2.57                     | 0.40              |
| 1:K:83:LYS:HZ2  | 1:K:111:GLU:HB3  | 1.87                     | 0.40              |
| 1:K:98:LYS:HE3  | 1:K:100:ASN:CA   | 2.36                     | 0.40              |
| 1:L:38:VAL:O    | 1:L:44:TYR:CE1   | 2.75                     | 0.40              |
| 1:M:38:VAL:O    | 1:M:44:TYR:CE1   | 2.75                     | 0.40              |
| 1:M:100:ASN:HA  | 1:M:100:ASN:HD22 | 1.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers  | Percentiles |   |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|---|
| 1   | A     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | B     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | C     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | D     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | E     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | F     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | G     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | H     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | I     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | J     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | K     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | L     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | M     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| 1   | N     | 110/112 (98%)   | 70 (64%)  | 26 (24%)  | 14 (13%)  | 0           | 4 |
| All | All   | 1540/1568 (98%) | 980 (64%) | 364 (24%) | 196 (13%) | 0           | 4 |

All (196) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | VAL  |
| 1   | A     | 14  | LYS  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 28  | ALA  |
| 1   | A     | 33  | ALA  |
| 1   | A     | 38  | VAL  |
| 1   | A     | 83  | LYS  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 14  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 21  | VAL  |
| 1   | B     | 28  | ALA  |
| 1   | B     | 33  | ALA  |
| 1   | B     | 38  | VAL  |
| 1   | B     | 83  | LYS  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 14  | LYS  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 28  | ALA  |
| 1   | C     | 33  | ALA  |
| 1   | C     | 38  | VAL  |
| 1   | C     | 83  | LYS  |
| 1   | D     | 3   | VAL  |
| 1   | D     | 14  | LYS  |
| 1   | D     | 21  | VAL  |
| 1   | D     | 28  | ALA  |
| 1   | D     | 33  | ALA  |
| 1   | D     | 38  | VAL  |
| 1   | D     | 83  | LYS  |
| 1   | E     | 3   | VAL  |
| 1   | E     | 14  | LYS  |
| 1   | E     | 21  | VAL  |
| 1   | E     | 28  | ALA  |
| 1   | E     | 33  | ALA  |
| 1   | E     | 38  | VAL  |
| 1   | E     | 83  | LYS  |
| 1   | F     | 3   | VAL  |
| 1   | F     | 14  | LYS  |
| 1   | F     | 21  | VAL  |
| 1   | F     | 28  | ALA  |
| 1   | F     | 33  | ALA  |
| 1   | F     | 38  | VAL  |
| 1   | F     | 83  | LYS  |
| 1   | G     | 3   | VAL  |
| 1   | G     | 14  | LYS  |
| 1   | G     | 21  | VAL  |
| 1   | G     | 28  | ALA  |
| 1   | G     | 33  | ALA  |
| 1   | G     | 38  | VAL  |
| 1   | G     | 83  | LYS  |
| 1   | H     | 3   | VAL  |
| 1   | H     | 14  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 21  | VAL  |
| 1   | H     | 28  | ALA  |
| 1   | H     | 33  | ALA  |
| 1   | H     | 38  | VAL  |
| 1   | H     | 83  | LYS  |
| 1   | I     | 3   | VAL  |
| 1   | I     | 14  | LYS  |
| 1   | I     | 21  | VAL  |
| 1   | I     | 28  | ALA  |
| 1   | I     | 33  | ALA  |
| 1   | I     | 38  | VAL  |
| 1   | I     | 83  | LYS  |
| 1   | J     | 3   | VAL  |
| 1   | J     | 14  | LYS  |
| 1   | J     | 21  | VAL  |
| 1   | J     | 28  | ALA  |
| 1   | J     | 33  | ALA  |
| 1   | J     | 38  | VAL  |
| 1   | J     | 83  | LYS  |
| 1   | K     | 3   | VAL  |
| 1   | K     | 14  | LYS  |
| 1   | K     | 21  | VAL  |
| 1   | K     | 28  | ALA  |
| 1   | K     | 33  | ALA  |
| 1   | K     | 38  | VAL  |
| 1   | K     | 83  | LYS  |
| 1   | L     | 3   | VAL  |
| 1   | L     | 14  | LYS  |
| 1   | L     | 21  | VAL  |
| 1   | L     | 28  | ALA  |
| 1   | L     | 33  | ALA  |
| 1   | L     | 38  | VAL  |
| 1   | L     | 83  | LYS  |
| 1   | M     | 3   | VAL  |
| 1   | M     | 14  | LYS  |
| 1   | M     | 21  | VAL  |
| 1   | M     | 28  | ALA  |
| 1   | M     | 33  | ALA  |
| 1   | M     | 38  | VAL  |
| 1   | M     | 83  | LYS  |
| 1   | N     | 3   | VAL  |
| 1   | N     | 14  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 21  | VAL  |
| 1   | N     | 28  | ALA  |
| 1   | N     | 33  | ALA  |
| 1   | N     | 38  | VAL  |
| 1   | N     | 83  | LYS  |
| 1   | A     | 35  | HIS  |
| 1   | A     | 37  | VAL  |
| 1   | A     | 109 | PHE  |
| 1   | B     | 35  | HIS  |
| 1   | B     | 37  | VAL  |
| 1   | B     | 109 | PHE  |
| 1   | C     | 35  | HIS  |
| 1   | C     | 37  | VAL  |
| 1   | C     | 109 | PHE  |
| 1   | D     | 35  | HIS  |
| 1   | D     | 37  | VAL  |
| 1   | D     | 109 | PHE  |
| 1   | E     | 35  | HIS  |
| 1   | E     | 37  | VAL  |
| 1   | E     | 109 | PHE  |
| 1   | F     | 35  | HIS  |
| 1   | F     | 37  | VAL  |
| 1   | F     | 109 | PHE  |
| 1   | G     | 35  | HIS  |
| 1   | G     | 37  | VAL  |
| 1   | G     | 109 | PHE  |
| 1   | H     | 35  | HIS  |
| 1   | H     | 37  | VAL  |
| 1   | H     | 109 | PHE  |
| 1   | I     | 35  | HIS  |
| 1   | I     | 37  | VAL  |
| 1   | I     | 109 | PHE  |
| 1   | J     | 35  | HIS  |
| 1   | J     | 37  | VAL  |
| 1   | J     | 109 | PHE  |
| 1   | K     | 35  | HIS  |
| 1   | K     | 37  | VAL  |
| 1   | K     | 109 | PHE  |
| 1   | L     | 35  | HIS  |
| 1   | L     | 37  | VAL  |
| 1   | L     | 109 | PHE  |
| 1   | M     | 35  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 37  | VAL  |
| 1   | M     | 109 | PHE  |
| 1   | N     | 35  | HIS  |
| 1   | N     | 37  | VAL  |
| 1   | N     | 109 | PHE  |
| 1   | A     | 62  | ASN  |
| 1   | A     | 70  | GLN  |
| 1   | A     | 93  | ILE  |
| 1   | B     | 62  | ASN  |
| 1   | B     | 70  | GLN  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 70  | GLN  |
| 1   | C     | 93  | ILE  |
| 1   | D     | 62  | ASN  |
| 1   | D     | 70  | GLN  |
| 1   | D     | 93  | ILE  |
| 1   | E     | 62  | ASN  |
| 1   | E     | 70  | GLN  |
| 1   | E     | 93  | ILE  |
| 1   | F     | 62  | ASN  |
| 1   | F     | 70  | GLN  |
| 1   | G     | 62  | ASN  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 93  | ILE  |
| 1   | H     | 62  | ASN  |
| 1   | H     | 70  | GLN  |
| 1   | H     | 93  | ILE  |
| 1   | I     | 62  | ASN  |
| 1   | I     | 70  | GLN  |
| 1   | J     | 62  | ASN  |
| 1   | J     | 70  | GLN  |
| 1   | J     | 93  | ILE  |
| 1   | K     | 62  | ASN  |
| 1   | K     | 70  | GLN  |
| 1   | K     | 93  | ILE  |
| 1   | L     | 62  | ASN  |
| 1   | L     | 70  | GLN  |
| 1   | L     | 93  | ILE  |
| 1   | M     | 62  | ASN  |
| 1   | M     | 70  | GLN  |
| 1   | N     | 62  | ASN  |
| 1   | N     | 70  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 93  | ILE  |
| 1   | B     | 93  | ILE  |
| 1   | F     | 93  | ILE  |
| 1   | I     | 93  | ILE  |
| 1   | M     | 93  | ILE  |
| 1   | A     | 80  | VAL  |
| 1   | B     | 80  | VAL  |
| 1   | C     | 80  | VAL  |
| 1   | D     | 80  | VAL  |
| 1   | E     | 80  | VAL  |
| 1   | F     | 80  | VAL  |
| 1   | G     | 80  | VAL  |
| 1   | H     | 80  | VAL  |
| 1   | I     | 80  | VAL  |
| 1   | J     | 80  | VAL  |
| 1   | K     | 80  | VAL  |
| 1   | L     | 80  | VAL  |
| 1   | M     | 80  | VAL  |
| 1   | N     | 80  | VAL  |

### 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     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | B     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | C     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | D     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | E     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | F     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | G     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | H     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |
| 1   | I     | 99/99 (100%) | 67 (68%)  | 32 (32%) | 0           | 2 |

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| Mol | Chain | Analysed         | Rotameric | Outliers  | Percentiles |   |
|-----|-------|------------------|-----------|-----------|-------------|---|
| 1   | J     | 99/99 (100%)     | 67 (68%)  | 32 (32%)  | 0           | 2 |
| 1   | K     | 99/99 (100%)     | 67 (68%)  | 32 (32%)  | 0           | 2 |
| 1   | L     | 99/99 (100%)     | 67 (68%)  | 32 (32%)  | 0           | 2 |
| 1   | M     | 99/99 (100%)     | 67 (68%)  | 32 (32%)  | 0           | 2 |
| 1   | N     | 99/99 (100%)     | 67 (68%)  | 32 (32%)  | 0           | 2 |
| All | All   | 1386/1386 (100%) | 938 (68%) | 448 (32%) | 1           | 2 |

All (448) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | LEU  |
| 1   | A     | 3   | VAL  |
| 1   | A     | 9   | TYR  |
| 1   | A     | 11  | TYR  |
| 1   | A     | 14  | LYS  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 25  | LYS  |
| 1   | A     | 26  | ILE  |
| 1   | A     | 43  | THR  |
| 1   | A     | 45  | ILE  |
| 1   | A     | 49  | PHE  |
| 1   | A     | 53  | GLU  |
| 1   | A     | 55  | ARG  |
| 1   | A     | 59  | HIS  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 61  | MET  |
| 1   | A     | 62  | ASN  |
| 1   | A     | 64  | PHE  |
| 1   | A     | 66  | VAL  |
| 1   | A     | 69  | LYS  |
| 1   | A     | 70  | GLN  |
| 1   | A     | 73  | SER  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 78  | VAL  |
| 1   | A     | 84  | ARG  |
| 1   | A     | 89  | VAL  |
| 1   | A     | 93  | ILE  |
| 1   | A     | 98  | LYS  |
| 1   | A     | 105 | VAL  |
| 1   | A     | 109 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | ILE  |
| 1   | A     | 111 | GLU  |
| 1   | B     | 1   | LEU  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 9   | TYR  |
| 1   | B     | 11  | TYR  |
| 1   | B     | 14  | LYS  |
| 1   | B     | 17  | VAL  |
| 1   | B     | 25  | LYS  |
| 1   | B     | 26  | ILE  |
| 1   | B     | 43  | THR  |
| 1   | B     | 45  | ILE  |
| 1   | B     | 49  | PHE  |
| 1   | B     | 53  | GLU  |
| 1   | B     | 55  | ARG  |
| 1   | B     | 59  | HIS  |
| 1   | B     | 60  | LYS  |
| 1   | B     | 61  | MET  |
| 1   | B     | 62  | ASN  |
| 1   | B     | 64  | PHE  |
| 1   | B     | 66  | VAL  |
| 1   | B     | 69  | LYS  |
| 1   | B     | 70  | GLN  |
| 1   | B     | 73  | SER  |
| 1   | B     | 76  | ASN  |
| 1   | B     | 78  | VAL  |
| 1   | B     | 84  | ARG  |
| 1   | B     | 89  | VAL  |
| 1   | B     | 93  | ILE  |
| 1   | B     | 98  | LYS  |
| 1   | B     | 105 | VAL  |
| 1   | B     | 109 | PHE  |
| 1   | B     | 110 | ILE  |
| 1   | B     | 111 | GLU  |
| 1   | C     | 1   | LEU  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 9   | TYR  |
| 1   | C     | 11  | TYR  |
| 1   | C     | 14  | LYS  |
| 1   | C     | 17  | VAL  |
| 1   | C     | 25  | LYS  |
| 1   | C     | 26  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 43  | THR  |
| 1   | C     | 45  | ILE  |
| 1   | C     | 49  | PHE  |
| 1   | C     | 53  | GLU  |
| 1   | C     | 55  | ARG  |
| 1   | C     | 59  | HIS  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 61  | MET  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 64  | PHE  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 69  | LYS  |
| 1   | C     | 70  | GLN  |
| 1   | C     | 73  | SER  |
| 1   | C     | 76  | ASN  |
| 1   | C     | 78  | VAL  |
| 1   | C     | 84  | ARG  |
| 1   | C     | 89  | VAL  |
| 1   | C     | 93  | ILE  |
| 1   | C     | 98  | LYS  |
| 1   | C     | 105 | VAL  |
| 1   | C     | 109 | PHE  |
| 1   | C     | 110 | ILE  |
| 1   | C     | 111 | GLU  |
| 1   | D     | 1   | LEU  |
| 1   | D     | 3   | VAL  |
| 1   | D     | 9   | TYR  |
| 1   | D     | 11  | TYR  |
| 1   | D     | 14  | LYS  |
| 1   | D     | 17  | VAL  |
| 1   | D     | 25  | LYS  |
| 1   | D     | 26  | ILE  |
| 1   | D     | 43  | THR  |
| 1   | D     | 45  | ILE  |
| 1   | D     | 49  | PHE  |
| 1   | D     | 53  | GLU  |
| 1   | D     | 55  | ARG  |
| 1   | D     | 59  | HIS  |
| 1   | D     | 60  | LYS  |
| 1   | D     | 61  | MET  |
| 1   | D     | 62  | ASN  |
| 1   | D     | 64  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 66  | VAL  |
| 1   | D     | 69  | LYS  |
| 1   | D     | 70  | GLN  |
| 1   | D     | 73  | SER  |
| 1   | D     | 76  | ASN  |
| 1   | D     | 78  | VAL  |
| 1   | D     | 84  | ARG  |
| 1   | D     | 89  | VAL  |
| 1   | D     | 93  | ILE  |
| 1   | D     | 98  | LYS  |
| 1   | D     | 105 | VAL  |
| 1   | D     | 109 | PHE  |
| 1   | D     | 110 | ILE  |
| 1   | D     | 111 | GLU  |
| 1   | E     | 1   | LEU  |
| 1   | E     | 3   | VAL  |
| 1   | E     | 9   | TYR  |
| 1   | E     | 11  | TYR  |
| 1   | E     | 14  | LYS  |
| 1   | E     | 17  | VAL  |
| 1   | E     | 25  | LYS  |
| 1   | E     | 26  | ILE  |
| 1   | E     | 43  | THR  |
| 1   | E     | 45  | ILE  |
| 1   | E     | 49  | PHE  |
| 1   | E     | 53  | GLU  |
| 1   | E     | 55  | ARG  |
| 1   | E     | 59  | HIS  |
| 1   | E     | 60  | LYS  |
| 1   | E     | 61  | MET  |
| 1   | E     | 62  | ASN  |
| 1   | E     | 64  | PHE  |
| 1   | E     | 66  | VAL  |
| 1   | E     | 69  | LYS  |
| 1   | E     | 70  | GLN  |
| 1   | E     | 73  | SER  |
| 1   | E     | 76  | ASN  |
| 1   | E     | 78  | VAL  |
| 1   | E     | 84  | ARG  |
| 1   | E     | 89  | VAL  |
| 1   | E     | 93  | ILE  |
| 1   | E     | 98  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 105 | VAL  |
| 1   | E     | 109 | PHE  |
| 1   | E     | 110 | ILE  |
| 1   | E     | 111 | GLU  |
| 1   | F     | 1   | LEU  |
| 1   | F     | 3   | VAL  |
| 1   | F     | 9   | TYR  |
| 1   | F     | 11  | TYR  |
| 1   | F     | 14  | LYS  |
| 1   | F     | 17  | VAL  |
| 1   | F     | 25  | LYS  |
| 1   | F     | 26  | ILE  |
| 1   | F     | 43  | THR  |
| 1   | F     | 45  | ILE  |
| 1   | F     | 49  | PHE  |
| 1   | F     | 53  | GLU  |
| 1   | F     | 55  | ARG  |
| 1   | F     | 59  | HIS  |
| 1   | F     | 60  | LYS  |
| 1   | F     | 61  | MET  |
| 1   | F     | 62  | ASN  |
| 1   | F     | 64  | PHE  |
| 1   | F     | 66  | VAL  |
| 1   | F     | 69  | LYS  |
| 1   | F     | 70  | GLN  |
| 1   | F     | 73  | SER  |
| 1   | F     | 76  | ASN  |
| 1   | F     | 78  | VAL  |
| 1   | F     | 84  | ARG  |
| 1   | F     | 89  | VAL  |
| 1   | F     | 93  | ILE  |
| 1   | F     | 98  | LYS  |
| 1   | F     | 105 | VAL  |
| 1   | F     | 109 | PHE  |
| 1   | F     | 110 | ILE  |
| 1   | F     | 111 | GLU  |
| 1   | G     | 1   | LEU  |
| 1   | G     | 3   | VAL  |
| 1   | G     | 9   | TYR  |
| 1   | G     | 11  | TYR  |
| 1   | G     | 14  | LYS  |
| 1   | G     | 17  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 25  | LYS  |
| 1   | G     | 26  | ILE  |
| 1   | G     | 43  | THR  |
| 1   | G     | 45  | ILE  |
| 1   | G     | 49  | PHE  |
| 1   | G     | 53  | GLU  |
| 1   | G     | 55  | ARG  |
| 1   | G     | 59  | HIS  |
| 1   | G     | 60  | LYS  |
| 1   | G     | 61  | MET  |
| 1   | G     | 62  | ASN  |
| 1   | G     | 64  | PHE  |
| 1   | G     | 66  | VAL  |
| 1   | G     | 69  | LYS  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 73  | SER  |
| 1   | G     | 76  | ASN  |
| 1   | G     | 78  | VAL  |
| 1   | G     | 84  | ARG  |
| 1   | G     | 89  | VAL  |
| 1   | G     | 93  | ILE  |
| 1   | G     | 98  | LYS  |
| 1   | G     | 105 | VAL  |
| 1   | G     | 109 | PHE  |
| 1   | G     | 110 | ILE  |
| 1   | G     | 111 | GLU  |
| 1   | H     | 1   | LEU  |
| 1   | H     | 3   | VAL  |
| 1   | H     | 9   | TYR  |
| 1   | H     | 11  | TYR  |
| 1   | H     | 14  | LYS  |
| 1   | H     | 17  | VAL  |
| 1   | H     | 25  | LYS  |
| 1   | H     | 26  | ILE  |
| 1   | H     | 43  | THR  |
| 1   | H     | 45  | ILE  |
| 1   | H     | 49  | PHE  |
| 1   | H     | 53  | GLU  |
| 1   | H     | 55  | ARG  |
| 1   | H     | 59  | HIS  |
| 1   | H     | 60  | LYS  |
| 1   | H     | 61  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 62  | ASN  |
| 1   | H     | 64  | PHE  |
| 1   | H     | 66  | VAL  |
| 1   | H     | 69  | LYS  |
| 1   | H     | 70  | GLN  |
| 1   | H     | 73  | SER  |
| 1   | H     | 76  | ASN  |
| 1   | H     | 78  | VAL  |
| 1   | H     | 84  | ARG  |
| 1   | H     | 89  | VAL  |
| 1   | H     | 93  | ILE  |
| 1   | H     | 98  | LYS  |
| 1   | H     | 105 | VAL  |
| 1   | H     | 109 | PHE  |
| 1   | H     | 110 | ILE  |
| 1   | H     | 111 | GLU  |
| 1   | I     | 1   | LEU  |
| 1   | I     | 3   | VAL  |
| 1   | I     | 9   | TYR  |
| 1   | I     | 11  | TYR  |
| 1   | I     | 14  | LYS  |
| 1   | I     | 17  | VAL  |
| 1   | I     | 25  | LYS  |
| 1   | I     | 26  | ILE  |
| 1   | I     | 43  | THR  |
| 1   | I     | 45  | ILE  |
| 1   | I     | 49  | PHE  |
| 1   | I     | 53  | GLU  |
| 1   | I     | 55  | ARG  |
| 1   | I     | 59  | HIS  |
| 1   | I     | 60  | LYS  |
| 1   | I     | 61  | MET  |
| 1   | I     | 62  | ASN  |
| 1   | I     | 64  | PHE  |
| 1   | I     | 66  | VAL  |
| 1   | I     | 69  | LYS  |
| 1   | I     | 70  | GLN  |
| 1   | I     | 73  | SER  |
| 1   | I     | 76  | ASN  |
| 1   | I     | 78  | VAL  |
| 1   | I     | 84  | ARG  |
| 1   | I     | 89  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 93  | ILE  |
| 1   | I     | 98  | LYS  |
| 1   | I     | 105 | VAL  |
| 1   | I     | 109 | PHE  |
| 1   | I     | 110 | ILE  |
| 1   | I     | 111 | GLU  |
| 1   | J     | 1   | LEU  |
| 1   | J     | 3   | VAL  |
| 1   | J     | 9   | TYR  |
| 1   | J     | 11  | TYR  |
| 1   | J     | 14  | LYS  |
| 1   | J     | 17  | VAL  |
| 1   | J     | 25  | LYS  |
| 1   | J     | 26  | ILE  |
| 1   | J     | 43  | THR  |
| 1   | J     | 45  | ILE  |
| 1   | J     | 49  | PHE  |
| 1   | J     | 53  | GLU  |
| 1   | J     | 55  | ARG  |
| 1   | J     | 59  | HIS  |
| 1   | J     | 60  | LYS  |
| 1   | J     | 61  | MET  |
| 1   | J     | 62  | ASN  |
| 1   | J     | 64  | PHE  |
| 1   | J     | 66  | VAL  |
| 1   | J     | 69  | LYS  |
| 1   | J     | 70  | GLN  |
| 1   | J     | 73  | SER  |
| 1   | J     | 76  | ASN  |
| 1   | J     | 78  | VAL  |
| 1   | J     | 84  | ARG  |
| 1   | J     | 89  | VAL  |
| 1   | J     | 93  | ILE  |
| 1   | J     | 98  | LYS  |
| 1   | J     | 105 | VAL  |
| 1   | J     | 109 | PHE  |
| 1   | J     | 110 | ILE  |
| 1   | J     | 111 | GLU  |
| 1   | K     | 1   | LEU  |
| 1   | K     | 3   | VAL  |
| 1   | K     | 9   | TYR  |
| 1   | K     | 11  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 14  | LYS  |
| 1   | K     | 17  | VAL  |
| 1   | K     | 25  | LYS  |
| 1   | K     | 26  | ILE  |
| 1   | K     | 43  | THR  |
| 1   | K     | 45  | ILE  |
| 1   | K     | 49  | PHE  |
| 1   | K     | 53  | GLU  |
| 1   | K     | 55  | ARG  |
| 1   | K     | 59  | HIS  |
| 1   | K     | 60  | LYS  |
| 1   | K     | 61  | MET  |
| 1   | K     | 62  | ASN  |
| 1   | K     | 64  | PHE  |
| 1   | K     | 66  | VAL  |
| 1   | K     | 69  | LYS  |
| 1   | K     | 70  | GLN  |
| 1   | K     | 73  | SER  |
| 1   | K     | 76  | ASN  |
| 1   | K     | 78  | VAL  |
| 1   | K     | 84  | ARG  |
| 1   | K     | 89  | VAL  |
| 1   | K     | 93  | ILE  |
| 1   | K     | 98  | LYS  |
| 1   | K     | 105 | VAL  |
| 1   | K     | 109 | PHE  |
| 1   | K     | 110 | ILE  |
| 1   | K     | 111 | GLU  |
| 1   | L     | 1   | LEU  |
| 1   | L     | 3   | VAL  |
| 1   | L     | 9   | TYR  |
| 1   | L     | 11  | TYR  |
| 1   | L     | 14  | LYS  |
| 1   | L     | 17  | VAL  |
| 1   | L     | 25  | LYS  |
| 1   | L     | 26  | ILE  |
| 1   | L     | 43  | THR  |
| 1   | L     | 45  | ILE  |
| 1   | L     | 49  | PHE  |
| 1   | L     | 53  | GLU  |
| 1   | L     | 55  | ARG  |
| 1   | L     | 59  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 60  | LYS  |
| 1   | L     | 61  | MET  |
| 1   | L     | 62  | ASN  |
| 1   | L     | 64  | PHE  |
| 1   | L     | 66  | VAL  |
| 1   | L     | 69  | LYS  |
| 1   | L     | 70  | GLN  |
| 1   | L     | 73  | SER  |
| 1   | L     | 76  | ASN  |
| 1   | L     | 78  | VAL  |
| 1   | L     | 84  | ARG  |
| 1   | L     | 89  | VAL  |
| 1   | L     | 93  | ILE  |
| 1   | L     | 98  | LYS  |
| 1   | L     | 105 | VAL  |
| 1   | L     | 109 | PHE  |
| 1   | L     | 110 | ILE  |
| 1   | L     | 111 | GLU  |
| 1   | M     | 1   | LEU  |
| 1   | M     | 3   | VAL  |
| 1   | M     | 9   | TYR  |
| 1   | M     | 11  | TYR  |
| 1   | M     | 14  | LYS  |
| 1   | M     | 17  | VAL  |
| 1   | M     | 25  | LYS  |
| 1   | M     | 26  | ILE  |
| 1   | M     | 43  | THR  |
| 1   | M     | 45  | ILE  |
| 1   | M     | 49  | PHE  |
| 1   | M     | 53  | GLU  |
| 1   | M     | 55  | ARG  |
| 1   | M     | 59  | HIS  |
| 1   | M     | 60  | LYS  |
| 1   | M     | 61  | MET  |
| 1   | M     | 62  | ASN  |
| 1   | M     | 64  | PHE  |
| 1   | M     | 66  | VAL  |
| 1   | M     | 69  | LYS  |
| 1   | M     | 70  | GLN  |
| 1   | M     | 73  | SER  |
| 1   | M     | 76  | ASN  |
| 1   | M     | 78  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 84  | ARG  |
| 1   | M     | 89  | VAL  |
| 1   | M     | 93  | ILE  |
| 1   | M     | 98  | LYS  |
| 1   | M     | 105 | VAL  |
| 1   | M     | 109 | PHE  |
| 1   | M     | 110 | ILE  |
| 1   | M     | 111 | GLU  |
| 1   | N     | 1   | LEU  |
| 1   | N     | 3   | VAL  |
| 1   | N     | 9   | TYR  |
| 1   | N     | 11  | TYR  |
| 1   | N     | 14  | LYS  |
| 1   | N     | 17  | VAL  |
| 1   | N     | 25  | LYS  |
| 1   | N     | 26  | ILE  |
| 1   | N     | 43  | THR  |
| 1   | N     | 45  | ILE  |
| 1   | N     | 49  | PHE  |
| 1   | N     | 53  | GLU  |
| 1   | N     | 55  | ARG  |
| 1   | N     | 59  | HIS  |
| 1   | N     | 60  | LYS  |
| 1   | N     | 61  | MET  |
| 1   | N     | 62  | ASN  |
| 1   | N     | 64  | PHE  |
| 1   | N     | 66  | VAL  |
| 1   | N     | 69  | LYS  |
| 1   | N     | 70  | GLN  |
| 1   | N     | 73  | SER  |
| 1   | N     | 76  | ASN  |
| 1   | N     | 78  | VAL  |
| 1   | N     | 84  | ARG  |
| 1   | N     | 89  | VAL  |
| 1   | N     | 93  | ILE  |
| 1   | N     | 98  | LYS  |
| 1   | N     | 105 | VAL  |
| 1   | N     | 109 | PHE  |
| 1   | N     | 110 | ILE  |
| 1   | N     | 111 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | HIS  |
| 1   | A     | 70  | GLN  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 91  | HIS  |
| 1   | A     | 100 | ASN  |
| 1   | B     | 59  | HIS  |
| 1   | B     | 70  | GLN  |
| 1   | B     | 76  | ASN  |
| 1   | B     | 87  | ASN  |
| 1   | B     | 91  | HIS  |
| 1   | B     | 100 | ASN  |
| 1   | C     | 59  | HIS  |
| 1   | C     | 70  | GLN  |
| 1   | C     | 76  | ASN  |
| 1   | C     | 87  | ASN  |
| 1   | C     | 91  | HIS  |
| 1   | C     | 100 | ASN  |
| 1   | D     | 59  | HIS  |
| 1   | D     | 70  | GLN  |
| 1   | D     | 76  | ASN  |
| 1   | D     | 87  | ASN  |
| 1   | D     | 91  | HIS  |
| 1   | D     | 100 | ASN  |
| 1   | E     | 59  | HIS  |
| 1   | E     | 70  | GLN  |
| 1   | E     | 76  | ASN  |
| 1   | E     | 87  | ASN  |
| 1   | E     | 91  | HIS  |
| 1   | E     | 100 | ASN  |
| 1   | F     | 59  | HIS  |
| 1   | F     | 70  | GLN  |
| 1   | F     | 76  | ASN  |
| 1   | F     | 87  | ASN  |
| 1   | F     | 91  | HIS  |
| 1   | F     | 100 | ASN  |
| 1   | G     | 59  | HIS  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 76  | ASN  |
| 1   | G     | 87  | ASN  |
| 1   | G     | 91  | HIS  |
| 1   | G     | 100 | ASN  |
| 1   | H     | 59  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 70  | GLN  |
| 1   | H     | 76  | ASN  |
| 1   | H     | 87  | ASN  |
| 1   | H     | 91  | HIS  |
| 1   | H     | 100 | ASN  |
| 1   | I     | 59  | HIS  |
| 1   | I     | 70  | GLN  |
| 1   | I     | 76  | ASN  |
| 1   | I     | 87  | ASN  |
| 1   | I     | 91  | HIS  |
| 1   | I     | 100 | ASN  |
| 1   | J     | 70  | GLN  |
| 1   | J     | 76  | ASN  |
| 1   | J     | 87  | ASN  |
| 1   | J     | 91  | HIS  |
| 1   | J     | 100 | ASN  |
| 1   | K     | 59  | HIS  |
| 1   | K     | 70  | GLN  |
| 1   | K     | 76  | ASN  |
| 1   | K     | 87  | ASN  |
| 1   | K     | 91  | HIS  |
| 1   | K     | 100 | ASN  |
| 1   | L     | 59  | HIS  |
| 1   | L     | 70  | GLN  |
| 1   | L     | 76  | ASN  |
| 1   | L     | 87  | ASN  |
| 1   | L     | 91  | HIS  |
| 1   | L     | 100 | ASN  |
| 1   | M     | 59  | HIS  |
| 1   | M     | 70  | GLN  |
| 1   | M     | 76  | ASN  |
| 1   | M     | 87  | ASN  |
| 1   | M     | 91  | HIS  |
| 1   | M     | 100 | ASN  |
| 1   | N     | 59  | HIS  |
| 1   | N     | 70  | GLN  |
| 1   | N     | 76  | ASN  |
| 1   | N     | 87  | ASN  |
| 1   | N     | 91  | HIS  |
| 1   | N     | 100 | ASN  |

### 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-2233. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

#### 6.1.1 Primary map



X



Y



Z

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

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

#### 6.2.1 Primary map



X Index: 80



Y Index: 80



Z Index: 80

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: 97



Y Index: 103

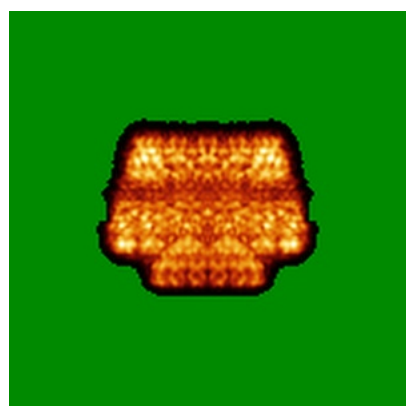


Z Index: 66

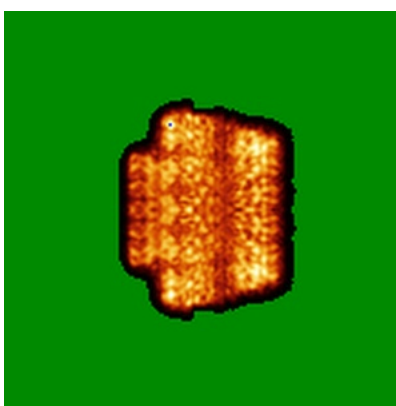
The images above show the largest variance slices of the map in three orthogonal directions.

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

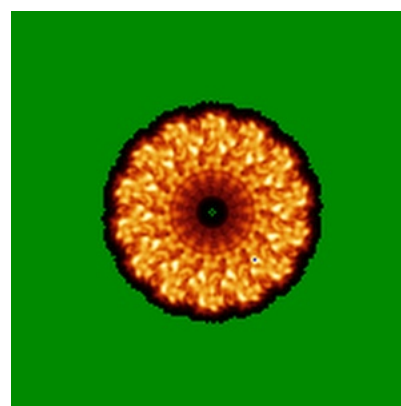
### 6.4.1 Primary map



X



Y

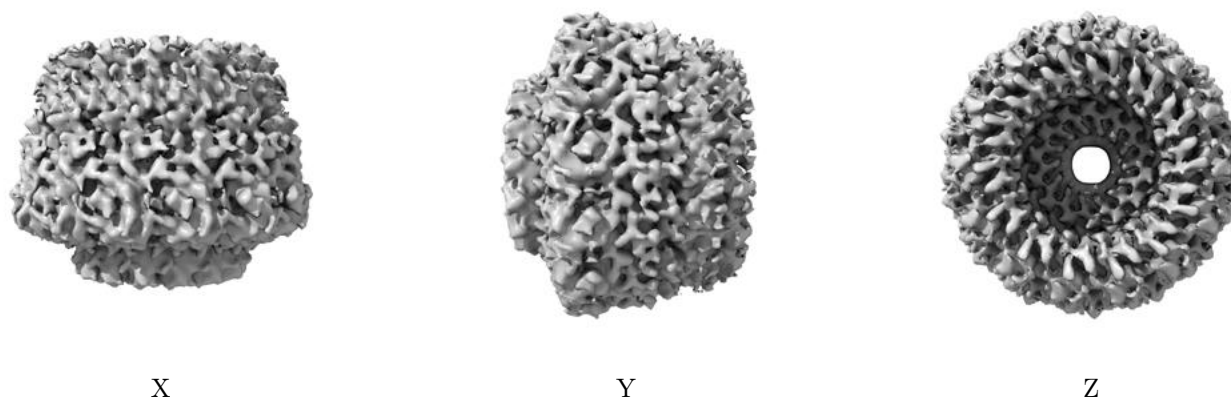


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

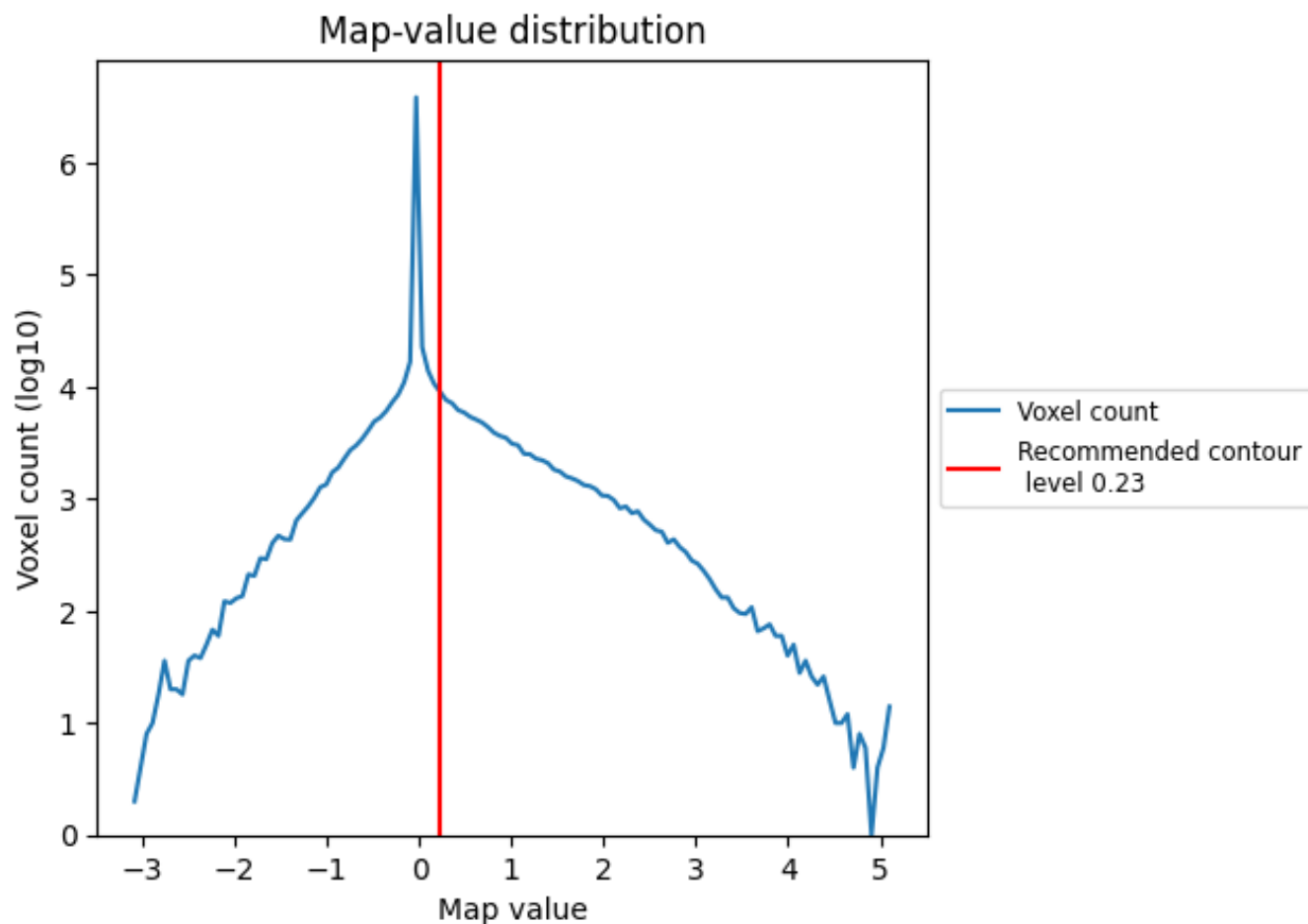
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

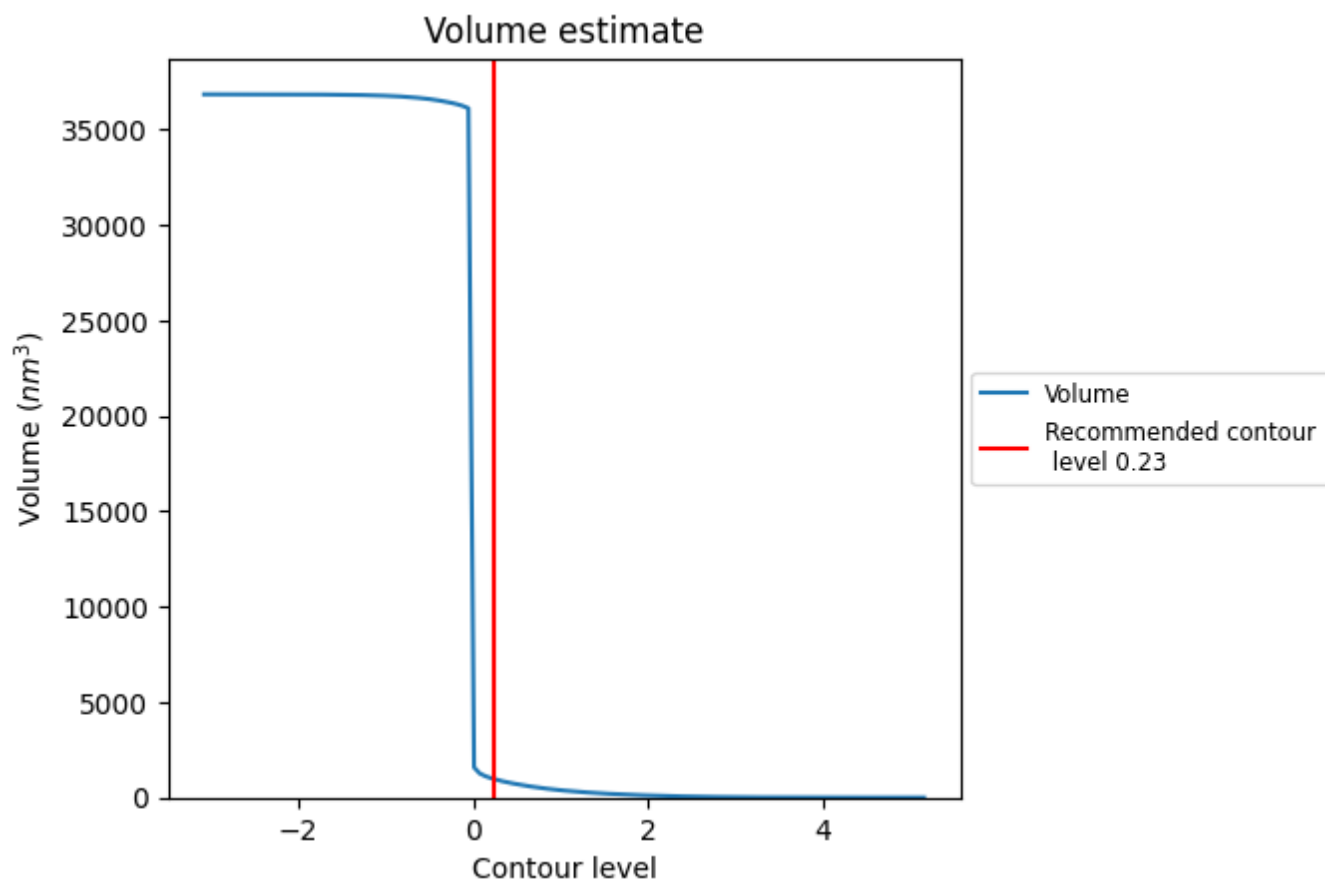
This section contains the results of statistical analysis of the map.

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



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

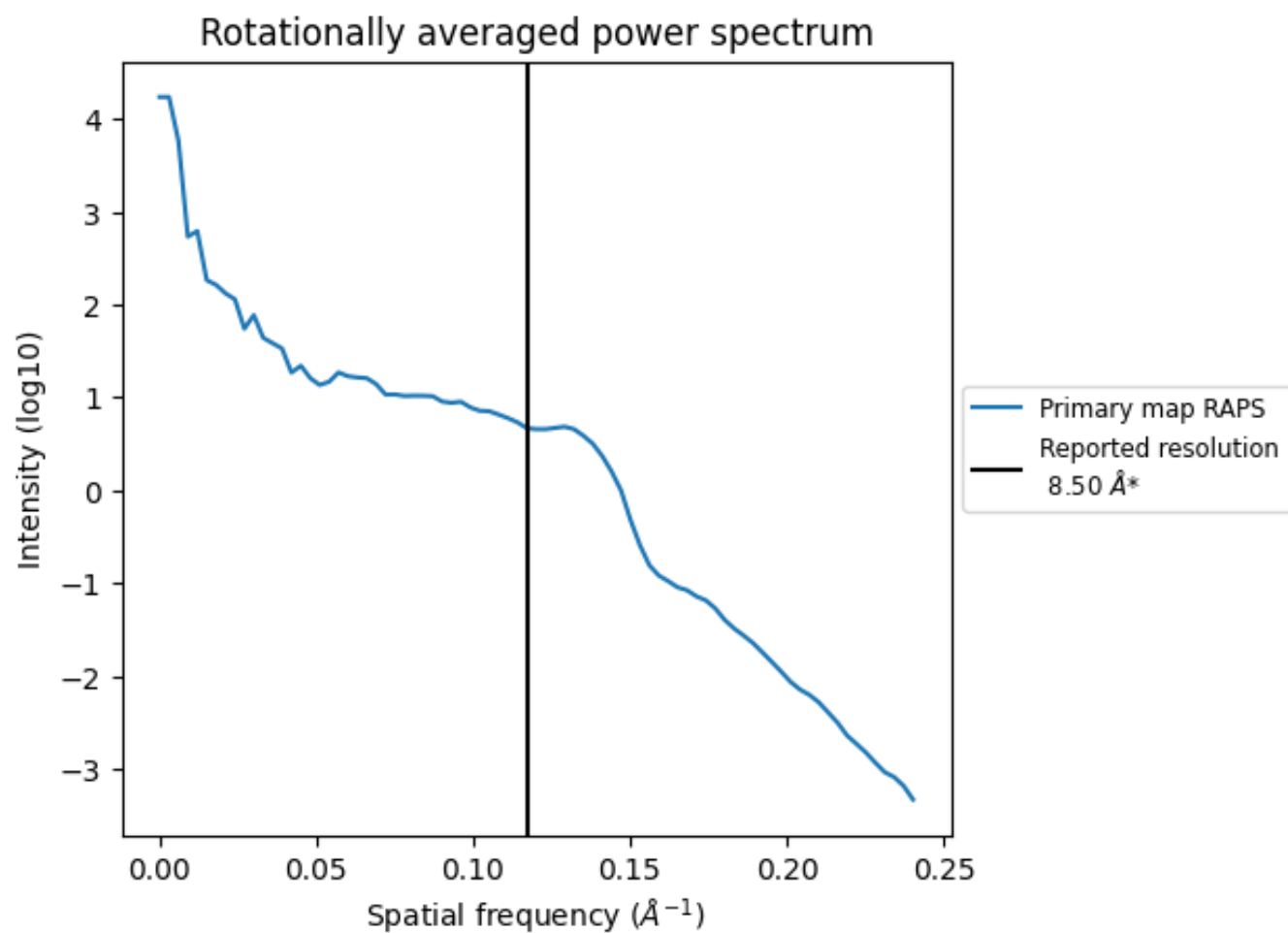
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $983 \text{ nm}^3$ ; this corresponds to an approximate mass of 888 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 0.118 Å<sup>-1</sup>

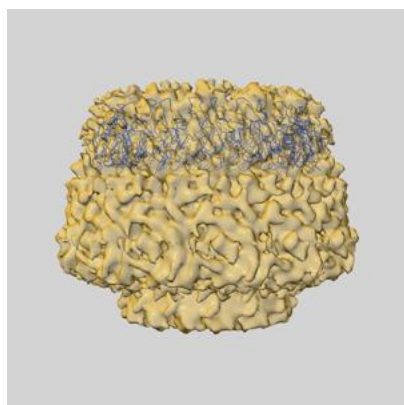
## 8 Fourier-Shell correlation

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

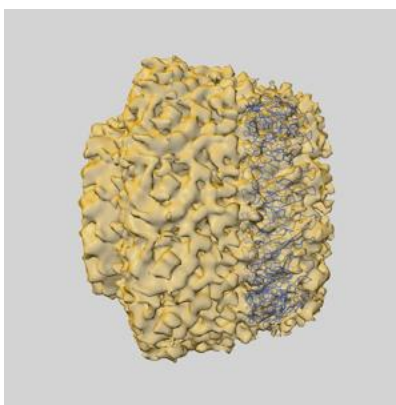
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2233 and PDB model 3ZBJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

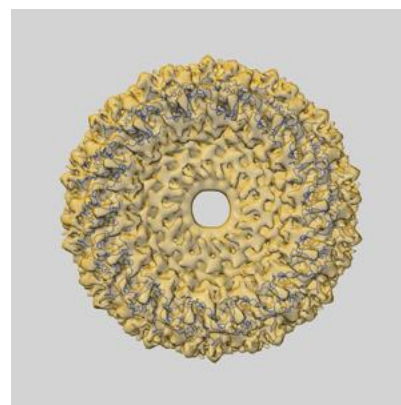
### 9.1 Map-model overlay [i](#)



X



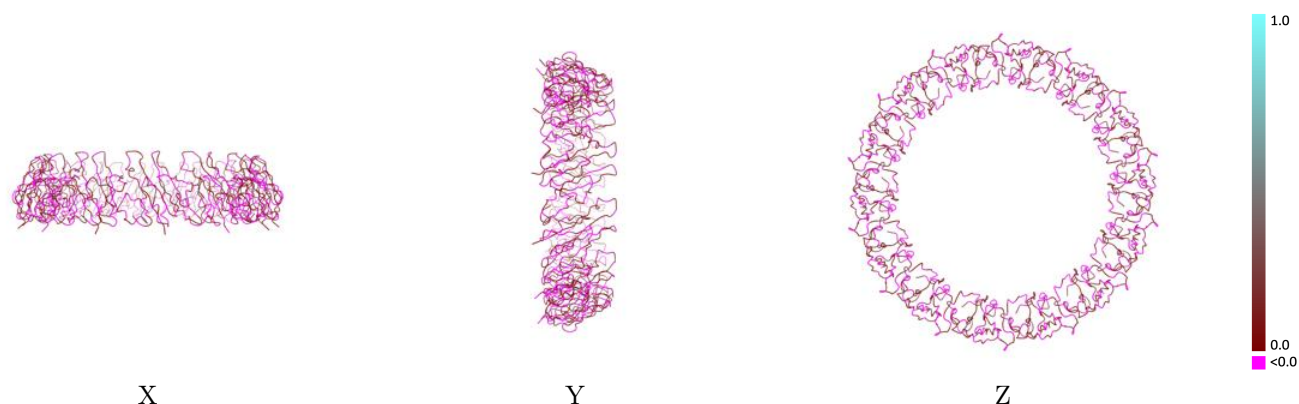
Y



Z

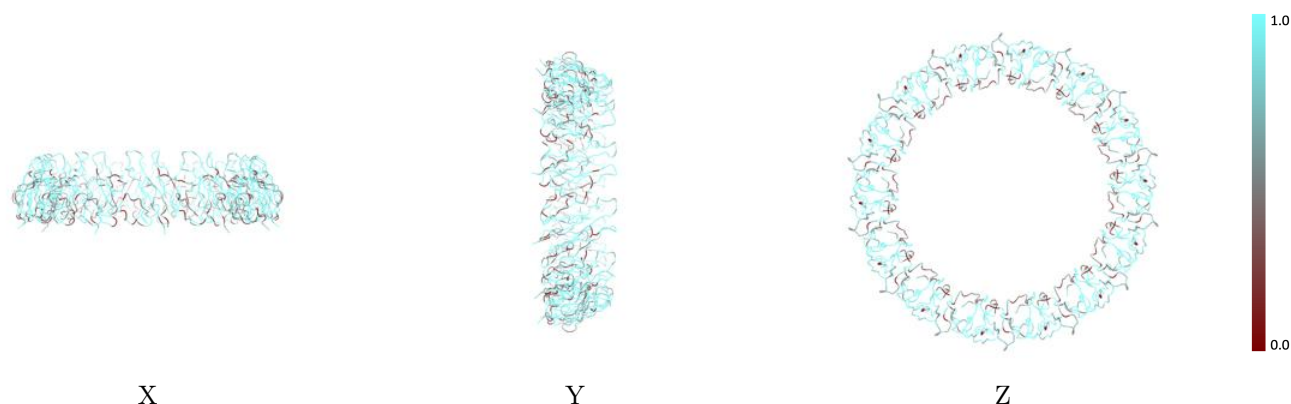
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



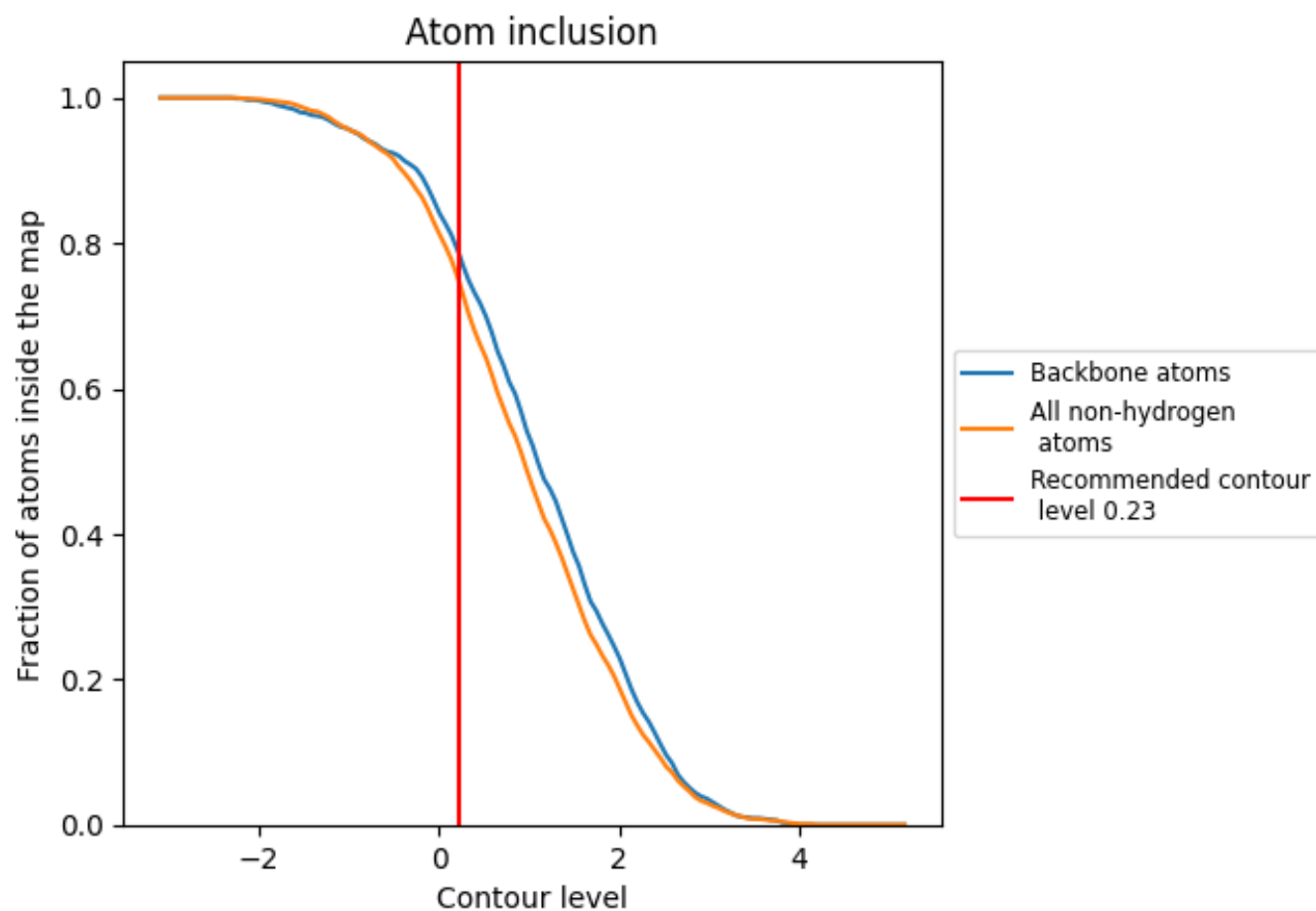
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.23) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.7460</div> | <div><div></div>0.0290</div> |
| A     | <div><div></div>0.7430</div> | <div><div></div>0.0280</div> |
| B     | <div><div></div>0.7450</div> | <div><div></div>0.0330</div> |
| C     | <div><div></div>0.7460</div> | <div><div></div>0.0290</div> |
| D     | <div><div></div>0.7470</div> | <div><div></div>0.0280</div> |
| E     | <div><div></div>0.7410</div> | <div><div></div>0.0260</div> |
| F     | <div><div></div>0.7480</div> | <div><div></div>0.0280</div> |
| G     | <div><div></div>0.7490</div> | <div><div></div>0.0280</div> |
| H     | <div><div></div>0.7430</div> | <div><div></div>0.0300</div> |
| I     | <div><div></div>0.7450</div> | <div><div></div>0.0310</div> |
| J     | <div><div></div>0.7460</div> | <div><div></div>0.0310</div> |
| K     | <div><div></div>0.7470</div> | <div><div></div>0.0270</div> |
| L     | <div><div></div>0.7410</div> | <div><div></div>0.0300</div> |
| M     | <div><div></div>0.7480</div> | <div><div></div>0.0300</div> |
| N     | <div><div></div>0.7490</div> | <div><div></div>0.0310</div> |

