



## Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 11:39 PM EDT

PDB ID : 7LFH  
EMDB ID : EMD-23302  
Title : Cryo-EM structure of NLRP3 double-ring cage, 6-fold (12-mer)  
Authors : Andreeva, L.; Rawson, S.; Wu, H.  
Deposited on : 2021-01-17  
Resolution : 4.20 Å (reported)  
Based on initial model : 6NPY

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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

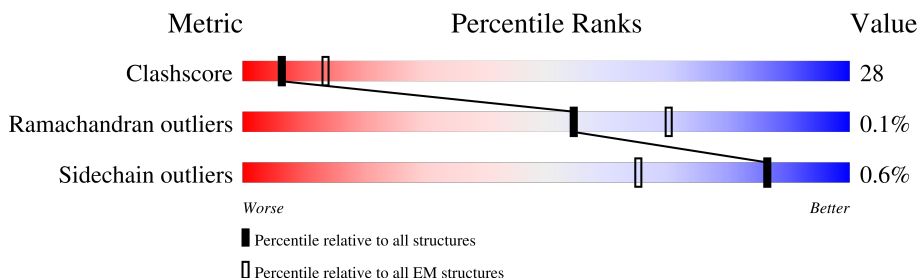
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

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     | 1037   | <div> <div>24%</div> <div>38%</div> <div>39%</div> <div>22%</div> </div> |
| 1   | B     | 1037   | <div> <div>23%</div> <div>39%</div> <div>38%</div> <div>22%</div> </div> |
| 1   | C     | 1037   | <div> <div>27%</div> <div>38%</div> <div>39%</div> <div>22%</div> </div> |
| 1   | D     | 1037   | <div> <div>22%</div> <div>39%</div> <div>38%</div> <div>22%</div> </div> |
| 1   | E     | 1037   | <div> <div>25%</div> <div>38%</div> <div>39%</div> <div>22%</div> </div> |
| 1   | F     | 1037   | <div> <div>21%</div> <div>38%</div> <div>39%</div> <div>22%</div> </div> |
| 1   | G     | 1037   | <div> <div>25%</div> <div>39%</div> <div>39%</div> <div>22%</div> </div> |
| 1   | H     | 1037   | <div> <div>24%</div> <div>38%</div> <div>39%</div> <div>22%</div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | I     | 1037   | <div><div>24%</div><div><div></div><div>39%</div><div>38%</div><div>22%</div></div></div> |
| 1   | J     | 1037   | <div><div>22%</div><div><div></div><div>38%</div><div>39%</div><div>22%</div></div></div> |
| 1   | K     | 1037   | <div><div>23%</div><div><div></div><div>39%</div><div>39%</div><div>22%</div></div></div> |
| 1   | L     | 1037   | <div><div>20%</div><div><div></div><div>38%</div><div>39%</div><div>22%</div></div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 76884 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 NACHT, LRR and PYD domains-containing protein 3.

| Mol | Chain | Residues | Atoms         |           |           |           |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|---------|-------|
| 1   | A     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | B     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | C     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | D     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | E     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | F     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | G     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | H     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | I     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | J     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | K     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |
| 1   | L     | 806      | Total<br>6407 | C<br>4099 | N<br>1089 | O<br>1166 | S<br>53 | 0       | 0     |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| A     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| A     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| A     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| B     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| B     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |

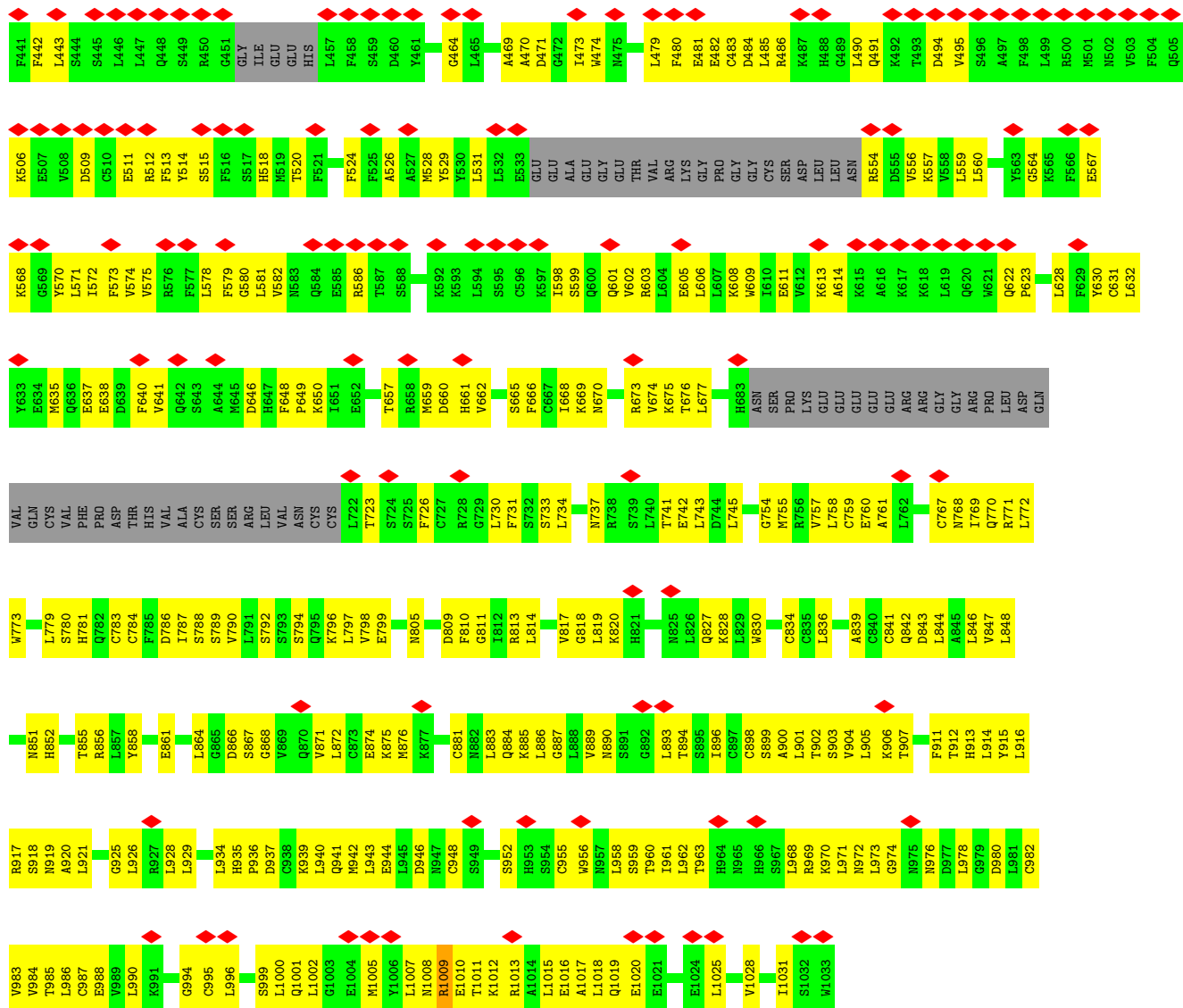
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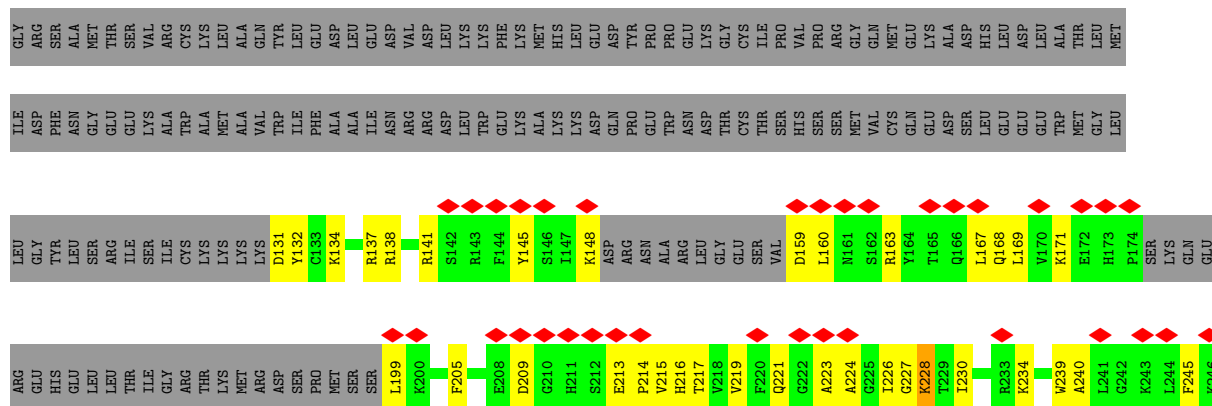
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| B     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| C     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| C     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| C     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| C     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| D     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| D     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| D     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| D     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| E     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| E     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| E     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| E     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| F     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| F     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| F     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| F     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| G     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| G     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| G     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| G     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| H     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| H     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| H     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| H     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| I     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| I     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| I     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| I     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| J     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| J     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| J     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| J     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| K     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| K     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| K     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| K     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |
| L     | -3      | GLY      | -      | expression tag | UNP Q8R4B8 |
| L     | -2      | ARG      | -      | expression tag | UNP Q8R4B8 |
| L     | -1      | SER      | -      | expression tag | UNP Q8R4B8 |
| L     | 0       | ALA      | -      | expression tag | UNP Q8R4B8 |



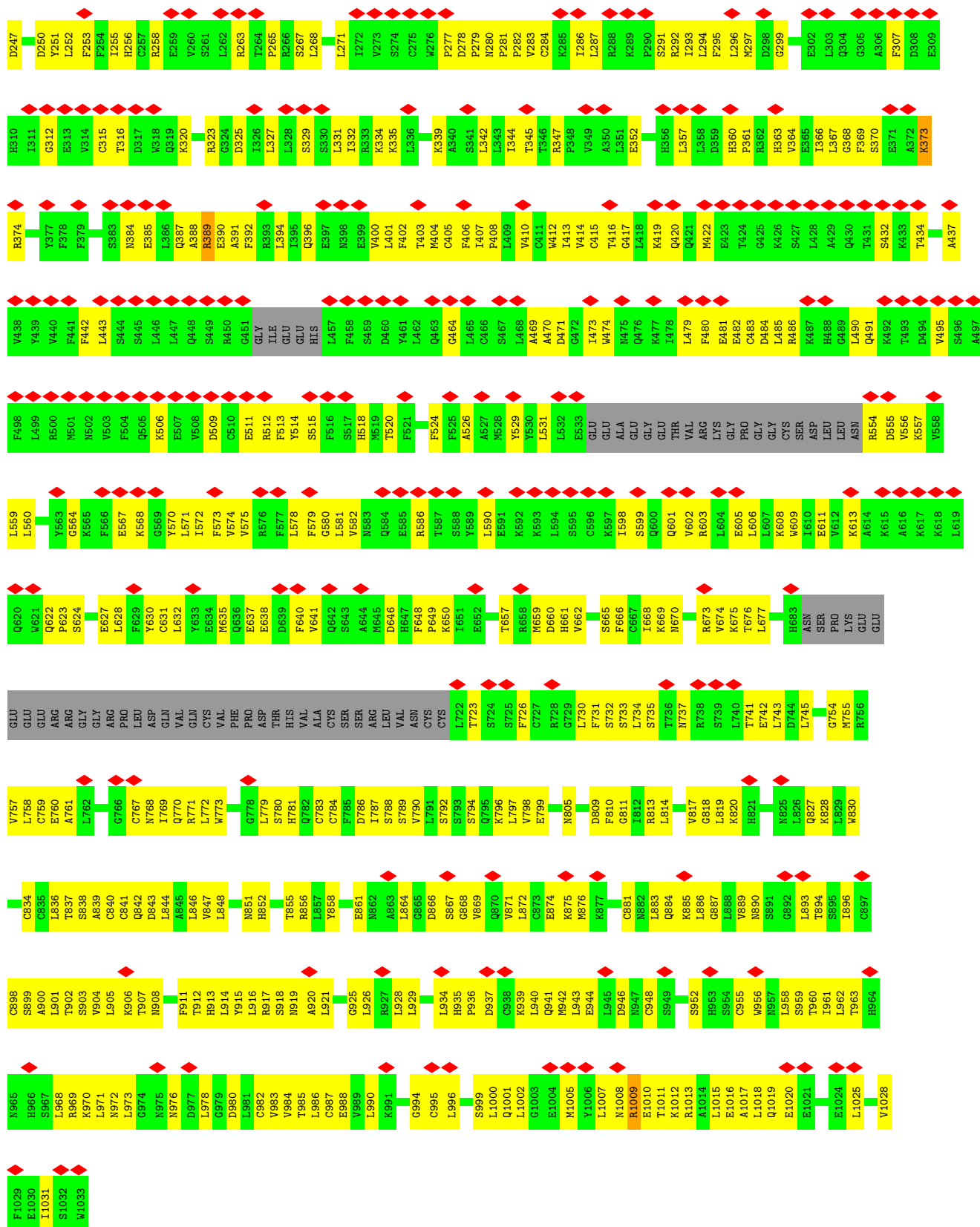


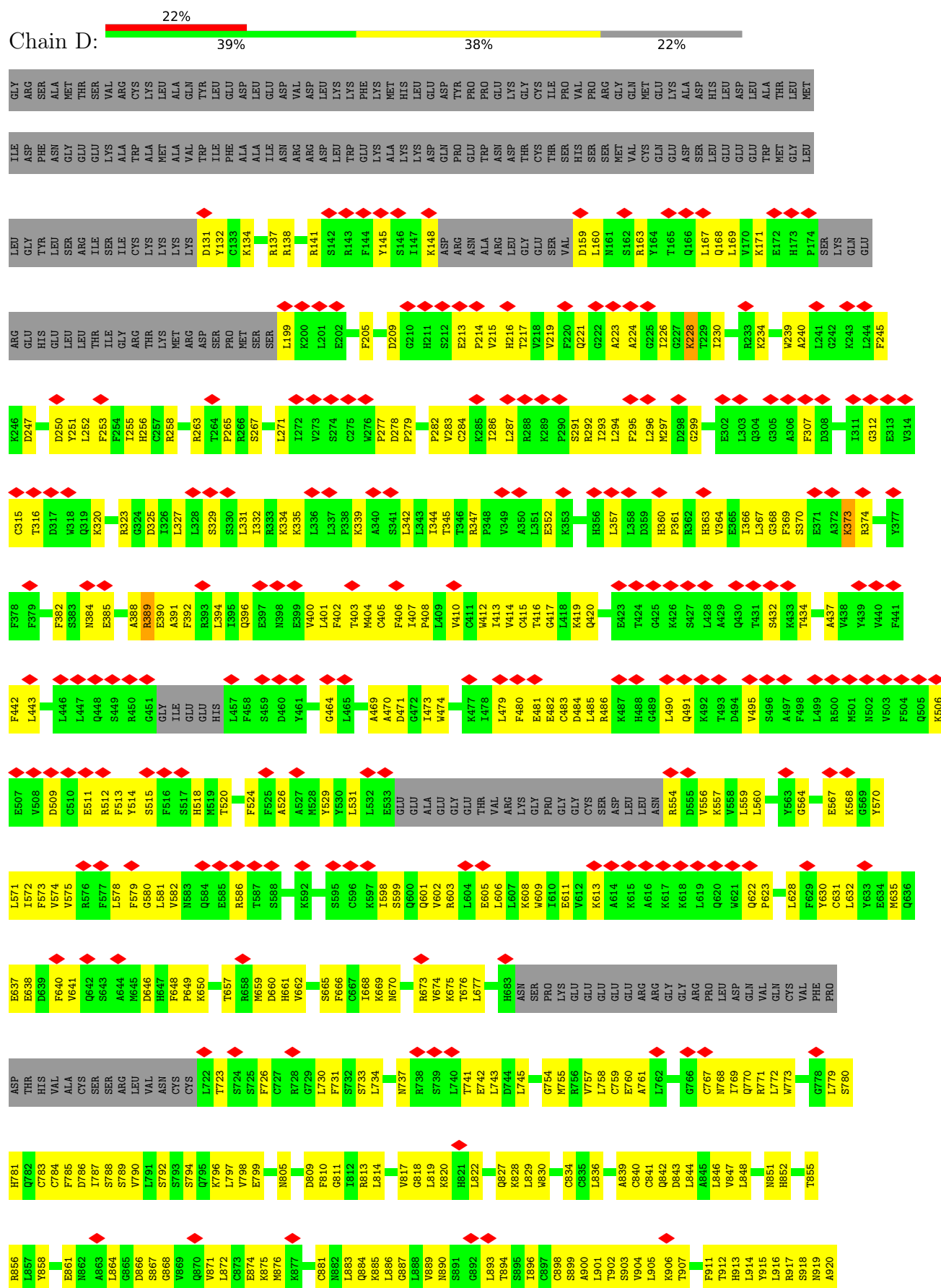


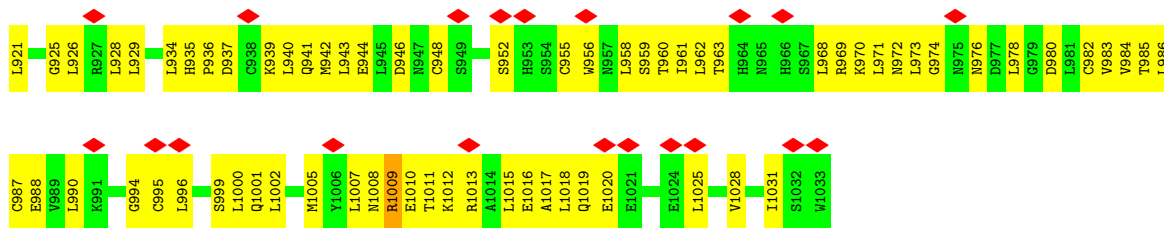
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



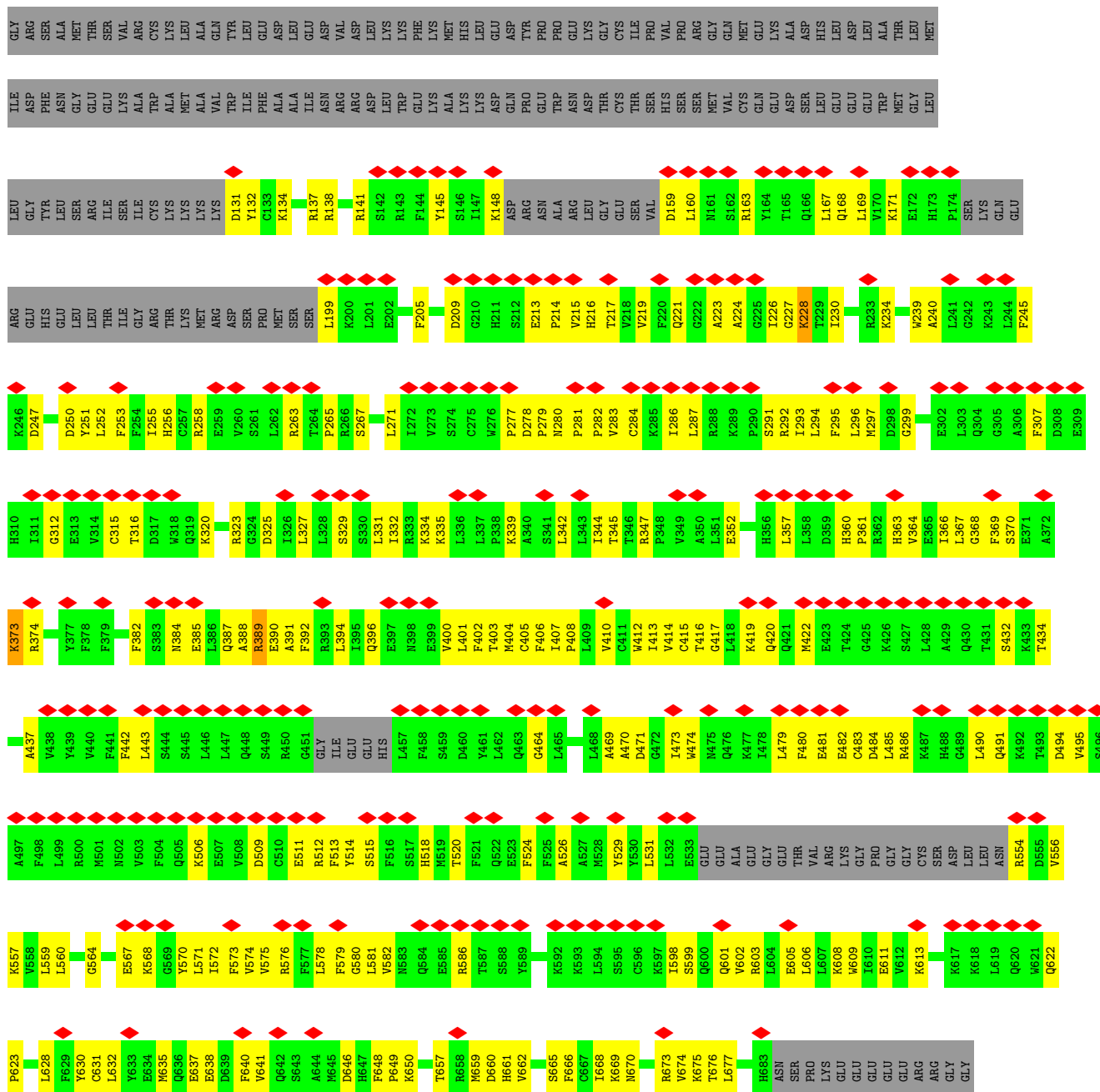






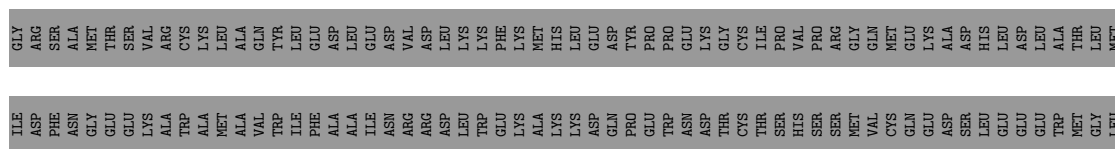


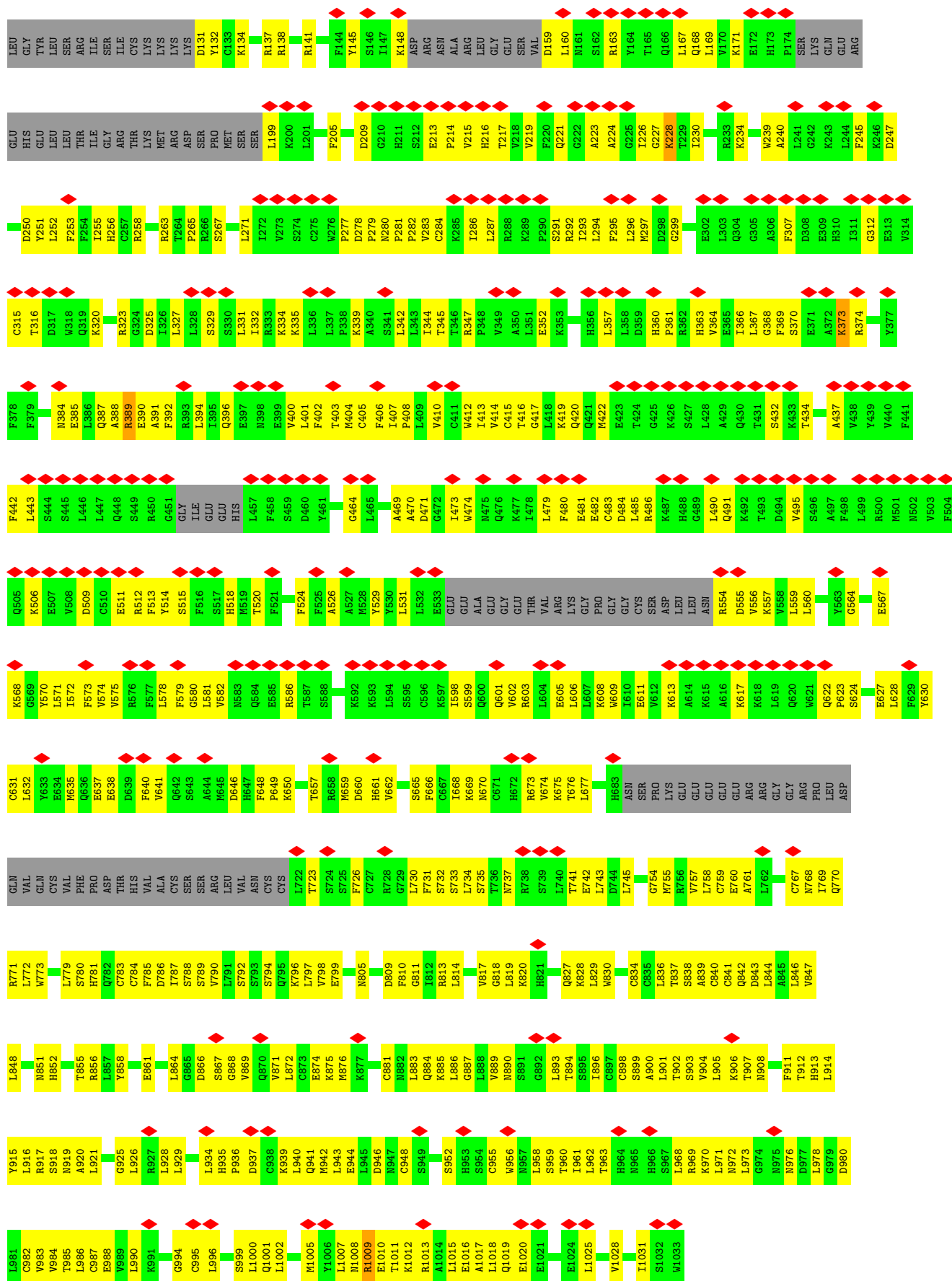
● Molecule 1: NACHT, LRR and PYD domains-containing protein 3







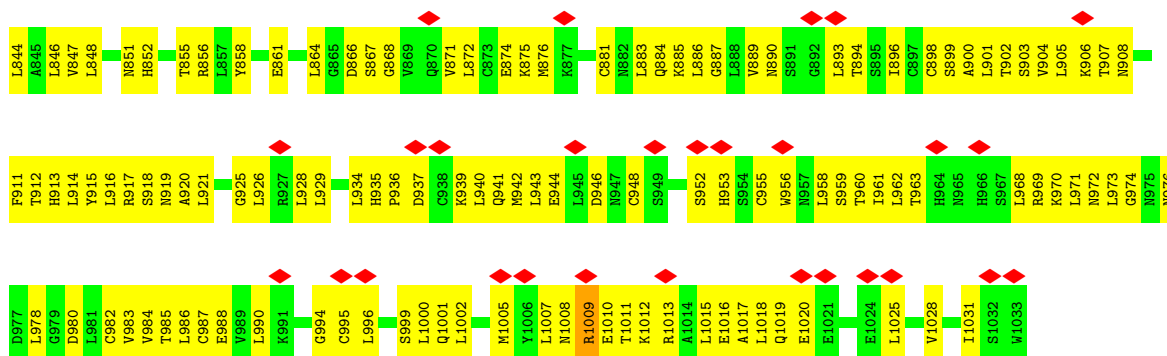




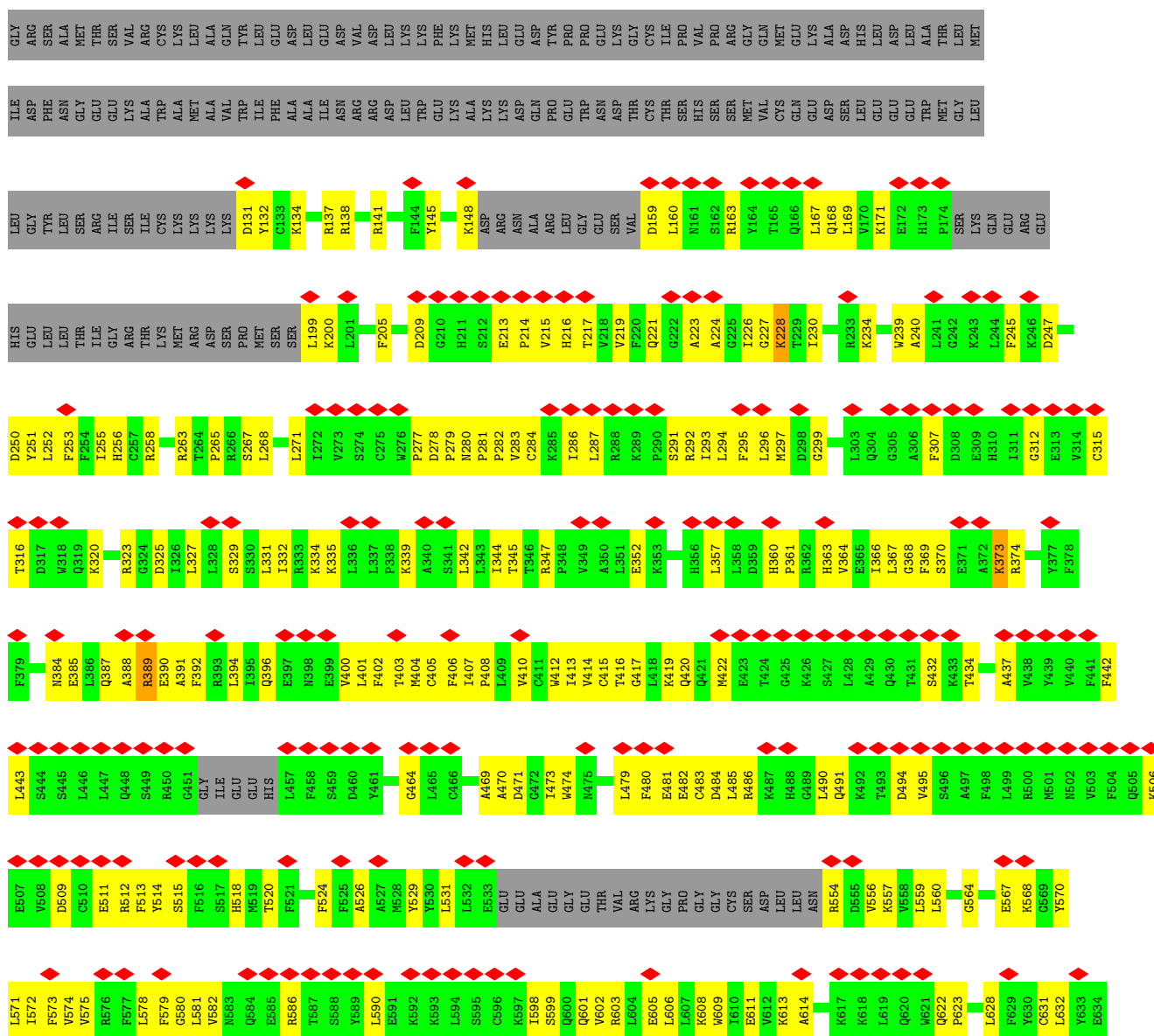
- Chain I:

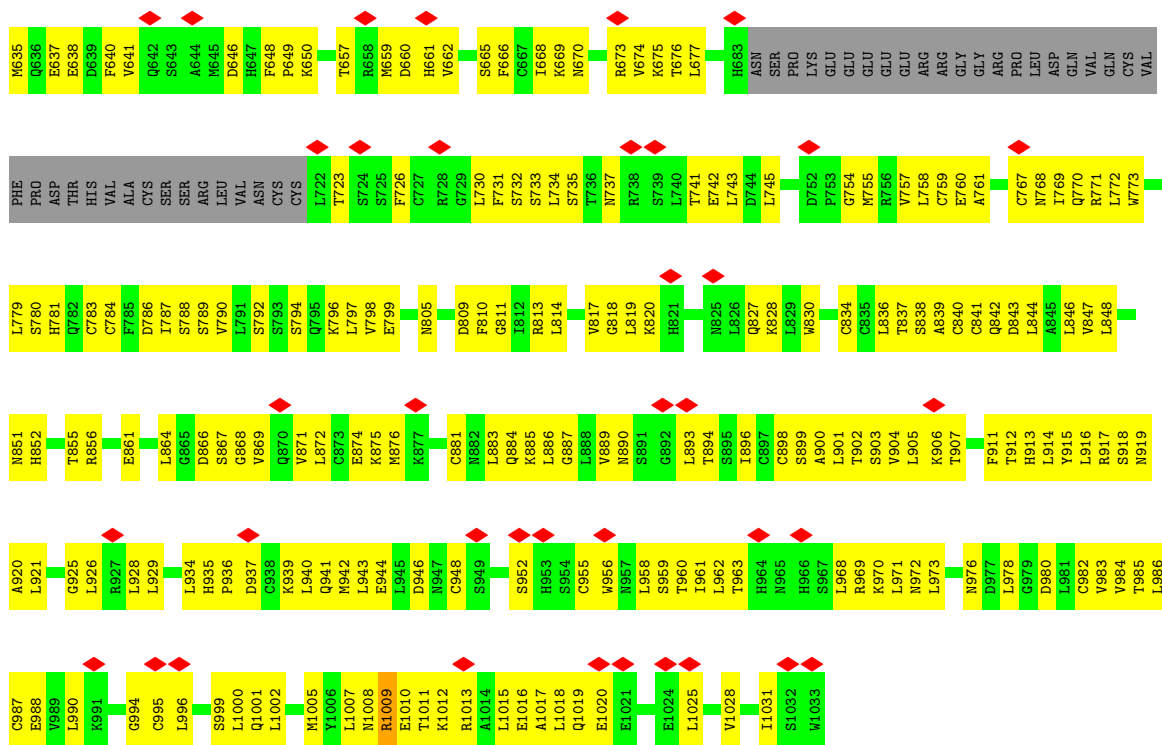




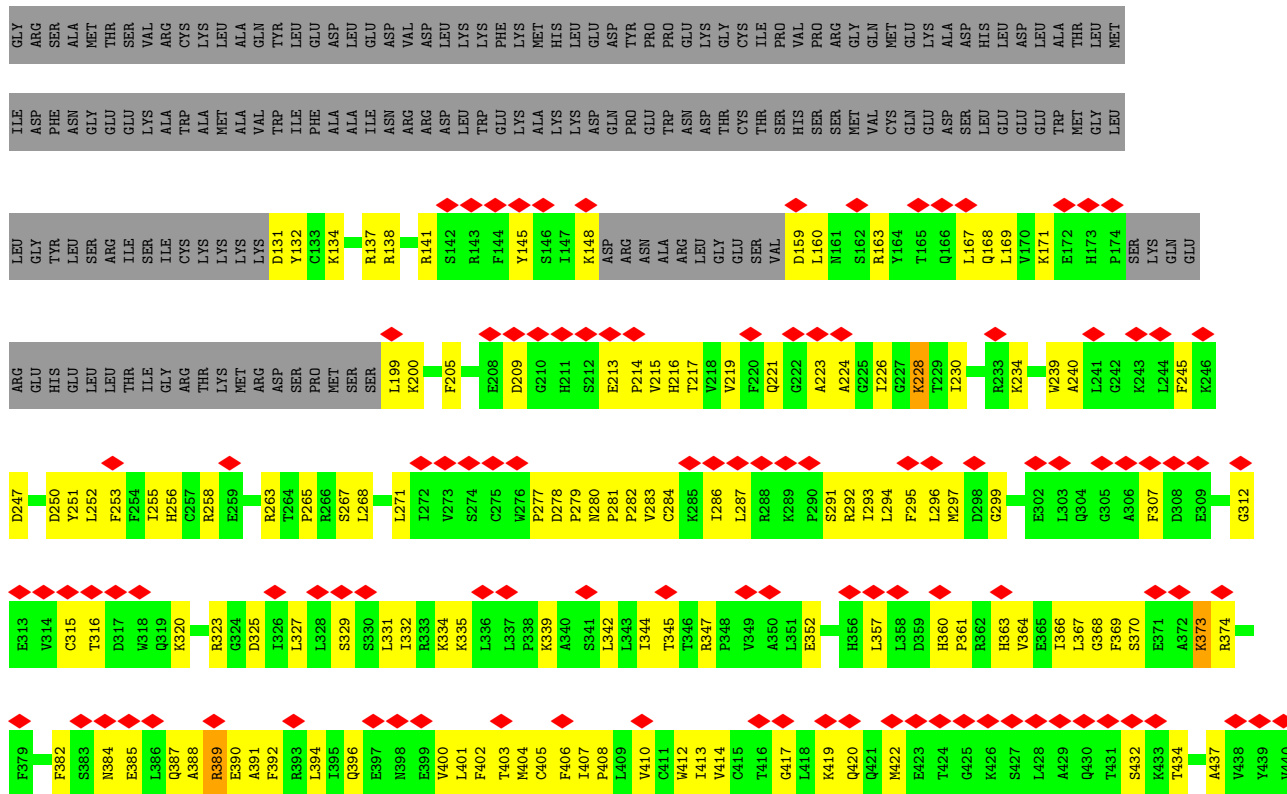


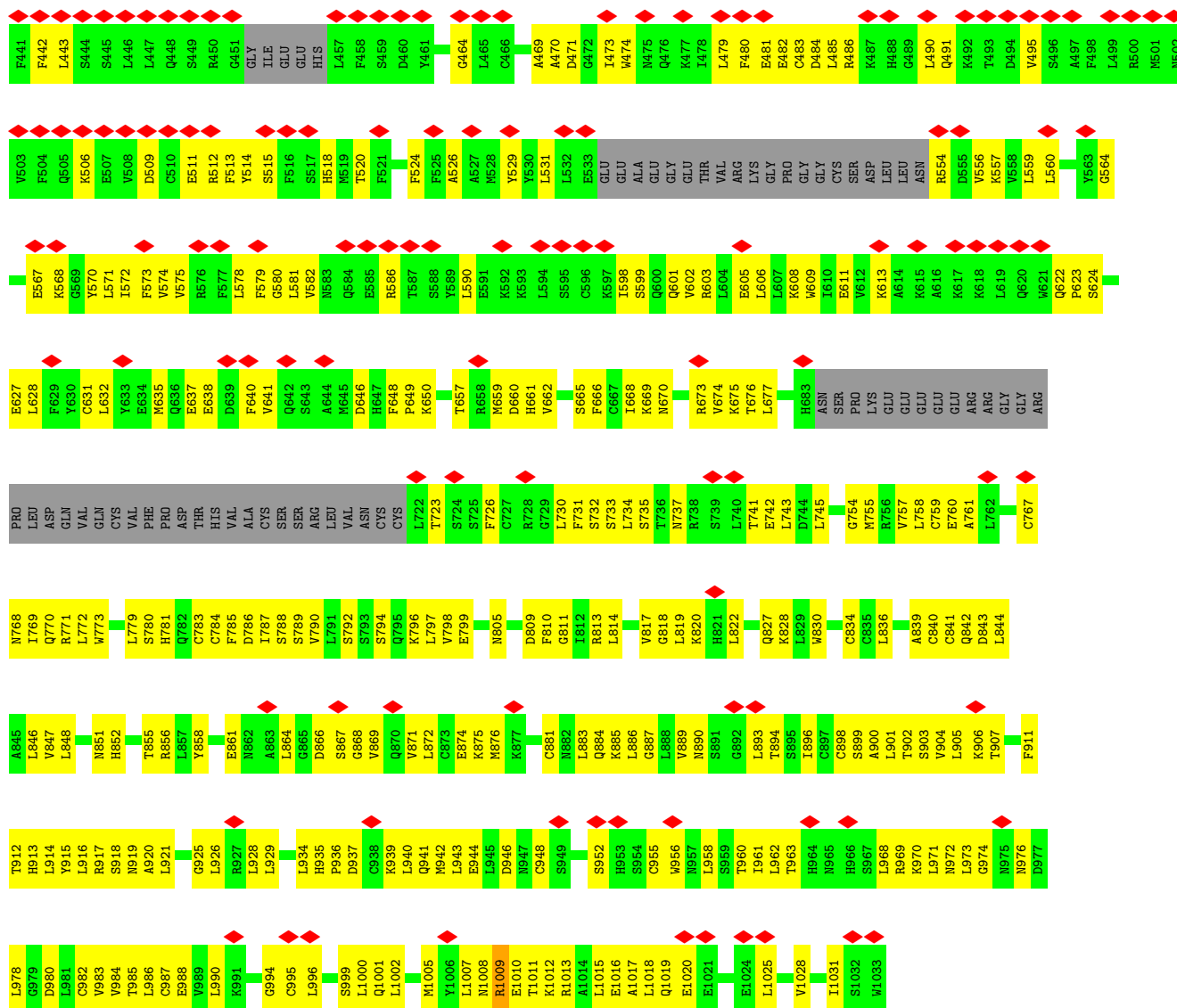
● Molecule 1: NACHT, LRR and PYD domains-containing protein 3



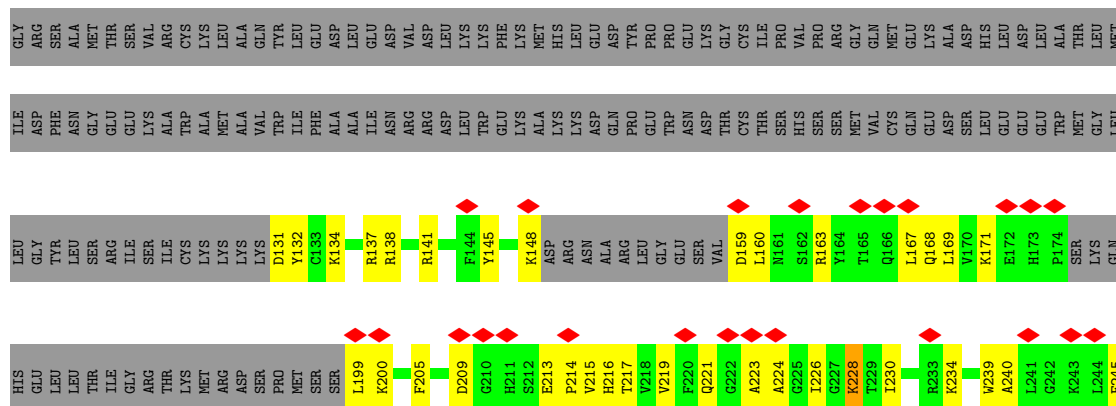


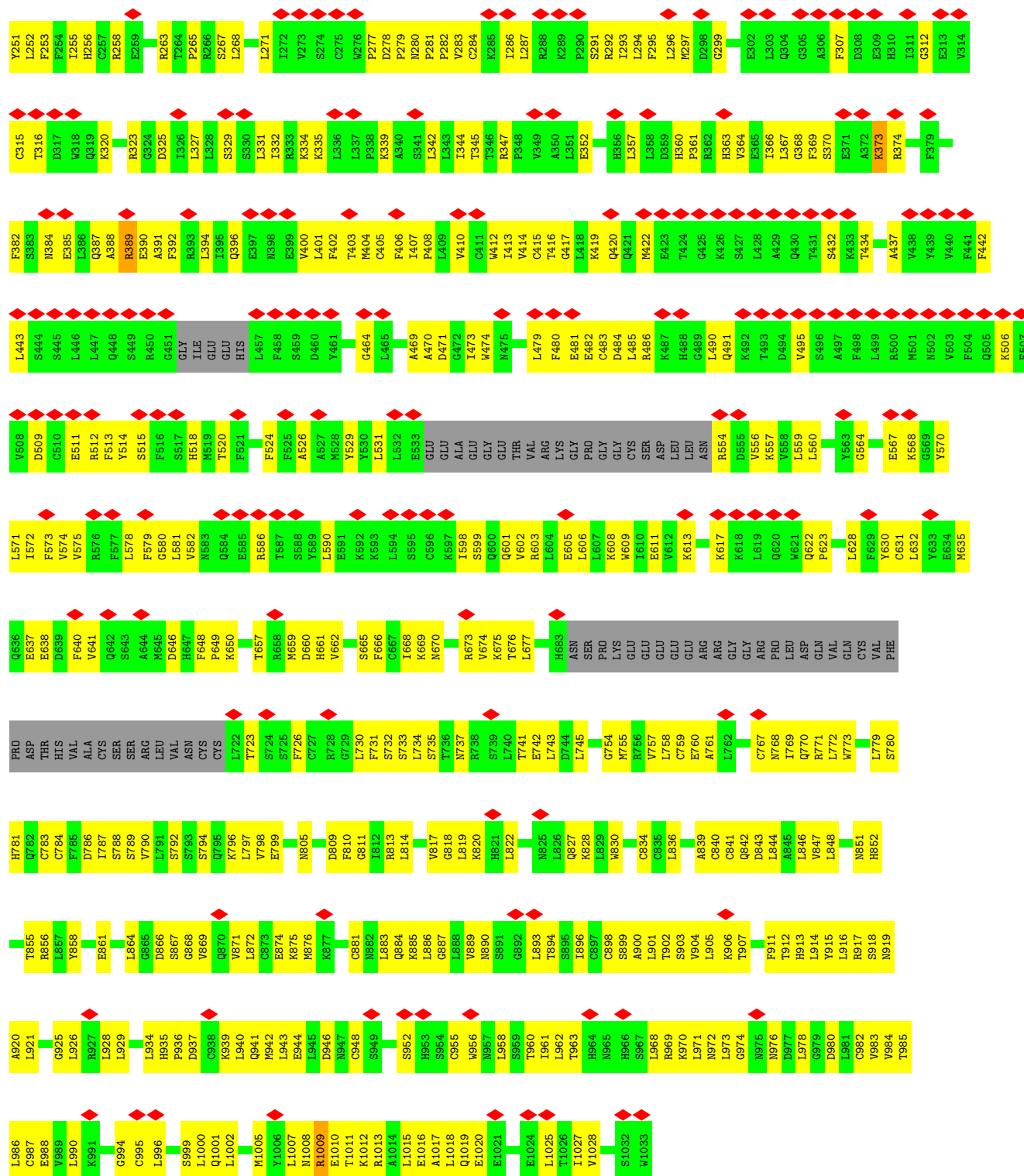
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3





• Molecule 1: NACHT, LRR and PYD domains-containing protein 3





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, D6                               | Depositor |
| Number of particles used             | 122941                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 53.225                                  | Depositor |
| Minimum defocus (nm)                 | -800                                    | Depositor |
| Maximum defocus (nm)                 | -2400                                   | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.730                                   | Depositor |
| Minimum map value                    | -0.002                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.031                                   | Depositor |
| Recommended contour level            | 0.09                                    | Depositor |
| Map size (Å)                         | 422.4, 422.4, 422.4                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.825, 0.825, 0.825                     | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | A     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | B     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | C     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | D     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | E     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | F     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | G     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | H     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | I     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | J     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | K     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| 1   | L     | 0.28         | 0/6527  | 0.56        | 0/8804   |
| All | All   | 0.28         | 0/78324 | 0.56        | 0/105648 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6407  | 0        | 6446     | 367     | 0            |
| 1   | B     | 6407  | 0        | 6446     | 365     | 0            |
| 1   | C     | 6407  | 0        | 6446     | 370     | 0            |
| 1   | D     | 6407  | 0        | 6446     | 365     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 6407  | 0        | 6446     | 368     | 0            |
| 1   | F     | 6407  | 0        | 6446     | 374     | 0            |
| 1   | G     | 6407  | 0        | 6446     | 371     | 0            |
| 1   | H     | 6407  | 0        | 6446     | 370     | 0            |
| 1   | I     | 6407  | 0        | 6446     | 366     | 0            |
| 1   | J     | 6407  | 0        | 6446     | 367     | 0            |
| 1   | K     | 6407  | 0        | 6446     | 361     | 0            |
| 1   | L     | 6407  | 0        | 6446     | 367     | 0            |
| All | All   | 76884 | 0        | 77352    | 4371    | 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 28.

All (4371) 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:K:785:PHE:HB3 | 1:L:810:PHE:HZ   | 1.35                     | 0.92              |
| 1:C:810:PHE:HZ  | 1:D:785:PHE:HB3  | 1.31                     | 0.91              |
| 1:A:773:TRP:HH2 | 1:L:1013:ARG:HG2 | 1.39                     | 0.88              |
| 1:A:385:GLU:HA  | 1:A:389:ARG:HH12 | 1.44                     | 0.83              |
| 1:J:385:GLU:HA  | 1:J:389:ARG:HH12 | 1.44                     | 0.83              |
| 1:C:385:GLU:HA  | 1:C:389:ARG:HH12 | 1.44                     | 0.83              |
| 1:H:385:GLU:HA  | 1:H:389:ARG:HH12 | 1.44                     | 0.83              |
| 1:F:385:GLU:HA  | 1:F:389:ARG:HH12 | 1.44                     | 0.83              |
| 1:E:385:GLU:HA  | 1:E:389:ARG:HH12 | 1.44                     | 0.82              |
| 1:L:385:GLU:HA  | 1:L:389:ARG:HH12 | 1.44                     | 0.82              |
| 1:K:385:GLU:HA  | 1:K:389:ARG:HH12 | 1.44                     | 0.82              |
| 1:B:385:GLU:HA  | 1:B:389:ARG:HH12 | 1.44                     | 0.82              |
| 1:D:385:GLU:HA  | 1:D:389:ARG:HH12 | 1.44                     | 0.81              |
| 1:I:385:GLU:HA  | 1:I:389:ARG:HH12 | 1.44                     | 0.81              |
| 1:G:385:GLU:HA  | 1:G:389:ARG:HH12 | 1.44                     | 0.81              |
| 1:A:785:PHE:HB3 | 1:B:810:PHE:HZ   | 1.46                     | 0.81              |
| 1:E:810:PHE:HZ  | 1:F:785:PHE:HB3  | 1.47                     | 0.80              |
| 1:C:810:PHE:CZ  | 1:D:785:PHE:HB3  | 2.17                     | 0.78              |
| 1:A:134:LYS:HB3 | 1:A:138:ARG:HH12 | 1.49                     | 0.78              |
| 1:J:134:LYS:HB3 | 1:J:138:ARG:HH12 | 1.49                     | 0.78              |
| 1:L:134:LYS:HB3 | 1:L:138:ARG:HH12 | 1.49                     | 0.77              |
| 1:K:134:LYS:HB3 | 1:K:138:ARG:HH12 | 1.49                     | 0.77              |
| 1:D:134:LYS:HB3 | 1:D:138:ARG:HH12 | 1.49                     | 0.76              |
| 1:B:773:TRP:HH2 | 1:C:1013:ARG:HG2 | 1.48                     | 0.76              |
| 1:G:134:LYS:HB3 | 1:G:138:ARG:HH12 | 1.49                     | 0.76              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:168:GLN:HB3 | 1:C:367:LEU:HB2  | 1.68                     | 0.76              |
| 1:B:134:LYS:HB3 | 1:B:138:ARG:HH12 | 1.49                     | 0.76              |
| 1:C:944:GLU:HG2 | 1:C:972:ASN:HB2  | 1.68                     | 0.76              |
| 1:E:134:LYS:HB3 | 1:E:138:ARG:HH12 | 1.49                     | 0.76              |
| 1:J:168:GLN:HB3 | 1:J:367:LEU:HB2  | 1.68                     | 0.76              |
| 1:A:168:GLN:HB3 | 1:A:367:LEU:HB2  | 1.68                     | 0.76              |
| 1:E:168:GLN:HB3 | 1:E:367:LEU:HB2  | 1.68                     | 0.76              |
| 1:H:944:GLU:HG2 | 1:H:972:ASN:HB2  | 1.68                     | 0.76              |
| 1:B:944:GLU:HG2 | 1:B:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:E:937:ASP:OD1 | 1:E:939:LYS:NZ   | 2.19                     | 0.75              |
| 1:F:134:LYS:HB3 | 1:F:138:ARG:HH12 | 1.49                     | 0.75              |
| 1:H:134:LYS:HB3 | 1:H:138:ARG:HH12 | 1.49                     | 0.75              |
| 1:K:944:GLU:HG2 | 1:K:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:L:944:GLU:HG2 | 1:L:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:F:168:GLN:HB3 | 1:F:367:LEU:HB2  | 1.68                     | 0.75              |
| 1:F:937:ASP:OD1 | 1:F:939:LYS:NZ   | 2.19                     | 0.75              |
| 1:I:134:LYS:HB3 | 1:I:138:ARG:HH12 | 1.49                     | 0.75              |
| 1:G:937:ASP:OD1 | 1:G:939:LYS:NZ   | 2.19                     | 0.75              |
| 1:H:168:GLN:HB3 | 1:H:367:LEU:HB2  | 1.68                     | 0.75              |
| 1:I:944:GLU:HG2 | 1:I:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:A:944:GLU:HG2 | 1:A:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:C:134:LYS:HB3 | 1:C:138:ARG:HH12 | 1.49                     | 0.75              |
| 1:D:937:ASP:OD1 | 1:D:939:LYS:NZ   | 2.19                     | 0.75              |
| 1:J:944:GLU:HG2 | 1:J:972:ASN:HB2  | 1.68                     | 0.75              |
| 1:J:937:ASP:OD1 | 1:J:939:LYS:NZ   | 2.19                     | 0.75              |
| 1:E:944:GLU:HG2 | 1:E:972:ASN:HB2  | 1.68                     | 0.74              |
| 1:F:944:GLU:HG2 | 1:F:972:ASN:HB2  | 1.68                     | 0.74              |
| 1:C:937:ASP:OD1 | 1:C:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:H:937:ASP:OD1 | 1:H:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:A:937:ASP:OD1 | 1:A:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:G:168:GLN:HB3 | 1:G:367:LEU:HB2  | 1.68                     | 0.74              |
| 1:C:134:LYS:HB3 | 1:C:138:ARG:NH1  | 2.03                     | 0.74              |
| 1:D:944:GLU:HG2 | 1:D:972:ASN:HB2  | 1.68                     | 0.74              |
| 1:G:944:GLU:HG2 | 1:G:972:ASN:HB2  | 1.68                     | 0.74              |
| 1:L:168:GLN:HB3 | 1:L:367:LEU:HB2  | 1.68                     | 0.74              |
| 1:D:134:LYS:HB3 | 1:D:138:ARG:NH1  | 2.03                     | 0.74              |
| 1:D:168:GLN:HB3 | 1:D:367:LEU:HB2  | 1.68                     | 0.74              |
| 1:G:134:LYS:HB3 | 1:G:138:ARG:NH1  | 2.03                     | 0.74              |
| 1:H:134:LYS:HB3 | 1:H:138:ARG:NH1  | 2.03                     | 0.74              |
| 1:K:168:GLN:HB3 | 1:K:367:LEU:HB2  | 1.68                     | 0.74              |
| 1:L:937:ASP:OD1 | 1:L:939:LYS:NZ   | 2.19                     | 0.74              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:937:ASP:OD1 | 1:B:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:H:279:PRO:HB2 | 1:H:282:PRO:HG2  | 1.70                     | 0.74              |
| 1:I:168:GLN:HB3 | 1:I:367:LEU:HB2  | 1.68                     | 0.74              |
| 1:I:937:ASP:OD1 | 1:I:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:K:937:ASP:OD1 | 1:K:939:LYS:NZ   | 2.19                     | 0.74              |
| 1:F:134:LYS:HB3 | 1:F:138:ARG:NH1  | 2.03                     | 0.73              |
| 1:B:134:LYS:HB3 | 1:B:138:ARG:NH1  | 2.03                     | 0.73              |
| 1:C:279:PRO:HB2 | 1:C:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:I:134:LYS:HB3 | 1:I:138:ARG:NH1  | 2.03                     | 0.73              |
| 1:K:279:PRO:HB2 | 1:K:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:B:479:LEU:HB2 | 1:B:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:F:479:LEU:HB2 | 1:F:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:L:279:PRO:HB2 | 1:L:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:B:168:GLN:HB3 | 1:B:367:LEU:HB2  | 1.68                     | 0.73              |
| 1:B:279:PRO:HB2 | 1:B:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:I:479:LEU:HB2 | 1:I:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:J:479:LEU:HB2 | 1:J:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:J:646:ASP:HA  | 1:J:673:ARG:HB2  | 1.71                     | 0.73              |
| 1:L:479:LEU:HB2 | 1:L:513:PHE:HZ   | 1.53                     | 0.73              |
| 1:E:279:PRO:HB2 | 1:E:282:PRO:HG2  | 1.71                     | 0.73              |
| 1:E:479:LEU:HB2 | 1:E:513:PHE:HZ   | 1.53                     | 0.73              |
| 1:A:479:LEU:HB2 | 1:A:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:A:646:ASP:HA  | 1:A:673:ARG:HB2  | 1.71                     | 0.73              |
| 1:G:279:PRO:HB2 | 1:G:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:H:479:LEU:HB2 | 1:H:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:I:279:PRO:HB2 | 1:I:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:K:479:LEU:HB2 | 1:K:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:A:279:PRO:HB2 | 1:A:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:C:479:LEU:HB2 | 1:C:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:E:134:LYS:HB3 | 1:E:138:ARG:NH1  | 2.03                     | 0.73              |
| 1:G:1009:ARG:HA | 1:G:1012:LYS:HG2 | 1.71                     | 0.73              |
| 1:J:279:PRO:HB2 | 1:J:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:E:646:ASP:HA  | 1:E:673:ARG:HB2  | 1.71                     | 0.73              |
| 1:F:279:PRO:HB2 | 1:F:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:F:646:ASP:HA  | 1:F:673:ARG:HB2  | 1.71                     | 0.73              |
| 1:I:1009:ARG:HA | 1:I:1012:LYS:HG2 | 1.71                     | 0.73              |
| 1:B:1009:ARG:HA | 1:B:1012:LYS:HG2 | 1.71                     | 0.73              |
| 1:D:279:PRO:HB2 | 1:D:282:PRO:HG2  | 1.70                     | 0.73              |
| 1:G:479:LEU:HB2 | 1:G:513:PHE:HZ   | 1.54                     | 0.73              |
| 1:C:646:ASP:HA  | 1:C:673:ARG:HB2  | 1.71                     | 0.73              |
| 1:D:479:LEU:HB2 | 1:D:513:PHE:HZ   | 1.54                     | 0.73              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:1009:ARG:HA | 1:D:1012:LYS:HG2 | 1.71                     | 0.73              |
| 1:F:1009:ARG:HA | 1:F:1012:LYS:HG2 | 1.71                     | 0.73              |
| 1:H:646:ASP:HA  | 1:H:673:ARG:HB2  | 1.71                     | 0.72              |
| 1:L:646:ASP:HA  | 1:L:673:ARG:HB2  | 1.71                     | 0.72              |
| 1:A:134:LYS:HB3 | 1:A:138:ARG:NH1  | 2.03                     | 0.72              |
| 1:J:134:LYS:HB3 | 1:J:138:ARG:NH1  | 2.03                     | 0.72              |
| 1:K:646:ASP:HA  | 1:K:673:ARG:HB2  | 1.71                     | 0.72              |
| 1:C:730:LEU:O   | 1:C:733:SER:OG   | 2.08                     | 0.72              |
| 1:E:1009:ARG:HA | 1:E:1012:LYS:HG2 | 1.71                     | 0.72              |
| 1:B:666:PHE:O   | 1:B:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:D:666:PHE:O   | 1:D:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:E:730:LEU:O   | 1:E:733:SER:OG   | 2.08                     | 0.72              |
| 1:H:666:PHE:O   | 1:H:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:H:730:LEU:O   | 1:H:733:SER:OG   | 2.08                     | 0.72              |
| 1:K:666:PHE:O   | 1:K:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:C:666:PHE:O   | 1:C:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:G:666:PHE:O   | 1:G:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:H:1009:ARG:HA | 1:H:1012:LYS:HG2 | 1.71                     | 0.72              |
| 1:I:666:PHE:O   | 1:I:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:K:1009:ARG:HA | 1:K:1012:LYS:HG2 | 1.71                     | 0.72              |
| 1:L:666:PHE:O   | 1:L:670:ASN:ND2  | 2.23                     | 0.72              |
| 1:B:646:ASP:HA  | 1:B:673:ARG:HB2  | 1.71                     | 0.72              |
| 1:C:531:LEU:HA  | 1:C:598:ILE:HD13 | 1.71                     | 0.72              |
| 1:A:972:ASN:OD1 | 1:A:1001:GLN:NE2 | 2.22                     | 0.71              |
| 1:F:666:PHE:O   | 1:F:670:ASN:ND2  | 2.23                     | 0.71              |
| 1:H:531:LEU:HA  | 1:H:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:I:934:LEU:HA  | 1:I:961:ILE:HD11 | 1.72                     | 0.71              |
| 1:A:730:LEU:O   | 1:A:733:SER:OG   | 2.08                     | 0.71              |
| 1:D:646:ASP:HA  | 1:D:673:ARG:HB2  | 1.71                     | 0.71              |
| 1:E:531:LEU:HA  | 1:E:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:I:646:ASP:HA  | 1:I:673:ARG:HB2  | 1.71                     | 0.71              |
| 1:J:730:LEU:O   | 1:J:733:SER:OG   | 2.08                     | 0.71              |
| 1:J:972:ASN:OD1 | 1:J:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:L:1009:ARG:HA | 1:L:1012:LYS:HG2 | 1.71                     | 0.71              |
| 1:A:1009:ARG:HA | 1:A:1012:LYS:HG2 | 1.71                     | 0.71              |
| 1:B:934:LEU:HA  | 1:B:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:C:1009:ARG:HA | 1:C:1012:LYS:HG2 | 1.71                     | 0.71              |
| 1:E:934:LEU:HA  | 1:E:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:F:730:LEU:O   | 1:F:733:SER:OG   | 2.08                     | 0.71              |
| 1:F:934:LEU:HA  | 1:F:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:G:646:ASP:HA  | 1:G:673:ARG:HB2  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:531:LEU:HA   | 1:J:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:K:531:LEU:HA   | 1:K:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:L:531:LEU:HA   | 1:L:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:D:531:LEU:HA   | 1:D:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:E:666:PHE:O    | 1:E:670:ASN:ND2  | 2.23                     | 0.71              |
| 1:H:972:ASN:OD1  | 1:H:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:K:134:LYS:HB3  | 1:K:138:ARG:NH1  | 2.03                     | 0.71              |
| 1:L:134:LYS:HB3  | 1:L:138:ARG:NH1  | 2.03                     | 0.71              |
| 1:A:531:LEU:HA   | 1:A:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:D:809:ASP:OD1  | 1:D:810:PHE:N    | 2.24                     | 0.71              |
| 1:E:809:ASP:OD1  | 1:E:810:PHE:N    | 2.24                     | 0.71              |
| 1:E:972:ASN:OD1  | 1:E:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:G:809:ASP:OD1  | 1:G:810:PHE:N    | 2.24                     | 0.71              |
| 1:K:934:LEU:HA   | 1:K:961:ILE:HD11 | 1.72                     | 0.71              |
| 1:L:934:LEU:HA   | 1:L:961:ILE:HD11 | 1.72                     | 0.71              |
| 1:B:1013:ARG:HG2 | 1:C:773:TRP:HH2  | 1.54                     | 0.71              |
| 1:F:531:LEU:HA   | 1:F:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:G:531:LEU:HA   | 1:G:598:ILE:HD13 | 1.71                     | 0.71              |
| 1:J:1009:ARG:HA  | 1:J:1012:LYS:HG2 | 1.71                     | 0.71              |
| 1:A:675:LYS:O    | 1:A:742:GLU:N    | 2.24                     | 0.71              |
| 1:C:809:ASP:OD1  | 1:C:810:PHE:N    | 2.24                     | 0.71              |
| 1:C:972:ASN:OD1  | 1:C:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:F:675:LYS:O    | 1:F:742:GLU:N    | 2.24                     | 0.71              |
| 1:F:809:ASP:OD1  | 1:F:810:PHE:N    | 2.24                     | 0.71              |
| 1:G:934:LEU:HA   | 1:G:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:I:972:ASN:OD1  | 1:I:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:J:675:LYS:O    | 1:J:742:GLU:N    | 2.24                     | 0.71              |
| 1:L:335:LYS:HE2  | 1:L:357:LEU:HD11 | 1.73                     | 0.71              |
| 1:D:730:LEU:O    | 1:D:733:SER:OG   | 2.08                     | 0.71              |
| 1:F:972:ASN:OD1  | 1:F:1001:GLN:NE2 | 2.22                     | 0.71              |
| 1:G:730:LEU:O    | 1:G:733:SER:OG   | 2.08                     | 0.71              |
| 1:H:809:ASP:OD1  | 1:H:810:PHE:N    | 2.24                     | 0.71              |
| 1:K:335:LYS:HE2  | 1:K:357:LEU:HD11 | 1.73                     | 0.71              |
| 1:A:666:PHE:O    | 1:A:670:ASN:ND2  | 2.23                     | 0.71              |
| 1:A:809:ASP:OD1  | 1:A:810:PHE:N    | 2.24                     | 0.71              |
| 1:C:335:LYS:HE2  | 1:C:357:LEU:HD11 | 1.73                     | 0.71              |
| 1:K:972:ASN:OD1  | 1:K:1001:GLN:NE2 | 2.23                     | 0.71              |
| 1:D:675:LYS:O    | 1:D:742:GLU:N    | 2.24                     | 0.71              |
| 1:D:934:LEU:HA   | 1:D:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:F:335:LYS:HE2  | 1:F:357:LEU:HD11 | 1.73                     | 0.71              |
| 1:G:675:LYS:O    | 1:G:742:GLU:N    | 2.24                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:335:LYS:HE2  | 1:H:357:LEU:HD11 | 1.73                     | 0.71              |
| 1:H:934:LEU:HA   | 1:H:961:ILE:HD11 | 1.73                     | 0.71              |
| 1:B:675:LYS:O    | 1:B:742:GLU:N    | 2.24                     | 0.70              |
| 1:E:675:LYS:O    | 1:E:742:GLU:N    | 2.24                     | 0.70              |
| 1:H:228:LYS:NZ   | 1:H:299:GLY:H    | 1.89                     | 0.70              |
| 1:I:809:ASP:OD1  | 1:I:810:PHE:N    | 2.24                     | 0.70              |
| 1:J:228:LYS:NZ   | 1:J:299:GLY:H    | 1.90                     | 0.70              |
| 1:J:666:PHE:O    | 1:J:670:ASN:ND2  | 2.23                     | 0.70              |
| 1:L:972:ASN:OD1  | 1:L:1001:GLN:NE2 | 2.22                     | 0.70              |
| 1:A:228:LYS:NZ   | 1:A:299:GLY:H    | 1.90                     | 0.70              |
| 1:B:972:ASN:OD1  | 1:B:1001:GLN:NE2 | 2.23                     | 0.70              |
| 1:C:228:LYS:NZ   | 1:C:299:GLY:H    | 1.89                     | 0.70              |
| 1:E:335:LYS:HE2  | 1:E:357:LEU:HD11 | 1.73                     | 0.70              |
| 1:I:675:LYS:O    | 1:I:742:GLU:N    | 2.24                     | 0.70              |
| 1:J:809:ASP:OD1  | 1:J:810:PHE:N    | 2.24                     | 0.70              |
| 1:K:228:LYS:NZ   | 1:K:299:GLY:H    | 1.90                     | 0.70              |
| 1:L:228:LYS:NZ   | 1:L:299:GLY:H    | 1.90                     | 0.70              |
| 1:L:730:LEU:O    | 1:L:733:SER:OG   | 2.08                     | 0.70              |
| 1:A:934:LEU:HA   | 1:A:961:ILE:HD11 | 1.73                     | 0.70              |
| 1:B:809:ASP:OD1  | 1:B:810:PHE:N    | 2.24                     | 0.70              |
| 1:C:934:LEU:HA   | 1:C:961:ILE:HD11 | 1.73                     | 0.70              |
| 1:F:228:LYS:NZ   | 1:F:299:GLY:H    | 1.89                     | 0.70              |
| 1:K:809:ASP:OD1  | 1:K:810:PHE:N    | 2.24                     | 0.70              |
| 1:L:809:ASP:OD1  | 1:L:810:PHE:N    | 2.24                     | 0.70              |
| 1:D:734:LEU:HD23 | 1:D:737:ASN:HD22 | 1.57                     | 0.70              |
| 1:G:734:LEU:HD23 | 1:G:737:ASN:HD22 | 1.57                     | 0.70              |
| 1:I:531:LEU:HA   | 1:I:598:ILE:HD13 | 1.71                     | 0.70              |
| 1:K:730:LEU:O    | 1:K:733:SER:OG   | 2.08                     | 0.70              |
| 1:B:228:LYS:NZ   | 1:B:299:GLY:H    | 1.90                     | 0.70              |
| 1:E:228:LYS:NZ   | 1:E:299:GLY:H    | 1.90                     | 0.70              |
| 1:H:675:LYS:O    | 1:H:742:GLU:N    | 2.24                     | 0.70              |
| 1:I:730:LEU:O    | 1:I:733:SER:OG   | 2.08                     | 0.70              |
| 1:K:675:LYS:O    | 1:K:742:GLU:N    | 2.24                     | 0.70              |
| 1:L:675:LYS:O    | 1:L:742:GLU:N    | 2.24                     | 0.70              |
| 1:I:228:LYS:NZ   | 1:I:299:GLY:H    | 1.89                     | 0.70              |
| 1:J:934:LEU:HA   | 1:J:961:ILE:HD11 | 1.73                     | 0.70              |
| 1:B:531:LEU:HA   | 1:B:598:ILE:HD13 | 1.71                     | 0.70              |
| 1:D:972:ASN:OD1  | 1:D:1001:GLN:NE2 | 2.23                     | 0.70              |
| 1:B:730:LEU:O    | 1:B:733:SER:OG   | 2.08                     | 0.70              |
| 1:C:675:LYS:O    | 1:C:742:GLU:N    | 2.24                     | 0.70              |
| 1:K:734:LEU:HD23 | 1:K:737:ASN:HD22 | 1.57                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:335:LYS:HE2  | 1:B:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:E:443:LEU:HD22 | 1:E:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:G:228:LYS:NZ   | 1:G:299:GLY:H    | 1.89                     | 0.69              |
| 1:G:972:ASN:OD1  | 1:G:1001:GLN:NE2 | 2.22                     | 0.69              |
| 1:J:335:LYS:HE2  | 1:J:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:A:335:LYS:HE2  | 1:A:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:A:443:LEU:HD22 | 1:A:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:C:734:LEU:HD23 | 1:C:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:D:228:LYS:NZ   | 1:D:299:GLY:H    | 1.90                     | 0.69              |
| 1:F:443:LEU:HD22 | 1:F:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:H:734:LEU:HD23 | 1:H:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:L:734:LEU:HD23 | 1:L:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:D:335:LYS:HE2  | 1:D:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:I:335:LYS:HE2  | 1:I:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:J:443:LEU:HD22 | 1:J:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:K:443:LEU:HD22 | 1:K:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:L:443:LEU:HD22 | 1:L:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:B:734:LEU:HD23 | 1:B:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:I:734:LEU:HD23 | 1:I:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:G:443:LEU:HD22 | 1:G:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:H:443:LEU:HD22 | 1:H:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:C:443:LEU:HD22 | 1:C:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:G:335:LYS:HE2  | 1:G:357:LEU:HD11 | 1.73                     | 0.69              |
| 1:I:443:LEU:HD22 | 1:I:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:A:734:LEU:HD23 | 1:A:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:B:443:LEU:HD22 | 1:B:524:PHE:HE2  | 1.57                     | 0.69              |
| 1:I:479:LEU:HB2  | 1:I:513:PHE:CZ   | 2.28                     | 0.69              |
| 1:K:785:PHE:HB3  | 1:L:810:PHE:CZ   | 2.23                     | 0.69              |
| 1:B:479:LEU:HB2  | 1:B:513:PHE:CZ   | 2.28                     | 0.69              |
| 1:H:479:LEU:HB2  | 1:H:513:PHE:CZ   | 2.28                     | 0.69              |
| 1:J:734:LEU:HD23 | 1:J:737:ASN:HD22 | 1.57                     | 0.69              |
| 1:D:443:LEU:HD22 | 1:D:524:PHE:HE2  | 1.57                     | 0.68              |
| 1:E:810:PHE:CZ   | 1:F:785:PHE:HB3  | 2.28                     | 0.68              |
| 1:G:479:LEU:HB2  | 1:G:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:C:839:ALA:O    | 1:C:842:GLN:NE2  | 2.25                     | 0.68              |
| 1:D:479:LEU:HB2  | 1:D:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:E:369:PHE:HB3  | 1:E:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:F:734:LEU:HD23 | 1:F:737:ASN:HD22 | 1.57                     | 0.68              |
| 1:A:369:PHE:HB3  | 1:A:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:D:786:ASP:O    | 1:D:789:SER:OG   | 2.11                     | 0.68              |
| 1:E:734:LEU:HD23 | 1:E:737:ASN:HD22 | 1.57                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:369:PHE:HB3  | 1:F:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:J:369:PHE:HB3  | 1:J:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:K:369:PHE:HB3  | 1:K:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:L:369:PHE:HB3  | 1:L:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:C:479:LEU:HB2  | 1:C:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:G:786:ASP:O    | 1:G:789:SER:OG   | 2.11                     | 0.68              |
| 1:I:384:ASN:O    | 1:I:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:A:856:ARG:HD3  | 1:A:885:LYS:HB2  | 1.76                     | 0.68              |
| 1:B:384:ASN:O    | 1:B:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:D:369:PHE:HB3  | 1:D:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:D:384:ASN:O    | 1:D:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:D:990:LEU:HA   | 1:D:994:GLY:HA2  | 1.75                     | 0.68              |
| 1:E:271:LEU:HD11 | 1:E:278:ASP:H    | 1.59                     | 0.68              |
| 1:F:271:LEU:HD11 | 1:F:278:ASP:H    | 1.59                     | 0.68              |
| 1:F:384:ASN:O    | 1:F:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:G:990:LEU:HA   | 1:G:994:GLY:HA2  | 1.75                     | 0.68              |
| 1:I:990:LEU:HA   | 1:I:994:GLY:HA2  | 1.75                     | 0.68              |
| 1:L:479:LEU:HB2  | 1:L:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:C:271:LEU:HD11 | 1:C:278:ASP:H    | 1.59                     | 0.68              |
| 1:J:856:ARG:HD3  | 1:J:885:LYS:HB2  | 1.76                     | 0.68              |
| 1:K:479:LEU:HB2  | 1:K:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:G:369:PHE:HB3  | 1:G:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:G:384:ASN:O    | 1:G:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:K:384:ASN:O    | 1:K:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:B:369:PHE:HB3  | 1:B:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:E:486:ARG:NH1  | 1:E:491:GLN:OE1  | 2.27                     | 0.68              |
| 1:F:486:ARG:NH1  | 1:F:491:GLN:OE1  | 2.27                     | 0.68              |
| 1:A:479:LEU:HB2  | 1:A:513:PHE:CZ   | 2.28                     | 0.68              |
| 1:D:486:ARG:NH1  | 1:D:491:GLN:OE1  | 2.27                     | 0.68              |
| 1:E:384:ASN:O    | 1:E:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:K:856:ARG:HD3  | 1:K:885:LYS:HB2  | 1.76                     | 0.68              |
| 1:L:384:ASN:O    | 1:L:389:ARG:NH1  | 2.27                     | 0.68              |
| 1:L:856:ARG:HD3  | 1:L:885:LYS:HB2  | 1.76                     | 0.68              |
| 1:A:1005:MET:HB3 | 1:A:1007:LEU:HG  | 1.76                     | 0.68              |
| 1:B:990:LEU:HA   | 1:B:994:GLY:HA2  | 1.76                     | 0.68              |
| 1:F:773:TRP:HH2  | 1:G:1013:ARG:HG2 | 1.59                     | 0.68              |
| 1:G:486:ARG:NH1  | 1:G:491:GLN:OE1  | 2.27                     | 0.68              |
| 1:I:369:PHE:HB3  | 1:I:374:ARG:HB2  | 1.75                     | 0.68              |
| 1:J:1005:MET:HB3 | 1:J:1007:LEU:HG  | 1.76                     | 0.68              |
| 1:L:1005:MET:HB3 | 1:L:1007:LEU:HG  | 1.76                     | 0.68              |
| 1:A:271:LEU:HD11 | 1:A:278:ASP:H    | 1.59                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:486:ARG:NH1  | 1:A:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:B:1005:MET:HB3 | 1:B:1007:LEU:HG   | 1.77                     | 0.67              |
| 1:C:369:PHE:HB3  | 1:C:374:ARG:HB2   | 1.75                     | 0.67              |
| 1:C:856:ARG:HD3  | 1:C:885:LYS:HB2   | 1.76                     | 0.67              |
| 1:H:271:LEU:HD11 | 1:H:278:ASP:H     | 1.59                     | 0.67              |
| 1:H:856:ARG:HD3  | 1:H:885:LYS:HB2   | 1.75                     | 0.67              |
| 1:I:798:VAL:O    | 1:I:827:GLN:N     | 2.26                     | 0.67              |
| 1:I:1005:MET:HB3 | 1:I:1007:LEU:HG   | 1.77                     | 0.67              |
| 1:J:486:ARG:NH1  | 1:J:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:K:486:ARG:NH1  | 1:K:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:L:271:LEU:HD11 | 1:L:278:ASP:H     | 1.59                     | 0.67              |
| 1:L:486:ARG:NH1  | 1:L:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:A:990:LEU:HD11 | 1:A:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:C:962:LEU:HD11 | 1:C:968:LEU:HG    | 1.77                     | 0.67              |
| 1:J:271:LEU:HD11 | 1:J:278:ASP:H     | 1.59                     | 0.67              |
| 1:K:271:LEU:HD11 | 1:K:278:ASP:H     | 1.59                     | 0.67              |
| 1:K:990:LEU:HD11 | 1:K:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:K:990:LEU:HA   | 1:K:994:GLY:HA2   | 1.75                     | 0.67              |
| 1:K:1005:MET:HB3 | 1:K:1007:LEU:HG   | 1.77                     | 0.67              |
| 1:L:990:LEU:HD11 | 1:L:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:A:384:ASN:O    | 1:A:389:ARG:NH1   | 2.27                     | 0.67              |
| 1:E:479:LEU:HB2  | 1:E:513:PHE:CZ    | 2.28                     | 0.67              |
| 1:E:962:LEU:HD11 | 1:E:968:LEU:HG    | 1.77                     | 0.67              |
| 1:H:962:LEU:HD11 | 1:H:968:LEU:HG    | 1.77                     | 0.67              |
| 1:I:486:ARG:NH1  | 1:I:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:J:479:LEU:HB2  | 1:J:513:PHE:CZ    | 2.28                     | 0.67              |
| 1:J:990:LEU:HD11 | 1:J:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:J:990:LEU:HA   | 1:J:994:GLY:HA2   | 1.75                     | 0.67              |
| 1:B:486:ARG:NH1  | 1:B:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:C:384:ASN:O    | 1:C:389:ARG:NH1   | 2.27                     | 0.67              |
| 1:C:990:LEU:HD11 | 1:C:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:E:990:LEU:HD11 | 1:E:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:F:479:LEU:HB2  | 1:F:513:PHE:CZ    | 2.28                     | 0.67              |
| 1:F:962:LEU:HD11 | 1:F:968:LEU:HG    | 1.77                     | 0.67              |
| 1:H:369:PHE:HB3  | 1:H:374:ARG:HB2   | 1.75                     | 0.67              |
| 1:H:384:ASN:O    | 1:H:389:ARG:NH1   | 2.27                     | 0.67              |
| 1:J:384:ASN:O    | 1:J:389:ARG:NH1   | 2.27                     | 0.67              |
| 1:A:990:LEU:HA   | 1:A:994:GLY:HA2   | 1.75                     | 0.67              |
| 1:B:999:SER:OG   | 1:B:1001:GLN:OE1  | 2.13                     | 0.67              |
| 1:C:486:ARG:NH1  | 1:C:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:J:962:LEU:HD11 | 1:J:968:LEU:HG    | 1.77                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:799:GLU:HB2  | 1:F:828:LYS:HB2   | 1.77                     | 0.67              |
| 1:H:1005:MET:HB3 | 1:H:1007:LEU:HG   | 1.76                     | 0.67              |
| 1:I:999:SER:OG   | 1:I:1001:GLN:OE1  | 2.13                     | 0.67              |
| 1:L:990:LEU:HA   | 1:L:994:GLY:HA2   | 1.76                     | 0.67              |
| 1:A:962:LEU:HD11 | 1:A:968:LEU:HG    | 1.77                     | 0.67              |
| 1:B:271:LEU:HD11 | 1:B:278:ASP:H     | 1.59                     | 0.67              |
| 1:B:990:LEU:HD11 | 1:B:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:C:1005:MET:HB3 | 1:C:1007:LEU:HG   | 1.77                     | 0.67              |
| 1:G:856:ARG:HD3  | 1:G:885:LYS:HB2   | 1.76                     | 0.67              |
| 1:H:990:LEU:HD11 | 1:H:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:J:773:TRP:HH2  | 1:K:1013:ARG:HG2  | 1.59                     | 0.67              |
| 1:B:856:ARG:HD3  | 1:B:885:LYS:HB2   | 1.76                     | 0.67              |
| 1:D:856:ARG:HD3  | 1:D:885:LYS:HB2   | 1.76                     | 0.67              |
| 1:E:799:GLU:HB2  | 1:E:828:LYS:HB2   | 1.77                     | 0.67              |
| 1:F:990:LEU:HD11 | 1:F:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:H:486:ARG:NH1  | 1:H:491:GLN:OE1   | 2.27                     | 0.67              |
| 1:I:252:LEU:HD22 | 1:I:294:LEU:HD23  | 1.77                     | 0.67              |
| 1:I:786:ASP:O    | 1:I:789:SER:OG    | 2.12                     | 0.67              |
| 1:I:990:LEU:HD11 | 1:I:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:K:999:SER:OG   | 1:K:1001:GLN:OE1  | 2.13                     | 0.67              |
| 1:B:252:LEU:HD22 | 1:B:294:LEU:HD23  | 1.77                     | 0.67              |
| 1:C:999:SER:OG   | 1:C:1001:GLN:OE1  | 2.13                     | 0.67              |
| 1:D:990:LEU:HD11 | 1:D:1018:LEU:HD22 | 1.77                     | 0.67              |
| 1:F:990:LEU:HA   | 1:F:994:GLY:HA2   | 1.75                     | 0.67              |
| 1:G:1005:MET:HB3 | 1:G:1007:LEU:HG   | 1.76                     | 0.67              |
| 1:I:856:ARG:HD3  | 1:I:885:LYS:HB2   | 1.76                     | 0.67              |
| 1:K:252:LEU:HD22 | 1:K:294:LEU:HD23  | 1.77                     | 0.67              |
| 1:D:1005:MET:HB3 | 1:D:1007:LEU:HG   | 1.76                     | 0.66              |
| 1:E:990:LEU:HA   | 1:E:994:GLY:HA2   | 1.75                     | 0.66              |
| 1:E:1005:MET:HB3 | 1:E:1007:LEU:HG   | 1.76                     | 0.66              |
| 1:G:990:LEU:HD11 | 1:G:1018:LEU:HD22 | 1.77                     | 0.66              |
| 1:L:252:LEU:HD22 | 1:L:294:LEU:HD23  | 1.76                     | 0.66              |
| 1:L:999:SER:OG   | 1:L:1001:GLN:OE1  | 2.13                     | 0.66              |
| 1:G:798:VAL:O    | 1:G:827:GLN:N     | 2.26                     | 0.66              |
| 1:H:999:SER:OG   | 1:H:1001:GLN:OE1  | 2.13                     | 0.66              |
| 1:D:271:LEU:HD11 | 1:D:278:ASP:H     | 1.59                     | 0.66              |
| 1:D:839:ALA:O    | 1:D:842:GLN:NE2   | 2.25                     | 0.66              |
| 1:D:962:LEU:HD11 | 1:D:968:LEU:HG    | 1.77                     | 0.66              |
| 1:F:856:ARG:HD3  | 1:F:885:LYS:HB2   | 1.76                     | 0.66              |
| 1:G:271:LEU:HD11 | 1:G:278:ASP:H     | 1.59                     | 0.66              |
| 1:G:962:LEU:HD11 | 1:G:968:LEU:HG    | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:271:LEU:HD11 | 1:I:278:ASP:H    | 1.59                     | 0.66              |
| 1:D:798:VAL:O    | 1:D:827:GLN:N    | 2.26                     | 0.66              |
| 1:F:999:SER:OG   | 1:F:1001:GLN:OE1 | 2.13                     | 0.66              |
| 1:G:839:ALA:O    | 1:G:842:GLN:NE2  | 2.25                     | 0.66              |
| 1:H:252:LEU:HD22 | 1:H:294:LEU:HD23 | 1.77                     | 0.66              |
| 1:H:799:GLU:HB2  | 1:H:828:LYS:HB2  | 1.77                     | 0.66              |
| 1:L:948:CYS:SG   | 1:L:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:A:948:CYS:SG   | 1:A:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:C:252:LEU:HD22 | 1:C:294:LEU:HD23 | 1.77                     | 0.66              |
| 1:D:252:LEU:HD22 | 1:D:294:LEU:HD23 | 1.77                     | 0.66              |
| 1:E:856:ARG:HD3  | 1:E:885:LYS:HB2  | 1.76                     | 0.66              |
| 1:F:1005:MET:HB3 | 1:F:1007:LEU:HG  | 1.77                     | 0.66              |
| 1:J:948:CYS:SG   | 1:J:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:K:334:LYS:HG3  | 1:K:342:LEU:HD11 | 1.78                     | 0.66              |
| 1:K:948:CYS:SG   | 1:K:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:C:990:LEU:HA   | 1:C:994:GLY:HA2  | 1.75                     | 0.66              |
| 1:E:999:SER:OG   | 1:E:1001:GLN:OE1 | 2.13                     | 0.66              |
| 1:G:223:ALA:O    | 1:G:347:ARG:NH1  | 2.29                     | 0.66              |
| 1:G:252:LEU:HD22 | 1:G:294:LEU:HD23 | 1.77                     | 0.66              |
| 1:I:839:ALA:O    | 1:I:842:GLN:NE2  | 2.25                     | 0.66              |
| 1:C:786:ASP:O    | 1:C:789:SER:OG   | 2.11                     | 0.66              |
| 1:L:334:LYS:HG3  | 1:L:342:LEU:HD11 | 1.78                     | 0.66              |
| 1:B:839:ALA:O    | 1:B:842:GLN:NE2  | 2.25                     | 0.66              |
| 1:C:799:GLU:HB2  | 1:C:828:LYS:HB2  | 1.77                     | 0.66              |
| 1:D:223:ALA:O    | 1:D:347:ARG:NH1  | 2.29                     | 0.66              |
| 1:I:799:GLU:HB2  | 1:I:828:LYS:HB2  | 1.77                     | 0.66              |
| 1:B:948:CYS:SG   | 1:B:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:H:374:ARG:NH1  | 1:H:396:GLN:OE1  | 2.29                     | 0.66              |
| 1:H:1010:GLU:O   | 1:H:1013:ARG:HG3 | 1.96                     | 0.66              |
| 1:J:334:LYS:HG3  | 1:J:342:LEU:HD11 | 1.78                     | 0.66              |
| 1:K:374:ARG:NH1  | 1:K:396:GLN:OE1  | 2.29                     | 0.66              |
| 1:A:334:LYS:HG3  | 1:A:342:LEU:HD11 | 1.78                     | 0.66              |
| 1:B:799:GLU:HB2  | 1:B:828:LYS:HB2  | 1.77                     | 0.66              |
| 1:D:228:LYS:HD3  | 1:D:345:THR:HB   | 1.78                     | 0.66              |
| 1:D:799:GLU:HB2  | 1:D:828:LYS:HB2  | 1.77                     | 0.66              |
| 1:F:325:ASP:O    | 1:F:329:SER:N    | 2.29                     | 0.66              |
| 1:H:948:CYS:SG   | 1:H:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:H:990:LEU:HA   | 1:H:994:GLY:HA2  | 1.76                     | 0.66              |
| 1:I:948:CYS:SG   | 1:I:976:ASN:ND2  | 2.69                     | 0.66              |
| 1:A:252:LEU:HD22 | 1:A:294:LEU:HD23 | 1.77                     | 0.65              |
| 1:B:962:LEU:HD11 | 1:B:968:LEU:HG   | 1.77                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:374:ARG:NH1  | 1:C:396:GLN:OE1   | 2.29                     | 0.65              |
| 1:C:866:ASP:OD1  | 1:C:867:SER:N     | 2.29                     | 0.65              |
| 1:C:1010:GLU:O   | 1:C:1013:ARG:HG3  | 1.97                     | 0.65              |
| 1:E:325:ASP:O    | 1:E:329:SER:N     | 2.30                     | 0.65              |
| 1:J:799:GLU:HB2  | 1:J:828:LYS:HB2   | 1.77                     | 0.65              |
| 1:L:374:ARG:NH1  | 1:L:396:GLN:OE1   | 2.29                     | 0.65              |
| 1:L:962:LEU:HD11 | 1:L:968:LEU:HG    | 1.77                     | 0.65              |
| 1:A:786:ASP:O    | 1:A:789:SER:OG    | 2.11                     | 0.65              |
| 1:A:1010:GLU:O   | 1:A:1013:ARG:HG3  | 1.96                     | 0.65              |
| 1:C:948:CYS:SG   | 1:C:976:ASN:ND2   | 2.69                     | 0.65              |
| 1:D:141:ARG:NH1  | 1:D:240:ALA:O     | 2.30                     | 0.65              |
| 1:D:374:ARG:NH1  | 1:D:396:GLN:OE1   | 2.29                     | 0.65              |
| 1:G:141:ARG:NH1  | 1:G:240:ALA:O     | 2.30                     | 0.65              |
| 1:G:228:LYS:HD3  | 1:G:345:THR:HB    | 1.79                     | 0.65              |
| 1:G:799:GLU:HB2  | 1:G:828:LYS:HB2   | 1.77                     | 0.65              |
| 1:I:962:LEU:HD11 | 1:I:968:LEU:HG    | 1.77                     | 0.65              |
| 1:J:786:ASP:O    | 1:J:789:SER:OG    | 2.12                     | 0.65              |
| 1:J:1010:GLU:O   | 1:J:1013:ARG:HG3  | 1.96                     | 0.65              |
| 1:A:799:GLU:HB2  | 1:A:828:LYS:HB2   | 1.77                     | 0.65              |
| 1:E:141:ARG:NH1  | 1:E:240:ALA:O     | 2.30                     | 0.65              |
| 1:F:141:ARG:NH1  | 1:F:240:ALA:O     | 2.30                     | 0.65              |
| 1:G:374:ARG:NH1  | 1:G:396:GLN:OE1   | 2.29                     | 0.65              |
| 1:H:866:ASP:OD1  | 1:H:867:SER:N     | 2.29                     | 0.65              |
| 1:I:223:ALA:O    | 1:I:347:ARG:NH1   | 2.29                     | 0.65              |
| 1:K:962:LEU:HD11 | 1:K:968:LEU:HG    | 1.77                     | 0.65              |
| 1:L:996:LEU:HD11 | 1:L:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:D:325:ASP:O    | 1:D:329:SER:N     | 2.30                     | 0.65              |
| 1:G:999:SER:OG   | 1:G:1001:GLN:OE1  | 2.13                     | 0.65              |
| 1:H:325:ASP:O    | 1:H:329:SER:N     | 2.30                     | 0.65              |
| 1:C:334:LYS:HG3  | 1:C:342:LEU:HD11  | 1.78                     | 0.65              |
| 1:G:325:ASP:O    | 1:G:329:SER:N     | 2.30                     | 0.65              |
| 1:J:252:LEU:HD22 | 1:J:294:LEU:HD23  | 1.77                     | 0.65              |
| 1:K:996:LEU:HD11 | 1:K:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:B:223:ALA:O    | 1:B:347:ARG:NH1   | 2.29                     | 0.65              |
| 1:B:334:LYS:HG3  | 1:B:342:LEU:HD11  | 1.78                     | 0.65              |
| 1:C:325:ASP:O    | 1:C:329:SER:N     | 2.29                     | 0.65              |
| 1:D:948:CYS:SG   | 1:D:976:ASN:ND2   | 2.69                     | 0.65              |
| 1:E:252:LEU:HD22 | 1:E:294:LEU:HD23  | 1.76                     | 0.65              |
| 1:E:1010:GLU:O   | 1:E:1013:ARG:HG3  | 1.96                     | 0.65              |
| 1:F:252:LEU:HD22 | 1:F:294:LEU:HD23  | 1.76                     | 0.65              |
| 1:F:334:LYS:HG3  | 1:F:342:LEU:HD11  | 1.78                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:786:ASP:O    | 1:F:789:SER:OG    | 2.11                     | 0.65              |
| 1:F:948:CYS:SG   | 1:F:976:ASN:ND2   | 2.69                     | 0.65              |
| 1:I:334:LYS:HG3  | 1:I:342:LEU:HD11  | 1.78                     | 0.65              |
| 1:J:996:LEU:HD11 | 1:J:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:K:1010:GLU:O   | 1:K:1013:ARG:HG3  | 1.96                     | 0.65              |
| 1:A:996:LEU:HD11 | 1:A:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:B:141:ARG:NH1  | 1:B:240:ALA:O     | 2.30                     | 0.65              |
| 1:C:141:ARG:NH1  | 1:C:240:ALA:O     | 2.30                     | 0.65              |
| 1:I:141:ARG:NH1  | 1:I:240:ALA:O     | 2.30                     | 0.65              |
| 1:I:1010:GLU:O   | 1:I:1013:ARG:HG3  | 1.97                     | 0.65              |
| 1:J:223:ALA:O    | 1:J:347:ARG:NH1   | 2.29                     | 0.65              |
| 1:L:226:ILE:HG23 | 1:L:408:PRO:HG2   | 1.79                     | 0.65              |
| 1:C:996:LEU:HD11 | 1:C:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:D:999:SER:OG   | 1:D:1001:GLN:OE1  | 2.13                     | 0.65              |
| 1:E:223:ALA:O    | 1:E:347:ARG:NH1   | 2.29                     | 0.65              |
| 1:E:374:ARG:NH1  | 1:E:396:GLN:OE1   | 2.29                     | 0.65              |
| 1:E:948:CYS:SG   | 1:E:976:ASN:ND2   | 2.69                     | 0.65              |
| 1:E:996:LEU:HD11 | 1:E:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:F:223:ALA:O    | 1:F:347:ARG:NH1   | 2.29                     | 0.65              |
| 1:G:948:CYS:SG   | 1:G:976:ASN:ND2   | 2.69                     | 0.65              |
| 1:H:141:ARG:NH1  | 1:H:240:ALA:O     | 2.30                     | 0.65              |
| 1:J:1009:ARG:NH1 | 1:J:1012:LYS:HB2  | 2.12                     | 0.65              |
| 1:K:226:ILE:HG23 | 1:K:408:PRO:HG2   | 1.79                     | 0.65              |
| 1:L:1009:ARG:NH1 | 1:L:1012:LYS:HB2  | 2.12                     | 0.65              |
| 1:L:1010:GLU:O   | 1:L:1013:ARG:HG3  | 1.97                     | 0.65              |
| 1:A:1009:ARG:NH1 | 1:A:1012:LYS:HB2  | 2.12                     | 0.65              |
| 1:H:572:ILE:HG13 | 1:H:573:PHE:H     | 1.62                     | 0.65              |
| 1:H:599:SER:O    | 1:H:603:ARG:NH1   | 2.30                     | 0.65              |
| 1:A:325:ASP:O    | 1:A:329:SER:N     | 2.29                     | 0.65              |
| 1:B:325:ASP:O    | 1:B:329:SER:N     | 2.30                     | 0.65              |
| 1:B:1010:GLU:O   | 1:B:1013:ARG:HG3  | 1.96                     | 0.65              |
| 1:C:572:ILE:HG13 | 1:C:573:PHE:H     | 1.62                     | 0.65              |
| 1:C:599:SER:O    | 1:C:603:ARG:NH1   | 2.30                     | 0.65              |
| 1:E:334:LYS:HG3  | 1:E:342:LEU:HD11  | 1.78                     | 0.65              |
| 1:F:599:SER:O    | 1:F:603:ARG:NH1   | 2.30                     | 0.65              |
| 1:F:996:LEU:HD11 | 1:F:1025:LEU:HD13 | 1.79                     | 0.65              |
| 1:G:866:ASP:OD1  | 1:G:867:SER:N     | 2.29                     | 0.65              |
| 1:I:325:ASP:O    | 1:I:329:SER:N     | 2.29                     | 0.65              |
| 1:J:325:ASP:O    | 1:J:329:SER:N     | 2.29                     | 0.65              |
| 1:J:999:SER:OG   | 1:J:1001:GLN:OE1  | 2.13                     | 0.65              |
| 1:K:1009:ARG:NH1 | 1:K:1012:LYS:HB2  | 2.12                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:223:ALA:O    | 1:A:347:ARG:NH1   | 2.29                     | 0.64              |
| 1:A:599:SER:O    | 1:A:603:ARG:NH1   | 2.30                     | 0.64              |
| 1:B:374:ARG:NH1  | 1:B:396:GLN:OE1   | 2.29                     | 0.64              |
| 1:B:798:VAL:O    | 1:B:827:GLN:N     | 2.26                     | 0.64              |
| 1:C:223:ALA:O    | 1:C:347:ARG:NH1   | 2.29                     | 0.64              |
| 1:F:866:ASP:OD1  | 1:F:867:SER:N     | 2.29                     | 0.64              |
| 1:J:226:ILE:HG23 | 1:J:408:PRO:HG2   | 1.79                     | 0.64              |
| 1:J:599:SER:O    | 1:J:603:ARG:NH1   | 2.30                     | 0.64              |
| 1:L:799:GLU:HB2  | 1:L:828:LYS:HB2   | 1.77                     | 0.64              |
| 1:A:374:ARG:NH1  | 1:A:396:GLN:OE1   | 2.29                     | 0.64              |
| 1:H:334:LYS:HG3  | 1:H:342:LEU:HD11  | 1.78                     | 0.64              |
| 1:I:374:ARG:NH1  | 1:I:396:GLN:OE1   | 2.29                     | 0.64              |
| 1:J:572:ILE:HG13 | 1:J:573:PHE:H     | 1.62                     | 0.64              |
| 1:J:839:ALA:O    | 1:J:842:GLN:NE2   | 2.25                     | 0.64              |
| 1:A:226:ILE:HG23 | 1:A:408:PRO:HG2   | 1.79                     | 0.64              |
| 1:F:1010:GLU:O   | 1:F:1013:ARG:HG3  | 1.97                     | 0.64              |
| 1:H:996:LEU:HD11 | 1:H:1025:LEU:HD13 | 1.79                     | 0.64              |
| 1:H:1009:ARG:NH1 | 1:H:1012:LYS:HB2  | 2.12                     | 0.64              |
| 1:K:799:GLU:HB2  | 1:K:828:LYS:HB2   | 1.77                     | 0.64              |
| 1:L:223:ALA:O    | 1:L:347:ARG:NH1   | 2.29                     | 0.64              |
| 1:A:572:ILE:HG13 | 1:A:573:PHE:H     | 1.62                     | 0.64              |
| 1:A:999:SER:OG   | 1:A:1001:GLN:OE1  | 2.13                     | 0.64              |
| 1:C:1009:ARG:NH1 | 1:C:1012:LYS:HB2  | 2.12                     | 0.64              |
| 1:F:572:ILE:HG13 | 1:F:573:PHE:H     | 1.62                     | 0.64              |
| 1:G:599:SER:O    | 1:G:603:ARG:NH1   | 2.30                     | 0.64              |
| 1:J:374:ARG:NH1  | 1:J:396:GLN:OE1   | 2.29                     | 0.64              |
| 1:K:223:ALA:O    | 1:K:347:ARG:NH1   | 2.29                     | 0.64              |
| 1:K:572:ILE:HG13 | 1:K:573:PHE:H     | 1.62                     | 0.64              |
| 1:K:839:ALA:O    | 1:K:842:GLN:NE2   | 2.25                     | 0.64              |
| 1:L:141:ARG:NH1  | 1:L:240:ALA:O     | 2.30                     | 0.64              |
| 1:A:839:ALA:O    | 1:A:842:GLN:NE2   | 2.25                     | 0.64              |
| 1:D:334:LYS:HG3  | 1:D:342:LEU:HD11  | 1.78                     | 0.64              |
| 1:D:1010:GLU:O   | 1:D:1013:ARG:HG3  | 1.97                     | 0.64              |
| 1:E:572:ILE:HG13 | 1:E:573:PHE:H     | 1.62                     | 0.64              |
| 1:E:599:SER:O    | 1:E:603:ARG:NH1   | 2.30                     | 0.64              |
| 1:F:374:ARG:NH1  | 1:F:396:GLN:OE1   | 2.29                     | 0.64              |
| 1:H:223:ALA:O    | 1:H:347:ARG:NH1   | 2.29                     | 0.64              |
| 1:J:228:LYS:HD3  | 1:J:345:THR:HB    | 1.78                     | 0.64              |
| 1:K:141:ARG:NH1  | 1:K:240:ALA:O     | 2.30                     | 0.64              |
| 1:L:325:ASP:O    | 1:L:329:SER:N     | 2.29                     | 0.64              |
| 1:L:572:ILE:HG13 | 1:L:573:PHE:H     | 1.62                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:ARG:NH1  | 1:A:240:ALA:O    | 2.30                     | 0.64              |
| 1:B:1009:ARG:NH1 | 1:B:1012:LYS:HB2 | 2.12                     | 0.64              |
| 1:C:169:LEU:O    | 1:C:199:LEU:N    | 2.31                     | 0.64              |
| 1:D:599:SER:O    | 1:D:603:ARG:NH1  | 2.30                     | 0.64              |
| 1:E:630:TYR:OH   | 1:E:660:ASP:OD1  | 2.12                     | 0.64              |
| 1:E:866:ASP:OD1  | 1:E:867:SER:N    | 2.29                     | 0.64              |
| 1:G:630:TYR:OH   | 1:G:660:ASP:OD1  | 2.12                     | 0.64              |
| 1:H:169:LEU:O    | 1:H:199:LEU:N    | 2.31                     | 0.64              |
| 1:I:599:SER:O    | 1:I:603:ARG:NH1  | 2.30                     | 0.64              |
| 1:J:141:ARG:NH1  | 1:J:240:ALA:O    | 2.30                     | 0.64              |
| 1:J:169:LEU:O    | 1:J:199:LEU:N    | 2.31                     | 0.64              |
| 1:K:325:ASP:O    | 1:K:329:SER:N    | 2.29                     | 0.64              |
| 1:L:786:ASP:O    | 1:L:789:SER:OG   | 2.11                     | 0.64              |
| 1:A:169:LEU:O    | 1:A:199:LEU:N    | 2.31                     | 0.64              |
| 1:D:572:ILE:HG13 | 1:D:573:PHE:H    | 1.62                     | 0.64              |
| 1:F:228:LYS:HD3  | 1:F:345:THR:HB   | 1.78                     | 0.64              |
| 1:G:334:LYS:HG3  | 1:G:342:LEU:HD11 | 1.78                     | 0.64              |
| 1:I:228:LYS:HD3  | 1:I:345:THR:HB   | 1.78                     | 0.64              |
| 1:J:556:VAL:HG11 | 1:J:605:GLU:HG3  | 1.80                     | 0.64              |
| 1:L:995:CYS:SG   | 1:L:996:LEU:N    | 2.71                     | 0.64              |
| 1:B:572:ILE:HG13 | 1:B:573:PHE:H    | 1.62                     | 0.64              |
| 1:F:169:LEU:O    | 1:F:199:LEU:N    | 2.31                     | 0.64              |
| 1:G:1010:GLU:O   | 1:G:1013:ARG:HG3 | 1.97                     | 0.64              |
| 1:K:228:LYS:HD3  | 1:K:345:THR:HB   | 1.78                     | 0.64              |
| 1:K:995:CYS:SG   | 1:K:996:LEU:N    | 2.71                     | 0.64              |
| 1:L:839:ALA:O    | 1:L:842:GLN:NE2  | 2.25                     | 0.64              |
| 1:A:228:LYS:HD3  | 1:A:345:THR:HB   | 1.79                     | 0.64              |
| 1:D:630:TYR:OH   | 1:D:660:ASP:OD1  | 2.12                     | 0.64              |
| 1:E:786:ASP:O    | 1:E:789:SER:OG   | 2.12                     | 0.64              |
| 1:F:1009:ARG:NH1 | 1:F:1012:LYS:HB2 | 2.12                     | 0.64              |
| 1:K:786:ASP:O    | 1:K:789:SER:OG   | 2.11                     | 0.64              |
| 1:K:798:VAL:O    | 1:K:827:GLN:N    | 2.26                     | 0.64              |
| 1:L:798:VAL:O    | 1:L:827:GLN:N    | 2.26                     | 0.64              |
| 1:B:226:ILE:HG23 | 1:B:408:PRO:HG2  | 1.79                     | 0.64              |
| 1:B:599:SER:O    | 1:B:603:ARG:NH1  | 2.30                     | 0.64              |
| 1:B:773:TRP:CH2  | 1:C:1013:ARG:HG2 | 2.32                     | 0.64              |
| 1:C:556:VAL:HG11 | 1:C:605:GLU:HG3  | 1.80                     | 0.64              |
| 1:D:995:CYS:SG   | 1:D:996:LEU:N    | 2.71                     | 0.64              |
| 1:E:995:CYS:SG   | 1:E:996:LEU:N    | 2.71                     | 0.64              |
| 1:G:572:ILE:HG13 | 1:G:573:PHE:H    | 1.62                     | 0.64              |
| 1:I:572:ILE:HG13 | 1:I:573:PHE:H    | 1.62                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:1009:ARG:NH1 | 1:I:1012:LYS:HB2  | 2.12                     | 0.64              |
| 1:K:599:SER:O    | 1:K:603:ARG:NH1   | 2.30                     | 0.64              |
| 1:A:556:VAL:HG11 | 1:A:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:B:228:LYS:HD3  | 1:B:345:THR:HB    | 1.79                     | 0.63              |
| 1:B:913:HIS:CD2  | 1:B:942:MET:HB2   | 2.33                     | 0.63              |
| 1:C:913:HIS:CD2  | 1:C:942:MET:HB2   | 2.33                     | 0.63              |
| 1:G:995:CYS:SG   | 1:G:996:LEU:N     | 2.71                     | 0.63              |
| 1:H:228:LYS:HD3  | 1:H:345:THR:HB    | 1.79                     | 0.63              |
| 1:H:556:VAL:HG11 | 1:H:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:H:913:HIS:CD2  | 1:H:942:MET:HB2   | 2.34                     | 0.63              |
| 1:I:913:HIS:CD2  | 1:I:942:MET:HB2   | 2.34                     | 0.63              |
| 1:L:228:LYS:HD3  | 1:L:345:THR:HB    | 1.79                     | 0.63              |
| 1:L:599:SER:O    | 1:L:603:ARG:NH1   | 2.30                     | 0.63              |
| 1:E:169:LEU:O    | 1:E:199:LEU:N     | 2.31                     | 0.63              |
| 1:I:556:VAL:HG11 | 1:I:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:A:885:LYS:HE3  | 1:A:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:D:996:LEU:HD11 | 1:D:1025:LEU:HD13 | 1.79                     | 0.63              |
| 1:E:839:ALA:O    | 1:E:842:GLN:NE2   | 2.25                     | 0.63              |
| 1:F:839:ALA:O    | 1:F:842:GLN:NE2   | 2.25                     | 0.63              |
| 1:G:913:HIS:CD2  | 1:G:942:MET:HB2   | 2.33                     | 0.63              |
| 1:J:885:LYS:HE3  | 1:J:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:K:885:LYS:HE3  | 1:K:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:B:556:VAL:HG11 | 1:B:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:B:995:CYS:SG   | 1:B:996:LEU:N     | 2.71                     | 0.63              |
| 1:C:885:LYS:HE3  | 1:C:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:E:1009:ARG:NH1 | 1:E:1012:LYS:HB2  | 2.12                     | 0.63              |
| 1:H:885:LYS:HE3  | 1:H:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:I:226:ILE:HG23 | 1:I:408:PRO:HG2   | 1.79                     | 0.63              |
| 1:J:995:CYS:SG   | 1:J:996:LEU:N     | 2.71                     | 0.63              |
| 1:L:885:LYS:HE3  | 1:L:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:A:995:CYS:SG   | 1:A:996:LEU:N     | 2.71                     | 0.63              |
| 1:B:996:LEU:HD11 | 1:B:1025:LEU:HD13 | 1.79                     | 0.63              |
| 1:C:226:ILE:HG23 | 1:C:408:PRO:HG2   | 1.79                     | 0.63              |
| 1:C:228:LYS:HD3  | 1:C:345:THR:HB    | 1.78                     | 0.63              |
| 1:D:913:HIS:CD2  | 1:D:942:MET:HB2   | 2.34                     | 0.63              |
| 1:E:226:ILE:HG23 | 1:E:408:PRO:HG2   | 1.79                     | 0.63              |
| 1:E:228:LYS:HD3  | 1:E:345:THR:HB    | 1.79                     | 0.63              |
| 1:A:913:HIS:CD2  | 1:A:942:MET:HB2   | 2.33                     | 0.63              |
| 1:D:1009:ARG:NH1 | 1:D:1012:LYS:HB2  | 2.12                     | 0.63              |
| 1:E:885:LYS:HE3  | 1:E:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:G:996:LEU:HD11 | 1:G:1025:LEU:HD13 | 1.79                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:556:VAL:HG11 | 1:L:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:B:786:ASP:O    | 1:B:789:SER:OG    | 2.11                     | 0.63              |
| 1:E:913:HIS:CD2  | 1:E:942:MET:HB2   | 2.34                     | 0.63              |
| 1:F:995:CYS:SG   | 1:F:996:LEU:N     | 2.71                     | 0.63              |
| 1:G:556:VAL:HG11 | 1:G:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:K:556:VAL:HG11 | 1:K:605:GLU:HG3   | 1.80                     | 0.63              |
| 1:A:773:TRP:CH2  | 1:L:1013:ARG:HG2  | 2.29                     | 0.63              |
| 1:B:769:ILE:HG22 | 1:B:771:ARG:H     | 1.64                     | 0.63              |
| 1:D:885:LYS:HE3  | 1:D:913:HIS:CE1   | 2.34                     | 0.63              |
| 1:F:226:ILE:HG23 | 1:F:408:PRO:HG2   | 1.79                     | 0.63              |
| 1:H:786:ASP:O    | 1:H:789:SER:OG    | 2.12                     | 0.63              |
| 1:H:917:ARG:HD2  | 1:H:946:ASP:HB2   | 1.81                     | 0.63              |
| 1:I:769:ILE:HG22 | 1:I:771:ARG:H     | 1.64                     | 0.63              |
| 1:L:817:VAL:HG12 | 1:L:820:LYS:HZ3   | 1.64                     | 0.63              |
| 1:L:856:ARG:CD   | 1:L:885:LYS:HB2   | 2.29                     | 0.63              |
| 1:B:169:LEU:O    | 1:B:199:LEU:N     | 2.31                     | 0.63              |
| 1:D:866:ASP:OD1  | 1:D:867:SER:N     | 2.29                     | 0.63              |
| 1:G:1009:ARG:NH1 | 1:G:1012:LYS:HB2  | 2.12                     | 0.63              |
| 1:I:995:CYS:SG   | 1:I:996:LEU:N     | 2.71                     | 0.63              |
| 1:J:913:HIS:CD2  | 1:J:942:MET:HB2   | 2.34                     | 0.63              |
| 1:C:917:ARG:HD2  | 1:C:946:ASP:HB2   | 1.81                     | 0.62              |
| 1:D:226:ILE:HG23 | 1:D:408:PRO:HG2   | 1.79                     | 0.62              |
| 1:D:556:VAL:HG11 | 1:D:605:GLU:HG3   | 1.80                     | 0.62              |
| 1:F:913:HIS:CD2  | 1:F:942:MET:HB2   | 2.34                     | 0.62              |
| 1:G:169:LEU:O    | 1:G:199:LEU:N     | 2.31                     | 0.62              |
| 1:G:885:LYS:HE3  | 1:G:913:HIS:CE1   | 2.34                     | 0.62              |
| 1:K:856:ARG:CD   | 1:K:885:LYS:HB2   | 2.29                     | 0.62              |
| 1:L:169:LEU:O    | 1:L:199:LEU:N     | 2.31                     | 0.62              |
| 1:B:255:ILE:HB   | 1:B:297:MET:HA    | 1.81                     | 0.62              |
| 1:D:769:ILE:HG22 | 1:D:771:ARG:H     | 1.64                     | 0.62              |
| 1:E:917:ARG:HD2  | 1:E:946:ASP:HB2   | 1.81                     | 0.62              |
| 1:F:885:LYS:HE3  | 1:F:913:HIS:CE1   | 2.34                     | 0.62              |
| 1:H:226:ILE:HG23 | 1:H:408:PRO:HG2   | 1.79                     | 0.62              |
| 1:H:995:CYS:SG   | 1:H:996:LEU:N     | 2.71                     | 0.62              |
| 1:I:169:LEU:O    | 1:I:199:LEU:N     | 2.31                     | 0.62              |
| 1:I:255:ILE:HB   | 1:I:297:MET:HA    | 1.81                     | 0.62              |
| 1:K:169:LEU:O    | 1:K:199:LEU:N     | 2.31                     | 0.62              |
| 1:D:169:LEU:O    | 1:D:199:LEU:N     | 2.31                     | 0.62              |
| 1:H:255:ILE:HB   | 1:H:297:MET:HA    | 1.81                     | 0.62              |
| 1:I:996:LEU:HD11 | 1:I:1025:LEU:HD13 | 1.79                     | 0.62              |
| 1:J:917:ARG:HD2  | 1:J:946:ASP:HB2   | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:913:HIS:CD2  | 1:K:942:MET:HB2  | 2.33                     | 0.62              |
| 1:L:913:HIS:CD2  | 1:L:942:MET:HB2  | 2.33                     | 0.62              |
| 1:A:917:ARG:HD2  | 1:A:946:ASP:HB2  | 1.81                     | 0.62              |
| 1:B:885:LYS:HE3  | 1:B:913:HIS:CE1  | 2.34                     | 0.62              |
| 1:C:798:VAL:O    | 1:C:827:GLN:N    | 2.26                     | 0.62              |
| 1:E:255:ILE:HB   | 1:E:297:MET:HA   | 1.81                     | 0.62              |
| 1:F:556:VAL:HG11 | 1:F:605:GLU:HG3  | 1.80                     | 0.62              |
| 1:F:917:ARG:HD2  | 1:F:946:ASP:HB2  | 1.81                     | 0.62              |
| 1:G:255:ILE:HB   | 1:G:297:MET:HA   | 1.81                     | 0.62              |
| 1:G:769:ILE:HG22 | 1:G:771:ARG:H    | 1.64                     | 0.62              |
| 1:I:885:LYS:HE3  | 1:I:913:HIS:CE1  | 2.34                     | 0.62              |
| 1:J:798:VAL:O    | 1:J:827:GLN:N    | 2.26                     | 0.62              |
| 1:J:866:ASP:OD1  | 1:J:867:SER:N    | 2.29                     | 0.62              |
| 1:A:856:ARG:CD   | 1:A:885:LYS:HB2  | 2.29                     | 0.62              |
| 1:C:787:ILE:HA   | 1:C:790:VAL:HG22 | 1.82                     | 0.62              |
| 1:D:255:ILE:HB   | 1:D:297:MET:HA   | 1.81                     | 0.62              |
| 1:D:650:LYS:HG3  | 1:D:676:THR:HB   | 1.82                     | 0.62              |
| 1:F:255:ILE:HB   | 1:F:297:MET:HA   | 1.81                     | 0.62              |
| 1:G:226:ILE:HG23 | 1:G:408:PRO:HG2  | 1.79                     | 0.62              |
| 1:J:856:ARG:CD   | 1:J:885:LYS:HB2  | 2.29                     | 0.62              |
| 1:A:771:ARG:HB2  | 1:A:799:GLU:OE2  | 2.00                     | 0.62              |
| 1:G:650:LYS:HG3  | 1:G:676:THR:HB   | 1.82                     | 0.62              |
| 1:L:255:ILE:HB   | 1:L:297:MET:HA   | 1.81                     | 0.62              |
| 1:A:267:SER:OG   | 1:A:320:LYS:O    | 2.18                     | 0.62              |
| 1:B:267:SER:OG   | 1:B:320:LYS:O    | 2.18                     | 0.62              |
| 1:B:650:LYS:HG3  | 1:B:676:THR:HB   | 1.82                     | 0.62              |
| 1:B:771:ARG:HB2  | 1:B:799:GLU:OE2  | 2.00                     | 0.62              |
| 1:B:866:ASP:OD1  | 1:B:867:SER:N    | 2.29                     | 0.62              |
| 1:H:787:ILE:HA   | 1:H:790:VAL:HG22 | 1.82                     | 0.62              |
| 1:J:771:ARG:HB2  | 1:J:799:GLU:OE2  | 2.00                     | 0.62              |
| 1:K:255:ILE:HB   | 1:K:297:MET:HA   | 1.81                     | 0.62              |
| 1:B:856:ARG:CD   | 1:B:885:LYS:HB2  | 2.29                     | 0.62              |
| 1:E:556:VAL:HG11 | 1:E:605:GLU:HG3  | 1.79                     | 0.62              |
| 1:E:769:ILE:HG22 | 1:E:771:ARG:H    | 1.64                     | 0.62              |
| 1:F:856:ARG:CD   | 1:F:885:LYS:HB2  | 2.29                     | 0.62              |
| 1:I:650:LYS:HG3  | 1:I:676:THR:HB   | 1.82                     | 0.62              |
| 1:I:866:ASP:OD1  | 1:I:867:SER:N    | 2.29                     | 0.62              |
| 1:A:798:VAL:O    | 1:A:827:GLN:N    | 2.26                     | 0.62              |
| 1:C:255:ILE:HB   | 1:C:297:MET:HA   | 1.81                     | 0.62              |
| 1:C:856:ARG:CD   | 1:C:885:LYS:HB2  | 2.29                     | 0.62              |
| 1:E:771:ARG:HB2  | 1:E:799:GLU:OE2  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:856:ARG:CD   | 1:E:885:LYS:HB2   | 2.29                     | 0.62              |
| 1:H:798:VAL:O    | 1:H:827:GLN:N     | 2.26                     | 0.62              |
| 1:I:267:SER:OG   | 1:I:320:LYS:O     | 2.18                     | 0.62              |
| 1:J:267:SER:OG   | 1:J:320:LYS:O     | 2.18                     | 0.62              |
| 1:J:787:ILE:HA   | 1:J:790:VAL:HG22  | 1.82                     | 0.62              |
| 1:K:267:SER:OG   | 1:K:320:LYS:O     | 2.18                     | 0.62              |
| 1:L:267:SER:OG   | 1:L:320:LYS:O     | 2.18                     | 0.62              |
| 1:L:769:ILE:HG22 | 1:L:771:ARG:H     | 1.64                     | 0.62              |
| 1:A:866:ASP:OD1  | 1:A:867:SER:N     | 2.29                     | 0.62              |
| 1:C:267:SER:OG   | 1:C:320:LYS:O     | 2.18                     | 0.62              |
| 1:F:769:ILE:HG22 | 1:F:771:ARG:H     | 1.64                     | 0.62              |
| 1:G:856:ARG:CD   | 1:G:885:LYS:HB2   | 2.29                     | 0.62              |
| 1:I:771:ARG:HB2  | 1:I:799:GLU:OE2   | 2.00                     | 0.62              |
| 1:J:137:ARG:HG3  | 1:J:141:ARG:NH2   | 2.15                     | 0.62              |
| 1:K:769:ILE:HG22 | 1:K:771:ARG:H     | 1.64                     | 0.62              |
| 1:L:866:ASP:OD1  | 1:L:867:SER:N     | 2.29                     | 0.62              |
| 1:A:255:ILE:HB   | 1:A:297:MET:HA    | 1.81                     | 0.61              |
| 1:B:263:ARG:NH2  | 1:B:325:ASP:OD2   | 2.33                     | 0.61              |
| 1:C:531:LEU:HD11 | 1:C:581:LEU:HD13  | 1.82                     | 0.61              |
| 1:E:267:SER:OG   | 1:E:320:LYS:O     | 2.18                     | 0.61              |
| 1:G:267:SER:OG   | 1:G:320:LYS:O     | 2.18                     | 0.61              |
| 1:H:267:SER:OG   | 1:H:320:LYS:O     | 2.18                     | 0.61              |
| 1:I:856:ARG:CD   | 1:I:885:LYS:HB2   | 2.29                     | 0.61              |
| 1:J:255:ILE:HB   | 1:J:297:MET:HA    | 1.81                     | 0.61              |
| 1:K:866:ASP:OD1  | 1:K:867:SER:N     | 2.29                     | 0.61              |
| 1:A:137:ARG:HG3  | 1:A:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:A:970:LYS:HD2  | 1:A:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:B:759:CYS:SG   | 1:B:760:GLU:N     | 2.73                     | 0.61              |
| 1:D:267:SER:OG   | 1:D:320:LYS:O     | 2.18                     | 0.61              |
| 1:D:856:ARG:CD   | 1:D:885:LYS:HB2   | 2.29                     | 0.61              |
| 1:E:650:LYS:HG3  | 1:E:676:THR:HB    | 1.82                     | 0.61              |
| 1:F:970:LYS:HD2  | 1:F:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:H:856:ARG:CD   | 1:H:885:LYS:HB2   | 2.29                     | 0.61              |
| 1:I:263:ARG:NH2  | 1:I:325:ASP:OD2   | 2.33                     | 0.61              |
| 1:I:759:CYS:SG   | 1:I:760:GLU:N     | 2.73                     | 0.61              |
| 1:I:970:LYS:HD2  | 1:I:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:J:769:ILE:HG22 | 1:J:771:ARG:H     | 1.64                     | 0.61              |
| 1:J:970:LYS:HD2  | 1:J:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:K:817:VAL:HG12 | 1:K:820:LYS:HZ3   | 1.65                     | 0.61              |
| 1:L:137:ARG:HG3  | 1:L:141:ARG:NH2   | 2.15                     | 0.61              |
| 1:A:787:ILE:HA   | 1:A:790:VAL:HG22  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:771:ARG:HB2  | 1:D:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:D:917:ARG:HD2  | 1:D:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:E:263:ARG:NH2  | 1:E:325:ASP:OD2   | 2.33                     | 0.61              |
| 1:F:137:ARG:HG3  | 1:F:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:F:267:SER:OG   | 1:F:320:LYS:O     | 2.18                     | 0.61              |
| 1:H:769:ILE:HG22 | 1:H:771:ARG:H     | 1.64                     | 0.61              |
| 1:H:839:ALA:O    | 1:H:842:GLN:NE2   | 2.25                     | 0.61              |
| 1:J:531:LEU:HD11 | 1:J:581:LEU:HD13  | 1.82                     | 0.61              |
| 1:K:137:ARG:HG3  | 1:K:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:K:759:CYS:SG   | 1:K:760:GLU:N     | 2.73                     | 0.61              |
| 1:K:970:LYS:HD2  | 1:K:1001:GLN:HE22 | 1.66                     | 0.61              |
| 1:L:759:CYS:SG   | 1:L:760:GLU:N     | 2.73                     | 0.61              |
| 1:L:970:LYS:HD2  | 1:L:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:A:650:LYS:HG3  | 1:A:676:THR:HB    | 1.82                     | 0.61              |
| 1:B:970:LYS:HD2  | 1:B:1001:GLN:HE22 | 1.66                     | 0.61              |
| 1:C:769:ILE:HG22 | 1:C:771:ARG:H     | 1.64                     | 0.61              |
| 1:C:890:ASN:ND2  | 1:C:918:SER:OG    | 2.34                     | 0.61              |
| 1:C:995:CYS:SG   | 1:C:996:LEU:N     | 2.71                     | 0.61              |
| 1:D:970:LYS:HD2  | 1:D:1001:GLN:HE22 | 1.65                     | 0.61              |
| 1:E:759:CYS:SG   | 1:E:760:GLU:N     | 2.73                     | 0.61              |
| 1:F:263:ARG:NH2  | 1:F:325:ASP:OD2   | 2.33                     | 0.61              |
| 1:F:650:LYS:HG3  | 1:F:676:THR:HB    | 1.82                     | 0.61              |
| 1:H:531:LEU:HD11 | 1:H:581:LEU:HD13  | 1.82                     | 0.61              |
| 1:I:890:ASN:ND2  | 1:I:918:SER:OG    | 2.34                     | 0.61              |
| 1:L:917:ARG:HD2  | 1:L:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:A:531:LEU:HD11 | 1:A:581:LEU:HD13  | 1.82                     | 0.61              |
| 1:A:759:CYS:SG   | 1:A:760:GLU:N     | 2.73                     | 0.61              |
| 1:B:890:ASN:ND2  | 1:B:918:SER:OG    | 2.34                     | 0.61              |
| 1:D:890:ASN:ND2  | 1:D:918:SER:OG    | 2.34                     | 0.61              |
| 1:E:787:ILE:HA   | 1:E:790:VAL:HG22  | 1.82                     | 0.61              |
| 1:F:771:ARG:HB2  | 1:F:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:G:780:SER:OG   | 1:G:781:HIS:N     | 2.34                     | 0.61              |
| 1:G:917:ARG:HD2  | 1:G:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:H:771:ARG:HB2  | 1:H:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:B:917:ARG:HD2  | 1:B:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:D:780:SER:OG   | 1:D:781:HIS:N     | 2.34                     | 0.61              |
| 1:F:759:CYS:SG   | 1:F:760:GLU:N     | 2.73                     | 0.61              |
| 1:F:848:LEU:HD23 | 1:F:875:LYS:HB3   | 1.82                     | 0.61              |
| 1:G:771:ARG:HB2  | 1:G:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:G:890:ASN:ND2  | 1:G:918:SER:OG    | 2.34                     | 0.61              |
| 1:G:970:LYS:HD2  | 1:G:1001:GLN:HE22 | 1.66                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:890:ASN:ND2  | 1:H:918:SER:OG    | 2.34                     | 0.61              |
| 1:J:650:LYS:HG3  | 1:J:676:THR:HB    | 1.82                     | 0.61              |
| 1:A:769:ILE:HG22 | 1:A:771:ARG:H     | 1.64                     | 0.61              |
| 1:A:890:ASN:ND2  | 1:A:918:SER:OG    | 2.34                     | 0.61              |
| 1:D:137:ARG:HG3  | 1:D:141:ARG:NH2   | 2.15                     | 0.61              |
| 1:E:137:ARG:HG3  | 1:E:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:F:734:LEU:HD22 | 1:F:741:THR:HG21  | 1.83                     | 0.61              |
| 1:I:848:LEU:HD23 | 1:I:875:LYS:HB3   | 1.82                     | 0.61              |
| 1:J:759:CYS:SG   | 1:J:760:GLU:N     | 2.74                     | 0.61              |
| 1:K:787:ILE:HA   | 1:K:790:VAL:HG22  | 1.82                     | 0.61              |
| 1:K:917:ARG:HD2  | 1:K:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:L:771:ARG:HB2  | 1:L:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:L:787:ILE:HA   | 1:L:790:VAL:HG22  | 1.82                     | 0.61              |
| 1:D:557:LYS:NZ   | 1:D:605:GLU:OE1   | 2.28                     | 0.61              |
| 1:D:759:CYS:SG   | 1:D:760:GLU:N     | 2.74                     | 0.61              |
| 1:H:137:ARG:HG3  | 1:H:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:I:780:SER:OG   | 1:I:781:HIS:N     | 2.34                     | 0.61              |
| 1:I:917:ARG:HD2  | 1:I:946:ASP:HB2   | 1.81                     | 0.61              |
| 1:J:734:LEU:HD22 | 1:J:741:THR:HG21  | 1.83                     | 0.61              |
| 1:J:890:ASN:ND2  | 1:J:918:SER:OG    | 2.34                     | 0.61              |
| 1:K:771:ARG:HB2  | 1:K:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:A:734:LEU:HD22 | 1:A:741:THR:HG21  | 1.83                     | 0.61              |
| 1:B:780:SER:OG   | 1:B:781:HIS:N     | 2.34                     | 0.61              |
| 1:C:771:ARG:HB2  | 1:C:799:GLU:OE2   | 2.00                     | 0.61              |
| 1:E:734:LEU:HD22 | 1:E:741:THR:HG21  | 1.83                     | 0.61              |
| 1:E:970:LYS:HD2  | 1:E:1001:GLN:HE22 | 1.66                     | 0.61              |
| 1:F:787:ILE:HA   | 1:F:790:VAL:HG22  | 1.82                     | 0.61              |
| 1:H:650:LYS:HG3  | 1:H:676:THR:HB    | 1.82                     | 0.61              |
| 1:A:785:PHE:HB3  | 1:B:810:PHE:CZ    | 2.32                     | 0.61              |
| 1:B:848:LEU:HD23 | 1:B:875:LYS:HB3   | 1.82                     | 0.61              |
| 1:B:1013:ARG:HG2 | 1:C:773:TRP:CH2   | 2.36                     | 0.61              |
| 1:D:471:ASP:HA   | 1:D:474:TRP:HB3   | 1.83                     | 0.61              |
| 1:G:137:ARG:HG3  | 1:G:141:ARG:NH2   | 2.16                     | 0.61              |
| 1:G:471:ASP:HA   | 1:G:474:TRP:HB3   | 1.83                     | 0.61              |
| 1:I:531:LEU:HD11 | 1:I:581:LEU:HD13  | 1.82                     | 0.61              |
| 1:L:890:ASN:ND2  | 1:L:918:SER:OG    | 2.34                     | 0.61              |
| 1:C:759:CYS:SG   | 1:C:760:GLU:N     | 2.73                     | 0.60              |
| 1:D:848:LEU:HD23 | 1:D:875:LYS:HB3   | 1.82                     | 0.60              |
| 1:E:848:LEU:HD23 | 1:E:875:LYS:HB3   | 1.82                     | 0.60              |
| 1:G:759:CYS:SG   | 1:G:760:GLU:N     | 2.73                     | 0.60              |
| 1:H:970:LYS:HD2  | 1:H:1001:GLN:HE22 | 1.65                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:417:GLY:HA3  | 1:J:442:PHE:CE2  | 2.36                     | 0.60              |
| 1:K:890:ASN:ND2  | 1:K:918:SER:OG   | 2.34                     | 0.60              |
| 1:B:531:LEU:HD11 | 1:B:581:LEU:HD13 | 1.82                     | 0.60              |
| 1:D:787:ILE:HA   | 1:D:790:VAL:HG22 | 1.82                     | 0.60              |
| 1:E:531:LEU:HD11 | 1:E:581:LEU:HD13 | 1.82                     | 0.60              |
| 1:F:486:ARG:HD3  | 1:F:495:VAL:HG21 | 1.83                     | 0.60              |
| 1:F:890:ASN:ND2  | 1:F:918:SER:OG   | 2.34                     | 0.60              |
| 1:G:787:ILE:HA   | 1:G:790:VAL:HG22 | 1.82                     | 0.60              |
| 1:A:471:ASP:HA   | 1:A:474:TRP:HB3  | 1.83                     | 0.60              |
| 1:B:137:ARG:HG3  | 1:B:141:ARG:NH2  | 2.15                     | 0.60              |
| 1:C:572:ILE:HG13 | 1:C:573:PHE:N    | 2.16                     | 0.60              |
| 1:E:798:VAL:O    | 1:E:827:GLN:N    | 2.26                     | 0.60              |
| 1:L:531:LEU:HD11 | 1:L:581:LEU:HD13 | 1.82                     | 0.60              |
| 1:A:817:VAL:HG12 | 1:A:820:LYS:HZ3  | 1.65                     | 0.60              |
| 1:A:848:LEU:HD23 | 1:A:875:LYS:HB3  | 1.82                     | 0.60              |
| 1:F:531:LEU:HD11 | 1:F:581:LEU:HD13 | 1.82                     | 0.60              |
| 1:F:780:SER:OG   | 1:F:781:HIS:N    | 2.34                     | 0.60              |
| 1:G:848:LEU:HD23 | 1:G:875:LYS:HB3  | 1.82                     | 0.60              |
| 1:J:471:ASP:HA   | 1:J:474:TRP:HB3  | 1.83                     | 0.60              |
| 1:J:848:LEU:HD23 | 1:J:875:LYS:HB3  | 1.82                     | 0.60              |
| 1:A:263:ARG:NH2  | 1:A:325:ASP:OD2  | 2.33                     | 0.60              |
| 1:A:417:GLY:HA3  | 1:A:442:PHE:CE2  | 2.36                     | 0.60              |
| 1:C:137:ARG:HG3  | 1:C:141:ARG:NH2  | 2.16                     | 0.60              |
| 1:C:650:LYS:HG3  | 1:C:676:THR:HB   | 1.82                     | 0.60              |
| 1:D:486:ARG:HD3  | 1:D:495:VAL:HG21 | 1.83                     | 0.60              |
| 1:E:417:GLY:HA3  | 1:E:442:PHE:CE2  | 2.36                     | 0.60              |
| 1:E:486:ARG:HD3  | 1:E:495:VAL:HG21 | 1.83                     | 0.60              |
| 1:E:890:ASN:ND2  | 1:E:918:SER:OG   | 2.34                     | 0.60              |
| 1:I:137:ARG:HG3  | 1:I:141:ARG:NH2  | 2.15                     | 0.60              |
| 1:K:848:LEU:HD23 | 1:K:875:LYS:HB3  | 1.82                     | 0.60              |
| 1:L:734:LEU:HD22 | 1:L:741:THR:HG21 | 1.83                     | 0.60              |
| 1:B:787:ILE:HA   | 1:B:790:VAL:HG22 | 1.82                     | 0.60              |
| 1:C:471:ASP:HA   | 1:C:474:TRP:HB3  | 1.83                     | 0.60              |
| 1:F:417:GLY:HA3  | 1:F:442:PHE:CE2  | 2.36                     | 0.60              |
| 1:H:471:ASP:HA   | 1:H:474:TRP:HB3  | 1.83                     | 0.60              |
| 1:H:759:CYS:SG   | 1:H:760:GLU:N    | 2.73                     | 0.60              |
| 1:I:787:ILE:HA   | 1:I:790:VAL:HG22 | 1.82                     | 0.60              |
| 1:K:531:LEU:HD11 | 1:K:581:LEU:HD13 | 1.82                     | 0.60              |
| 1:K:734:LEU:HD22 | 1:K:741:THR:HG21 | 1.83                     | 0.60              |
| 1:E:780:SER:OG   | 1:E:781:HIS:N    | 2.34                     | 0.60              |
| 1:G:417:GLY:HA3  | 1:G:442:PHE:CE2  | 2.36                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:486:ARG:HD3  | 1:G:495:VAL:HG21  | 1.83                     | 0.60              |
| 1:H:486:ARG:HD3  | 1:H:495:VAL:HG21  | 1.83                     | 0.60              |
| 1:H:572:ILE:HG13 | 1:H:573:PHE:N     | 2.16                     | 0.60              |
| 1:K:650:LYS:HG3  | 1:K:676:THR:HB    | 1.82                     | 0.60              |
| 1:L:650:LYS:HG3  | 1:L:676:THR:HB    | 1.82                     | 0.60              |
| 1:C:417:GLY:HA3  | 1:C:442:PHE:CE2   | 2.36                     | 0.60              |
| 1:C:486:ARG:HD3  | 1:C:495:VAL:HG21  | 1.83                     | 0.60              |
| 1:E:572:ILE:HG13 | 1:E:573:PHE:N     | 2.16                     | 0.60              |
| 1:F:798:VAL:O    | 1:F:827:GLN:N     | 2.26                     | 0.60              |
| 1:I:417:GLY:HA3  | 1:I:442:PHE:CE2   | 2.36                     | 0.60              |
| 1:L:848:LEU:HD23 | 1:L:875:LYS:HB3   | 1.82                     | 0.60              |
| 1:B:417:GLY:HA3  | 1:B:442:PHE:CE2   | 2.36                     | 0.60              |
| 1:C:848:LEU:HD23 | 1:C:875:LYS:HB3   | 1.82                     | 0.60              |
| 1:C:970:LYS:HD2  | 1:C:1001:GLN:HE22 | 1.66                     | 0.60              |
| 1:F:572:ILE:HG13 | 1:F:573:PHE:N     | 2.16                     | 0.60              |
| 1:G:572:ILE:HG13 | 1:G:573:PHE:N     | 2.16                     | 0.60              |
| 1:J:263:ARG:NH2  | 1:J:325:ASP:OD2   | 2.33                     | 0.60              |
| 1:K:780:SER:OG   | 1:K:781:HIS:N     | 2.34                     | 0.60              |
| 1:L:780:SER:OG   | 1:L:781:HIS:N     | 2.34                     | 0.60              |
| 1:B:471:ASP:HA   | 1:B:474:TRP:HB3   | 1.83                     | 0.60              |
| 1:D:417:GLY:HA3  | 1:D:442:PHE:CE2   | 2.36                     | 0.60              |
| 1:D:734:LEU:HD22 | 1:D:741:THR:HG21  | 1.83                     | 0.60              |
| 1:I:471:ASP:HA   | 1:I:474:TRP:HB3   | 1.83                     | 0.60              |
| 1:K:417:GLY:HA3  | 1:K:442:PHE:CE2   | 2.36                     | 0.60              |
| 1:L:572:ILE:HG13 | 1:L:573:PHE:N     | 2.16                     | 0.60              |
| 1:B:734:LEU:HD22 | 1:B:741:THR:HG21  | 1.83                     | 0.59              |
| 1:C:134:LYS:HA   | 1:C:137:ARG:HG2   | 1.84                     | 0.59              |
| 1:D:572:ILE:HG13 | 1:D:573:PHE:N     | 2.16                     | 0.59              |
| 1:E:471:ASP:HA   | 1:E:474:TRP:HB3   | 1.83                     | 0.59              |
| 1:I:486:ARG:HD3  | 1:I:495:VAL:HG21  | 1.83                     | 0.59              |
| 1:I:734:LEU:HD22 | 1:I:741:THR:HG21  | 1.83                     | 0.59              |
| 1:I:1008:ASN:ND2 | 1:I:1010:GLU:OE2  | 2.35                     | 0.59              |
| 1:J:572:ILE:HG13 | 1:J:573:PHE:N     | 2.16                     | 0.59              |
| 1:J:817:VAL:HG12 | 1:J:820:LYS:HZ3   | 1.66                     | 0.59              |
| 1:B:1008:ASN:ND2 | 1:B:1010:GLU:OE2  | 2.35                     | 0.59              |
| 1:E:145:TYR:O    | 1:E:159:ASP:N     | 2.36                     | 0.59              |
| 1:G:263:ARG:NH2  | 1:G:325:ASP:OD2   | 2.33                     | 0.59              |
| 1:H:134:LYS:HA   | 1:H:137:ARG:HG2   | 1.84                     | 0.59              |
| 1:H:145:TYR:O    | 1:H:159:ASP:N     | 2.36                     | 0.59              |
| 1:I:572:ILE:HG13 | 1:I:573:PHE:N     | 2.16                     | 0.59              |
| 1:J:780:SER:OG   | 1:J:781:HIS:N     | 2.34                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:572:ILE:HG13 | 1:K:573:PHE:N    | 2.16                     | 0.59              |
| 1:L:145:TYR:O    | 1:L:159:ASP:N    | 2.36                     | 0.59              |
| 1:L:417:GLY:HA3  | 1:L:442:PHE:CE2  | 2.36                     | 0.59              |
| 1:B:486:ARG:HD3  | 1:B:495:VAL:HG21 | 1.83                     | 0.59              |
| 1:B:572:ILE:HG13 | 1:B:573:PHE:N    | 2.16                     | 0.59              |
| 1:C:145:TYR:O    | 1:C:159:ASP:N    | 2.36                     | 0.59              |
| 1:C:734:LEU:HD22 | 1:C:741:THR:HG21 | 1.83                     | 0.59              |
| 1:G:734:LEU:HD22 | 1:G:741:THR:HG21 | 1.83                     | 0.59              |
| 1:H:417:GLY:HA3  | 1:H:442:PHE:CE2  | 2.36                     | 0.59              |
| 1:J:789:SER:O    | 1:J:792:SER:OG   | 2.19                     | 0.59              |
| 1:K:145:TYR:O    | 1:K:159:ASP:N    | 2.36                     | 0.59              |
| 1:A:145:TYR:O    | 1:A:159:ASP:N    | 2.36                     | 0.59              |
| 1:A:572:ILE:HG13 | 1:A:573:PHE:N    | 2.16                     | 0.59              |
| 1:A:789:SER:O    | 1:A:792:SER:OG   | 2.19                     | 0.59              |
| 1:D:940:LEU:HD21 | 1:D:943:LEU:HD13 | 1.85                     | 0.59              |
| 1:E:976:ASN:HB3  | 1:E:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:F:145:TYR:O    | 1:F:159:ASP:N    | 2.36                     | 0.59              |
| 1:F:471:ASP:HA   | 1:F:474:TRP:HB3  | 1.83                     | 0.59              |
| 1:G:531:LEU:HD11 | 1:G:581:LEU:HD13 | 1.82                     | 0.59              |
| 1:H:848:LEU:HD23 | 1:H:875:LYS:HB3  | 1.82                     | 0.59              |
| 1:J:145:TYR:O    | 1:J:159:ASP:N    | 2.36                     | 0.59              |
| 1:J:976:ASN:HB3  | 1:J:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:486:ARG:HD3  | 1:A:495:VAL:HG21 | 1.83                     | 0.59              |
| 1:B:145:TYR:O    | 1:B:159:ASP:N    | 2.35                     | 0.59              |
| 1:B:413:ILE:HG12 | 1:B:442:PHE:CD1  | 2.38                     | 0.59              |
| 1:G:940:LEU:HD21 | 1:G:943:LEU:HD13 | 1.85                     | 0.59              |
| 1:I:413:ILE:HG12 | 1:I:442:PHE:CD1  | 2.38                     | 0.59              |
| 1:L:263:ARG:NH2  | 1:L:325:ASP:OD2  | 2.33                     | 0.59              |
| 1:A:134:LYS:HA   | 1:A:137:ARG:HG2  | 1.84                     | 0.59              |
| 1:A:780:SER:OG   | 1:A:781:HIS:N    | 2.34                     | 0.59              |
| 1:A:976:ASN:HB3  | 1:A:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:C:131:ASP:N    | 1:C:134:LYS:HZ3  | 2.00                     | 0.59              |
| 1:C:263:ARG:NH2  | 1:C:325:ASP:OD2  | 2.33                     | 0.59              |
| 1:D:263:ARG:NH2  | 1:D:325:ASP:OD2  | 2.33                     | 0.59              |
| 1:G:413:ILE:HG12 | 1:G:442:PHE:CD1  | 2.38                     | 0.59              |
| 1:H:1013:ARG:HG2 | 1:I:773:TRP:HH2  | 1.67                     | 0.59              |
| 1:I:145:TYR:O    | 1:I:159:ASP:N    | 2.36                     | 0.59              |
| 1:J:134:LYS:HA   | 1:J:137:ARG:HG2  | 1.84                     | 0.59              |
| 1:J:486:ARG:HD3  | 1:J:495:VAL:HG21 | 1.83                     | 0.59              |
| 1:L:471:ASP:HA   | 1:L:474:TRP:HB3  | 1.83                     | 0.59              |
| 1:D:413:ILE:HG12 | 1:D:442:PHE:CD1  | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:976:ASN:HB3  | 1:F:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:H:734:LEU:HD22 | 1:H:741:THR:HG21 | 1.83                     | 0.59              |
| 1:K:263:ARG:NH2  | 1:K:325:ASP:OD2  | 2.33                     | 0.59              |
| 1:K:471:ASP:HA   | 1:K:474:TRP:HB3  | 1.83                     | 0.59              |
| 1:A:940:LEU:HD21 | 1:A:943:LEU:HD13 | 1.85                     | 0.59              |
| 1:D:131:ASP:N    | 1:D:134:LYS:HZ3  | 2.01                     | 0.59              |
| 1:D:531:LEU:HD11 | 1:D:581:LEU:HD13 | 1.82                     | 0.59              |
| 1:I:400:VAL:HG13 | 1:I:401:LEU:HD23 | 1.84                     | 0.59              |
| 1:K:413:ILE:HG12 | 1:K:442:PHE:CD1  | 2.38                     | 0.59              |
| 1:A:131:ASP:N    | 1:A:134:LYS:HZ3  | 2.01                     | 0.59              |
| 1:D:145:TYR:O    | 1:D:159:ASP:N    | 2.36                     | 0.59              |
| 1:F:388:ALA:HB3  | 1:F:389:ARG:HH11 | 1.68                     | 0.59              |
| 1:G:145:TYR:O    | 1:G:159:ASP:N    | 2.36                     | 0.59              |
| 1:G:1008:ASN:ND2 | 1:G:1010:GLU:OE2 | 2.35                     | 0.59              |
| 1:I:940:LEU:HD21 | 1:I:943:LEU:HD13 | 1.85                     | 0.59              |
| 1:J:131:ASP:N    | 1:J:134:LYS:HZ3  | 2.00                     | 0.59              |
| 1:L:976:ASN:HB3  | 1:L:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:1008:ASN:ND2 | 1:A:1010:GLU:OE2 | 2.35                     | 0.59              |
| 1:C:413:ILE:HG12 | 1:C:442:PHE:CD1  | 2.38                     | 0.59              |
| 1:D:1008:ASN:ND2 | 1:D:1010:GLU:OE2 | 2.35                     | 0.59              |
| 1:I:134:LYS:HA   | 1:I:137:ARG:HG2  | 1.84                     | 0.59              |
| 1:J:400:VAL:HG13 | 1:J:401:LEU:HD23 | 1.84                     | 0.59              |
| 1:K:976:ASN:HB3  | 1:K:978:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:400:VAL:HG13 | 1:A:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:B:940:LEU:HD21 | 1:B:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:G:131:ASP:N    | 1:G:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:H:388:ALA:HB3  | 1:H:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:J:940:LEU:HD21 | 1:J:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:J:1008:ASN:ND2 | 1:J:1010:GLU:OE2 | 2.36                     | 0.58              |
| 1:L:413:ILE:HG12 | 1:L:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:B:331:LEU:HA   | 1:B:334:LYS:HE2  | 1.85                     | 0.58              |
| 1:B:400:VAL:HG13 | 1:B:401:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:388:ALA:HB3  | 1:C:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:E:134:LYS:HA   | 1:E:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:E:413:ILE:HG12 | 1:E:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:E:1008:ASN:ND2 | 1:E:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:H:131:ASP:N    | 1:H:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:I:131:ASP:N    | 1:I:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:I:331:LEU:HA   | 1:I:334:LYS:HE2  | 1.86                     | 0.58              |
| 1:K:1008:ASN:ND2 | 1:K:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:B:131:ASP:N    | 1:B:134:LYS:HZ3  | 2.01                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:134:LYS:HA   | 1:D:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:D:400:VAL:HG13 | 1:D:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:D:976:ASN:HB3  | 1:D:978:LEU:HD21 | 1.85                     | 0.58              |
| 1:E:388:ALA:HB3  | 1:E:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:E:400:VAL:HG13 | 1:E:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:F:134:LYS:HA   | 1:F:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:G:134:LYS:HA   | 1:G:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:G:400:VAL:HG13 | 1:G:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:H:400:VAL:HG13 | 1:H:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:I:976:ASN:HB3  | 1:I:978:LEU:HD21 | 1.85                     | 0.58              |
| 1:L:486:ARG:HD3  | 1:L:495:VAL:HG21 | 1.83                     | 0.58              |
| 1:B:976:ASN:HB3  | 1:B:978:LEU:HD21 | 1.85                     | 0.58              |
| 1:C:400:VAL:HG13 | 1:C:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:F:1008:ASN:ND2 | 1:F:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:H:263:ARG:NH2  | 1:H:325:ASP:OD2  | 2.33                     | 0.58              |
| 1:H:1008:ASN:ND2 | 1:H:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:J:413:ILE:HG12 | 1:J:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:L:134:LYS:HA   | 1:L:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:L:1008:ASN:ND2 | 1:L:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:A:413:ILE:HG12 | 1:A:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:B:134:LYS:HA   | 1:B:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:C:1008:ASN:O   | 1:C:1011:THR:OG1 | 2.21                     | 0.58              |
| 1:H:413:ILE:HG12 | 1:H:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:K:486:ARG:HD3  | 1:K:495:VAL:HG21 | 1.83                     | 0.58              |
| 1:L:131:ASP:N    | 1:L:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:A:331:LEU:HA   | 1:A:334:LYS:HE2  | 1.86                     | 0.58              |
| 1:B:557:LYS:NZ   | 1:B:605:GLU:OE1  | 2.28                     | 0.58              |
| 1:C:1008:ASN:ND2 | 1:C:1010:GLU:OE2 | 2.35                     | 0.58              |
| 1:E:940:LEU:HD21 | 1:E:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:G:976:ASN:HB3  | 1:G:978:LEU:HD21 | 1.85                     | 0.58              |
| 1:H:940:LEU:HD21 | 1:H:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:K:134:LYS:HA   | 1:K:137:ARG:HG2  | 1.84                     | 0.58              |
| 1:K:331:LEU:HA   | 1:K:334:LYS:HE2  | 1.86                     | 0.58              |
| 1:K:810:PHE:CD1  | 1:K:813:ARG:HD3  | 2.39                     | 0.58              |
| 1:L:331:LEU:HA   | 1:L:334:LYS:HE2  | 1.86                     | 0.58              |
| 1:L:940:LEU:HD21 | 1:L:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:F:131:ASP:N    | 1:F:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:F:400:VAL:HG13 | 1:F:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:F:413:ILE:HG12 | 1:F:442:PHE:CD1  | 2.38                     | 0.58              |
| 1:J:331:LEU:HA   | 1:J:334:LYS:HE2  | 1.86                     | 0.58              |
| 1:K:131:ASP:N    | 1:K:134:LYS:HZ3  | 2.01                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:940:LEU:HD21 | 1:K:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:L:810:PHE:CD1  | 1:L:813:ARG:HD3  | 2.39                     | 0.58              |
| 1:D:388:ALA:HB3  | 1:D:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:E:137:ARG:HG3  | 1:E:141:ARG:HH22 | 1.69                     | 0.58              |
| 1:G:331:LEU:HA   | 1:G:334:LYS:HE2  | 1.85                     | 0.58              |
| 1:K:400:VAL:HG13 | 1:K:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:C:885:LYS:HG2  | 1:C:913:HIS:HB2  | 1.86                     | 0.58              |
| 1:D:331:LEU:HA   | 1:D:334:LYS:HE2  | 1.85                     | 0.58              |
| 1:F:137:ARG:HG3  | 1:F:141:ARG:HH22 | 1.69                     | 0.58              |
| 1:F:789:SER:O    | 1:F:792:SER:OG   | 2.19                     | 0.58              |
| 1:G:388:ALA:HB3  | 1:G:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:L:400:VAL:HG13 | 1:L:401:LEU:HD23 | 1.84                     | 0.58              |
| 1:B:810:PHE:CD1  | 1:B:813:ARG:HD3  | 2.39                     | 0.58              |
| 1:E:131:ASP:N    | 1:E:134:LYS:HZ3  | 2.01                     | 0.58              |
| 1:F:940:LEU:HD21 | 1:F:943:LEU:HD13 | 1.85                     | 0.58              |
| 1:H:976:ASN:HB3  | 1:H:978:LEU:HD21 | 1.85                     | 0.58              |
| 1:H:1008:ASN:O   | 1:H:1011:THR:OG1 | 2.21                     | 0.58              |
| 1:I:810:PHE:CD1  | 1:I:813:ARG:HD3  | 2.39                     | 0.58              |
| 1:L:388:ALA:HB3  | 1:L:389:ARG:HH11 | 1.68                     | 0.58              |
| 1:B:388:ALA:HB3  | 1:B:389:ARG:HH11 | 1.68                     | 0.57              |
| 1:C:940:LEU:HD21 | 1:C:943:LEU:HD13 | 1.85                     | 0.57              |
| 1:C:976:ASN:HB3  | 1:C:978:LEU:HD21 | 1.85                     | 0.57              |
| 1:H:557:LYS:NZ   | 1:H:605:GLU:OE1  | 2.28                     | 0.57              |
| 1:H:810:PHE:CD1  | 1:H:813:ARG:HD3  | 2.39                     | 0.57              |
| 1:H:885:LYS:HG2  | 1:H:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:H:906:LYS:HG3  | 1:H:907:THR:HG23 | 1.87                     | 0.57              |
| 1:J:400:VAL:HG22 | 1:J:401:LEU:H    | 1.69                     | 0.57              |
| 1:J:885:LYS:HG2  | 1:J:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:K:388:ALA:HB3  | 1:K:389:ARG:HH11 | 1.68                     | 0.57              |
| 1:A:885:LYS:HG2  | 1:A:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:I:388:ALA:HB3  | 1:I:389:ARG:HH11 | 1.68                     | 0.57              |
| 1:I:630:TYR:OH   | 1:I:660:ASP:OD1  | 2.12                     | 0.57              |
| 1:A:400:VAL:HG22 | 1:A:401:LEU:H    | 1.69                     | 0.57              |
| 1:A:810:PHE:CD1  | 1:A:813:ARG:HD3  | 2.39                     | 0.57              |
| 1:C:331:LEU:HA   | 1:C:334:LYS:HE2  | 1.85                     | 0.57              |
| 1:C:817:VAL:HG12 | 1:C:820:LYS:HZ3  | 1.69                     | 0.57              |
| 1:H:331:LEU:HA   | 1:H:334:LYS:HE2  | 1.85                     | 0.57              |
| 1:C:779:LEU:HB3  | 1:C:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:C:810:PHE:CD1  | 1:C:813:ARG:HD3  | 2.39                     | 0.57              |
| 1:D:137:ARG:HG3  | 1:D:141:ARG:HH22 | 1.69                     | 0.57              |
| 1:E:307:PHE:HD2  | 1:E:567:GLU:HB2  | 1.69                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:137:ARG:HG3  | 1:G:141:ARG:HH22 | 1.69                     | 0.57              |
| 1:H:400:VAL:HG22 | 1:H:401:LEU:H    | 1.69                     | 0.57              |
| 1:H:630:TYR:OH   | 1:H:660:ASP:OD1  | 2.12                     | 0.57              |
| 1:I:906:LYS:HG3  | 1:I:907:THR:HG23 | 1.87                     | 0.57              |
| 1:J:810:PHE:CD1  | 1:J:813:ARG:HD3  | 2.39                     | 0.57              |
| 1:C:906:LYS:HG3  | 1:C:907:THR:HG23 | 1.87                     | 0.57              |
| 1:E:810:PHE:CD1  | 1:E:813:ARG:HD3  | 2.39                     | 0.57              |
| 1:H:779:LEU:HB3  | 1:H:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:B:906:LYS:HG3  | 1:B:907:THR:HG23 | 1.87                     | 0.57              |
| 1:C:608:LYS:HA   | 1:C:611:GLU:CD   | 2.25                     | 0.57              |
| 1:D:779:LEU:HB3  | 1:D:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:E:779:LEU:HB3  | 1:E:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:F:307:PHE:HD2  | 1:F:567:GLU:HB2  | 1.70                     | 0.57              |
| 1:G:906:LYS:HG3  | 1:G:907:THR:HG23 | 1.87                     | 0.57              |
| 1:I:779:LEU:HB3  | 1:I:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:L:137:ARG:HG3  | 1:L:141:ARG:HH22 | 1.69                     | 0.57              |
| 1:C:810:PHE:HZ   | 1:D:785:PHE:CB   | 2.12                     | 0.57              |
| 1:D:307:PHE:HD2  | 1:D:567:GLU:HB2  | 1.69                     | 0.57              |
| 1:E:608:LYS:HA   | 1:E:611:GLU:CD   | 2.25                     | 0.57              |
| 1:E:789:SER:O    | 1:E:792:SER:OG   | 2.19                     | 0.57              |
| 1:F:400:VAL:HG22 | 1:F:401:LEU:H    | 1.69                     | 0.57              |
| 1:F:608:LYS:HA   | 1:F:611:GLU:CD   | 2.25                     | 0.57              |
| 1:F:779:LEU:HB3  | 1:F:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:G:779:LEU:HB3  | 1:G:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:G:885:LYS:HG2  | 1:G:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:H:608:LYS:HA   | 1:H:611:GLU:CD   | 2.25                     | 0.57              |
| 1:K:137:ARG:HG3  | 1:K:141:ARG:HH22 | 1.69                     | 0.57              |
| 1:K:608:LYS:HA   | 1:K:611:GLU:CD   | 2.25                     | 0.57              |
| 1:L:608:LYS:HA   | 1:L:611:GLU:CD   | 2.25                     | 0.57              |
| 1:L:885:LYS:HG2  | 1:L:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:A:608:LYS:HA   | 1:A:611:GLU:CD   | 2.25                     | 0.57              |
| 1:B:779:LEU:HB3  | 1:B:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:C:134:LYS:HG3  | 1:C:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:C:780:SER:OG   | 1:C:781:HIS:N    | 2.34                     | 0.57              |
| 1:D:885:LYS:HG2  | 1:D:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:D:906:LYS:HG3  | 1:D:907:THR:HG23 | 1.87                     | 0.57              |
| 1:E:403:THR:HG21 | 1:E:662:VAL:HG11 | 1.87                     | 0.57              |
| 1:F:403:THR:HG21 | 1:F:662:VAL:HG11 | 1.87                     | 0.57              |
| 1:H:134:LYS:HG3  | 1:H:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:H:307:PHE:HD2  | 1:H:567:GLU:HB2  | 1.70                     | 0.57              |
| 1:J:608:LYS:HA   | 1:J:611:GLU:CD   | 2.25                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:1008:ASN:O   | 1:J:1011:THR:OG1 | 2.21                     | 0.57              |
| 1:A:779:LEU:HB3  | 1:A:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:C:400:VAL:HG22 | 1:C:401:LEU:H    | 1.69                     | 0.57              |
| 1:E:885:LYS:HG2  | 1:E:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:F:331:LEU:HA   | 1:F:334:LYS:HE2  | 1.85                     | 0.57              |
| 1:G:307:PHE:HD2  | 1:G:567:GLU:HB2  | 1.69                     | 0.57              |
| 1:H:403:THR:HG21 | 1:H:662:VAL:HG11 | 1.87                     | 0.57              |
| 1:H:780:SER:OG   | 1:H:781:HIS:N    | 2.34                     | 0.57              |
| 1:J:307:PHE:HD2  | 1:J:567:GLU:HB2  | 1.69                     | 0.57              |
| 1:J:779:LEU:HB3  | 1:J:805:ASN:HB2  | 1.87                     | 0.57              |
| 1:L:1008:ASN:O   | 1:L:1011:THR:OG1 | 2.21                     | 0.57              |
| 1:A:134:LYS:HG3  | 1:A:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:A:388:ALA:HB3  | 1:A:389:ARG:HH11 | 1.68                     | 0.57              |
| 1:B:134:LYS:HG3  | 1:B:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:G:134:LYS:HG3  | 1:G:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:K:134:LYS:HG3  | 1:K:137:ARG:HH21 | 1.70                     | 0.57              |
| 1:K:885:LYS:HG2  | 1:K:913:HIS:HB2  | 1.86                     | 0.57              |
| 1:K:1008:ASN:O   | 1:K:1011:THR:OG1 | 2.21                     | 0.57              |
| 1:A:906:LYS:HG3  | 1:A:907:THR:HG23 | 1.87                     | 0.56              |
| 1:B:608:LYS:HA   | 1:B:611:GLU:CD   | 2.25                     | 0.56              |
| 1:D:134:LYS:HG3  | 1:D:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:D:400:VAL:HG22 | 1:D:401:LEU:H    | 1.69                     | 0.56              |
| 1:D:810:PHE:CD1  | 1:D:813:ARG:HD3  | 2.39                     | 0.56              |
| 1:E:134:LYS:HG3  | 1:E:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:E:331:LEU:HA   | 1:E:334:LYS:HE2  | 1.85                     | 0.56              |
| 1:E:400:VAL:HG22 | 1:E:401:LEU:H    | 1.69                     | 0.56              |
| 1:F:810:PHE:CD1  | 1:F:813:ARG:HD3  | 2.39                     | 0.56              |
| 1:G:810:PHE:CD1  | 1:G:813:ARG:HD3  | 2.39                     | 0.56              |
| 1:H:817:VAL:HG12 | 1:H:820:LYS:HZ3  | 1.70                     | 0.56              |
| 1:J:134:LYS:HG3  | 1:J:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:J:388:ALA:HB3  | 1:J:389:ARG:HH11 | 1.68                     | 0.56              |
| 1:L:134:LYS:HG3  | 1:L:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:307:PHE:HD2  | 1:A:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:A:1008:ASN:O   | 1:A:1011:THR:OG1 | 2.21                     | 0.56              |
| 1:C:307:PHE:HD2  | 1:C:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:C:403:THR:HG21 | 1:C:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:D:817:VAL:HG12 | 1:D:820:LYS:HZ3  | 1.69                     | 0.56              |
| 1:F:885:LYS:HG2  | 1:F:913:HIS:HB2  | 1.86                     | 0.56              |
| 1:F:906:LYS:HG3  | 1:F:907:THR:HG23 | 1.87                     | 0.56              |
| 1:I:134:LYS:HG3  | 1:I:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:557:LYS:NZ   | 1:A:605:GLU:OE1  | 2.28                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:768:ASN:H    | 1:A:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:B:307:PHE:HD2  | 1:B:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:B:768:ASN:H    | 1:B:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:C:941:GLN:OE1  | 1:C:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:D:608:LYS:HA   | 1:D:611:GLU:CD   | 2.25                     | 0.56              |
| 1:E:1008:ASN:O   | 1:E:1011:THR:OG1 | 2.21                     | 0.56              |
| 1:F:134:LYS:HG3  | 1:F:137:ARG:HH21 | 1.70                     | 0.56              |
| 1:G:400:VAL:HG22 | 1:G:401:LEU:H    | 1.69                     | 0.56              |
| 1:G:817:VAL:HG12 | 1:G:820:LYS:HZ3  | 1.69                     | 0.56              |
| 1:I:294:LEU:HD12 | 1:I:295:PHE:H    | 1.70                     | 0.56              |
| 1:I:307:PHE:HD2  | 1:I:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:I:608:LYS:HA   | 1:I:611:GLU:CD   | 2.25                     | 0.56              |
| 1:I:768:ASN:H    | 1:I:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:J:906:LYS:HG3  | 1:J:907:THR:HG23 | 1.87                     | 0.56              |
| 1:L:400:VAL:HG22 | 1:L:401:LEU:H    | 1.69                     | 0.56              |
| 1:L:779:LEU:HB3  | 1:L:805:ASN:HB2  | 1.87                     | 0.56              |
| 1:B:137:ARG:HG3  | 1:B:141:ARG:HH22 | 1.69                     | 0.56              |
| 1:B:294:LEU:HD12 | 1:B:295:PHE:H    | 1.70                     | 0.56              |
| 1:D:768:ASN:H    | 1:D:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:E:256:HIS:CD2  | 1:E:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:E:407:ILE:HG23 | 1:E:410:VAL:HB   | 1.87                     | 0.56              |
| 1:F:256:HIS:CD2  | 1:F:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:F:1008:ASN:O   | 1:F:1011:THR:OG1 | 2.21                     | 0.56              |
| 1:G:608:LYS:HA   | 1:G:611:GLU:CD   | 2.25                     | 0.56              |
| 1:G:768:ASN:H    | 1:G:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:H:789:SER:O    | 1:H:792:SER:OG   | 2.19                     | 0.56              |
| 1:I:137:ARG:HG3  | 1:I:141:ARG:HH22 | 1.69                     | 0.56              |
| 1:I:885:LYS:HG2  | 1:I:913:HIS:HB2  | 1.86                     | 0.56              |
| 1:J:137:ARG:HG3  | 1:J:141:ARG:HH22 | 1.69                     | 0.56              |
| 1:J:557:LYS:NZ   | 1:J:605:GLU:OE1  | 2.28                     | 0.56              |
| 1:K:779:LEU:HB3  | 1:K:805:ASN:HB2  | 1.87                     | 0.56              |
| 1:A:137:ARG:HG3  | 1:A:141:ARG:HH22 | 1.69                     | 0.56              |
| 1:A:579:PHE:CG   | 1:A:631:CYS:HB3  | 2.41                     | 0.56              |
| 1:A:602:VAL:O    | 1:A:606:LEU:HG   | 2.06                     | 0.56              |
| 1:A:941:GLN:OE1  | 1:A:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:B:602:VAL:O    | 1:B:606:LEU:HG   | 2.06                     | 0.56              |
| 1:C:256:HIS:CD2  | 1:C:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:C:557:LYS:NZ   | 1:C:605:GLU:OE1  | 2.28                     | 0.56              |
| 1:D:407:ILE:HG23 | 1:D:410:VAL:HB   | 1.87                     | 0.56              |
| 1:D:602:VAL:O    | 1:D:606:LEU:HG   | 2.06                     | 0.56              |
| 1:E:768:ASN:H    | 1:E:796:LYS:HG3  | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:407:ILE:HG23 | 1:F:410:VAL:HB   | 1.88                     | 0.56              |
| 1:F:768:ASN:H    | 1:F:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:G:407:ILE:HG23 | 1:G:410:VAL:HB   | 1.88                     | 0.56              |
| 1:G:602:VAL:O    | 1:G:606:LEU:HG   | 2.06                     | 0.56              |
| 1:H:941:GLN:OE1  | 1:H:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:I:400:VAL:HG22 | 1:I:401:LEU:H    | 1.69                     | 0.56              |
| 1:J:602:VAL:O    | 1:J:606:LEU:HG   | 2.06                     | 0.56              |
| 1:J:768:ASN:H    | 1:J:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:J:941:GLN:OE1  | 1:J:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:K:307:PHE:HD2  | 1:K:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:K:400:VAL:HG22 | 1:K:401:LEU:H    | 1.69                     | 0.56              |
| 1:L:579:PHE:CG   | 1:L:631:CYS:HB3  | 2.41                     | 0.56              |
| 1:B:400:VAL:HG22 | 1:B:401:LEU:H    | 1.69                     | 0.56              |
| 1:C:810:PHE:HD1  | 1:C:813:ARG:HD3  | 1.71                     | 0.56              |
| 1:E:294:LEU:HD12 | 1:E:295:PHE:H    | 1.70                     | 0.56              |
| 1:E:906:LYS:HG3  | 1:E:907:THR:HG23 | 1.87                     | 0.56              |
| 1:I:256:HIS:CD2  | 1:I:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:I:602:VAL:O    | 1:I:606:LEU:HG   | 2.06                     | 0.56              |
| 1:J:403:THR:HG21 | 1:J:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:L:307:PHE:HD2  | 1:L:567:GLU:HB2  | 1.69                     | 0.56              |
| 1:A:294:LEU:HD12 | 1:A:295:PHE:H    | 1.70                     | 0.56              |
| 1:A:810:PHE:HD1  | 1:A:813:ARG:HD3  | 1.71                     | 0.56              |
| 1:B:885:LYS:HG2  | 1:B:913:HIS:HB2  | 1.86                     | 0.56              |
| 1:D:294:LEU:HD12 | 1:D:295:PHE:H    | 1.70                     | 0.56              |
| 1:D:403:THR:HG21 | 1:D:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:F:941:GLN:OE1  | 1:F:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:G:265:PRO:HA   | 1:G:325:ASP:HA   | 1.88                     | 0.56              |
| 1:G:403:THR:HG21 | 1:G:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:I:265:PRO:HA   | 1:I:325:ASP:HA   | 1.88                     | 0.56              |
| 1:J:294:LEU:HD12 | 1:J:295:PHE:H    | 1.70                     | 0.56              |
| 1:J:768:ASN:H    | 1:J:796:LYS:HZ2  | 1.54                     | 0.56              |
| 1:J:810:PHE:HD1  | 1:J:813:ARG:HD3  | 1.71                     | 0.56              |
| 1:K:579:PHE:CG   | 1:K:631:CYS:HB3  | 2.41                     | 0.56              |
| 1:L:602:VAL:O    | 1:L:606:LEU:HG   | 2.06                     | 0.56              |
| 1:B:265:PRO:HA   | 1:B:325:ASP:HA   | 1.88                     | 0.56              |
| 1:D:265:PRO:HA   | 1:D:325:ASP:HA   | 1.88                     | 0.56              |
| 1:D:941:GLN:OE1  | 1:D:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:E:817:VAL:HG12 | 1:E:820:LYS:HZ3  | 1.71                     | 0.56              |
| 1:G:215:VAL:HG23 | 1:G:360:HIS:O    | 2.06                     | 0.56              |
| 1:G:941:GLN:OE1  | 1:G:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:H:256:HIS:CD2  | 1:H:258:ARG:HB3  | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:768:ASN:H    | 1:H:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:J:579:PHE:CG   | 1:J:631:CYS:HB3  | 2.41                     | 0.56              |
| 1:K:602:VAL:O    | 1:K:606:LEU:HG   | 2.06                     | 0.56              |
| 1:K:768:ASN:H    | 1:K:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:L:768:ASN:H    | 1:L:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:A:403:THR:HG21 | 1:A:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:C:294:LEU:HD12 | 1:C:295:PHE:H    | 1.70                     | 0.56              |
| 1:C:768:ASN:H    | 1:C:796:LYS:HG3  | 1.71                     | 0.56              |
| 1:D:215:VAL:HG23 | 1:D:360:HIS:O    | 2.06                     | 0.56              |
| 1:D:404:MET:O    | 1:D:407:ILE:HG22 | 2.06                     | 0.56              |
| 1:E:602:VAL:O    | 1:E:606:LEU:HG   | 2.06                     | 0.56              |
| 1:E:941:GLN:OE1  | 1:E:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:F:579:PHE:CG   | 1:F:631:CYS:HB3  | 2.41                     | 0.56              |
| 1:G:256:HIS:CD2  | 1:G:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:G:294:LEU:HD12 | 1:G:295:PHE:H    | 1.70                     | 0.56              |
| 1:G:404:MET:O    | 1:G:407:ILE:HG22 | 2.06                     | 0.56              |
| 1:J:215:VAL:HG23 | 1:J:360:HIS:O    | 2.06                     | 0.56              |
| 1:A:215:VAL:HG23 | 1:A:360:HIS:O    | 2.06                     | 0.56              |
| 1:A:768:ASN:H    | 1:A:796:LYS:HZ2  | 1.54                     | 0.56              |
| 1:D:256:HIS:CD2  | 1:D:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:E:404:MET:O    | 1:E:407:ILE:HG22 | 2.06                     | 0.56              |
| 1:F:817:VAL:HG12 | 1:F:820:LYS:HZ3  | 1.71                     | 0.56              |
| 1:H:137:ARG:HG3  | 1:H:141:ARG:HH22 | 1.69                     | 0.56              |
| 1:H:294:LEU:HD12 | 1:H:295:PHE:H    | 1.70                     | 0.56              |
| 1:H:810:PHE:HD1  | 1:H:813:ARG:HD3  | 1.71                     | 0.56              |
| 1:I:215:VAL:HG23 | 1:I:360:HIS:O    | 2.06                     | 0.56              |
| 1:I:403:THR:HG21 | 1:I:662:VAL:HG11 | 1.87                     | 0.56              |
| 1:I:785:PHE:HB3  | 1:J:810:PHE:HZ   | 1.70                     | 0.56              |
| 1:J:871:VAL:HG12 | 1:J:875:LYS:NZ   | 2.21                     | 0.56              |
| 1:K:256:HIS:CD2  | 1:K:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:K:265:PRO:HA   | 1:K:325:ASP:HA   | 1.88                     | 0.56              |
| 1:K:941:GLN:OE1  | 1:K:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:L:256:HIS:CD2  | 1:L:258:ARG:HB3  | 2.41                     | 0.56              |
| 1:L:941:GLN:OE1  | 1:L:969:ARG:NH1  | 2.39                     | 0.56              |
| 1:A:871:VAL:HG12 | 1:A:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:B:256:HIS:CD2  | 1:B:258:ARG:HB3  | 2.41                     | 0.55              |
| 1:B:403:THR:HG21 | 1:B:662:VAL:HG11 | 1.87                     | 0.55              |
| 1:C:404:MET:O    | 1:C:407:ILE:HG22 | 2.06                     | 0.55              |
| 1:C:789:SER:O    | 1:C:792:SER:OG   | 2.19                     | 0.55              |
| 1:E:926:LEU:HA   | 1:E:929:LEU:HD12 | 1.88                     | 0.55              |
| 1:H:407:ILE:HG23 | 1:H:410:VAL:HB   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:579:PHE:CG   | 1:H:631:CYS:HB3   | 2.41                     | 0.55              |
| 1:K:899:SER:O    | 1:K:902:THR:OG1   | 2.22                     | 0.55              |
| 1:L:215:VAL:HG23 | 1:L:360:HIS:O     | 2.06                     | 0.55              |
| 1:L:557:LYS:NZ   | 1:L:605:GLU:OE1   | 2.28                     | 0.55              |
| 1:A:649:PRO:O    | 1:A:675:LYS:N     | 2.36                     | 0.55              |
| 1:A:970:LYS:HE2  | 1:L:1027:ILE:HD13 | 1.87                     | 0.55              |
| 1:B:1008:ASN:O   | 1:B:1011:THR:OG1  | 2.21                     | 0.55              |
| 1:C:630:TYR:OH   | 1:C:660:ASP:OD1   | 2.12                     | 0.55              |
| 1:F:294:LEU:HD12 | 1:F:295:PHE:H     | 1.70                     | 0.55              |
| 1:F:404:MET:O    | 1:F:407:ILE:HG22  | 2.06                     | 0.55              |
| 1:H:404:MET:O    | 1:H:407:ILE:HG22  | 2.06                     | 0.55              |
| 1:H:732:SER:O    | 1:H:735:SER:OG    | 2.20                     | 0.55              |
| 1:I:579:PHE:CG   | 1:I:631:CYS:HB3   | 2.41                     | 0.55              |
| 1:I:941:GLN:OE1  | 1:I:969:ARG:NH1   | 2.39                     | 0.55              |
| 1:J:256:HIS:CD2  | 1:J:258:ARG:HB3   | 2.41                     | 0.55              |
| 1:J:404:MET:O    | 1:J:407:ILE:HG22  | 2.06                     | 0.55              |
| 1:K:215:VAL:HG23 | 1:K:360:HIS:O     | 2.06                     | 0.55              |
| 1:K:407:ILE:HG23 | 1:K:410:VAL:HB    | 1.87                     | 0.55              |
| 1:K:557:LYS:NZ   | 1:K:605:GLU:OE1   | 2.28                     | 0.55              |
| 1:K:906:LYS:HG3  | 1:K:907:THR:HG23  | 1.87                     | 0.55              |
| 1:L:294:LEU:HD12 | 1:L:295:PHE:H     | 1.70                     | 0.55              |
| 1:L:407:ILE:HG23 | 1:L:410:VAL:HB    | 1.88                     | 0.55              |
| 1:L:906:LYS:HG3  | 1:L:907:THR:HG23  | 1.87                     | 0.55              |
| 1:A:256:HIS:CD2  | 1:A:258:ARG:HB3   | 2.41                     | 0.55              |
| 1:A:404:MET:O    | 1:A:407:ILE:HG22  | 2.06                     | 0.55              |
| 1:B:215:VAL:HG23 | 1:B:360:HIS:O     | 2.06                     | 0.55              |
| 1:B:579:PHE:CG   | 1:B:631:CYS:HB3   | 2.41                     | 0.55              |
| 1:C:401:LEU:HD22 | 1:C:404:MET:HE3   | 1.89                     | 0.55              |
| 1:D:926:LEU:HA   | 1:D:929:LEU:HD12  | 1.88                     | 0.55              |
| 1:E:215:VAL:HG23 | 1:E:360:HIS:O     | 2.06                     | 0.55              |
| 1:F:926:LEU:HA   | 1:F:929:LEU:HD12  | 1.89                     | 0.55              |
| 1:I:404:MET:O    | 1:I:407:ILE:HG22  | 2.06                     | 0.55              |
| 1:I:926:LEU:HA   | 1:I:929:LEU:HD12  | 1.88                     | 0.55              |
| 1:K:871:VAL:HG12 | 1:K:875:LYS:NZ    | 2.21                     | 0.55              |
| 1:L:871:VAL:HG12 | 1:L:875:LYS:NZ    | 2.21                     | 0.55              |
| 1:L:899:SER:O    | 1:L:902:THR:OG1   | 2.22                     | 0.55              |
| 1:B:926:LEU:HA   | 1:B:929:LEU:HD12  | 1.88                     | 0.55              |
| 1:B:941:GLN:OE1  | 1:B:969:ARG:NH1   | 2.39                     | 0.55              |
| 1:C:137:ARG:HG3  | 1:C:141:ARG:HH22  | 1.69                     | 0.55              |
| 1:C:215:VAL:HG23 | 1:C:360:HIS:O     | 2.06                     | 0.55              |
| 1:C:407:ILE:HG23 | 1:C:410:VAL:HB    | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:579:PHE:CG   | 1:C:631:CYS:HB3  | 2.41                     | 0.55              |
| 1:C:602:VAL:O    | 1:C:606:LEU:HG   | 2.06                     | 0.55              |
| 1:E:579:PHE:CG   | 1:E:631:CYS:HB3  | 2.41                     | 0.55              |
| 1:E:768:ASN:H    | 1:E:796:LYS:HZ2  | 1.54                     | 0.55              |
| 1:F:602:VAL:O    | 1:F:606:LEU:HG   | 2.06                     | 0.55              |
| 1:G:926:LEU:HA   | 1:G:929:LEU:HD12 | 1.88                     | 0.55              |
| 1:L:265:PRO:HA   | 1:L:325:ASP:HA   | 1.88                     | 0.55              |
| 1:C:871:VAL:HG12 | 1:C:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:E:265:PRO:HA   | 1:E:325:ASP:HA   | 1.88                     | 0.55              |
| 1:H:926:LEU:HA   | 1:H:929:LEU:HD12 | 1.88                     | 0.55              |
| 1:I:407:ILE:HG23 | 1:I:410:VAL:HB   | 1.87                     | 0.55              |
| 1:I:871:VAL:HG12 | 1:I:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:K:294:LEU:HD12 | 1:K:295:PHE:H    | 1.70                     | 0.55              |
| 1:L:404:MET:O    | 1:L:407:ILE:HG22 | 2.06                     | 0.55              |
| 1:B:404:MET:O    | 1:B:407:ILE:HG22 | 2.06                     | 0.55              |
| 1:C:1007:LEU:HB2 | 1:C:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:D:919:ASN:HB2  | 1:D:921:LEU:HG   | 1.89                     | 0.55              |
| 1:E:758:LEU:HA   | 1:E:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:E:1007:LEU:HB2 | 1:E:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:G:810:PHE:HD1  | 1:G:813:ARG:HD3  | 1.71                     | 0.55              |
| 1:H:871:VAL:HG12 | 1:H:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:K:404:MET:O    | 1:K:407:ILE:HG22 | 2.06                     | 0.55              |
| 1:B:407:ILE:HG23 | 1:B:410:VAL:HB   | 1.87                     | 0.55              |
| 1:B:758:LEU:HA   | 1:B:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:E:251:TYR:HB2  | 1:E:293:ILE:HD12 | 1.89                     | 0.55              |
| 1:E:810:PHE:HD1  | 1:E:813:ARG:HD3  | 1.71                     | 0.55              |
| 1:F:215:VAL:HG23 | 1:F:360:HIS:O    | 2.06                     | 0.55              |
| 1:F:265:PRO:HA   | 1:F:325:ASP:HA   | 1.88                     | 0.55              |
| 1:F:758:LEU:HA   | 1:F:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:G:919:ASN:HB2  | 1:G:921:LEU:HG   | 1.89                     | 0.55              |
| 1:A:265:PRO:HA   | 1:A:325:ASP:HA   | 1.88                     | 0.55              |
| 1:B:871:VAL:HG12 | 1:B:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:D:758:LEU:HA   | 1:D:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:D:810:PHE:HD1  | 1:D:813:ARG:HD3  | 1.71                     | 0.55              |
| 1:F:630:TYR:OH   | 1:F:660:ASP:OD1  | 2.12                     | 0.55              |
| 1:F:1007:LEU:HB2 | 1:F:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:G:1007:LEU:HB2 | 1:G:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:H:602:VAL:O    | 1:H:606:LEU:HG   | 2.06                     | 0.55              |
| 1:I:758:LEU:HA   | 1:I:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:J:407:ILE:HG23 | 1:J:410:VAL:HB   | 1.88                     | 0.55              |
| 1:K:403:THR:HG21 | 1:K:662:VAL:HG11 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:758:LEU:HA   | 1:K:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:L:403:THR:HG21 | 1:L:662:VAL:HG11 | 1.87                     | 0.55              |
| 1:A:407:ILE:HG23 | 1:A:410:VAL:HB   | 1.87                     | 0.55              |
| 1:D:1007:LEU:HB2 | 1:D:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:F:251:TYR:HB2  | 1:F:293:ILE:HD12 | 1.89                     | 0.55              |
| 1:H:215:VAL:HG23 | 1:H:360:HIS:O    | 2.06                     | 0.55              |
| 1:I:919:ASN:HB2  | 1:I:921:LEU:HG   | 1.89                     | 0.55              |
| 1:I:1008:ASN:O   | 1:I:1011:THR:OG1 | 2.21                     | 0.55              |
| 1:L:758:LEU:HA   | 1:L:761:ALA:HB3  | 1.89                     | 0.55              |
| 1:A:734:LEU:HA   | 1:A:737:ASN:HB2  | 1.90                     | 0.55              |
| 1:A:1007:LEU:HB2 | 1:A:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:C:732:SER:O    | 1:C:735:SER:OG   | 2.20                     | 0.55              |
| 1:C:926:LEU:HA   | 1:C:929:LEU:HD12 | 1.89                     | 0.55              |
| 1:D:579:PHE:CG   | 1:D:631:CYS:HB3  | 2.41                     | 0.55              |
| 1:G:579:PHE:CG   | 1:G:631:CYS:HB3  | 2.41                     | 0.55              |
| 1:G:871:VAL:HG12 | 1:G:875:LYS:NZ   | 2.21                     | 0.55              |
| 1:H:265:PRO:HA   | 1:H:325:ASP:HA   | 1.88                     | 0.55              |
| 1:H:1007:LEU:HB2 | 1:H:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:J:734:LEU:HA   | 1:J:737:ASN:HB2  | 1.89                     | 0.55              |
| 1:J:1007:LEU:HB2 | 1:J:1012:LYS:NZ  | 2.21                     | 0.55              |
| 1:B:919:ASN:HB2  | 1:B:921:LEU:HG   | 1.89                     | 0.54              |
| 1:B:1007:LEU:HB2 | 1:B:1012:LYS:NZ  | 2.22                     | 0.54              |
| 1:C:265:PRO:HA   | 1:C:325:ASP:HA   | 1.88                     | 0.54              |
| 1:D:871:VAL:HG12 | 1:D:875:LYS:NZ   | 2.21                     | 0.54              |
| 1:G:734:LEU:HA   | 1:G:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:I:1007:LEU:HB2 | 1:I:1012:LYS:NZ  | 2.22                     | 0.54              |
| 1:C:251:TYR:HB2  | 1:C:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:D:734:LEU:HA   | 1:D:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:G:758:LEU:HA   | 1:G:761:ALA:HB3  | 1.89                     | 0.54              |
| 1:L:810:PHE:HD1  | 1:L:813:ARG:HD3  | 1.71                     | 0.54              |
| 1:H:251:TYR:HB2  | 1:H:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:J:265:PRO:HA   | 1:J:325:ASP:HA   | 1.88                     | 0.54              |
| 1:J:919:ASN:HB2  | 1:J:921:LEU:HG   | 1.89                     | 0.54              |
| 1:K:1007:LEU:HB2 | 1:K:1012:LYS:NZ  | 2.21                     | 0.54              |
| 1:L:1007:LEU:HB2 | 1:L:1012:LYS:NZ  | 2.21                     | 0.54              |
| 1:A:926:LEU:HA   | 1:A:929:LEU:HD12 | 1.88                     | 0.54              |
| 1:B:810:PHE:HD1  | 1:B:813:ARG:HD3  | 1.71                     | 0.54              |
| 1:C:209:ASP:HA   | 1:C:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:F:734:LEU:HA   | 1:F:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:H:734:LEU:HA   | 1:H:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:K:810:PHE:HD1  | 1:K:813:ARG:HD3  | 1.71                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:209:ASP:HA   | 1:D:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:E:209:ASP:HA   | 1:E:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:E:871:VAL:HG12 | 1:E:875:LYS:NZ   | 2.21                     | 0.54              |
| 1:F:810:PHE:HD1  | 1:F:813:ARG:HD3  | 1.71                     | 0.54              |
| 1:H:209:ASP:HA   | 1:H:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:J:926:LEU:HA   | 1:J:929:LEU:HD12 | 1.88                     | 0.54              |
| 1:K:734:LEU:HA   | 1:K:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:K:926:LEU:HA   | 1:K:929:LEU:HD12 | 1.88                     | 0.54              |
| 1:L:734:LEU:HA   | 1:L:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:L:926:LEU:HA   | 1:L:929:LEU:HD12 | 1.88                     | 0.54              |
| 1:A:919:ASN:HB2  | 1:A:921:LEU:HG   | 1.89                     | 0.54              |
| 1:B:734:LEU:HA   | 1:B:737:ASN:HB2  | 1.89                     | 0.54              |
| 1:B:899:SER:O    | 1:B:902:THR:OG1  | 2.22                     | 0.54              |
| 1:C:734:LEU:HA   | 1:C:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:E:734:LEU:HA   | 1:E:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:G:209:ASP:HA   | 1:G:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:I:734:LEU:HA   | 1:I:737:ASN:HB2  | 1.90                     | 0.54              |
| 1:I:810:PHE:HD1  | 1:I:813:ARG:HD3  | 1.71                     | 0.54              |
| 1:J:209:ASP:HA   | 1:J:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:209:ASP:HA   | 1:A:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:890:ASN:HA   | 1:A:919:ASN:HD22 | 1.73                     | 0.54              |
| 1:D:251:TYR:HB2  | 1:D:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:D:890:ASN:HA   | 1:D:919:ASN:HD22 | 1.73                     | 0.54              |
| 1:F:209:ASP:HA   | 1:F:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:G:890:ASN:HA   | 1:G:919:ASN:HD22 | 1.73                     | 0.54              |
| 1:I:899:SER:O    | 1:I:902:THR:OG1  | 2.22                     | 0.54              |
| 1:B:209:ASP:HA   | 1:B:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:D:649:PRO:O    | 1:D:675:LYS:N    | 2.36                     | 0.54              |
| 1:E:919:ASN:HB2  | 1:E:921:LEU:HG   | 1.89                     | 0.54              |
| 1:G:251:TYR:HB2  | 1:G:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:H:247:ASP:O    | 1:H:292:ARG:NH2  | 2.31                     | 0.54              |
| 1:J:251:TYR:HB2  | 1:J:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:J:890:ASN:HA   | 1:J:919:ASN:HD22 | 1.73                     | 0.54              |
| 1:C:758:LEU:HA   | 1:C:761:ALA:HB3  | 1.89                     | 0.54              |
| 1:C:919:ASN:HB2  | 1:C:921:LEU:HG   | 1.89                     | 0.54              |
| 1:F:871:VAL:HG12 | 1:F:875:LYS:NZ   | 2.21                     | 0.54              |
| 1:F:919:ASN:HB2  | 1:F:921:LEU:HG   | 1.89                     | 0.54              |
| 1:G:872:LEU:HD23 | 1:G:875:LYS:HZ1  | 1.72                     | 0.54              |
| 1:H:919:ASN:HB2  | 1:H:921:LEU:HG   | 1.89                     | 0.54              |
| 1:I:209:ASP:HA   | 1:I:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:251:TYR:HB2  | 1:A:293:ILE:HD12 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:171:LYS:HG2  | 1:D:363:HIS:O    | 2.09                     | 0.54              |
| 1:E:148:LYS:HB3  | 1:E:159:ASP:HB2  | 1.90                     | 0.54              |
| 1:G:171:LYS:HG2  | 1:G:363:HIS:O    | 2.08                     | 0.54              |
| 1:H:758:LEU:HA   | 1:H:761:ALA:HB3  | 1.89                     | 0.54              |
| 1:K:209:ASP:HA   | 1:K:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:K:251:TYR:HB2  | 1:K:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:L:209:ASP:HA   | 1:L:213:GLU:HG3  | 1.90                     | 0.54              |
| 1:L:251:TYR:HB2  | 1:L:293:ILE:HD12 | 1.89                     | 0.54              |
| 1:A:899:SER:O    | 1:A:902:THR:OG1  | 2.22                     | 0.53              |
| 1:B:734:LEU:HA   | 1:B:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:B:890:ASN:HA   | 1:B:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:C:160:LEU:HA   | 1:C:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:F:171:LYS:HG2  | 1:F:363:HIS:O    | 2.08                     | 0.53              |
| 1:H:160:LEU:HA   | 1:H:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:H:890:ASN:HA   | 1:H:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:J:758:LEU:HA   | 1:J:761:ALA:HB3  | 1.89                     | 0.53              |
| 1:K:160:LEU:HA   | 1:K:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:K:732:SER:O    | 1:K:735:SER:OG   | 2.20                     | 0.53              |
| 1:K:919:ASN:HB2  | 1:K:921:LEU:HG   | 1.89                     | 0.53              |
| 1:L:789:SER:O    | 1:L:792:SER:OG   | 2.19                     | 0.53              |
| 1:L:890:ASN:HA   | 1:L:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:A:758:LEU:HA   | 1:A:761:ALA:HB3  | 1.89                     | 0.53              |
| 1:A:842:GLN:O    | 1:A:846:LEU:HG   | 2.09                     | 0.53              |
| 1:B:171:LYS:HG2  | 1:B:363:HIS:O    | 2.09                     | 0.53              |
| 1:B:529:TYR:OH   | 1:B:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:C:890:ASN:HA   | 1:C:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:E:401:LEU:HD22 | 1:E:404:MET:HE3  | 1.89                     | 0.53              |
| 1:E:890:ASN:HA   | 1:E:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:E:934:LEU:CA   | 1:E:961:ILE:HD11 | 2.39                     | 0.53              |
| 1:F:890:ASN:HA   | 1:F:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:G:649:PRO:O    | 1:G:675:LYS:N    | 2.36                     | 0.53              |
| 1:H:414:VAL:HA   | 1:H:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:I:890:ASN:HA   | 1:I:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:K:890:ASN:HA   | 1:K:919:ASN:HD22 | 1.73                     | 0.53              |
| 1:L:160:LEU:HA   | 1:L:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:L:919:ASN:HB2  | 1:L:921:LEU:HG   | 1.89                     | 0.53              |
| 1:A:529:TYR:OH   | 1:A:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:B:160:LEU:HA   | 1:B:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:B:817:VAL:HG12 | 1:B:820:LYS:HZ3  | 1.71                     | 0.53              |
| 1:D:788:SER:HB2  | 1:D:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:E:723:THR:HA   | 1:E:726:PHE:CD2  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:734:LEU:HA   | 1:E:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:F:934:LEU:CA   | 1:F:961:ILE:HD11 | 2.39                     | 0.53              |
| 1:G:788:SER:HB2  | 1:G:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:H:148:LYS:HB3  | 1:H:159:ASP:HB2  | 1.90                     | 0.53              |
| 1:I:529:TYR:OH   | 1:I:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:I:734:LEU:HA   | 1:I:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:J:160:LEU:HA   | 1:J:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:J:734:LEU:HA   | 1:J:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:J:842:GLN:O    | 1:J:846:LEU:HG   | 2.09                     | 0.53              |
| 1:A:160:LEU:HA   | 1:A:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:A:734:LEU:HA   | 1:A:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:A:788:SER:HB2  | 1:A:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:B:955:CYS:HB3  | 1:B:986:LEU:HD21 | 1.91                     | 0.53              |
| 1:C:414:VAL:HA   | 1:C:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:E:414:VAL:HA   | 1:E:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:F:734:LEU:HA   | 1:F:737:ASN:HD22 | 1.74                     | 0.53              |
| 1:G:1008:ASN:O   | 1:G:1011:THR:OG1 | 2.21                     | 0.53              |
| 1:I:557:LYS:NZ   | 1:I:605:GLU:OE1  | 2.28                     | 0.53              |
| 1:J:529:TYR:OH   | 1:J:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:J:743:LEU:HD21 | 1:J:745:LEU:HG   | 1.91                     | 0.53              |
| 1:J:788:SER:HB2  | 1:J:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:J:899:SER:O    | 1:J:902:THR:OG1  | 2.22                     | 0.53              |
| 1:K:789:SER:O    | 1:K:792:SER:OG   | 2.19                     | 0.53              |
| 1:L:171:LYS:HG2  | 1:L:363:HIS:O    | 2.09                     | 0.53              |
| 1:A:743:LEU:HD21 | 1:A:745:LEU:HG   | 1.91                     | 0.53              |
| 1:C:506:LYS:HG2  | 1:C:513:PHE:O    | 2.09                     | 0.53              |
| 1:C:637:GLU:OE2  | 1:C:640:PHE:N    | 2.28                     | 0.53              |
| 1:C:723:THR:HA   | 1:C:726:PHE:CD2  | 2.43                     | 0.53              |
| 1:E:171:LYS:HG2  | 1:E:363:HIS:O    | 2.09                     | 0.53              |
| 1:E:239:TRP:CE3  | 1:E:252:LEU:HG   | 2.44                     | 0.53              |
| 1:F:148:LYS:HB3  | 1:F:159:ASP:HB2  | 1.90                     | 0.53              |
| 1:F:239:TRP:CE3  | 1:F:252:LEU:HG   | 2.44                     | 0.53              |
| 1:G:557:LYS:NZ   | 1:G:605:GLU:OE1  | 2.28                     | 0.53              |
| 1:H:788:SER:HB2  | 1:H:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:I:160:LEU:HA   | 1:I:163:ARG:HB2  | 1.90                     | 0.53              |
| 1:I:247:ASP:O    | 1:I:292:ARG:NH2  | 2.31                     | 0.53              |
| 1:I:789:SER:O    | 1:I:792:SER:OG   | 2.19                     | 0.53              |
| 1:I:955:CYS:HB3  | 1:I:986:LEU:HD21 | 1.91                     | 0.53              |
| 1:K:171:LYS:HG2  | 1:K:363:HIS:O    | 2.09                     | 0.53              |
| 1:K:529:TYR:OH   | 1:K:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:K:723:THR:HA   | 1:K:726:PHE:CD2  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:529:TYR:OH   | 1:L:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:L:732:SER:O    | 1:L:735:SER:OG   | 2.20                     | 0.53              |
| 1:C:743:LEU:HD21 | 1:C:745:LEU:HG   | 1.91                     | 0.53              |
| 1:D:1008:ASN:O   | 1:D:1011:THR:OG1 | 2.21                     | 0.53              |
| 1:E:872:LEU:HD23 | 1:E:875:LYS:HZ1  | 1.74                     | 0.53              |
| 1:F:414:VAL:HA   | 1:F:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:H:506:LYS:HG2  | 1:H:513:PHE:O    | 2.09                     | 0.53              |
| 1:H:768:ASN:H    | 1:H:796:LYS:HZ3  | 1.56                     | 0.53              |
| 1:I:171:LYS:HG2  | 1:I:363:HIS:O    | 2.09                     | 0.53              |
| 1:I:723:THR:HA   | 1:I:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:K:842:GLN:O    | 1:K:846:LEU:HG   | 2.09                     | 0.53              |
| 1:L:723:THR:HA   | 1:L:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:A:955:CYS:HB3  | 1:A:986:LEU:HD21 | 1.91                     | 0.53              |
| 1:B:723:THR:HA   | 1:B:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:C:148:LYS:HB3  | 1:C:159:ASP:HB2  | 1.90                     | 0.53              |
| 1:C:239:TRP:CE3  | 1:C:252:LEU:HG   | 2.44                     | 0.53              |
| 1:C:327:LEU:HA   | 1:C:331:LEU:HG   | 1.91                     | 0.53              |
| 1:C:759:CYS:HA   | 1:C:790:VAL:HG11 | 1.91                     | 0.53              |
| 1:D:506:LYS:HG2  | 1:D:513:PHE:O    | 2.09                     | 0.53              |
| 1:E:167:LEU:HD22 | 1:E:368:GLY:HA2  | 1.91                     | 0.53              |
| 1:F:723:THR:HA   | 1:F:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:G:327:LEU:HA   | 1:G:331:LEU:HG   | 1.91                     | 0.53              |
| 1:H:239:TRP:CE3  | 1:H:252:LEU:HG   | 2.44                     | 0.53              |
| 1:H:723:THR:HA   | 1:H:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:I:252:LEU:HB3  | 1:I:296:LEU:HD13 | 1.90                     | 0.53              |
| 1:L:842:GLN:O    | 1:L:846:LEU:HG   | 2.09                     | 0.53              |
| 1:A:506:LYS:HG2  | 1:A:513:PHE:O    | 2.09                     | 0.53              |
| 1:B:252:LEU:HB3  | 1:B:296:LEU:HD13 | 1.90                     | 0.53              |
| 1:B:789:SER:O    | 1:B:792:SER:OG   | 2.19                     | 0.53              |
| 1:C:307:PHE:CD2  | 1:C:567:GLU:HB2  | 2.44                     | 0.53              |
| 1:D:327:LEU:HA   | 1:D:331:LEU:HG   | 1.91                     | 0.53              |
| 1:D:529:TYR:OH   | 1:D:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:D:668:ILE:HG22 | 1:D:737:ASN:HD21 | 1.74                     | 0.53              |
| 1:E:327:LEU:HA   | 1:E:331:LEU:HG   | 1.91                     | 0.53              |
| 1:F:167:LEU:HD22 | 1:F:368:GLY:HA2  | 1.91                     | 0.53              |
| 1:F:872:LEU:HD23 | 1:F:875:LYS:HZ1  | 1.74                     | 0.53              |
| 1:H:307:PHE:CD2  | 1:H:567:GLU:HB2  | 2.44                     | 0.53              |
| 1:H:743:LEU:HD21 | 1:H:745:LEU:HG   | 1.91                     | 0.53              |
| 1:H:759:CYS:HA   | 1:H:790:VAL:HG11 | 1.91                     | 0.53              |
| 1:J:167:LEU:HD22 | 1:J:368:GLY:HA2  | 1.91                     | 0.53              |
| 1:J:414:VAL:HA   | 1:J:442:PHE:CZ   | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:955:CYS:HB3  | 1:J:986:LEU:HD21 | 1.91                     | 0.53              |
| 1:L:506:LYS:HG2  | 1:L:513:PHE:O    | 2.09                     | 0.53              |
| 1:A:167:LEU:HD22 | 1:A:368:GLY:HA2  | 1.91                     | 0.53              |
| 1:A:414:VAL:HA   | 1:A:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:B:251:TYR:HB2  | 1:B:293:ILE:HD12 | 1.89                     | 0.53              |
| 1:C:788:SER:HB2  | 1:C:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:D:148:LYS:HB3  | 1:D:159:ASP:HB2  | 1.90                     | 0.53              |
| 1:D:239:TRP:CE3  | 1:D:252:LEU:HG   | 2.44                     | 0.53              |
| 1:D:789:SER:O    | 1:D:792:SER:OG   | 2.19                     | 0.53              |
| 1:E:876:MET:HA   | 1:E:881:CYS:SG   | 2.49                     | 0.53              |
| 1:F:557:LYS:NZ   | 1:F:605:GLU:OE1  | 2.28                     | 0.53              |
| 1:G:506:LYS:HG2  | 1:G:513:PHE:O    | 2.09                     | 0.53              |
| 1:H:252:LEU:HB3  | 1:H:296:LEU:HD13 | 1.91                     | 0.53              |
| 1:H:934:LEU:CA   | 1:H:961:ILE:HD11 | 2.39                     | 0.53              |
| 1:I:251:TYR:HB2  | 1:I:293:ILE:HD12 | 1.89                     | 0.53              |
| 1:J:506:LYS:HG2  | 1:J:513:PHE:O    | 2.09                     | 0.53              |
| 1:K:506:LYS:HG2  | 1:K:513:PHE:O    | 2.09                     | 0.53              |
| 1:K:768:ASN:H    | 1:K:796:LYS:HZ3  | 1.56                     | 0.53              |
| 1:K:871:VAL:HG12 | 1:K:875:LYS:HZ2  | 1.74                     | 0.53              |
| 1:A:327:LEU:HA   | 1:A:331:LEU:HG   | 1.91                     | 0.53              |
| 1:B:788:SER:HB2  | 1:B:818:GLY:HA3  | 1.91                     | 0.53              |
| 1:B:842:GLN:O    | 1:B:846:LEU:HG   | 2.09                     | 0.53              |
| 1:B:861:GLU:OE1  | 1:B:918:SER:OG   | 2.27                     | 0.53              |
| 1:C:252:LEU:HB3  | 1:C:296:LEU:HD13 | 1.91                     | 0.53              |
| 1:D:723:THR:HA   | 1:D:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:F:327:LEU:HA   | 1:F:331:LEU:HG   | 1.91                     | 0.53              |
| 1:F:529:TYR:OH   | 1:F:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:G:239:TRP:CE3  | 1:G:252:LEU:HG   | 2.44                     | 0.53              |
| 1:G:529:TYR:OH   | 1:G:554:ARG:NH1  | 2.42                     | 0.53              |
| 1:G:668:ILE:HG22 | 1:G:737:ASN:HD21 | 1.74                     | 0.53              |
| 1:G:723:THR:HA   | 1:G:726:PHE:CD2  | 2.44                     | 0.53              |
| 1:H:327:LEU:HA   | 1:H:331:LEU:HG   | 1.91                     | 0.53              |
| 1:H:861:GLU:OE1  | 1:H:918:SER:OG   | 2.27                     | 0.53              |
| 1:I:414:VAL:HA   | 1:I:442:PHE:CZ   | 2.44                     | 0.53              |
| 1:I:861:GLU:OE1  | 1:I:918:SER:OG   | 2.27                     | 0.53              |
| 1:J:307:PHE:CD2  | 1:J:567:GLU:HB2  | 2.44                     | 0.53              |
| 1:J:327:LEU:HA   | 1:J:331:LEU:HG   | 1.91                     | 0.53              |
| 1:L:871:VAL:HG12 | 1:L:875:LYS:HZ2  | 1.74                     | 0.53              |
| 1:A:307:PHE:CD2  | 1:A:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:B:876:MET:HA   | 1:B:881:CYS:SG   | 2.49                     | 0.52              |
| 1:C:167:LEU:HD22 | 1:C:368:GLY:HA2  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:734:LEU:HA   | 1:C:737:ASN:HD22 | 1.74                     | 0.52              |
| 1:E:160:LEU:HA   | 1:E:163:ARG:HB2  | 1.90                     | 0.52              |
| 1:E:307:PHE:CD2  | 1:E:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:E:529:TYR:OH   | 1:E:554:ARG:NH1  | 2.42                     | 0.52              |
| 1:E:743:LEU:HD21 | 1:E:745:LEU:HG   | 1.91                     | 0.52              |
| 1:F:985:THR:O    | 1:F:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:G:148:LYS:HB3  | 1:G:159:ASP:HB2  | 1.90                     | 0.52              |
| 1:I:788:SER:HB2  | 1:I:818:GLY:HA3  | 1.91                     | 0.52              |
| 1:J:148:LYS:HB3  | 1:J:159:ASP:HB2  | 1.90                     | 0.52              |
| 1:J:677:LEU:HD22 | 1:J:734:LEU:HD21 | 1.91                     | 0.52              |
| 1:J:759:CYS:HA   | 1:J:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:L:167:LEU:HD22 | 1:L:368:GLY:HA2  | 1.91                     | 0.52              |
| 1:L:743:LEU:HD21 | 1:L:745:LEU:HG   | 1.91                     | 0.52              |
| 1:L:768:ASN:H    | 1:L:796:LYS:HZ3  | 1.56                     | 0.52              |
| 1:L:876:MET:HA   | 1:L:881:CYS:SG   | 2.49                     | 0.52              |
| 1:A:148:LYS:HB3  | 1:A:159:ASP:HB2  | 1.90                     | 0.52              |
| 1:A:171:LYS:HG2  | 1:A:363:HIS:O    | 2.09                     | 0.52              |
| 1:A:608:LYS:HA   | 1:A:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:861:GLU:OE1  | 1:A:918:SER:OG   | 2.27                     | 0.52              |
| 1:C:767:CYS:SG   | 1:C:796:LYS:NZ   | 2.82                     | 0.52              |
| 1:C:861:GLU:OE1  | 1:C:918:SER:OG   | 2.27                     | 0.52              |
| 1:E:788:SER:HB2  | 1:E:818:GLY:HA3  | 1.91                     | 0.52              |
| 1:F:160:LEU:HA   | 1:F:163:ARG:HB2  | 1.90                     | 0.52              |
| 1:F:876:MET:HA   | 1:F:881:CYS:SG   | 2.49                     | 0.52              |
| 1:G:307:PHE:CD2  | 1:G:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:H:529:TYR:OH   | 1:H:554:ARG:NH1  | 2.42                     | 0.52              |
| 1:H:842:GLN:O    | 1:H:846:LEU:HG   | 2.09                     | 0.52              |
| 1:I:327:LEU:HA   | 1:I:331:LEU:HG   | 1.91                     | 0.52              |
| 1:J:171:LYS:HG2  | 1:J:363:HIS:O    | 2.08                     | 0.52              |
| 1:J:861:GLU:OE1  | 1:J:918:SER:OG   | 2.27                     | 0.52              |
| 1:K:167:LEU:HD22 | 1:K:368:GLY:HA2  | 1.91                     | 0.52              |
| 1:K:252:LEU:HB3  | 1:K:296:LEU:HD13 | 1.90                     | 0.52              |
| 1:K:668:ILE:HG22 | 1:K:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:K:743:LEU:HD21 | 1:K:745:LEU:HG   | 1.91                     | 0.52              |
| 1:K:876:MET:HA   | 1:K:881:CYS:SG   | 2.49                     | 0.52              |
| 1:L:608:LYS:HA   | 1:L:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:L:668:ILE:HG22 | 1:L:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:A:677:LEU:HD22 | 1:A:734:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:723:THR:HA   | 1:A:726:PHE:CD2  | 2.43                     | 0.52              |
| 1:A:917:ARG:N    | 1:A:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:B:327:LEU:HA   | 1:B:331:LEU:HG   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:213:GLU:HB2  | 1:C:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:C:608:LYS:HA   | 1:C:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:C:934:LEU:CA   | 1:C:961:ILE:HD11 | 2.39                     | 0.52              |
| 1:F:759:CYS:HA   | 1:F:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:I:817:VAL:HG12 | 1:I:820:LYS:HZ3  | 1.72                     | 0.52              |
| 1:I:842:GLN:O    | 1:I:846:LEU:HG   | 2.09                     | 0.52              |
| 1:J:252:LEU:HB3  | 1:J:296:LEU:HD13 | 1.91                     | 0.52              |
| 1:J:608:LYS:HA   | 1:J:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:J:723:THR:HA   | 1:J:726:PHE:CD2  | 2.43                     | 0.52              |
| 1:K:414:VAL:HA   | 1:K:442:PHE:CZ   | 2.44                     | 0.52              |
| 1:K:608:LYS:HA   | 1:K:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:K:734:LEU:HD13 | 1:K:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:L:252:LEU:HB3  | 1:L:296:LEU:HD13 | 1.90                     | 0.52              |
| 1:A:252:LEU:HB3  | 1:A:296:LEU:HD13 | 1.90                     | 0.52              |
| 1:C:171:LYS:HG2  | 1:C:363:HIS:O    | 2.08                     | 0.52              |
| 1:E:608:LYS:HA   | 1:E:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:E:759:CYS:HA   | 1:E:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:F:955:CYS:HB3  | 1:F:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:G:789:SER:O    | 1:G:792:SER:OG   | 2.19                     | 0.52              |
| 1:H:171:LYS:HG2  | 1:H:363:HIS:O    | 2.08                     | 0.52              |
| 1:H:213:GLU:HB2  | 1:H:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:H:608:LYS:HA   | 1:H:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:H:876:MET:HA   | 1:H:881:CYS:SG   | 2.49                     | 0.52              |
| 1:I:743:LEU:HD21 | 1:I:745:LEU:HG   | 1.91                     | 0.52              |
| 1:K:917:ARG:N    | 1:K:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:K:955:CYS:HB3  | 1:K:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:L:327:LEU:HA   | 1:L:331:LEU:HG   | 1.91                     | 0.52              |
| 1:A:668:ILE:HG22 | 1:A:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:A:759:CYS:HA   | 1:A:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:B:239:TRP:CE3  | 1:B:252:LEU:HG   | 2.44                     | 0.52              |
| 1:B:414:VAL:HA   | 1:B:442:PHE:CZ   | 2.44                     | 0.52              |
| 1:B:506:LYS:HG2  | 1:B:513:PHE:O    | 2.09                     | 0.52              |
| 1:C:529:TYR:OH   | 1:C:554:ARG:NH1  | 2.42                     | 0.52              |
| 1:C:842:GLN:O    | 1:C:846:LEU:HG   | 2.09                     | 0.52              |
| 1:C:985:THR:O    | 1:C:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:D:307:PHE:CD2  | 1:D:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:D:876:MET:HA   | 1:D:881:CYS:SG   | 2.49                     | 0.52              |
| 1:D:914:LEU:HB3  | 1:D:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:E:985:THR:O    | 1:E:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:F:307:PHE:CD2  | 1:F:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:G:160:LEU:HA   | 1:G:163:ARG:HB2  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:876:MET:HA   | 1:G:881:CYS:SG   | 2.49                     | 0.52              |
| 1:G:914:LEU:HB3  | 1:G:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:H:167:LEU:HD22 | 1:H:368:GLY:HA2  | 1.91                     | 0.52              |
| 1:H:734:LEU:HA   | 1:H:737:ASN:HD22 | 1.74                     | 0.52              |
| 1:H:985:THR:O    | 1:H:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:I:148:LYS:HB3  | 1:I:159:ASP:HB2  | 1.90                     | 0.52              |
| 1:I:506:LYS:HG2  | 1:I:513:PHE:O    | 2.09                     | 0.52              |
| 1:I:734:LEU:HD13 | 1:I:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:I:914:LEU:HB3  | 1:I:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:J:213:GLU:HB2  | 1:J:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:J:239:TRP:CE3  | 1:J:252:LEU:HG   | 2.44                     | 0.52              |
| 1:J:917:ARG:N    | 1:J:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:L:414:VAL:HA   | 1:L:442:PHE:CZ   | 2.44                     | 0.52              |
| 1:L:734:LEU:HD13 | 1:L:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:L:759:CYS:HA   | 1:L:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:L:872:LEU:HA   | 1:L:875:LYS:HZ3  | 1.74                     | 0.52              |
| 1:L:917:ARG:N    | 1:L:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:A:876:MET:HA   | 1:A:881:CYS:SG   | 2.49                     | 0.52              |
| 1:B:247:ASP:O    | 1:B:292:ARG:NH2  | 2.31                     | 0.52              |
| 1:B:307:PHE:CD2  | 1:B:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:B:734:LEU:HD13 | 1:B:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:B:917:ARG:N    | 1:B:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:E:958:LEU:O    | 1:E:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:F:213:GLU:HB2  | 1:F:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:F:608:LYS:HA   | 1:F:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:F:743:LEU:HD21 | 1:F:745:LEU:HG   | 1.91                     | 0.52              |
| 1:F:958:LEU:O    | 1:F:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:G:414:VAL:HA   | 1:G:442:PHE:CZ   | 2.44                     | 0.52              |
| 1:H:649:PRO:O    | 1:H:675:LYS:N    | 2.36                     | 0.52              |
| 1:H:914:LEU:HB3  | 1:H:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:I:239:TRP:CE3  | 1:I:252:LEU:HG   | 2.44                     | 0.52              |
| 1:I:876:MET:HA   | 1:I:881:CYS:SG   | 2.49                     | 0.52              |
| 1:I:985:THR:O    | 1:I:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:K:239:TRP:CE3  | 1:K:252:LEU:HG   | 2.44                     | 0.52              |
| 1:K:327:LEU:HA   | 1:K:331:LEU:HG   | 1.91                     | 0.52              |
| 1:K:649:PRO:O    | 1:K:675:LYS:N    | 2.36                     | 0.52              |
| 1:K:872:LEU:HA   | 1:K:875:LYS:HZ3  | 1.75                     | 0.52              |
| 1:L:239:TRP:CE3  | 1:L:252:LEU:HG   | 2.44                     | 0.52              |
| 1:L:788:SER:HB2  | 1:L:818:GLY:HA3  | 1.91                     | 0.52              |
| 1:L:955:CYS:HB3  | 1:L:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:934:LEU:CA   | 1:A:961:ILE:HD11 | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:148:LYS:HB3  | 1:B:159:ASP:HB2  | 1.90                     | 0.52              |
| 1:B:608:LYS:HA   | 1:B:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:B:914:LEU:HB3  | 1:B:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:B:985:THR:O    | 1:B:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:C:958:LEU:O    | 1:C:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:D:160:LEU:HA   | 1:D:163:ARG:HB2  | 1.90                     | 0.52              |
| 1:E:668:ILE:HG22 | 1:E:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:F:252:LEU:HB3  | 1:F:296:LEU:HD13 | 1.90                     | 0.52              |
| 1:F:861:GLU:OE1  | 1:F:918:SER:OG   | 2.27                     | 0.52              |
| 1:F:914:LEU:HB3  | 1:F:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:G:861:GLU:OE1  | 1:G:918:SER:OG   | 2.27                     | 0.52              |
| 1:H:137:ARG:NH1  | 1:H:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:H:677:LEU:HD22 | 1:H:734:LEU:HD21 | 1.91                     | 0.52              |
| 1:H:830:TRP:CZ3  | 1:I:1009:ARG:NE  | 2.77                     | 0.52              |
| 1:H:917:ARG:N    | 1:H:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:I:307:PHE:CD2  | 1:I:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:I:917:ARG:N    | 1:I:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:I:934:LEU:CA   | 1:I:961:ILE:HD11 | 2.39                     | 0.52              |
| 1:J:137:ARG:NH1  | 1:J:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:K:307:PHE:CD2  | 1:K:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:K:759:CYS:HA   | 1:K:790:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:137:ARG:NH1  | 1:A:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:A:213:GLU:HB2  | 1:A:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:A:239:TRP:CE3  | 1:A:252:LEU:HG   | 2.44                     | 0.52              |
| 1:A:914:LEU:HB3  | 1:A:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:B:743:LEU:HD21 | 1:B:745:LEU:HG   | 1.91                     | 0.52              |
| 1:C:876:MET:HA   | 1:C:881:CYS:SG   | 2.49                     | 0.52              |
| 1:C:917:ARG:N    | 1:C:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:D:414:VAL:HA   | 1:D:442:PHE:CZ   | 2.44                     | 0.52              |
| 1:D:734:LEU:HA   | 1:D:737:ASN:HD22 | 1.74                     | 0.52              |
| 1:D:861:GLU:OE1  | 1:D:918:SER:OG   | 2.27                     | 0.52              |
| 1:E:213:GLU:HB2  | 1:E:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:E:252:LEU:HB3  | 1:E:296:LEU:HD13 | 1.91                     | 0.52              |
| 1:E:955:CYS:HB3  | 1:E:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:F:788:SER:HB2  | 1:F:818:GLY:HA3  | 1.91                     | 0.52              |
| 1:G:842:GLN:O    | 1:G:846:LEU:HG   | 2.09                     | 0.52              |
| 1:G:917:ARG:N    | 1:G:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:H:955:CYS:HB3  | 1:H:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:I:213:GLU:HB2  | 1:I:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:I:608:LYS:HA   | 1:I:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:J:871:VAL:HG12 | 1:J:875:LYS:HZ2  | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:934:LEU:CA   | 1:J:961:ILE:HD11 | 2.39                     | 0.52              |
| 1:K:788:SER:HB2  | 1:K:818:GLY:HA3  | 1.91                     | 0.52              |
| 1:K:958:LEU:O    | 1:K:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:L:307:PHE:CD2  | 1:L:567:GLU:HB2  | 2.44                     | 0.52              |
| 1:L:958:LEU:O    | 1:L:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:A:734:LEU:HD13 | 1:A:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:C:914:LEU:HB3  | 1:C:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:C:955:CYS:HB3  | 1:C:986:LEU:HD21 | 1.91                     | 0.52              |
| 1:D:559:LEU:HD12 | 1:D:560:LEU:N    | 2.25                     | 0.52              |
| 1:D:842:GLN:O    | 1:D:846:LEU:HG   | 2.09                     | 0.52              |
| 1:E:842:GLN:O    | 1:E:846:LEU:HG   | 2.09                     | 0.52              |
| 1:E:861:GLU:OE1  | 1:E:918:SER:OG   | 2.27                     | 0.52              |
| 1:E:914:LEU:HB3  | 1:E:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:E:917:ARG:N    | 1:E:919:ASN:OD1  | 2.43                     | 0.52              |
| 1:F:137:ARG:NH1  | 1:F:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:F:668:ILE:HG22 | 1:F:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:G:559:LEU:HD12 | 1:G:560:LEU:N    | 2.25                     | 0.52              |
| 1:G:734:LEU:HA   | 1:G:737:ASN:HD22 | 1.74                     | 0.52              |
| 1:H:637:GLU:OE2  | 1:H:640:PHE:N    | 2.28                     | 0.52              |
| 1:H:958:LEU:O    | 1:H:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:J:668:ILE:HG22 | 1:J:737:ASN:HD21 | 1.74                     | 0.52              |
| 1:J:876:MET:HA   | 1:J:881:CYS:SG   | 2.49                     | 0.52              |
| 1:J:914:LEU:HB3  | 1:J:943:LEU:HD12 | 1.92                     | 0.52              |
| 1:L:473:ILE:O    | 1:L:568:LYS:HA   | 2.10                     | 0.52              |
| 1:L:649:PRO:O    | 1:L:675:LYS:N    | 2.36                     | 0.52              |
| 1:B:137:ARG:NH1  | 1:B:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:B:213:GLU:HB2  | 1:B:214:PRO:HD3  | 1.91                     | 0.52              |
| 1:B:768:ASN:H    | 1:B:796:LYS:HZ3  | 1.57                     | 0.52              |
| 1:C:137:ARG:NH1  | 1:C:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:C:263:ARG:HH21 | 1:C:325:ASP:CG   | 2.13                     | 0.52              |
| 1:C:473:ILE:O    | 1:C:568:LYS:HA   | 2.10                     | 0.52              |
| 1:C:768:ASN:H    | 1:C:796:LYS:HZ3  | 1.57                     | 0.52              |
| 1:D:734:LEU:HD13 | 1:D:769:ILE:HD11 | 1.91                     | 0.52              |
| 1:D:743:LEU:HD21 | 1:D:745:LEU:HG   | 1.91                     | 0.52              |
| 1:D:958:LEU:O    | 1:D:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:G:608:LYS:HA   | 1:G:611:GLU:OE2  | 2.09                     | 0.52              |
| 1:G:743:LEU:HD21 | 1:G:745:LEU:HG   | 1.91                     | 0.52              |
| 1:G:958:LEU:O    | 1:G:961:ILE:HG22 | 2.10                     | 0.52              |
| 1:G:985:THR:O    | 1:G:988:GLU:HG3  | 2.10                     | 0.52              |
| 1:H:263:ARG:HH21 | 1:H:325:ASP:CG   | 2.13                     | 0.52              |
| 1:H:473:ILE:O    | 1:H:568:LYS:HA   | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:401:LEU:HD22 | 1:K:404:MET:HE3  | 1.92                     | 0.52              |
| 1:L:137:ARG:NH1  | 1:L:141:ARG:HH22 | 2.08                     | 0.52              |
| 1:B:473:ILE:O    | 1:B:568:LYS:HA   | 2.10                     | 0.51              |
| 1:B:851:ASN:OD1  | 1:B:852:HIS:N    | 2.44                     | 0.51              |
| 1:C:677:LEU:HD22 | 1:C:734:LEU:HD21 | 1.91                     | 0.51              |
| 1:D:473:ILE:O    | 1:D:568:LYS:HA   | 2.10                     | 0.51              |
| 1:D:608:LYS:HA   | 1:D:611:GLU:OE2  | 2.09                     | 0.51              |
| 1:D:917:ARG:N    | 1:D:919:ASN:OD1  | 2.43                     | 0.51              |
| 1:D:985:THR:O    | 1:D:988:GLU:HG3  | 2.10                     | 0.51              |
| 1:E:506:LYS:HG2  | 1:E:513:PHE:O    | 2.09                     | 0.51              |
| 1:F:559:LEU:HD12 | 1:F:560:LEU:N    | 2.25                     | 0.51              |
| 1:I:137:ARG:NH1  | 1:I:141:ARG:HH22 | 2.08                     | 0.51              |
| 1:I:759:CYS:HA   | 1:I:790:VAL:HG11 | 1.91                     | 0.51              |
| 1:J:559:LEU:HD12 | 1:J:560:LEU:N    | 2.25                     | 0.51              |
| 1:K:137:ARG:NH1  | 1:K:141:ARG:HH22 | 2.08                     | 0.51              |
| 1:K:734:LEU:HA   | 1:K:737:ASN:HD22 | 1.74                     | 0.51              |
| 1:A:473:ILE:O    | 1:A:568:LYS:HA   | 2.10                     | 0.51              |
| 1:A:559:LEU:HD12 | 1:A:560:LEU:N    | 2.25                     | 0.51              |
| 1:B:759:CYS:HA   | 1:B:790:VAL:HG11 | 1.91                     | 0.51              |
| 1:C:899:SER:O    | 1:C:902:THR:OG1  | 2.22                     | 0.51              |
| 1:D:851:ASN:OD1  | 1:D:852:HIS:N    | 2.44                     | 0.51              |
| 1:E:137:ARG:NH1  | 1:E:141:ARG:HH22 | 2.08                     | 0.51              |
| 1:E:247:ASP:O    | 1:E:292:ARG:NH2  | 2.31                     | 0.51              |
| 1:F:506:LYS:HG2  | 1:F:513:PHE:O    | 2.09                     | 0.51              |
| 1:F:851:ASN:OD1  | 1:F:852:HIS:N    | 2.44                     | 0.51              |
| 1:G:473:ILE:O    | 1:G:568:LYS:HA   | 2.10                     | 0.51              |
| 1:G:734:LEU:HD13 | 1:G:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:H:250:ASP:H    | 1:H:292:ARG:HB3  | 1.75                     | 0.51              |
| 1:I:473:ILE:O    | 1:I:568:LYS:HA   | 2.10                     | 0.51              |
| 1:I:851:ASN:OD1  | 1:I:852:HIS:N    | 2.44                     | 0.51              |
| 1:J:263:ARG:HH21 | 1:J:325:ASP:CG   | 2.13                     | 0.51              |
| 1:K:148:LYS:HB3  | 1:K:159:ASP:HB2  | 1.90                     | 0.51              |
| 1:K:473:ILE:O    | 1:K:568:LYS:HA   | 2.10                     | 0.51              |
| 1:K:914:LEU:HB3  | 1:K:943:LEU:HD12 | 1.92                     | 0.51              |
| 1:K:934:LEU:CA   | 1:K:961:ILE:HD11 | 2.39                     | 0.51              |
| 1:L:148:LYS:HB3  | 1:L:159:ASP:HB2  | 1.90                     | 0.51              |
| 1:L:250:ASP:H    | 1:L:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:L:914:LEU:HB3  | 1:L:943:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:613:LYS:HD2  | 1:A:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:934:LEU:CA   | 1:B:961:ILE:HD11 | 2.39                     | 0.51              |
| 1:C:851:ASN:OD1  | 1:C:852:HIS:N    | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:759:CYS:HA   | 1:D:790:VAL:HG11 | 1.91                     | 0.51              |
| 1:E:473:ILE:O    | 1:E:568:LYS:HA   | 2.10                     | 0.51              |
| 1:E:851:ASN:OD1  | 1:E:852:HIS:N    | 2.44                     | 0.51              |
| 1:F:473:ILE:O    | 1:F:568:LYS:HA   | 2.10                     | 0.51              |
| 1:F:917:ARG:N    | 1:F:919:ASN:OD1  | 2.43                     | 0.51              |
| 1:G:252:LEU:HB3  | 1:G:296:LEU:HD13 | 1.91                     | 0.51              |
| 1:G:759:CYS:HA   | 1:G:790:VAL:HG11 | 1.91                     | 0.51              |
| 1:J:473:ILE:O    | 1:J:568:LYS:HA   | 2.10                     | 0.51              |
| 1:J:613:LYS:HD2  | 1:J:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:K:250:ASP:H    | 1:K:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:K:470:ALA:HB2  | 1:K:526:ALA:HA   | 1.93                     | 0.51              |
| 1:L:934:LEU:CA   | 1:L:961:ILE:HD11 | 2.39                     | 0.51              |
| 1:A:250:ASP:H    | 1:A:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:B:250:ASP:H    | 1:B:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:B:613:LYS:HD2  | 1:B:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:773:TRP:NE1  | 1:B:799:GLU:OE2  | 2.44                     | 0.51              |
| 1:C:861:GLU:HA   | 1:C:889:VAL:HA   | 1.92                     | 0.51              |
| 1:E:559:LEU:HD12 | 1:E:560:LEU:N    | 2.25                     | 0.51              |
| 1:G:851:ASN:OD1  | 1:G:852:HIS:N    | 2.44                     | 0.51              |
| 1:H:401:LEU:HD22 | 1:H:404:MET:HE3  | 1.93                     | 0.51              |
| 1:H:559:LEU:HD12 | 1:H:560:LEU:N    | 2.25                     | 0.51              |
| 1:H:851:ASN:OD1  | 1:H:852:HIS:N    | 2.44                     | 0.51              |
| 1:H:861:GLU:HA   | 1:H:889:VAL:HA   | 1.92                     | 0.51              |
| 1:I:613:LYS:HD2  | 1:I:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:I:668:ILE:HG22 | 1:I:737:ASN:HD21 | 1.74                     | 0.51              |
| 1:I:773:TRP:NE1  | 1:I:799:GLU:OE2  | 2.44                     | 0.51              |
| 1:J:250:ASP:H    | 1:J:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:J:734:LEU:HD13 | 1:J:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:J:958:LEU:O    | 1:J:961:ILE:HG22 | 2.10                     | 0.51              |
| 1:K:851:ASN:OD1  | 1:K:852:HIS:N    | 2.44                     | 0.51              |
| 1:L:734:LEU:HA   | 1:L:737:ASN:HD22 | 1.74                     | 0.51              |
| 1:L:851:ASN:OD1  | 1:L:852:HIS:N    | 2.44                     | 0.51              |
| 1:A:958:LEU:O    | 1:A:961:ILE:HG22 | 2.10                     | 0.51              |
| 1:B:668:ILE:HG22 | 1:B:737:ASN:HD21 | 1.74                     | 0.51              |
| 1:C:470:ALA:HB2  | 1:C:526:ALA:HA   | 1.93                     | 0.51              |
| 1:D:137:ARG:NH1  | 1:D:141:ARG:HH22 | 2.08                     | 0.51              |
| 1:E:732:SER:O    | 1:E:735:SER:OG   | 2.20                     | 0.51              |
| 1:G:263:ARG:HH21 | 1:G:325:ASP:CG   | 2.13                     | 0.51              |
| 1:H:613:LYS:HD2  | 1:H:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:I:250:ASP:H    | 1:I:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:I:434:THR:H    | 1:I:437:ALA:HB3  | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:872:LEU:HA   | 1:J:875:LYS:HZ3  | 1.75                     | 0.51              |
| 1:K:985:THR:O    | 1:K:988:GLU:HG3  | 2.10                     | 0.51              |
| 1:L:470:ALA:HB2  | 1:L:526:ALA:HA   | 1.93                     | 0.51              |
| 1:L:559:LEU:HD12 | 1:L:560:LEU:N    | 2.25                     | 0.51              |
| 1:L:677:LEU:HD22 | 1:L:734:LEU:HD21 | 1.92                     | 0.51              |
| 1:L:985:THR:O    | 1:L:988:GLU:HG3  | 2.10                     | 0.51              |
| 1:A:263:ARG:HH21 | 1:A:325:ASP:CG   | 2.13                     | 0.51              |
| 1:A:851:ASN:OD1  | 1:A:852:HIS:N    | 2.44                     | 0.51              |
| 1:B:677:LEU:HD22 | 1:B:734:LEU:HD21 | 1.91                     | 0.51              |
| 1:C:250:ASP:H    | 1:C:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:D:167:LEU:HD22 | 1:D:368:GLY:HA2  | 1.91                     | 0.51              |
| 1:D:213:GLU:HB2  | 1:D:214:PRO:HD3  | 1.91                     | 0.51              |
| 1:D:252:LEU:HB3  | 1:D:296:LEU:HD13 | 1.90                     | 0.51              |
| 1:D:677:LEU:HD22 | 1:D:734:LEU:HD21 | 1.91                     | 0.51              |
| 1:D:899:SER:O    | 1:D:902:THR:OG1  | 2.22                     | 0.51              |
| 1:D:955:CYS:HB3  | 1:D:986:LEU:HD21 | 1.91                     | 0.51              |
| 1:E:677:LEU:HD22 | 1:E:734:LEU:HD21 | 1.92                     | 0.51              |
| 1:F:247:ASP:O    | 1:F:292:ARG:NH2  | 2.31                     | 0.51              |
| 1:F:842:GLN:O    | 1:F:846:LEU:HG   | 2.09                     | 0.51              |
| 1:G:137:ARG:NH1  | 1:G:141:ARG:HH22 | 2.08                     | 0.51              |
| 1:G:213:GLU:HB2  | 1:G:214:PRO:HD3  | 1.91                     | 0.51              |
| 1:G:677:LEU:HD22 | 1:G:734:LEU:HD21 | 1.91                     | 0.51              |
| 1:G:955:CYS:HB3  | 1:G:986:LEU:HD21 | 1.91                     | 0.51              |
| 1:I:167:LEU:HD22 | 1:I:368:GLY:HA2  | 1.91                     | 0.51              |
| 1:K:213:GLU:HB2  | 1:K:214:PRO:HD3  | 1.91                     | 0.51              |
| 1:K:559:LEU:HD12 | 1:K:560:LEU:N    | 2.25                     | 0.51              |
| 1:K:677:LEU:HD22 | 1:K:734:LEU:HD21 | 1.92                     | 0.51              |
| 1:L:213:GLU:HB2  | 1:L:214:PRO:HD3  | 1.91                     | 0.51              |
| 1:A:659:MET:HA   | 1:A:662:VAL:HG22 | 1.93                     | 0.51              |
| 1:B:958:LEU:O    | 1:B:961:ILE:HG22 | 2.10                     | 0.51              |
| 1:C:559:LEU:HD12 | 1:C:560:LEU:N    | 2.25                     | 0.51              |
| 1:D:263:ARG:HH21 | 1:D:325:ASP:CG   | 2.13                     | 0.51              |
| 1:D:434:THR:H    | 1:D:437:ALA:HB3  | 1.76                     | 0.51              |
| 1:E:263:ARG:HH21 | 1:E:325:ASP:CG   | 2.13                     | 0.51              |
| 1:E:734:LEU:HD13 | 1:E:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:F:250:ASP:H    | 1:F:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:F:734:LEU:HD13 | 1:F:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:G:434:THR:H    | 1:G:437:ALA:HB3  | 1.76                     | 0.51              |
| 1:G:773:TRP:NE1  | 1:G:799:GLU:OE2  | 2.44                     | 0.51              |
| 1:G:900:ALA:O    | 1:G:903:SER:OG   | 2.26                     | 0.51              |
| 1:J:659:MET:HA   | 1:J:662:VAL:HG22 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:851:ASN:OD1  | 1:J:852:HIS:N    | 2.44                     | 0.51              |
| 1:J:985:THR:O    | 1:J:988:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:167:LEU:HD22 | 1:B:368:GLY:HA2  | 1.91                     | 0.51              |
| 1:B:434:THR:H    | 1:B:437:ALA:HB3  | 1.76                     | 0.51              |
| 1:C:613:LYS:HD2  | 1:C:628:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:887:GLY:HA2  | 1:C:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:D:247:ASP:O    | 1:D:292:ARG:NH2  | 2.31                     | 0.51              |
| 1:E:861:GLU:HA   | 1:E:889:VAL:HA   | 1.92                     | 0.51              |
| 1:F:773:TRP:NE1  | 1:F:799:GLU:OE2  | 2.44                     | 0.51              |
| 1:G:247:ASP:O    | 1:G:292:ARG:NH2  | 2.31                     | 0.51              |
| 1:G:250:ASP:H    | 1:G:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:G:899:SER:O    | 1:G:902:THR:OG1  | 2.22                     | 0.51              |
| 1:H:470:ALA:HB2  | 1:H:526:ALA:HA   | 1.93                     | 0.51              |
| 1:H:668:ILE:HG22 | 1:H:737:ASN:HD21 | 1.74                     | 0.51              |
| 1:H:887:GLY:HA2  | 1:H:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:I:677:LEU:HD22 | 1:I:734:LEU:HD21 | 1.91                     | 0.51              |
| 1:J:861:GLU:HA   | 1:J:889:VAL:HA   | 1.93                     | 0.51              |
| 1:K:767:CYS:SG   | 1:K:796:LYS:NZ   | 2.82                     | 0.51              |
| 1:A:985:THR:O    | 1:A:988:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:887:GLY:HA2  | 1:B:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:C:668:ILE:HG22 | 1:C:737:ASN:HD21 | 1.74                     | 0.51              |
| 1:C:734:LEU:HD13 | 1:C:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:D:773:TRP:NE1  | 1:D:799:GLU:OE2  | 2.44                     | 0.51              |
| 1:E:659:MET:HA   | 1:E:662:VAL:HG22 | 1.93                     | 0.51              |
| 1:E:887:GLY:HA2  | 1:E:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:F:887:GLY:HA2  | 1:F:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:F:899:SER:O    | 1:F:902:THR:OG1  | 2.22                     | 0.51              |
| 1:G:167:LEU:HD22 | 1:G:368:GLY:HA2  | 1.91                     | 0.51              |
| 1:H:734:LEU:HD13 | 1:H:769:ILE:HD11 | 1.91                     | 0.51              |
| 1:I:559:LEU:HD12 | 1:I:560:LEU:N    | 2.25                     | 0.51              |
| 1:I:887:GLY:HA2  | 1:I:915:TYR:HB2  | 1.93                     | 0.51              |
| 1:J:291:SER:OG   | 1:J:339:LYS:O    | 2.28                     | 0.51              |
| 1:L:767:CYS:SG   | 1:L:796:LYS:NZ   | 2.82                     | 0.51              |
| 1:A:861:GLU:HA   | 1:A:889:VAL:HA   | 1.93                     | 0.51              |
| 1:D:250:ASP:H    | 1:D:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:D:934:LEU:CA   | 1:D:961:ILE:HD11 | 2.39                     | 0.51              |
| 1:E:250:ASP:H    | 1:E:292:ARG:HB3  | 1.76                     | 0.51              |
| 1:F:263:ARG:HH21 | 1:F:325:ASP:CG   | 2.13                     | 0.51              |
| 1:F:861:GLU:HA   | 1:F:889:VAL:HA   | 1.92                     | 0.51              |
| 1:H:659:MET:HA   | 1:H:662:VAL:HG22 | 1.93                     | 0.51              |
| 1:H:983:VAL:HA   | 1:H:986:LEU:HD12 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:649:PRO:O    | 1:I:675:LYS:N     | 2.36                     | 0.51              |
| 1:I:958:LEU:O    | 1:I:961:ILE:HG22  | 2.10                     | 0.51              |
| 1:K:861:GLU:HA   | 1:K:889:VAL:HA    | 1.92                     | 0.51              |
| 1:L:659:MET:HA   | 1:L:662:VAL:HG22  | 1.93                     | 0.51              |
| 1:L:917:ARG:O    | 1:L:919:ASN:ND2   | 2.44                     | 0.51              |
| 1:A:917:ARG:O    | 1:A:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:C:649:PRO:O    | 1:C:675:LYS:N     | 2.36                     | 0.50              |
| 1:D:887:GLY:HA2  | 1:D:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:E:773:TRP:NE1  | 1:E:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:F:900:ALA:O    | 1:F:903:SER:OG    | 2.26                     | 0.50              |
| 1:G:613:LYS:HD2  | 1:G:628:LEU:HD11  | 1.93                     | 0.50              |
| 1:G:983:VAL:HA   | 1:G:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:H:773:TRP:NE1  | 1:H:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:H:899:SER:O    | 1:H:902:THR:OG1   | 2.22                     | 0.50              |
| 1:K:659:MET:HA   | 1:K:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:K:917:ARG:O    | 1:K:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:A:773:TRP:NE1  | 1:A:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:B:559:LEU:HD12 | 1:B:560:LEU:N     | 2.25                     | 0.50              |
| 1:B:649:PRO:O    | 1:B:675:LYS:N     | 2.36                     | 0.50              |
| 1:B:861:GLU:HA   | 1:B:889:VAL:HA    | 1.92                     | 0.50              |
| 1:B:1016:GLU:HA  | 1:B:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:C:659:MET:HA   | 1:C:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:C:773:TRP:NE1  | 1:C:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:C:983:VAL:HA   | 1:C:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:D:613:LYS:HD2  | 1:D:628:LEU:HD11  | 1.93                     | 0.50              |
| 1:D:983:VAL:HA   | 1:D:986:LEU:HD12  | 1.94                     | 0.50              |
| 1:E:557:LYS:NZ   | 1:E:605:GLU:OE1   | 2.28                     | 0.50              |
| 1:E:731:PHE:CD2  | 1:E:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:E:917:ARG:O    | 1:E:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:E:960:THR:O    | 1:E:963:THR:OG1   | 2.24                     | 0.50              |
| 1:F:677:LEU:HD22 | 1:F:734:LEU:HD21  | 1.91                     | 0.50              |
| 1:F:731:PHE:CD2  | 1:F:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:G:580:GLY:O    | 1:G:586:ARG:NE    | 2.44                     | 0.50              |
| 1:G:887:GLY:HA2  | 1:G:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:I:960:THR:O    | 1:I:963:THR:OG1   | 2.24                     | 0.50              |
| 1:J:917:ARG:O    | 1:J:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:K:1016:GLU:HA  | 1:K:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:L:731:PHE:CD2  | 1:L:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:A:731:PHE:CD2  | 1:A:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:A:887:GLY:HA2  | 1:A:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:A:962:LEU:HD11 | 1:A:968:LEU:H     | 1.77                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:983:VAL:HA   | 1:A:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:B:263:ARG:HH21 | 1:B:325:ASP:CG    | 2.13                     | 0.50              |
| 1:B:369:PHE:O    | 1:B:406:PHE:HA    | 2.12                     | 0.50              |
| 1:B:470:ALA:HB2  | 1:B:526:ALA:HA    | 1.93                     | 0.50              |
| 1:C:580:GLY:O    | 1:C:586:ARG:NE    | 2.44                     | 0.50              |
| 1:C:731:PHE:CD2  | 1:C:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:C:962:LEU:HD11 | 1:C:968:LEU:H     | 1.77                     | 0.50              |
| 1:D:580:GLY:O    | 1:D:586:ARG:NE    | 2.44                     | 0.50              |
| 1:E:470:ALA:HB2  | 1:E:526:ALA:HA    | 1.93                     | 0.50              |
| 1:F:470:ALA:HB2  | 1:F:526:ALA:HA    | 1.93                     | 0.50              |
| 1:F:580:GLY:O    | 1:F:586:ARG:NE    | 2.45                     | 0.50              |
| 1:F:659:MET:HA   | 1:F:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:F:917:ARG:O    | 1:F:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:F:1016:GLU:HA  | 1:F:1019:GLN:HE22 | 1.77                     | 0.50              |
| 1:G:934:LEU:CA   | 1:G:961:ILE:HD11  | 2.39                     | 0.50              |
| 1:H:369:PHE:O    | 1:H:406:PHE:HA    | 2.12                     | 0.50              |
| 1:H:1016:GLU:HA  | 1:H:1019:GLN:HE22 | 1.77                     | 0.50              |
| 1:I:263:ARG:HH21 | 1:I:325:ASP:CG    | 2.13                     | 0.50              |
| 1:I:369:PHE:O    | 1:I:406:PHE:HA    | 2.12                     | 0.50              |
| 1:I:768:ASN:H    | 1:I:796:LYS:HZ3   | 1.59                     | 0.50              |
| 1:I:861:GLU:HA   | 1:I:889:VAL:HA    | 1.92                     | 0.50              |
| 1:I:1016:GLU:HA  | 1:I:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:J:580:GLY:O    | 1:J:586:ARG:NE    | 2.44                     | 0.50              |
| 1:J:773:TRP:NE1  | 1:J:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:J:887:GLY:HA2  | 1:J:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:K:369:PHE:O    | 1:K:406:PHE:HA    | 2.12                     | 0.50              |
| 1:L:369:PHE:O    | 1:L:406:PHE:HA    | 2.12                     | 0.50              |
| 1:L:1016:GLU:HA  | 1:L:1019:GLN:HE22 | 1.77                     | 0.50              |
| 1:A:580:GLY:O    | 1:A:586:ARG:NE    | 2.44                     | 0.50              |
| 1:A:1016:GLU:HA  | 1:A:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:D:369:PHE:O    | 1:D:406:PHE:HA    | 2.12                     | 0.50              |
| 1:D:637:GLU:OE2  | 1:D:640:PHE:N     | 2.28                     | 0.50              |
| 1:D:659:MET:HA   | 1:D:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:E:900:ALA:O    | 1:E:903:SER:OG    | 2.26                     | 0.50              |
| 1:E:1016:GLU:HA  | 1:E:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:F:434:THR:H    | 1:F:437:ALA:HB3   | 1.76                     | 0.50              |
| 1:G:401:LEU:HD22 | 1:G:404:MET:HE3   | 1.93                     | 0.50              |
| 1:I:983:VAL:HA   | 1:I:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:J:470:ALA:HB2  | 1:J:526:ALA:HA    | 1.93                     | 0.50              |
| 1:J:731:PHE:CD2  | 1:J:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:J:809:ASP:C    | 1:J:811:GLY:H     | 2.15                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:962:LEU:HD11 | 1:J:968:LEU:H     | 1.77                     | 0.50              |
| 1:K:731:PHE:CD2  | 1:K:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:K:887:GLY:HA2  | 1:K:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:K:900:ALA:O    | 1:K:903:SER:OG    | 2.26                     | 0.50              |
| 1:L:773:TRP:NE1  | 1:L:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:L:861:GLU:HA   | 1:L:889:VAL:HA    | 1.92                     | 0.50              |
| 1:L:887:GLY:HA2  | 1:L:915:TYR:HB2   | 1.93                     | 0.50              |
| 1:A:470:ALA:HB2  | 1:A:526:ALA:HA    | 1.93                     | 0.50              |
| 1:B:580:GLY:O    | 1:B:586:ARG:NE    | 2.44                     | 0.50              |
| 1:B:983:VAL:HA   | 1:B:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:E:369:PHE:O    | 1:E:406:PHE:HA    | 2.12                     | 0.50              |
| 1:E:434:THR:H    | 1:E:437:ALA:HB3   | 1.76                     | 0.50              |
| 1:E:580:GLY:O    | 1:E:586:ARG:NE    | 2.45                     | 0.50              |
| 1:F:401:LEU:HD22 | 1:F:404:MET:HE3   | 1.92                     | 0.50              |
| 1:G:369:PHE:O    | 1:G:406:PHE:HA    | 2.12                     | 0.50              |
| 1:H:580:GLY:O    | 1:H:586:ARG:NE    | 2.44                     | 0.50              |
| 1:H:731:PHE:CD2  | 1:H:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:I:580:GLY:O    | 1:I:586:ARG:NE    | 2.44                     | 0.50              |
| 1:J:1016:GLU:HA  | 1:J:1019:GLN:HE22 | 1.76                     | 0.50              |
| 1:K:580:GLY:O    | 1:K:586:ARG:NE    | 2.44                     | 0.50              |
| 1:L:291:SER:OG   | 1:L:339:LYS:O     | 2.28                     | 0.50              |
| 1:L:580:GLY:O    | 1:L:586:ARG:NE    | 2.44                     | 0.50              |
| 1:B:871:VAL:HG12 | 1:B:875:LYS:HZ2   | 1.76                     | 0.50              |
| 1:C:369:PHE:O    | 1:C:406:PHE:HA    | 2.12                     | 0.50              |
| 1:C:1016:GLU:HA  | 1:C:1019:GLN:HE22 | 1.77                     | 0.50              |
| 1:G:659:MET:HA   | 1:G:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:G:917:ARG:O    | 1:G:919:ASN:ND2   | 2.44                     | 0.50              |
| 1:H:809:ASP:C    | 1:H:811:GLY:H     | 2.15                     | 0.50              |
| 1:I:809:ASP:C    | 1:I:811:GLY:H     | 2.15                     | 0.50              |
| 1:I:872:LEU:HD23 | 1:I:875:LYS:HZ1   | 1.77                     | 0.50              |
| 1:J:983:VAL:HA   | 1:J:986:LEU:HD12  | 1.93                     | 0.50              |
| 1:K:434:THR:H    | 1:K:437:ALA:HB3   | 1.76                     | 0.50              |
| 1:K:773:TRP:NE1  | 1:K:799:GLU:OE2   | 2.44                     | 0.50              |
| 1:L:434:THR:H    | 1:L:437:ALA:HB3   | 1.76                     | 0.50              |
| 1:L:613:LYS:HD2  | 1:L:628:LEU:HD11  | 1.93                     | 0.50              |
| 1:L:900:ALA:O    | 1:L:903:SER:OG    | 2.26                     | 0.50              |
| 1:A:291:SER:OG   | 1:A:339:LYS:O     | 2.28                     | 0.50              |
| 1:A:369:PHE:O    | 1:A:406:PHE:HA    | 2.12                     | 0.50              |
| 1:B:659:MET:HA   | 1:B:662:VAL:HG22  | 1.93                     | 0.50              |
| 1:B:731:PHE:CD2  | 1:B:758:LEU:HD13  | 2.47                     | 0.50              |
| 1:C:434:THR:H    | 1:C:437:ALA:HB3   | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:883:LEU:HD21 | 1:E:886:LEU:HD13 | 1.94                     | 0.50              |
| 1:F:883:LEU:HD21 | 1:F:886:LEU:HD13 | 1.94                     | 0.50              |
| 1:H:962:LEU:HD11 | 1:H:968:LEU:H    | 1.77                     | 0.50              |
| 1:J:369:PHE:O    | 1:J:406:PHE:HA   | 2.12                     | 0.50              |
| 1:K:291:SER:OG   | 1:K:339:LYS:O    | 2.28                     | 0.50              |
| 1:K:770:GLN:O    | 1:K:798:VAL:HG22 | 2.12                     | 0.50              |
| 1:K:883:LEU:HD21 | 1:K:886:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:809:ASP:C    | 1:A:811:GLY:H    | 2.15                     | 0.50              |
| 1:B:883:LEU:HD21 | 1:B:886:LEU:HD13 | 1.94                     | 0.50              |
| 1:C:312:GLY:HA3  | 1:C:332:ILE:HD11 | 1.94                     | 0.50              |
| 1:D:770:GLN:O    | 1:D:798:VAL:HG22 | 2.12                     | 0.50              |
| 1:D:917:ARG:O    | 1:D:919:ASN:ND2  | 2.44                     | 0.50              |
| 1:F:914:LEU:HG   | 1:F:916:LEU:HD23 | 1.94                     | 0.50              |
| 1:H:312:GLY:HA3  | 1:H:332:ILE:HD11 | 1.94                     | 0.50              |
| 1:H:914:LEU:HG   | 1:H:916:LEU:HD23 | 1.94                     | 0.50              |
| 1:H:917:ARG:O    | 1:H:919:ASN:ND2  | 2.44                     | 0.50              |
| 1:I:470:ALA:HB2  | 1:I:526:ALA:HA   | 1.93                     | 0.50              |
| 1:I:659:MET:HA   | 1:I:662:VAL:HG22 | 1.93                     | 0.50              |
| 1:J:312:GLY:HA3  | 1:J:332:ILE:HD11 | 1.94                     | 0.50              |
| 1:J:434:THR:H    | 1:J:437:ALA:HB3  | 1.76                     | 0.50              |
| 1:K:613:LYS:HD2  | 1:K:628:LEU:HD11 | 1.93                     | 0.50              |
| 1:L:770:GLN:O    | 1:L:798:VAL:HG22 | 2.12                     | 0.50              |
| 1:A:434:THR:H    | 1:A:437:ALA:HB3  | 1.76                     | 0.50              |
| 1:A:1009:ARG:NE  | 1:L:830:TRP:CZ3  | 2.80                     | 0.50              |
| 1:B:914:LEU:HG   | 1:B:916:LEU:HD23 | 1.94                     | 0.50              |
| 1:B:917:ARG:O    | 1:B:919:ASN:ND2  | 2.44                     | 0.50              |
| 1:C:809:ASP:C    | 1:C:811:GLY:H    | 2.15                     | 0.50              |
| 1:C:872:LEU:HD23 | 1:C:875:LYS:HZ1  | 1.77                     | 0.50              |
| 1:C:914:LEU:HG   | 1:C:916:LEU:HD23 | 1.94                     | 0.50              |
| 1:E:312:GLY:HA3  | 1:E:332:ILE:HD11 | 1.94                     | 0.50              |
| 1:E:327:LEU:HD13 | 1:E:331:LEU:HD11 | 1.94                     | 0.50              |
| 1:E:613:LYS:HD2  | 1:E:628:LEU:HD11 | 1.93                     | 0.50              |
| 1:F:327:LEU:HD13 | 1:F:331:LEU:HD11 | 1.94                     | 0.50              |
| 1:F:369:PHE:O    | 1:F:406:PHE:HA   | 2.12                     | 0.50              |
| 1:F:770:GLN:O    | 1:F:798:VAL:HG22 | 2.12                     | 0.50              |
| 1:G:770:GLN:O    | 1:G:798:VAL:HG22 | 2.12                     | 0.50              |
| 1:H:434:THR:H    | 1:H:437:ALA:HB3  | 1.76                     | 0.50              |
| 1:L:883:LEU:HD21 | 1:L:886:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:312:GLY:HA3  | 1:A:332:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:755:MET:CG   | 1:A:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:C:291:SER:OG   | 1:C:339:LYS:O    | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:731:PHE:CD2  | 1:D:758:LEU:HD13 | 2.47                     | 0.49              |
| 1:D:809:ASP:C    | 1:D:811:GLY:H    | 2.15                     | 0.49              |
| 1:E:770:GLN:O    | 1:E:798:VAL:HG22 | 2.12                     | 0.49              |
| 1:G:809:ASP:C    | 1:G:811:GLY:H    | 2.15                     | 0.49              |
| 1:I:731:PHE:CD2  | 1:I:758:LEU:HD13 | 2.47                     | 0.49              |
| 1:I:883:LEU:HD21 | 1:I:886:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:770:GLN:O    | 1:A:798:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:912:THR:HG23 | 1:A:913:HIS:ND1  | 2.28                     | 0.49              |
| 1:B:770:GLN:O    | 1:B:798:VAL:HG22 | 2.12                     | 0.49              |
| 1:C:917:ARG:O    | 1:C:919:ASN:ND2  | 2.44                     | 0.49              |
| 1:D:291:SER:OG   | 1:D:339:LYS:O    | 2.28                     | 0.49              |
| 1:D:401:LEU:HD22 | 1:D:404:MET:HE3  | 1.94                     | 0.49              |
| 1:D:883:LEU:HD21 | 1:D:886:LEU:HD13 | 1.94                     | 0.49              |
| 1:E:755:MET:CG   | 1:E:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:F:983:VAL:HA   | 1:F:986:LEU:HD12 | 1.93                     | 0.49              |
| 1:H:407:ILE:HD12 | 1:H:408:PRO:HD2  | 1.94                     | 0.49              |
| 1:I:914:LEU:HG   | 1:I:916:LEU:HD23 | 1.94                     | 0.49              |
| 1:J:755:MET:CG   | 1:J:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:K:263:ARG:HH21 | 1:K:325:ASP:CG   | 2.13                     | 0.49              |
| 1:K:935:HIS:ND1  | 1:K:936:PRO:O    | 2.43                     | 0.49              |
| 1:L:263:ARG:HH21 | 1:L:325:ASP:CG   | 2.13                     | 0.49              |
| 1:L:327:LEU:HD13 | 1:L:331:LEU:HD11 | 1.94                     | 0.49              |
| 1:L:912:THR:HG23 | 1:L:913:HIS:ND1  | 2.27                     | 0.49              |
| 1:E:894:THR:OG1  | 1:E:921:LEU:HA   | 2.12                     | 0.49              |
| 1:F:312:GLY:HA3  | 1:F:332:ILE:HD11 | 1.94                     | 0.49              |
| 1:F:613:LYS:HD2  | 1:F:628:LEU:HD11 | 1.93                     | 0.49              |
| 1:F:767:CYS:SG   | 1:F:796:LYS:NZ   | 2.82                     | 0.49              |
| 1:F:918:SER:H    | 1:F:946:ASP:HB3  | 1.77                     | 0.49              |
| 1:G:637:GLU:OE2  | 1:G:640:PHE:N    | 2.28                     | 0.49              |
| 1:G:731:PHE:CD2  | 1:G:758:LEU:HD13 | 2.47                     | 0.49              |
| 1:G:883:LEU:HD21 | 1:G:886:LEU:HD13 | 1.94                     | 0.49              |
| 1:I:770:GLN:O    | 1:I:798:VAL:HG22 | 2.12                     | 0.49              |
| 1:J:912:THR:HG23 | 1:J:913:HIS:ND1  | 2.28                     | 0.49              |
| 1:K:962:LEU:HD11 | 1:K:968:LEU:H    | 1.77                     | 0.49              |
| 1:B:809:ASP:C    | 1:B:811:GLY:H    | 2.15                     | 0.49              |
| 1:C:407:ILE:HD12 | 1:C:408:PRO:HD2  | 1.94                     | 0.49              |
| 1:D:912:THR:HG23 | 1:D:913:HIS:ND1  | 2.28                     | 0.49              |
| 1:E:138:ARG:HD3  | 1:E:141:ARG:HH21 | 1.78                     | 0.49              |
| 1:E:912:THR:HG23 | 1:E:913:HIS:ND1  | 2.27                     | 0.49              |
| 1:E:914:LEU:HG   | 1:E:916:LEU:HD23 | 1.94                     | 0.49              |
| 1:F:138:ARG:HD3  | 1:F:141:ARG:HH21 | 1.78                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:755:MET:CG   | 1:F:783:CYS:HB3   | 2.42                     | 0.49              |
| 1:G:894:THR:OG1  | 1:G:921:LEU:HA    | 2.12                     | 0.49              |
| 1:G:912:THR:HG23 | 1:G:913:HIS:ND1   | 2.28                     | 0.49              |
| 1:H:770:GLN:O    | 1:H:798:VAL:HG22  | 2.12                     | 0.49              |
| 1:H:918:SER:H    | 1:H:946:ASP:HB3   | 1.77                     | 0.49              |
| 1:I:291:SER:OG   | 1:I:339:LYS:O     | 2.28                     | 0.49              |
| 1:J:770:GLN:O    | 1:J:798:VAL:HG22  | 2.12                     | 0.49              |
| 1:K:327:LEU:HD13 | 1:K:331:LEU:HD11  | 1.94                     | 0.49              |
| 1:L:962:LEU:HD11 | 1:L:968:LEU:H     | 1.77                     | 0.49              |
| 1:L:983:VAL:HA   | 1:L:986:LEU:HD12  | 1.93                     | 0.49              |
| 1:A:914:LEU:HG   | 1:A:916:LEU:HD23  | 1.94                     | 0.49              |
| 1:B:327:LEU:HD13 | 1:B:331:LEU:HD11  | 1.94                     | 0.49              |
| 1:C:894:THR:OG1  | 1:C:920:ALA:O     | 2.31                     | 0.49              |
| 1:D:894:THR:OG1  | 1:D:921:LEU:HA    | 2.12                     | 0.49              |
| 1:E:1002:LEU:HB3 | 1:E:1005:MET:HE1  | 1.95                     | 0.49              |
| 1:F:407:ILE:HD12 | 1:F:408:PRO:HD2   | 1.94                     | 0.49              |
| 1:F:894:THR:OG1  | 1:F:921:LEU:HA    | 2.12                     | 0.49              |
| 1:G:632:LEU:HB3  | 1:G:641:VAL:HG22  | 1.95                     | 0.49              |
| 1:G:1016:GLU:HA  | 1:G:1019:GLN:HE22 | 1.76                     | 0.49              |
| 1:I:407:ILE:HD12 | 1:I:408:PRO:HD2   | 1.94                     | 0.49              |
| 1:I:917:ARG:O    | 1:I:919:ASN:ND2   | 2.44                     | 0.49              |
| 1:K:809:ASP:C    | 1:K:811:GLY:H     | 2.15                     | 0.49              |
| 1:K:912:THR:HG23 | 1:K:913:HIS:ND1   | 2.28                     | 0.49              |
| 1:K:983:VAL:HA   | 1:K:986:LEU:HD12  | 1.93                     | 0.49              |
| 1:L:809:ASP:C    | 1:L:811:GLY:H     | 2.15                     | 0.49              |
| 1:A:327:LEU:HD13 | 1:A:331:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:410:VAL:HA   | 1:A:413:ILE:HG22  | 1.95                     | 0.49              |
| 1:B:755:MET:CG   | 1:B:783:CYS:HB3   | 2.42                     | 0.49              |
| 1:C:912:THR:HG23 | 1:C:913:HIS:ND1   | 2.28                     | 0.49              |
| 1:C:918:SER:H    | 1:C:946:ASP:HB3   | 1.77                     | 0.49              |
| 1:D:755:MET:CG   | 1:D:783:CYS:HB3   | 2.42                     | 0.49              |
| 1:D:1016:GLU:HA  | 1:D:1019:GLN:HE22 | 1.76                     | 0.49              |
| 1:E:918:SER:H    | 1:E:946:ASP:HB3   | 1.77                     | 0.49              |
| 1:G:327:LEU:HD13 | 1:G:331:LEU:HD11  | 1.94                     | 0.49              |
| 1:G:810:PHE:HZ   | 1:H:785:PHE:HB3   | 1.76                     | 0.49              |
| 1:H:894:THR:OG1  | 1:H:921:LEU:HA    | 2.12                     | 0.49              |
| 1:H:912:THR:HG23 | 1:H:913:HIS:ND1   | 2.28                     | 0.49              |
| 1:H:1002:LEU:HB3 | 1:H:1005:MET:HE1  | 1.95                     | 0.49              |
| 1:I:755:MET:CG   | 1:I:783:CYS:HB3   | 2.42                     | 0.49              |
| 1:C:410:VAL:HA   | 1:C:413:ILE:HG22  | 1.95                     | 0.49              |
| 1:C:770:GLN:O    | 1:C:798:VAL:HG22  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:470:ALA:HB2  | 1:D:526:ALA:HA   | 1.93                     | 0.49              |
| 1:D:632:LEU:HB3  | 1:D:641:VAL:HG22 | 1.95                     | 0.49              |
| 1:D:861:GLU:HA   | 1:D:889:VAL:HA   | 1.92                     | 0.49              |
| 1:D:962:LEU:HD11 | 1:D:968:LEU:H    | 1.77                     | 0.49              |
| 1:E:407:ILE:HD12 | 1:E:408:PRO:HD2  | 1.94                     | 0.49              |
| 1:G:483:CYS:HB3  | 1:G:486:ARG:HB3  | 1.95                     | 0.49              |
| 1:G:755:MET:CG   | 1:G:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:G:914:LEU:HG   | 1:G:916:LEU:HD23 | 1.94                     | 0.49              |
| 1:G:962:LEU:HD11 | 1:G:968:LEU:H    | 1.77                     | 0.49              |
| 1:H:327:LEU:HD13 | 1:H:331:LEU:HD11 | 1.94                     | 0.49              |
| 1:H:410:VAL:HA   | 1:H:413:ILE:HG22 | 1.95                     | 0.49              |
| 1:H:894:THR:OG1  | 1:H:920:ALA:O    | 2.31                     | 0.49              |
| 1:I:327:LEU:HD13 | 1:I:331:LEU:HD11 | 1.94                     | 0.49              |
| 1:I:935:HIS:ND1  | 1:I:936:PRO:O    | 2.43                     | 0.49              |
| 1:J:327:LEU:HD13 | 1:J:331:LEU:HD11 | 1.94                     | 0.49              |
| 1:J:410:VAL:HA   | 1:J:413:ILE:HG22 | 1.95                     | 0.49              |
| 1:J:894:THR:OG1  | 1:J:920:ALA:O    | 2.31                     | 0.49              |
| 1:J:914:LEU:HG   | 1:J:916:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:894:THR:OG1  | 1:A:920:ALA:O    | 2.31                     | 0.49              |
| 1:B:407:ILE:HD12 | 1:B:408:PRO:HD2  | 1.94                     | 0.49              |
| 1:B:960:THR:O    | 1:B:963:THR:OG1  | 2.24                     | 0.49              |
| 1:D:327:LEU:HD13 | 1:D:331:LEU:HD11 | 1.94                     | 0.49              |
| 1:E:901:LEU:HD22 | 1:E:914:LEU:HD11 | 1.95                     | 0.49              |
| 1:E:962:LEU:HD11 | 1:E:968:LEU:H    | 1.77                     | 0.49              |
| 1:F:649:PRO:O    | 1:F:675:LYS:N    | 2.36                     | 0.49              |
| 1:F:901:LEU:HD22 | 1:F:914:LEU:HD11 | 1.95                     | 0.49              |
| 1:F:912:THR:HG23 | 1:F:913:HIS:ND1  | 2.27                     | 0.49              |
| 1:F:1002:LEU:HB3 | 1:F:1005:MET:HE1 | 1.95                     | 0.49              |
| 1:G:861:GLU:HA   | 1:G:889:VAL:HA   | 1.92                     | 0.49              |
| 1:G:913:HIS:NE2  | 1:G:942:MET:HB2  | 2.28                     | 0.49              |
| 1:I:632:LEU:HB3  | 1:I:641:VAL:HG22 | 1.95                     | 0.49              |
| 1:I:912:THR:HG23 | 1:I:913:HIS:ND1  | 2.28                     | 0.49              |
| 1:L:894:THR:OG1  | 1:L:921:LEU:HA   | 2.12                     | 0.49              |
| 1:A:1002:LEU:HB3 | 1:A:1005:MET:HE1 | 1.95                     | 0.49              |
| 1:B:894:THR:OG1  | 1:B:921:LEU:HA   | 2.12                     | 0.49              |
| 1:B:912:THR:HG23 | 1:B:913:HIS:ND1  | 2.28                     | 0.49              |
| 1:C:913:HIS:NE2  | 1:C:942:MET:HB2  | 2.28                     | 0.49              |
| 1:D:138:ARG:HD3  | 1:D:141:ARG:HH21 | 1.78                     | 0.49              |
| 1:D:483:CYS:HB3  | 1:D:486:ARG:HB3  | 1.95                     | 0.49              |
| 1:D:767:CYS:SG   | 1:D:796:LYS:NZ   | 2.82                     | 0.49              |
| 1:D:894:THR:OG1  | 1:D:920:ALA:O    | 2.31                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:913:HIS:NE2  | 1:D:942:MET:HB2  | 2.28                     | 0.49              |
| 1:D:1013:ARG:HG2 | 1:E:773:TRP:HH2  | 1.77                     | 0.49              |
| 1:E:767:CYS:SG   | 1:E:796:LYS:NZ   | 2.82                     | 0.49              |
| 1:E:983:VAL:HA   | 1:E:986:LEU:HD12 | 1.93                     | 0.49              |
| 1:G:138:ARG:HD3  | 1:G:141:ARG:HH21 | 1.78                     | 0.49              |
| 1:G:767:CYS:SG   | 1:G:796:LYS:NZ   | 2.82                     | 0.49              |
| 1:G:894:THR:OG1  | 1:G:920:ALA:O    | 2.31                     | 0.49              |
| 1:H:221:GLN:O    | 1:H:366:ILE:N    | 2.45                     | 0.49              |
| 1:H:291:SER:OG   | 1:H:339:LYS:O    | 2.28                     | 0.49              |
| 1:H:913:HIS:NE2  | 1:H:942:MET:HB2  | 2.28                     | 0.49              |
| 1:K:483:CYS:HB3  | 1:K:486:ARG:HB3  | 1.95                     | 0.49              |
| 1:K:755:MET:CG   | 1:K:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:K:894:THR:OG1  | 1:K:921:LEU:HA   | 2.12                     | 0.49              |
| 1:L:312:GLY:HA3  | 1:L:332:ILE:HD11 | 1.94                     | 0.49              |
| 1:L:483:CYS:HB3  | 1:L:486:ARG:HB3  | 1.95                     | 0.49              |
| 1:L:755:MET:CG   | 1:L:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:L:871:VAL:HA   | 1:L:874:GLU:HG3  | 1.95                     | 0.49              |
| 1:B:575:VAL:HA   | 1:B:578:LEU:HD12 | 1.95                     | 0.49              |
| 1:C:883:LEU:HD21 | 1:C:886:LEU:HD13 | 1.94                     | 0.49              |
| 1:C:894:THR:OG1  | 1:C:921:LEU:HA   | 2.12                     | 0.49              |
| 1:C:1002:LEU:HB3 | 1:C:1005:MET:HE1 | 1.95                     | 0.49              |
| 1:D:914:LEU:HG   | 1:D:916:LEU:HD23 | 1.94                     | 0.49              |
| 1:E:899:SER:O    | 1:E:902:THR:OG1  | 2.22                     | 0.49              |
| 1:F:768:ASN:H    | 1:F:796:LYS:HZ3  | 1.60                     | 0.49              |
| 1:F:960:THR:O    | 1:F:963:THR:OG1  | 2.24                     | 0.49              |
| 1:G:407:ILE:HD12 | 1:G:408:PRO:HD2  | 1.94                     | 0.49              |
| 1:G:470:ALA:HB2  | 1:G:526:ALA:HA   | 1.93                     | 0.49              |
| 1:G:935:HIS:ND1  | 1:G:936:PRO:O    | 2.43                     | 0.49              |
| 1:H:755:MET:CG   | 1:H:783:CYS:HB3  | 2.42                     | 0.49              |
| 1:I:894:THR:OG1  | 1:I:920:ALA:O    | 2.31                     | 0.49              |
| 1:J:575:VAL:HG11 | 1:J:609:TRP:CZ3  | 2.48                     | 0.49              |
| 1:J:918:SER:H    | 1:J:946:ASP:HB3  | 1.78                     | 0.49              |
| 1:J:1002:LEU:HB3 | 1:J:1005:MET:HE1 | 1.95                     | 0.49              |
| 1:K:312:GLY:HA3  | 1:K:332:ILE:HD11 | 1.94                     | 0.49              |
| 1:K:339:LYS:O    | 1:K:339:LYS:HD3  | 2.13                     | 0.49              |
| 1:K:871:VAL:HA   | 1:K:874:GLU:HG3  | 1.95                     | 0.49              |
| 1:L:575:VAL:HG11 | 1:L:609:TRP:CZ3  | 2.48                     | 0.49              |
| 1:L:637:GLU:OE2  | 1:L:640:PHE:N    | 2.28                     | 0.49              |
| 1:L:960:THR:O    | 1:L:963:THR:OG1  | 2.24                     | 0.49              |
| 1:A:316:THR:HB   | 1:A:329:SER:HA   | 1.95                     | 0.48              |
| 1:A:575:VAL:HG11 | 1:A:609:TRP:CZ3  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:767:CYS:SG   | 1:A:796:LYS:NZ   | 2.82                     | 0.48              |
| 1:A:883:LEU:HD21 | 1:A:886:LEU:HD13 | 1.94                     | 0.48              |
| 1:A:918:SER:H    | 1:A:946:ASP:HB3  | 1.77                     | 0.48              |
| 1:B:312:GLY:HA3  | 1:B:332:ILE:HD11 | 1.94                     | 0.48              |
| 1:B:632:LEU:HB3  | 1:B:641:VAL:HG22 | 1.95                     | 0.48              |
| 1:C:316:THR:HB   | 1:C:329:SER:HA   | 1.95                     | 0.48              |
| 1:C:327:LEU:HD13 | 1:C:331:LEU:HD11 | 1.94                     | 0.48              |
| 1:D:407:ILE:HD12 | 1:D:408:PRO:HD2  | 1.94                     | 0.48              |
| 1:E:575:VAL:HG11 | 1:E:609:TRP:CZ3  | 2.48                     | 0.48              |
| 1:E:809:ASP:C    | 1:E:811:GLY:H    | 2.15                     | 0.48              |
| 1:F:410:VAL:HA   | 1:F:413:ILE:HG22 | 1.95                     | 0.48              |
| 1:F:809:ASP:C    | 1:F:811:GLY:H    | 2.15                     | 0.48              |
| 1:F:871:VAL:HA   | 1:F:874:GLU:HG3  | 1.95                     | 0.48              |
| 1:G:918:SER:H    | 1:G:946:ASP:HB3  | 1.77                     | 0.48              |
| 1:H:316:THR:HB   | 1:H:329:SER:HA   | 1.95                     | 0.48              |
| 1:H:339:LYS:O    | 1:H:339:LYS:HD3  | 2.13                     | 0.48              |
| 1:I:575:VAL:HA   | 1:I:578:LEU:HD12 | 1.95                     | 0.48              |
| 1:I:894:THR:OG1  | 1:I:921:LEU:HA   | 2.12                     | 0.48              |
| 1:J:316:THR:HB   | 1:J:329:SER:HA   | 1.95                     | 0.48              |
| 1:K:575:VAL:HG11 | 1:K:609:TRP:CZ3  | 2.48                     | 0.48              |
| 1:K:960:THR:O    | 1:K:963:THR:OG1  | 2.24                     | 0.48              |
| 1:L:339:LYS:O    | 1:L:339:LYS:HD3  | 2.13                     | 0.48              |
| 1:L:410:VAL:HA   | 1:L:413:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:483:CYS:HB3  | 1:A:486:ARG:HB3  | 1.95                     | 0.48              |
| 1:A:894:THR:OG1  | 1:A:921:LEU:HA   | 2.12                     | 0.48              |
| 1:B:894:THR:OG1  | 1:B:920:ALA:O    | 2.31                     | 0.48              |
| 1:C:339:LYS:O    | 1:C:339:LYS:HD3  | 2.14                     | 0.48              |
| 1:C:400:VAL:HG22 | 1:C:404:MET:HE1  | 1.95                     | 0.48              |
| 1:C:755:MET:CG   | 1:C:783:CYS:HB3  | 2.42                     | 0.48              |
| 1:D:312:GLY:HA3  | 1:D:332:ILE:HD11 | 1.94                     | 0.48              |
| 1:D:575:VAL:HG11 | 1:D:609:TRP:CZ3  | 2.48                     | 0.48              |
| 1:D:918:SER:H    | 1:D:946:ASP:HB3  | 1.77                     | 0.48              |
| 1:E:400:VAL:HG22 | 1:E:404:MET:HE1  | 1.95                     | 0.48              |
| 1:E:913:HIS:NE2  | 1:E:942:MET:HB2  | 2.28                     | 0.48              |
| 1:F:648:PHE:O    | 1:F:674:VAL:HG22 | 2.13                     | 0.48              |
| 1:F:913:HIS:NE2  | 1:F:942:MET:HB2  | 2.28                     | 0.48              |
| 1:G:312:GLY:HA3  | 1:G:332:ILE:HD11 | 1.94                     | 0.48              |
| 1:G:575:VAL:HG11 | 1:G:609:TRP:CZ3  | 2.48                     | 0.48              |
| 1:G:648:PHE:O    | 1:G:674:VAL:HG22 | 2.13                     | 0.48              |
| 1:H:872:LEU:HD23 | 1:H:875:LYS:HZ1  | 1.78                     | 0.48              |
| 1:H:883:LEU:HD21 | 1:H:886:LEU:HD13 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1013:ARG:HG2 | 1:I:773:TRP:CH2  | 2.47                     | 0.48              |
| 1:I:443:LEU:HD22 | 1:I:524:PHE:CE2  | 2.44                     | 0.48              |
| 1:I:962:LEU:HD11 | 1:I:968:LEU:H    | 1.77                     | 0.48              |
| 1:J:483:CYS:HB3  | 1:J:486:ARG:HB3  | 1.95                     | 0.48              |
| 1:J:883:LEU:HD21 | 1:J:886:LEU:HD13 | 1.94                     | 0.48              |
| 1:J:894:THR:OG1  | 1:J:921:LEU:HA   | 2.12                     | 0.48              |
| 1:J:913:HIS:NE2  | 1:J:942:MET:HB2  | 2.28                     | 0.48              |
| 1:K:637:GLU:OE2  | 1:K:640:PHE:N    | 2.28                     | 0.48              |
| 1:K:861:GLU:OE1  | 1:K:918:SER:OG   | 2.27                     | 0.48              |
| 1:K:1002:LEU:HB3 | 1:K:1005:MET:HE1 | 1.95                     | 0.48              |
| 1:L:861:GLU:OE1  | 1:L:918:SER:OG   | 2.27                     | 0.48              |
| 1:L:1002:LEU:HB3 | 1:L:1005:MET:HE1 | 1.95                     | 0.48              |
| 1:A:913:HIS:NE2  | 1:A:942:MET:HB2  | 2.28                     | 0.48              |
| 1:D:316:THR:HB   | 1:D:329:SER:HA   | 1.95                     | 0.48              |
| 1:D:648:PHE:O    | 1:D:674:VAL:HG22 | 2.13                     | 0.48              |
| 1:D:935:HIS:ND1  | 1:D:936:PRO:O    | 2.43                     | 0.48              |
| 1:E:410:VAL:HA   | 1:E:413:ILE:HG22 | 1.95                     | 0.48              |
| 1:E:871:VAL:HA   | 1:E:874:GLU:HG3  | 1.95                     | 0.48              |
| 1:F:575:VAL:HA   | 1:F:578:LEU:HD12 | 1.95                     | 0.48              |
| 1:F:575:VAL:HG11 | 1:F:609:TRP:CZ3  | 2.48                     | 0.48              |
| 1:G:369:PHE:HA   | 1:G:373:LYS:NZ   | 2.28                     | 0.48              |
| 1:G:443:LEU:HD22 | 1:G:524:PHE:CE2  | 2.44                     | 0.48              |
| 1:H:138:ARG:HD3  | 1:H:141:ARG:HH21 | 1.78                     | 0.48              |
| 1:J:407:ILE:HD12 | 1:J:408:PRO:HD2  | 1.94                     | 0.48              |
| 1:K:410:VAL:HA   | 1:K:413:ILE:HG22 | 1.95                     | 0.48              |
| 1:K:894:THR:OG1  | 1:K:920:ALA:O    | 2.31                     | 0.48              |
| 1:K:914:LEU:HG   | 1:K:916:LEU:HD23 | 1.94                     | 0.48              |
| 1:L:894:THR:OG1  | 1:L:920:ALA:O    | 2.31                     | 0.48              |
| 1:A:407:ILE:HD12 | 1:A:408:PRO:HD2  | 1.94                     | 0.48              |
| 1:B:410:VAL:HA   | 1:B:413:ILE:HG22 | 1.95                     | 0.48              |
| 1:B:962:LEU:HD11 | 1:B:968:LEU:H    | 1.77                     | 0.48              |
| 1:D:339:LYS:O    | 1:D:339:LYS:HD3  | 2.14                     | 0.48              |
| 1:D:369:PHE:HA   | 1:D:373:LYS:NZ   | 2.28                     | 0.48              |
| 1:D:1002:LEU:HB3 | 1:D:1005:MET:HE1 | 1.94                     | 0.48              |
| 1:E:648:PHE:O    | 1:E:674:VAL:HG22 | 2.13                     | 0.48              |
| 1:E:894:THR:OG1  | 1:E:920:ALA:O    | 2.31                     | 0.48              |
| 1:G:316:THR:HB   | 1:G:329:SER:HA   | 1.95                     | 0.48              |
| 1:G:339:LYS:O    | 1:G:339:LYS:HD3  | 2.14                     | 0.48              |
| 1:G:901:LEU:HD22 | 1:G:914:LEU:HD11 | 1.95                     | 0.48              |
| 1:H:228:LYS:HZ2  | 1:H:299:GLY:H    | 1.60                     | 0.48              |
| 1:I:312:GLY:HA3  | 1:I:332:ILE:HD11 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:483:CYS:HB3  | 1:I:486:ARG:HB3   | 1.95                     | 0.48              |
| 1:I:913:HIS:NE2  | 1:I:942:MET:HB2   | 2.28                     | 0.48              |
| 1:I:990:LEU:HD22 | 1:I:1025:LEU:HD22 | 1.96                     | 0.48              |
| 1:J:168:GLN:O    | 1:J:366:ILE:HD12  | 2.14                     | 0.48              |
| 1:K:575:VAL:HA   | 1:K:578:LEU:HD12  | 1.95                     | 0.48              |
| 1:L:914:LEU:HG   | 1:L:916:LEU:HD23  | 1.94                     | 0.48              |
| 1:B:339:LYS:O    | 1:B:339:LYS:HD3   | 2.13                     | 0.48              |
| 1:B:871:VAL:HA   | 1:B:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:B:913:HIS:NE2  | 1:B:942:MET:HB2   | 2.28                     | 0.48              |
| 1:C:138:ARG:HD3  | 1:C:141:ARG:HH21  | 1.78                     | 0.48              |
| 1:D:474:TRP:HH2  | 1:D:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:E:230:ILE:HG21 | 1:E:412:TRP:CH2   | 2.49                     | 0.48              |
| 1:E:784:CYS:HB3  | 1:E:814:LEU:HB2   | 1.96                     | 0.48              |
| 1:F:632:LEU:HB3  | 1:F:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:F:784:CYS:HB3  | 1:F:814:LEU:HB2   | 1.96                     | 0.48              |
| 1:G:1002:LEU:HB3 | 1:G:1005:MET:HE1  | 1.94                     | 0.48              |
| 1:H:901:LEU:HD22 | 1:H:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:I:339:LYS:O    | 1:I:339:LYS:HD3   | 2.13                     | 0.48              |
| 1:J:138:ARG:HD3  | 1:J:141:ARG:HH21  | 1.78                     | 0.48              |
| 1:J:767:CYS:SG   | 1:J:796:LYS:NZ    | 2.82                     | 0.48              |
| 1:K:168:GLN:O    | 1:K:366:ILE:HD12  | 2.14                     | 0.48              |
| 1:K:474:TRP:HH2  | 1:K:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:K:632:LEU:HB3  | 1:K:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:K:913:HIS:NE2  | 1:K:942:MET:HB2   | 2.28                     | 0.48              |
| 1:L:168:GLN:O    | 1:L:366:ILE:HD12  | 2.14                     | 0.48              |
| 1:L:913:HIS:NE2  | 1:L:942:MET:HB2   | 2.28                     | 0.48              |
| 1:L:935:HIS:ND1  | 1:L:936:PRO:O     | 2.43                     | 0.48              |
| 1:A:168:GLN:O    | 1:A:366:ILE:HD12  | 2.14                     | 0.48              |
| 1:A:901:LEU:HD22 | 1:A:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:B:443:LEU:HD22 | 1:B:524:PHE:CE2   | 2.44                     | 0.48              |
| 1:B:1002:LEU:HB3 | 1:B:1005:MET:HE1  | 1.95                     | 0.48              |
| 1:D:352:GLU:OE1  | 1:D:352:GLU:N     | 2.46                     | 0.48              |
| 1:D:410:VAL:HA   | 1:D:413:ILE:HG22  | 1.95                     | 0.48              |
| 1:D:768:ASN:H    | 1:D:796:LYS:HZ3   | 1.60                     | 0.48              |
| 1:E:443:LEU:HD22 | 1:E:524:PHE:CE2   | 2.44                     | 0.48              |
| 1:E:575:VAL:HA   | 1:E:578:LEU:HD12  | 1.95                     | 0.48              |
| 1:F:962:LEU:HD11 | 1:F:968:LEU:H     | 1.77                     | 0.48              |
| 1:H:575:VAL:HA   | 1:H:578:LEU:HD12  | 1.95                     | 0.48              |
| 1:I:369:PHE:HA   | 1:I:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:I:767:CYS:SG   | 1:I:796:LYS:NZ    | 2.82                     | 0.48              |
| 1:I:1002:LEU:HB3 | 1:I:1005:MET:HE1  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:369:PHE:HA   | 1:J:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:J:632:LEU:HB3  | 1:J:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:L:474:TRP:HH2  | 1:L:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:L:841:CYS:HA   | 1:L:844:LEU:HD13  | 1.96                     | 0.48              |
| 1:A:138:ARG:HD3  | 1:A:141:ARG:HH21  | 1.78                     | 0.48              |
| 1:A:871:VAL:HA   | 1:A:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:B:369:PHE:HA   | 1:B:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:B:872:LEU:HA   | 1:B:875:LYS:HZ3   | 1.78                     | 0.48              |
| 1:B:918:SER:H    | 1:B:946:ASP:HB3   | 1.77                     | 0.48              |
| 1:C:221:GLN:O    | 1:C:366:ILE:N     | 2.45                     | 0.48              |
| 1:D:901:LEU:HD22 | 1:D:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:F:894:THR:OG1  | 1:F:920:ALA:O     | 2.31                     | 0.48              |
| 1:F:1007:LEU:HB2 | 1:F:1012:LYS:HZ1  | 1.77                     | 0.48              |
| 1:G:410:VAL:HA   | 1:G:413:ILE:HG22  | 1.95                     | 0.48              |
| 1:G:755:MET:HG3  | 1:G:783:CYS:HB3   | 1.96                     | 0.48              |
| 1:G:768:ASN:H    | 1:G:796:LYS:HZ3   | 1.60                     | 0.48              |
| 1:H:900:ALA:O    | 1:H:903:SER:OG    | 2.26                     | 0.48              |
| 1:I:205:PHE:CZ   | 1:I:216:HIS:HA    | 2.49                     | 0.48              |
| 1:I:871:VAL:HA   | 1:I:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:J:871:VAL:HA   | 1:J:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:J:901:LEU:HD22 | 1:J:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:K:230:ILE:HG21 | 1:K:412:TRP:CH2   | 2.49                     | 0.48              |
| 1:K:841:CYS:HA   | 1:K:844:LEU:HD13  | 1.96                     | 0.48              |
| 1:K:901:LEU:HD22 | 1:K:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:L:632:LEU:HB3  | 1:L:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:392:PHE:O    | 1:A:396:GLN:HG2   | 2.14                     | 0.48              |
| 1:A:872:LEU:HD23 | 1:A:875:LYS:HZ1   | 1.78                     | 0.48              |
| 1:A:953:HIS:CD2  | 1:L:617:LYS:HD2   | 2.48                     | 0.48              |
| 1:A:960:THR:O    | 1:A:963:THR:OG1   | 2.24                     | 0.48              |
| 1:B:230:ILE:HG21 | 1:B:412:TRP:CH2   | 2.49                     | 0.48              |
| 1:B:483:CYS:HB3  | 1:B:486:ARG:HB3   | 1.95                     | 0.48              |
| 1:B:990:LEU:HD22 | 1:B:1025:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:369:PHE:HA   | 1:C:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:C:575:VAL:HA   | 1:C:578:LEU:HD12  | 1.95                     | 0.48              |
| 1:C:871:VAL:HA   | 1:C:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:D:443:LEU:HD22 | 1:D:524:PHE:CE2   | 2.44                     | 0.48              |
| 1:F:230:ILE:HG21 | 1:F:412:TRP:CH2   | 2.49                     | 0.48              |
| 1:F:339:LYS:O    | 1:F:339:LYS:HD3   | 2.14                     | 0.48              |
| 1:G:352:GLU:OE1  | 1:G:352:GLU:N     | 2.46                     | 0.48              |
| 1:G:474:TRP:HH2  | 1:G:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:G:990:LEU:HD22 | 1:G:1025:LEU:HD22 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:369:PHE:HA   | 1:H:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:H:575:VAL:HG11 | 1:H:609:TRP:CZ3   | 2.48                     | 0.48              |
| 1:H:648:PHE:O    | 1:H:674:VAL:HG22  | 2.13                     | 0.48              |
| 1:I:410:VAL:HA   | 1:I:413:ILE:HG22  | 1.95                     | 0.48              |
| 1:I:918:SER:H    | 1:I:946:ASP:HB3   | 1.77                     | 0.48              |
| 1:J:392:PHE:O    | 1:J:396:GLN:HG2   | 2.14                     | 0.48              |
| 1:K:221:GLN:O    | 1:K:366:ILE:N     | 2.45                     | 0.48              |
| 1:K:392:PHE:O    | 1:K:396:GLN:HG2   | 2.14                     | 0.48              |
| 1:K:407:ILE:HD12 | 1:K:408:PRO:HD2   | 1.94                     | 0.48              |
| 1:K:918:SER:H    | 1:K:946:ASP:HB3   | 1.77                     | 0.48              |
| 1:L:221:GLN:O    | 1:L:366:ILE:N     | 2.45                     | 0.48              |
| 1:L:575:VAL:HA   | 1:L:578:LEU:HD12  | 1.95                     | 0.48              |
| 1:L:901:LEU:HD22 | 1:L:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:B:575:VAL:HG11 | 1:B:609:TRP:CZ3   | 2.48                     | 0.48              |
| 1:D:755:MET:HG3  | 1:D:783:CYS:HB3   | 1.96                     | 0.48              |
| 1:D:784:CYS:HB3  | 1:D:814:LEU:HB2   | 1.96                     | 0.48              |
| 1:D:871:VAL:HA   | 1:D:874:GLU:HG3   | 1.95                     | 0.48              |
| 1:D:872:LEU:HD23 | 1:D:875:LYS:HZ1   | 1.78                     | 0.48              |
| 1:E:339:LYS:O    | 1:E:339:LYS:HD3   | 2.13                     | 0.48              |
| 1:E:632:LEU:HB3  | 1:E:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:F:474:TRP:HH2  | 1:F:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:G:205:PHE:CZ   | 1:G:216:HIS:HA    | 2.49                     | 0.48              |
| 1:G:291:SER:OG   | 1:G:339:LYS:O     | 2.28                     | 0.48              |
| 1:H:474:TRP:HH2  | 1:H:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:J:871:VAL:O    | 1:J:875:LYS:HG3   | 2.14                     | 0.48              |
| 1:L:230:ILE:HG21 | 1:L:412:TRP:CH2   | 2.49                     | 0.48              |
| 1:L:407:ILE:HD12 | 1:L:408:PRO:HD2   | 1.94                     | 0.48              |
| 1:L:918:SER:H    | 1:L:946:ASP:HB3   | 1.77                     | 0.48              |
| 1:A:369:PHE:HA   | 1:A:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:A:632:LEU:HB3  | 1:A:641:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:871:VAL:O    | 1:A:875:LYS:HG3   | 2.14                     | 0.48              |
| 1:B:205:PHE:CZ   | 1:B:216:HIS:HA    | 2.49                     | 0.48              |
| 1:B:871:VAL:O    | 1:B:875:LYS:HG3   | 2.14                     | 0.48              |
| 1:C:871:VAL:O    | 1:C:875:LYS:HG3   | 2.14                     | 0.48              |
| 1:C:901:LEU:HD22 | 1:C:914:LEU:HD11  | 1.95                     | 0.48              |
| 1:D:205:PHE:CZ   | 1:D:216:HIS:HA    | 2.49                     | 0.48              |
| 1:D:990:LEU:HD22 | 1:D:1025:LEU:HD22 | 1.96                     | 0.48              |
| 1:E:474:TRP:HH2  | 1:E:554:ARG:HD2   | 1.79                     | 0.48              |
| 1:F:369:PHE:HA   | 1:F:373:LYS:NZ    | 2.28                     | 0.48              |
| 1:F:392:PHE:O    | 1:F:396:GLN:HG2   | 2.14                     | 0.48              |
| 1:F:443:LEU:HD22 | 1:F:524:PHE:CE2   | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:230:ILE:HG21 | 1:I:412:TRP:CH2  | 2.49                     | 0.48              |
| 1:I:316:THR:HB   | 1:I:329:SER:HA   | 1.95                     | 0.48              |
| 1:K:138:ARG:HD3  | 1:K:141:ARG:HH21 | 1.78                     | 0.48              |
| 1:K:228:LYS:HZ2  | 1:K:299:GLY:H    | 1.60                     | 0.48              |
| 1:K:369:PHE:HA   | 1:K:373:LYS:NZ   | 2.28                     | 0.48              |
| 1:K:657:THR:O    | 1:K:660:ASP:HB2  | 2.14                     | 0.48              |
| 1:K:871:VAL:O    | 1:K:875:LYS:HG3  | 2.14                     | 0.48              |
| 1:L:228:LYS:HZ2  | 1:L:299:GLY:H    | 1.60                     | 0.48              |
| 1:L:392:PHE:O    | 1:L:396:GLN:HG2  | 2.14                     | 0.48              |
| 1:L:657:THR:O    | 1:L:660:ASP:HB2  | 2.14                     | 0.48              |
| 1:L:871:VAL:O    | 1:L:875:LYS:HG3  | 2.14                     | 0.48              |
| 1:A:935:HIS:ND1  | 1:A:936:PRO:O    | 2.43                     | 0.47              |
| 1:B:767:CYS:SG   | 1:B:796:LYS:NZ   | 2.82                     | 0.47              |
| 1:C:648:PHE:O    | 1:C:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:D:1007:LEU:HB2 | 1:D:1012:LYS:HZ1 | 1.76                     | 0.47              |
| 1:E:369:PHE:HA   | 1:E:373:LYS:NZ   | 2.28                     | 0.47              |
| 1:E:483:CYS:HB3  | 1:E:486:ARG:HB3  | 1.95                     | 0.47              |
| 1:G:784:CYS:HB3  | 1:G:814:LEU:HB2  | 1.96                     | 0.47              |
| 1:G:864:LEU:HG   | 1:G:889:VAL:HG11 | 1.96                     | 0.47              |
| 1:H:168:GLN:O    | 1:H:366:ILE:HD12 | 2.14                     | 0.47              |
| 1:H:871:VAL:O    | 1:H:875:LYS:HG3  | 2.14                     | 0.47              |
| 1:I:648:PHE:O    | 1:I:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:J:474:TRP:HH2  | 1:J:554:ARG:HD2  | 1.79                     | 0.47              |
| 1:J:960:THR:O    | 1:J:963:THR:OG1  | 2.24                     | 0.47              |
| 1:L:138:ARG:HD3  | 1:L:141:ARG:HH21 | 1.78                     | 0.47              |
| 1:L:369:PHE:HA   | 1:L:373:LYS:NZ   | 2.28                     | 0.47              |
| 1:A:474:TRP:HH2  | 1:A:554:ARG:HD2  | 1.79                     | 0.47              |
| 1:C:474:TRP:HH2  | 1:C:554:ARG:HD2  | 1.79                     | 0.47              |
| 1:C:575:VAL:HG11 | 1:C:609:TRP:CZ3  | 2.48                     | 0.47              |
| 1:D:230:ILE:HG21 | 1:D:412:TRP:CH2  | 2.49                     | 0.47              |
| 1:D:754:GLY:O    | 1:D:757:VAL:HG22 | 2.15                     | 0.47              |
| 1:E:316:THR:HB   | 1:E:329:SER:HA   | 1.95                     | 0.47              |
| 1:E:392:PHE:O    | 1:E:396:GLN:HG2  | 2.14                     | 0.47              |
| 1:E:649:PRO:O    | 1:E:675:LYS:N    | 2.36                     | 0.47              |
| 1:E:755:MET:HG3  | 1:E:783:CYS:HB3  | 1.96                     | 0.47              |
| 1:F:754:GLY:O    | 1:F:757:VAL:HG22 | 2.14                     | 0.47              |
| 1:F:1009:ARG:NE  | 1:G:830:TRP:CZ3  | 2.81                     | 0.47              |
| 1:G:754:GLY:O    | 1:G:757:VAL:HG22 | 2.14                     | 0.47              |
| 1:G:871:VAL:HA   | 1:G:874:GLU:HG3  | 1.95                     | 0.47              |
| 1:G:1000:LEU:O   | 1:G:1028:VAL:HA  | 2.14                     | 0.47              |
| 1:G:1007:LEU:HB2 | 1:G:1012:LYS:HZ1 | 1.76                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:871:VAL:HA   | 1:H:874:GLU:HG3  | 1.95                     | 0.47              |
| 1:I:575:VAL:HG11 | 1:I:609:TRP:CZ3  | 2.48                     | 0.47              |
| 1:I:1000:LEU:O   | 1:I:1028:VAL:HA  | 2.14                     | 0.47              |
| 1:K:648:PHE:O    | 1:K:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:A:575:VAL:HA   | 1:A:578:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:657:THR:O    | 1:A:660:ASP:HB2  | 2.14                     | 0.47              |
| 1:B:316:THR:HB   | 1:B:329:SER:HA   | 1.95                     | 0.47              |
| 1:B:630:TYR:OH   | 1:B:660:ASP:OD1  | 2.13                     | 0.47              |
| 1:B:841:CYS:HA   | 1:B:844:LEU:HD13 | 1.96                     | 0.47              |
| 1:C:168:GLN:O    | 1:C:366:ILE:HD12 | 2.14                     | 0.47              |
| 1:C:900:ALA:O    | 1:C:903:SER:OG   | 2.26                     | 0.47              |
| 1:D:864:LEU:HG   | 1:D:889:VAL:HG11 | 1.96                     | 0.47              |
| 1:D:1000:LEU:O   | 1:D:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:F:755:MET:HG3  | 1:F:783:CYS:HB3  | 1.96                     | 0.47              |
| 1:G:230:ILE:HG21 | 1:G:412:TRP:CH2  | 2.49                     | 0.47              |
| 1:H:483:CYS:HB3  | 1:H:486:ARG:HB3  | 1.95                     | 0.47              |
| 1:I:871:VAL:O    | 1:I:875:LYS:HG3  | 2.14                     | 0.47              |
| 1:J:657:THR:O    | 1:J:660:ASP:HB2  | 2.14                     | 0.47              |
| 1:J:773:TRP:CH2  | 1:K:1013:ARG:HG2 | 2.46                     | 0.47              |
| 1:J:864:LEU:HG   | 1:J:889:VAL:HG11 | 1.96                     | 0.47              |
| 1:K:205:PHE:CZ   | 1:K:216:HIS:HA   | 2.49                     | 0.47              |
| 1:K:1000:LEU:O   | 1:K:1028:VAL:HA  | 2.14                     | 0.47              |
| 1:L:205:PHE:CZ   | 1:L:216:HIS:HA   | 2.49                     | 0.47              |
| 1:L:316:THR:HB   | 1:L:329:SER:HA   | 1.95                     | 0.47              |
| 1:L:648:PHE:O    | 1:L:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:L:864:LEU:HG   | 1:L:889:VAL:HG11 | 1.96                     | 0.47              |
| 1:L:1000:LEU:O   | 1:L:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:A:352:GLU:OE1  | 1:A:352:GLU:N    | 2.46                     | 0.47              |
| 1:A:841:CYS:HA   | 1:A:844:LEU:HD13 | 1.96                     | 0.47              |
| 1:B:138:ARG:HD3  | 1:B:141:ARG:HH21 | 1.78                     | 0.47              |
| 1:B:648:PHE:O    | 1:B:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:B:1000:LEU:O   | 1:B:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:C:1000:LEU:O   | 1:C:1028:VAL:HA  | 2.14                     | 0.47              |
| 1:D:392:PHE:O    | 1:D:396:GLN:HG2  | 2.14                     | 0.47              |
| 1:E:836:LEU:HD11 | 1:E:864:LEU:HD23 | 1.97                     | 0.47              |
| 1:E:871:VAL:O    | 1:E:875:LYS:HG3  | 2.14                     | 0.47              |
| 1:E:1000:LEU:O   | 1:E:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:F:316:THR:HB   | 1:F:329:SER:HA   | 1.95                     | 0.47              |
| 1:G:392:PHE:O    | 1:G:396:GLN:HG2  | 2.14                     | 0.47              |
| 1:G:871:VAL:O    | 1:G:875:LYS:HG3  | 2.14                     | 0.47              |
| 1:I:168:GLN:O    | 1:I:366:ILE:HD12 | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:841:CYS:HA    | 1:I:844:LEU:HD13  | 1.96                     | 0.47              |
| 1:J:575:VAL:HA    | 1:J:578:LEU:HD12  | 1.95                     | 0.47              |
| 1:J:935:HIS:ND1   | 1:J:936:PRO:O     | 2.43                     | 0.47              |
| 1:K:864:LEU:HG    | 1:K:889:VAL:HG11  | 1.96                     | 0.47              |
| 1:L:784:CYS:HB3   | 1:L:814:LEU:HB2   | 1.96                     | 0.47              |
| 1:A:253:PHE:O     | 1:A:296:LEU:N     | 2.48                     | 0.47              |
| 1:A:864:LEU:HG    | 1:A:889:VAL:HG11  | 1.96                     | 0.47              |
| 1:A:973:LEU:HB2   | 1:A:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:B:168:GLN:O     | 1:B:366:ILE:HD12  | 2.14                     | 0.47              |
| 1:C:836:LEU:HD11  | 1:C:864:LEU:HD23  | 1.97                     | 0.47              |
| 1:D:871:VAL:O     | 1:D:875:LYS:HG3   | 2.14                     | 0.47              |
| 1:G:836:LEU:HD11  | 1:G:864:LEU:HD23  | 1.97                     | 0.47              |
| 1:G:973:LEU:HB2   | 1:G:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:J:253:PHE:O     | 1:J:296:LEU:N     | 2.48                     | 0.47              |
| 1:J:352:GLU:OE1   | 1:J:352:GLU:N     | 2.46                     | 0.47              |
| 1:J:841:CYS:HA    | 1:J:844:LEU:HD13  | 1.96                     | 0.47              |
| 1:J:973:LEU:HB2   | 1:J:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:K:784:CYS:HB3   | 1:K:814:LEU:HB2   | 1.96                     | 0.47              |
| 1:K:990:LEU:HD22  | 1:K:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:L:990:LEU:HD22  | 1:L:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:339:LYS:O     | 1:A:339:LYS:HD3   | 2.13                     | 0.47              |
| 1:A:758:LEU:HD21  | 1:A:772:LEU:HD11  | 1.97                     | 0.47              |
| 1:A:848:LEU:HD21  | 1:A:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:B:474:TRP:HH2   | 1:B:554:ARG:HD2   | 1.79                     | 0.47              |
| 1:B:657:THR:O     | 1:B:660:ASP:HB2   | 2.14                     | 0.47              |
| 1:B:755:MET:HG3   | 1:B:783:CYS:HB3   | 1.96                     | 0.47              |
| 1:C:205:PHE:CZ    | 1:C:216:HIS:HA    | 2.49                     | 0.47              |
| 1:C:848:LEU:HD21  | 1:C:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:C:855:THR:OG1   | 1:C:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:C:960:THR:O     | 1:C:963:THR:OG1   | 2.24                     | 0.47              |
| 1:D:973:LEU:HB2   | 1:D:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:205:PHE:CZ    | 1:E:216:HIS:HA    | 2.49                     | 0.47              |
| 1:E:754:GLY:O     | 1:E:757:VAL:HG22  | 2.15                     | 0.47              |
| 1:E:855:THR:OG1   | 1:E:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:E:1018:LEU:HD12 | 1:E:1019:GLN:N    | 2.30                     | 0.47              |
| 1:F:855:THR:OG1   | 1:F:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:F:973:LEU:HB2   | 1:F:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:G:575:VAL:HA    | 1:G:578:LEU:HD12  | 1.95                     | 0.47              |
| 1:H:836:LEU:HD11  | 1:H:864:LEU:HD23  | 1.97                     | 0.47              |
| 1:H:855:THR:OG1   | 1:H:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:I:755:MET:HG3   | 1:I:783:CYS:HB3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:871:VAL:HG12  | 1:I:875:LYS:HZ2  | 1.79                     | 0.47              |
| 1:J:848:LEU:HD21  | 1:J:883:LEU:HD22 | 1.97                     | 0.47              |
| 1:J:1000:LEU:O    | 1:J:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:K:316:THR:HB    | 1:K:329:SER:HA   | 1.95                     | 0.47              |
| 1:L:253:PHE:O     | 1:L:296:LEU:N    | 2.48                     | 0.47              |
| 1:A:570:TYR:HB3   | 1:A:572:ILE:HG23 | 1.97                     | 0.47              |
| 1:A:648:PHE:O     | 1:A:674:VAL:HG22 | 2.13                     | 0.47              |
| 1:A:898:CYS:SG    | 1:A:928:LEU:HD11 | 2.55                     | 0.47              |
| 1:A:1000:LEU:O    | 1:A:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:B:848:LEU:HD21  | 1:B:883:LEU:HD22 | 1.97                     | 0.47              |
| 1:B:898:CYS:SG    | 1:B:928:LEU:HD11 | 2.55                     | 0.47              |
| 1:C:230:ILE:HG21  | 1:C:412:TRP:CH2  | 2.49                     | 0.47              |
| 1:C:253:PHE:O     | 1:C:296:LEU:N    | 2.48                     | 0.47              |
| 1:C:392:PHE:O     | 1:C:396:GLN:HG2  | 2.14                     | 0.47              |
| 1:C:784:CYS:HB3   | 1:C:814:LEU:HB2  | 1.96                     | 0.47              |
| 1:C:864:LEU:HG    | 1:C:889:VAL:HG11 | 1.96                     | 0.47              |
| 1:D:575:VAL:HA    | 1:D:578:LEU:HD12 | 1.95                     | 0.47              |
| 1:D:836:LEU:HD11  | 1:D:864:LEU:HD23 | 1.97                     | 0.47              |
| 1:E:898:CYS:SG    | 1:E:928:LEU:HD11 | 2.55                     | 0.47              |
| 1:E:1007:LEU:HB2  | 1:E:1012:LYS:HZ1 | 1.79                     | 0.47              |
| 1:E:1012:LYS:HA   | 1:E:1015:LEU:HG  | 1.97                     | 0.47              |
| 1:F:1000:LEU:O    | 1:F:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:F:1018:LEU:HD12 | 1:F:1019:GLN:N   | 2.30                     | 0.47              |
| 1:H:230:ILE:HG21  | 1:H:412:TRP:CH2  | 2.49                     | 0.47              |
| 1:H:253:PHE:O     | 1:H:296:LEU:N    | 2.48                     | 0.47              |
| 1:H:392:PHE:O     | 1:H:396:GLN:HG2  | 2.14                     | 0.47              |
| 1:H:632:LEU:HB3   | 1:H:641:VAL:HG22 | 1.95                     | 0.47              |
| 1:H:784:CYS:HB3   | 1:H:814:LEU:HB2  | 1.96                     | 0.47              |
| 1:H:848:LEU:HD21  | 1:H:883:LEU:HD22 | 1.97                     | 0.47              |
| 1:H:1000:LEU:O    | 1:H:1028:VAL:HA  | 2.15                     | 0.47              |
| 1:I:132:TYR:OH    | 1:I:278:ASP:OD1  | 2.32                     | 0.47              |
| 1:I:138:ARG:HD3   | 1:I:141:ARG:HH21 | 1.78                     | 0.47              |
| 1:I:401:LEU:HD22  | 1:I:404:MET:HE3  | 1.96                     | 0.47              |
| 1:I:657:THR:O     | 1:I:660:ASP:HB2  | 2.14                     | 0.47              |
| 1:I:754:GLY:O     | 1:I:757:VAL:HG22 | 2.14                     | 0.47              |
| 1:I:848:LEU:HD21  | 1:I:883:LEU:HD22 | 1.97                     | 0.47              |
| 1:I:901:LEU:HD22  | 1:I:914:LEU:HD11 | 1.95                     | 0.47              |
| 1:J:339:LYS:O     | 1:J:339:LYS:HD3  | 2.14                     | 0.47              |
| 1:J:570:TYR:HB3   | 1:J:572:ILE:HG23 | 1.97                     | 0.47              |
| 1:J:758:LEU:HD21  | 1:J:772:LEU:HD11 | 1.97                     | 0.47              |
| 1:K:253:PHE:O     | 1:K:296:LEU:N    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:443:LEU:HD22  | 1:K:524:PHE:CE2   | 2.44                     | 0.47              |
| 1:K:848:LEU:HD21  | 1:K:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:L:848:LEU:HD21  | 1:L:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:L:973:LEU:HB2   | 1:L:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:1007:LEU:HB2  | 1:A:1012:LYS:HZ1  | 1.79                     | 0.47              |
| 1:A:1027:ILE:HD11 | 1:L:970:LYS:HE2   | 1.97                     | 0.47              |
| 1:B:392:PHE:O     | 1:B:396:GLN:HG2   | 2.14                     | 0.47              |
| 1:B:784:CYS:HB3   | 1:B:814:LEU:HB2   | 1.96                     | 0.47              |
| 1:B:901:LEU:HD22  | 1:B:914:LEU:HD11  | 1.95                     | 0.47              |
| 1:D:848:LEU:HD21  | 1:D:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:D:855:THR:OG1   | 1:D:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:E:990:LEU:HD22  | 1:E:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:F:221:GLN:O     | 1:F:366:ILE:N     | 2.45                     | 0.47              |
| 1:F:483:CYS:HB3   | 1:F:486:ARG:HB3   | 1.95                     | 0.47              |
| 1:F:665:SER:C     | 1:F:669:LYS:HZ2   | 2.19                     | 0.47              |
| 1:F:836:LEU:HD11  | 1:F:864:LEU:HD23  | 1.97                     | 0.47              |
| 1:F:848:LEU:HD21  | 1:F:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:F:871:VAL:O     | 1:F:875:LYS:HG3   | 2.14                     | 0.47              |
| 1:F:898:CYS:SG    | 1:F:928:LEU:HD11  | 2.55                     | 0.47              |
| 1:G:848:LEU:HD21  | 1:G:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:G:855:THR:OG1   | 1:G:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:G:1018:LEU:HD12 | 1:G:1019:GLN:N    | 2.30                     | 0.47              |
| 1:H:754:GLY:O     | 1:H:757:VAL:HG22  | 2.14                     | 0.47              |
| 1:I:898:CYS:SG    | 1:I:928:LEU:HD11  | 2.55                     | 0.47              |
| 1:J:205:PHE:CZ    | 1:J:216:HIS:HA    | 2.49                     | 0.47              |
| 1:J:228:LYS:HZ2   | 1:J:299:GLY:H     | 1.62                     | 0.47              |
| 1:J:230:ILE:HG21  | 1:J:412:TRP:CH2   | 2.49                     | 0.47              |
| 1:J:648:PHE:O     | 1:J:674:VAL:HG22  | 2.13                     | 0.47              |
| 1:J:898:CYS:SG    | 1:J:928:LEU:HD11  | 2.55                     | 0.47              |
| 1:K:973:LEU:HB2   | 1:K:1002:LEU:HD13 | 1.96                     | 0.47              |
| 1:K:1007:LEU:HB2  | 1:K:1012:LYS:HZ1  | 1.79                     | 0.47              |
| 1:K:1012:LYS:HA   | 1:K:1015:LEU:HG   | 1.97                     | 0.47              |
| 1:L:754:GLY:O     | 1:L:757:VAL:HG22  | 2.14                     | 0.47              |
| 1:A:205:PHE:CZ    | 1:A:216:HIS:HA    | 2.49                     | 0.47              |
| 1:A:230:ILE:HG21  | 1:A:412:TRP:CH2   | 2.49                     | 0.47              |
| 1:B:754:GLY:O     | 1:B:757:VAL:HG22  | 2.15                     | 0.47              |
| 1:C:632:LEU:HB3   | 1:C:641:VAL:HG22  | 1.95                     | 0.47              |
| 1:C:638:GLU:OE1   | 1:C:638:GLU:N     | 2.48                     | 0.47              |
| 1:C:990:LEU:HD22  | 1:C:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:D:168:GLN:O     | 1:D:366:ILE:HD12  | 2.14                     | 0.47              |
| 1:E:973:LEU:HB2   | 1:E:1002:LEU:HD13 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:168:GLN:O     | 1:F:366:ILE:HD12  | 2.14                     | 0.47              |
| 1:F:205:PHE:CZ    | 1:F:216:HIS:HA    | 2.49                     | 0.47              |
| 1:F:369:PHE:HA    | 1:F:373:LYS:HZ2   | 1.80                     | 0.47              |
| 1:G:1012:LYS:HA   | 1:G:1015:LEU:HG   | 1.97                     | 0.47              |
| 1:H:1018:LEU:HD12 | 1:H:1019:GLN:N    | 2.30                     | 0.47              |
| 1:I:474:TRP:HH2   | 1:I:554:ARG:HD2   | 1.79                     | 0.47              |
| 1:I:570:TYR:HB3   | 1:I:572:ILE:HG23  | 1.97                     | 0.47              |
| 1:I:836:LEU:HD11  | 1:I:864:LEU:HD23  | 1.97                     | 0.47              |
| 1:J:990:LEU:HD22  | 1:J:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:K:754:GLY:O     | 1:K:757:VAL:HG22  | 2.15                     | 0.47              |
| 1:L:401:LEU:HD22  | 1:L:404:MET:HE3   | 1.97                     | 0.47              |
| 1:L:638:GLU:OE1   | 1:L:638:GLU:N     | 2.48                     | 0.47              |
| 1:L:1012:LYS:HA   | 1:L:1015:LEU:HG   | 1.97                     | 0.47              |
| 1:A:637:GLU:OE2   | 1:A:640:PHE:N     | 2.28                     | 0.47              |
| 1:A:990:LEU:HD22  | 1:A:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:1012:LYS:HA   | 1:A:1015:LEU:HG   | 1.97                     | 0.47              |
| 1:B:291:SER:OG    | 1:B:339:LYS:O     | 2.28                     | 0.47              |
| 1:B:570:TYR:HB3   | 1:B:572:ILE:HG23  | 1.97                     | 0.47              |
| 1:C:483:CYS:HB3   | 1:C:486:ARG:HB3   | 1.95                     | 0.47              |
| 1:C:871:VAL:HG12  | 1:C:875:LYS:HZ2   | 1.79                     | 0.47              |
| 1:D:841:CYS:HA    | 1:D:844:LEU:HD13  | 1.96                     | 0.47              |
| 1:D:898:CYS:SG    | 1:D:928:LEU:HD11  | 2.55                     | 0.47              |
| 1:D:900:ALA:O     | 1:D:903:SER:OG    | 2.26                     | 0.47              |
| 1:D:1012:LYS:HA   | 1:D:1015:LEU:HG   | 1.97                     | 0.47              |
| 1:E:168:GLN:O     | 1:E:366:ILE:HD12  | 2.14                     | 0.47              |
| 1:E:848:LEU:HD21  | 1:E:883:LEU:HD22  | 1.97                     | 0.47              |
| 1:F:990:LEU:HD22  | 1:F:1025:LEU:HD22 | 1.96                     | 0.47              |
| 1:G:570:TYR:HB3   | 1:G:572:ILE:HG23  | 1.97                     | 0.47              |
| 1:G:841:CYS:HA    | 1:G:844:LEU:HD13  | 1.96                     | 0.47              |
| 1:G:898:CYS:SG    | 1:G:928:LEU:HD11  | 2.55                     | 0.47              |
| 1:H:205:PHE:CZ    | 1:H:216:HIS:HA    | 2.49                     | 0.47              |
| 1:H:767:CYS:SG    | 1:H:796:LYS:NZ    | 2.82                     | 0.47              |
| 1:I:221:GLN:O     | 1:I:366:ILE:N     | 2.45                     | 0.47              |
| 1:I:271:LEU:HD21  | 1:I:277:PRO:HA    | 1.98                     | 0.47              |
| 1:I:784:CYS:HB3   | 1:I:814:LEU:HB2   | 1.96                     | 0.47              |
| 1:I:855:THR:OG1   | 1:I:884:GLN:HG2   | 2.15                     | 0.47              |
| 1:I:864:LEU:HG    | 1:I:889:VAL:HG11  | 1.96                     | 0.47              |
| 1:K:638:GLU:OE1   | 1:K:638:GLU:N     | 2.48                     | 0.47              |
| 1:K:758:LEU:HD21  | 1:K:772:LEU:HD11  | 1.97                     | 0.47              |
| 1:L:758:LEU:HD21  | 1:L:772:LEU:HD11  | 1.97                     | 0.47              |
| 1:B:132:TYR:OH    | 1:B:278:ASP:OD1   | 2.33                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:250:ASP:N     | 1:B:292:ARG:HB3  | 2.30                     | 0.46              |
| 1:B:271:LEU:HD21  | 1:B:277:PRO:HA   | 1.98                     | 0.46              |
| 1:B:481:GLU:O     | 1:B:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:836:LEU:HD11  | 1:B:864:LEU:HD23 | 1.97                     | 0.46              |
| 1:B:1018:LEU:HD12 | 1:B:1019:GLN:N   | 2.30                     | 0.46              |
| 1:D:570:TYR:HB3   | 1:D:572:ILE:HG23 | 1.97                     | 0.46              |
| 1:D:1018:LEU:HD12 | 1:D:1019:GLN:N   | 2.30                     | 0.46              |
| 1:E:228:LYS:HZ2   | 1:E:299:GLY:H    | 1.60                     | 0.46              |
| 1:F:1012:LYS:HA   | 1:F:1015:LEU:HG  | 1.97                     | 0.46              |
| 1:G:168:GLN:O     | 1:G:366:ILE:HD12 | 2.14                     | 0.46              |
| 1:H:570:TYR:HB3   | 1:H:572:ILE:HG23 | 1.97                     | 0.46              |
| 1:H:841:CYS:HA    | 1:H:844:LEU:HD13 | 1.96                     | 0.46              |
| 1:K:855:THR:OG1   | 1:K:884:GLN:HG2  | 2.15                     | 0.46              |
| 1:L:443:LEU:HD22  | 1:L:524:PHE:CE2  | 2.44                     | 0.46              |
| 1:L:855:THR:OG1   | 1:L:884:GLN:HG2  | 2.15                     | 0.46              |
| 1:A:784:CYS:HB3   | 1:A:814:LEU:HB2  | 1.96                     | 0.46              |
| 1:A:836:LEU:HD11  | 1:A:864:LEU:HD23 | 1.97                     | 0.46              |
| 1:C:755:MET:HG3   | 1:C:783:CYS:HB3  | 1.96                     | 0.46              |
| 1:C:758:LEU:HD21  | 1:C:772:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:841:CYS:HA    | 1:C:844:LEU:HD13 | 1.96                     | 0.46              |
| 1:E:250:ASP:N     | 1:E:292:ARG:HB3  | 2.30                     | 0.46              |
| 1:E:291:SER:OG    | 1:E:339:LYS:O    | 2.28                     | 0.46              |
| 1:E:864:LEU:HG    | 1:E:889:VAL:HG11 | 1.96                     | 0.46              |
| 1:F:271:LEU:HD21  | 1:F:277:PRO:HA   | 1.98                     | 0.46              |
| 1:F:481:GLU:O     | 1:F:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:F:637:GLU:OE2   | 1:F:640:PHE:N    | 2.28                     | 0.46              |
| 1:F:657:THR:O     | 1:F:660:ASP:HB2  | 2.14                     | 0.46              |
| 1:G:253:PHE:O     | 1:G:296:LEU:N    | 2.48                     | 0.46              |
| 1:H:638:GLU:OE1   | 1:H:638:GLU:N    | 2.48                     | 0.46              |
| 1:H:657:THR:O     | 1:H:660:ASP:HB2  | 2.14                     | 0.46              |
| 1:H:758:LEU:HD21  | 1:H:772:LEU:HD11 | 1.97                     | 0.46              |
| 1:H:871:VAL:HG12  | 1:H:875:LYS:HZ2  | 1.79                     | 0.46              |
| 1:I:250:ASP:N     | 1:I:292:ARG:HB3  | 2.30                     | 0.46              |
| 1:I:481:GLU:O     | 1:I:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:J:247:ASP:O     | 1:J:292:ARG:NH2  | 2.31                     | 0.46              |
| 1:J:638:GLU:OE1   | 1:J:638:GLU:N    | 2.48                     | 0.46              |
| 1:J:836:LEU:HD11  | 1:J:864:LEU:HD23 | 1.97                     | 0.46              |
| 1:J:1012:LYS:HA   | 1:J:1015:LEU:HG  | 1.97                     | 0.46              |
| 1:L:898:CYS:SG    | 1:L:928:LEU:HD11 | 2.55                     | 0.46              |
| 1:L:1018:LEU:HD12 | 1:L:1019:GLN:N   | 2.30                     | 0.46              |
| 1:A:250:ASP:N     | 1:A:292:ARG:HB3  | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:638:GLU:OE1   | 1:A:638:GLU:N     | 2.48                     | 0.46              |
| 1:B:221:GLN:O     | 1:B:366:ILE:N     | 2.45                     | 0.46              |
| 1:B:253:PHE:O     | 1:B:296:LEU:N     | 2.48                     | 0.46              |
| 1:B:855:THR:OG1   | 1:B:884:GLN:HG2   | 2.15                     | 0.46              |
| 1:B:1012:LYS:HA   | 1:B:1015:LEU:HG   | 1.97                     | 0.46              |
| 1:C:657:THR:O     | 1:C:660:ASP:HB2   | 2.14                     | 0.46              |
| 1:E:481:GLU:O     | 1:E:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:E:570:TYR:HB3   | 1:E:572:ILE:HG23  | 1.97                     | 0.46              |
| 1:G:638:GLU:OE1   | 1:G:638:GLU:N     | 2.48                     | 0.46              |
| 1:G:732:SER:O     | 1:G:735:SER:OG    | 2.20                     | 0.46              |
| 1:H:250:ASP:N     | 1:H:292:ARG:HB3   | 2.30                     | 0.46              |
| 1:H:481:GLU:O     | 1:H:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:H:864:LEU:HG    | 1:H:889:VAL:HG11  | 1.96                     | 0.46              |
| 1:H:1012:LYS:HA   | 1:H:1015:LEU:HG   | 1.97                     | 0.46              |
| 1:I:392:PHE:O     | 1:I:396:GLN:HG2   | 2.14                     | 0.46              |
| 1:J:637:GLU:OE2   | 1:J:640:PHE:N     | 2.28                     | 0.46              |
| 1:J:784:CYS:HB3   | 1:J:814:LEU:HB2   | 1.96                     | 0.46              |
| 1:K:898:CYS:SG    | 1:K:928:LEU:HD11  | 2.55                     | 0.46              |
| 1:L:250:ASP:N     | 1:L:292:ARG:HB3   | 2.30                     | 0.46              |
| 1:L:755:MET:HG3   | 1:L:783:CYS:HB3   | 1.96                     | 0.46              |
| 1:D:638:GLU:OE1   | 1:D:638:GLU:N     | 2.48                     | 0.46              |
| 1:F:134:LYS:HG3   | 1:F:137:ARG:HE    | 1.81                     | 0.46              |
| 1:F:841:CYS:HA    | 1:F:844:LEU:HD13  | 1.96                     | 0.46              |
| 1:G:665:SER:C     | 1:G:669:LYS:HZ2   | 2.19                     | 0.46              |
| 1:H:755:MET:HG3   | 1:H:783:CYS:HB3   | 1.96                     | 0.46              |
| 1:H:990:LEU:HD22  | 1:H:1025:LEU:HD22 | 1.96                     | 0.46              |
| 1:I:1018:LEU:HD12 | 1:I:1019:GLN:N    | 2.30                     | 0.46              |
| 1:J:250:ASP:N     | 1:J:292:ARG:HB3   | 2.30                     | 0.46              |
| 1:K:250:ASP:N     | 1:K:292:ARG:HB3   | 2.31                     | 0.46              |
| 1:K:755:MET:HG3   | 1:K:783:CYS:HB3   | 1.96                     | 0.46              |
| 1:K:868:GLY:O     | 1:K:872:LEU:HG    | 2.16                     | 0.46              |
| 1:K:1018:LEU:HD12 | 1:K:1019:GLN:N    | 2.30                     | 0.46              |
| 1:L:868:GLY:O     | 1:L:872:LEU:HG    | 2.16                     | 0.46              |
| 1:A:247:ASP:O     | 1:A:292:ARG:NH2   | 2.31                     | 0.46              |
| 1:A:855:THR:OG1   | 1:A:884:GLN:HG2   | 2.15                     | 0.46              |
| 1:A:871:VAL:HG12  | 1:A:875:LYS:HZ2   | 1.79                     | 0.46              |
| 1:B:401:LEU:HD22  | 1:B:404:MET:HE3   | 1.96                     | 0.46              |
| 1:B:864:LEU:HG    | 1:B:889:VAL:HG11  | 1.96                     | 0.46              |
| 1:C:481:GLU:O     | 1:C:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:C:935:HIS:ND1   | 1:C:936:PRO:O     | 2.43                     | 0.46              |
| 1:C:1018:LEU:HD12 | 1:C:1019:GLN:N    | 2.30                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:253:PHE:O     | 1:D:296:LEU:N    | 2.48                     | 0.46              |
| 1:D:369:PHE:HA    | 1:D:373:LYS:HZ2  | 1.80                     | 0.46              |
| 1:D:758:LEU:HD21  | 1:D:772:LEU:HD11 | 1.97                     | 0.46              |
| 1:D:871:VAL:HG12  | 1:D:875:LYS:HZ2  | 1.79                     | 0.46              |
| 1:E:291:SER:HA    | 1:E:339:LYS:HZ3  | 1.80                     | 0.46              |
| 1:E:657:THR:O     | 1:E:660:ASP:HB2  | 2.14                     | 0.46              |
| 1:E:841:CYS:HA    | 1:E:844:LEU:HD13 | 1.96                     | 0.46              |
| 1:F:250:ASP:N     | 1:F:292:ARG:HB3  | 2.31                     | 0.46              |
| 1:F:253:PHE:O     | 1:F:296:LEU:N    | 2.48                     | 0.46              |
| 1:G:134:LYS:HG3   | 1:G:137:ARG:HE   | 1.81                     | 0.46              |
| 1:G:758:LEU:HD21  | 1:G:772:LEU:HD11 | 1.97                     | 0.46              |
| 1:H:132:TYR:OH    | 1:H:278:ASP:OD1  | 2.33                     | 0.46              |
| 1:I:1012:LYS:HA   | 1:I:1015:LEU:HG  | 1.97                     | 0.46              |
| 1:J:855:THR:OG1   | 1:J:884:GLN:HG2  | 2.15                     | 0.46              |
| 1:J:1018:LEU:HD12 | 1:J:1019:GLN:N   | 2.30                     | 0.46              |
| 1:K:481:GLU:O     | 1:K:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:L:1007:LEU:HB2  | 1:L:1012:LYS:HZ1 | 1.80                     | 0.46              |
| 1:A:754:GLY:O     | 1:A:757:VAL:HG22 | 2.15                     | 0.46              |
| 1:A:868:GLY:O     | 1:A:872:LEU:HG   | 2.16                     | 0.46              |
| 1:C:570:TYR:HB3   | 1:C:572:ILE:HG23 | 1.97                     | 0.46              |
| 1:C:754:GLY:O     | 1:C:757:VAL:HG22 | 2.15                     | 0.46              |
| 1:C:1012:LYS:HA   | 1:C:1015:LEU:HG  | 1.97                     | 0.46              |
| 1:D:657:THR:O     | 1:D:660:ASP:HB2  | 2.14                     | 0.46              |
| 1:D:665:SER:C     | 1:D:669:LYS:HZ2  | 2.19                     | 0.46              |
| 1:E:134:LYS:HG3   | 1:E:137:ARG:HE   | 1.81                     | 0.46              |
| 1:E:253:PHE:O     | 1:E:296:LEU:N    | 2.48                     | 0.46              |
| 1:I:253:PHE:O     | 1:I:296:LEU:N    | 2.48                     | 0.46              |
| 1:I:352:GLU:OE1   | 1:I:352:GLU:N    | 2.46                     | 0.46              |
| 1:J:481:GLU:O     | 1:J:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:J:649:PRO:O     | 1:J:675:LYS:N    | 2.36                     | 0.46              |
| 1:J:868:GLY:O     | 1:J:872:LEU:HG   | 2.16                     | 0.46              |
| 1:K:836:LEU:HD11  | 1:K:864:LEU:HD23 | 1.97                     | 0.46              |
| 1:L:481:GLU:O     | 1:L:482:GLU:HG2  | 2.15                     | 0.46              |
| 1:L:570:TYR:HB3   | 1:L:572:ILE:HG23 | 1.97                     | 0.46              |
| 1:L:630:TYR:OH    | 1:L:660:ASP:OD1  | 2.12                     | 0.46              |
| 1:L:836:LEU:HD11  | 1:L:864:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:1018:LEU:HD12 | 1:A:1019:GLN:N   | 2.30                     | 0.46              |
| 1:C:250:ASP:N     | 1:C:292:ARG:HB3  | 2.31                     | 0.46              |
| 1:C:898:CYS:SG    | 1:C:928:LEU:HD11 | 2.55                     | 0.46              |
| 1:D:901:LEU:HA    | 1:D:904:VAL:HG12 | 1.98                     | 0.46              |
| 1:E:271:LEU:HD21  | 1:E:277:PRO:HA   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:864:LEU:HG   | 1:F:889:VAL:HG11  | 1.96                     | 0.46              |
| 1:G:369:PHE:HA   | 1:G:373:LYS:HZ2   | 1.80                     | 0.46              |
| 1:H:973:LEU:HB2  | 1:H:1002:LEU:HD13 | 1.96                     | 0.46              |
| 1:I:638:GLU:N    | 1:I:638:GLU:OE1   | 2.48                     | 0.46              |
| 1:J:754:GLY:O    | 1:J:757:VAL:HG22  | 2.15                     | 0.46              |
| 1:K:570:TYR:HB3  | 1:K:572:ILE:HG23  | 1.97                     | 0.46              |
| 1:A:755:MET:HG3  | 1:A:783:CYS:HB3   | 1.96                     | 0.46              |
| 1:D:134:LYS:HG3  | 1:D:137:ARG:HE    | 1.81                     | 0.46              |
| 1:D:219:VAL:HG13 | 1:D:344:ILE:HG13  | 1.98                     | 0.46              |
| 1:D:868:GLY:O    | 1:D:872:LEU:HG    | 2.16                     | 0.46              |
| 1:F:228:LYS:HZ2  | 1:F:299:GLY:H     | 1.60                     | 0.46              |
| 1:F:638:GLU:N    | 1:F:638:GLU:OE1   | 2.48                     | 0.46              |
| 1:G:219:VAL:HG13 | 1:G:344:ILE:HG13  | 1.98                     | 0.46              |
| 1:G:657:THR:O    | 1:G:660:ASP:HB2   | 2.14                     | 0.46              |
| 1:I:973:LEU:HB2  | 1:I:1002:LEU:HD13 | 1.96                     | 0.46              |
| 1:J:401:LEU:HD22 | 1:J:404:MET:HE3   | 1.98                     | 0.46              |
| 1:A:481:GLU:O    | 1:A:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:B:973:LEU:HB2  | 1:B:1002:LEU:HD13 | 1.96                     | 0.46              |
| 1:C:228:LYS:HZ2  | 1:C:299:GLY:H     | 1.62                     | 0.46              |
| 1:C:291:SER:HA   | 1:C:339:LYS:HZ3   | 1.80                     | 0.46              |
| 1:D:332:ILE:HA   | 1:D:335:LYS:HB2   | 1.98                     | 0.46              |
| 1:D:481:GLU:O    | 1:D:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:E:935:HIS:ND1  | 1:E:936:PRO:O     | 2.43                     | 0.46              |
| 1:F:570:TYR:HB3  | 1:F:572:ILE:HG23  | 1.97                     | 0.46              |
| 1:G:469:ALA:HA   | 1:G:480:PHE:HZ    | 1.81                     | 0.46              |
| 1:G:481:GLU:O    | 1:G:482:GLU:HG2   | 2.15                     | 0.46              |
| 1:G:868:GLY:O    | 1:G:872:LEU:HG    | 2.16                     | 0.46              |
| 1:G:901:LEU:HA   | 1:G:904:VAL:HG12  | 1.98                     | 0.46              |
| 1:H:1007:LEU:HB2 | 1:H:1012:LYS:HZ1  | 1.80                     | 0.46              |
| 1:B:219:VAL:HG13 | 1:B:344:ILE:HG13  | 1.98                     | 0.46              |
| 1:B:469:ALA:HA   | 1:B:480:PHE:HZ    | 1.81                     | 0.46              |
| 1:B:638:GLU:OE1  | 1:B:638:GLU:N     | 2.48                     | 0.46              |
| 1:B:868:GLY:O    | 1:B:872:LEU:HG    | 2.16                     | 0.46              |
| 1:C:132:TYR:OH   | 1:C:278:ASP:OD1   | 2.33                     | 0.46              |
| 1:C:973:LEU:HB2  | 1:C:1002:LEU:HD13 | 1.96                     | 0.46              |
| 1:D:228:LYS:HZ2  | 1:D:299:GLY:H     | 1.62                     | 0.46              |
| 1:D:469:ALA:HA   | 1:D:480:PHE:HZ    | 1.81                     | 0.46              |
| 1:E:638:GLU:OE1  | 1:E:638:GLU:N     | 2.48                     | 0.46              |
| 1:F:773:TRP:CH2  | 1:G:1013:ARG:HG2  | 2.46                     | 0.46              |
| 1:I:219:VAL:HG13 | 1:I:344:ILE:HG13  | 1.98                     | 0.46              |
| 1:I:868:GLY:O    | 1:I:872:LEU:HG    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:469:ALA:HA   | 1:K:480:PHE:HZ   | 1.81                     | 0.46              |
| 1:K:601:GLN:O    | 1:K:605:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:134:LYS:HG3  | 1:A:137:ARG:HE   | 1.81                     | 0.45              |
| 1:B:332:ILE:HA   | 1:B:335:LYS:HB2  | 1.98                     | 0.45              |
| 1:B:352:GLU:OE1  | 1:B:352:GLU:N    | 2.46                     | 0.45              |
| 1:B:374:ARG:NE   | 1:B:405:CYS:HB2  | 2.31                     | 0.45              |
| 1:B:758:LEU:HD21 | 1:B:772:LEU:HD11 | 1.97                     | 0.45              |
| 1:B:901:LEU:HA   | 1:B:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:C:601:GLN:O    | 1:C:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:221:GLN:O    | 1:E:366:ILE:N    | 2.45                     | 0.45              |
| 1:E:868:GLY:O    | 1:E:872:LEU:HG   | 2.16                     | 0.45              |
| 1:F:400:VAL:HG22 | 1:F:404:MET:HE1  | 1.98                     | 0.45              |
| 1:G:271:LEU:HD21 | 1:G:277:PRO:HA   | 1.98                     | 0.45              |
| 1:G:332:ILE:HA   | 1:G:335:LYS:HB2  | 1.98                     | 0.45              |
| 1:H:271:LEU:HD21 | 1:H:277:PRO:HA   | 1.98                     | 0.45              |
| 1:H:400:VAL:HG22 | 1:H:404:MET:HE1  | 1.99                     | 0.45              |
| 1:I:469:ALA:HA   | 1:I:480:PHE:HZ   | 1.82                     | 0.45              |
| 1:I:901:LEU:HA   | 1:I:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:L:601:GLN:O    | 1:L:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:L:901:LEU:HA   | 1:L:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:C:271:LEU:HD21 | 1:C:277:PRO:HA   | 1.98                     | 0.45              |
| 1:C:868:GLY:O    | 1:C:872:LEU:HG   | 2.16                     | 0.45              |
| 1:D:271:LEU:HD21 | 1:D:277:PRO:HA   | 1.98                     | 0.45              |
| 1:F:291:SER:OG   | 1:F:339:LYS:O    | 2.28                     | 0.45              |
| 1:G:228:LYS:HZ2  | 1:G:299:GLY:H    | 1.61                     | 0.45              |
| 1:H:898:CYS:SG   | 1:H:928:LEU:HD11 | 2.55                     | 0.45              |
| 1:I:134:LYS:HG3  | 1:I:137:ARG:HE   | 1.81                     | 0.45              |
| 1:I:332:ILE:HA   | 1:I:335:LYS:HB2  | 1.98                     | 0.45              |
| 1:I:374:ARG:NE   | 1:I:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:J:601:GLN:O    | 1:J:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:J:755:MET:HG3  | 1:J:783:CYS:HB3  | 1.96                     | 0.45              |
| 1:K:400:VAL:HG22 | 1:K:404:MET:HE1  | 1.98                     | 0.45              |
| 1:K:901:LEU:HA   | 1:K:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:L:469:ALA:HA   | 1:L:480:PHE:HZ   | 1.82                     | 0.45              |
| 1:A:601:GLN:O    | 1:A:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:C:134:LYS:HG3  | 1:C:137:ARG:HE   | 1.81                     | 0.45              |
| 1:C:374:ARG:NE   | 1:C:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:C:813:ARG:NH1  | 1:C:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:E:637:GLU:OE2  | 1:E:640:PHE:N    | 2.28                     | 0.45              |
| 1:F:813:ARG:NH1  | 1:F:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:H:134:LYS:HG3  | 1:H:137:ARG:HE   | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:758:LEU:HD21 | 1:I:772:LEU:HD11 | 1.97                     | 0.45              |
| 1:D:872:LEU:HA   | 1:D:875:LYS:HZ3  | 1.82                     | 0.45              |
| 1:E:219:VAL:HG13 | 1:E:344:ILE:HG13 | 1.98                     | 0.45              |
| 1:E:758:LEU:HD21 | 1:E:772:LEU:HD11 | 1.97                     | 0.45              |
| 1:E:813:ARG:NH1  | 1:E:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:E:901:LEU:HA   | 1:E:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:F:469:ALA:HA   | 1:F:480:PHE:HZ   | 1.81                     | 0.45              |
| 1:H:960:THR:O    | 1:H:963:THR:OG1  | 2.24                     | 0.45              |
| 1:J:134:LYS:HG3  | 1:J:137:ARG:HE   | 1.81                     | 0.45              |
| 1:L:374:ARG:NE   | 1:L:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:F:219:VAL:HG13 | 1:F:344:ILE:HG13 | 1.98                     | 0.45              |
| 1:H:374:ARG:NE   | 1:H:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:H:813:ARG:NH1  | 1:H:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:K:374:ARG:NE   | 1:K:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:K:388:ALA:HB3  | 1:K:389:ARG:NH1  | 2.32                     | 0.45              |
| 1:L:388:ALA:HB3  | 1:L:389:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:968:LEU:HD13 | 1:A:970:LYS:O    | 2.17                     | 0.45              |
| 1:B:134:LYS:HG3  | 1:B:137:ARG:HE   | 1.81                     | 0.45              |
| 1:D:250:ASP:N    | 1:D:292:ARG:HB3  | 2.31                     | 0.45              |
| 1:E:469:ALA:HA   | 1:E:480:PHE:HZ   | 1.82                     | 0.45              |
| 1:E:665:SER:C    | 1:E:669:LYS:HZ2  | 2.20                     | 0.45              |
| 1:F:132:TYR:OH   | 1:F:278:ASP:OD1  | 2.33                     | 0.45              |
| 1:F:332:ILE:HA   | 1:F:335:LYS:HB2  | 1.98                     | 0.45              |
| 1:F:374:ARG:NE   | 1:F:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:F:868:GLY:O    | 1:F:872:LEU:HG   | 2.16                     | 0.45              |
| 1:F:901:LEU:HA   | 1:F:904:VAL:HG12 | 1.98                     | 0.45              |
| 1:H:352:GLU:OE1  | 1:H:352:GLU:N    | 2.46                     | 0.45              |
| 1:H:601:GLN:O    | 1:H:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:H:872:LEU:HA   | 1:H:875:LYS:HZ3  | 1.82                     | 0.45              |
| 1:I:894:THR:HG23 | 1:I:921:LEU:HD22 | 1.99                     | 0.45              |
| 1:J:768:ASN:N    | 1:J:796:LYS:HZ2  | 2.13                     | 0.45              |
| 1:K:134:LYS:HG3  | 1:K:137:ARG:HE   | 1.81                     | 0.45              |
| 1:K:271:LEU:HD21 | 1:K:277:PRO:HA   | 1.98                     | 0.45              |
| 1:K:726:PHE:O    | 1:K:730:LEU:HG   | 2.17                     | 0.45              |
| 1:L:726:PHE:O    | 1:L:730:LEU:HG   | 2.17                     | 0.45              |
| 1:A:768:ASN:N    | 1:A:796:LYS:HZ2  | 2.14                     | 0.45              |
| 1:B:258:ARG:HH22 | 1:B:515:SER:HB2  | 1.82                     | 0.45              |
| 1:B:894:THR:HG23 | 1:B:921:LEU:HD22 | 1.99                     | 0.45              |
| 1:E:352:GLU:OE1  | 1:E:352:GLU:N    | 2.46                     | 0.45              |
| 1:E:369:PHE:HA   | 1:E:373:LYS:HZ2  | 1.81                     | 0.45              |
| 1:G:250:ASP:N    | 1:G:292:ARG:HB3  | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:960:THR:O    | 1:G:963:THR:OG1  | 2.24                     | 0.45              |
| 1:H:868:GLY:O    | 1:H:872:LEU:HG   | 2.16                     | 0.45              |
| 1:I:258:ARG:HH22 | 1:I:515:SER:HB2  | 1.82                     | 0.45              |
| 1:I:813:ARG:NH1  | 1:I:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:J:370:SER:H    | 1:J:373:LYS:HE3  | 1.82                     | 0.45              |
| 1:J:813:ARG:NH1  | 1:J:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:J:968:LEU:HD13 | 1:J:970:LYS:O    | 2.17                     | 0.45              |
| 1:A:167:LEU:HB2  | 1:A:366:ILE:HD11 | 1.99                     | 0.45              |
| 1:A:370:SER:H    | 1:A:373:LYS:HE3  | 1.82                     | 0.45              |
| 1:A:401:LEU:HD22 | 1:A:404:MET:HE3  | 1.99                     | 0.45              |
| 1:A:813:ARG:NH1  | 1:A:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:B:813:ARG:NH1  | 1:B:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:C:810:PHE:CZ   | 1:D:785:PHE:CB   | 2.95                     | 0.45              |
| 1:D:167:LEU:HB2  | 1:D:366:ILE:HD11 | 1.98                     | 0.45              |
| 1:E:374:ARG:NE   | 1:E:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:G:649:PRO:HA   | 1:G:674:VAL:HA   | 1.99                     | 0.45              |
| 1:G:813:ARG:NH1  | 1:G:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:H:665:SER:C    | 1:H:669:LYS:HZ2  | 2.19                     | 0.45              |
| 1:H:935:HIS:ND1  | 1:H:936:PRO:O    | 2.43                     | 0.45              |
| 1:J:167:LEU:HB2  | 1:J:366:ILE:HD11 | 1.99                     | 0.45              |
| 1:K:167:LEU:HB2  | 1:K:366:ILE:HD11 | 1.98                     | 0.45              |
| 1:K:219:VAL:HG13 | 1:K:344:ILE:HG13 | 1.98                     | 0.45              |
| 1:L:134:LYS:HG3  | 1:L:137:ARG:HE   | 1.81                     | 0.45              |
| 1:L:167:LEU:HB2  | 1:L:366:ILE:HD11 | 1.99                     | 0.45              |
| 1:L:271:LEU:HD21 | 1:L:277:PRO:HA   | 1.98                     | 0.45              |
| 1:A:271:LEU:HD21 | 1:A:277:PRO:HA   | 1.98                     | 0.45              |
| 1:A:388:ALA:HB3  | 1:A:389:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:872:LEU:HA   | 1:A:875:LYS:HZ3  | 1.82                     | 0.45              |
| 1:B:250:ASP:N    | 1:B:292:ARG:O    | 2.46                     | 0.45              |
| 1:C:665:SER:C    | 1:C:669:LYS:HZ2  | 2.20                     | 0.45              |
| 1:D:649:PRO:HA   | 1:D:674:VAL:HA   | 1.99                     | 0.45              |
| 1:D:813:ARG:NH1  | 1:D:843:ASP:OD2  | 2.50                     | 0.45              |
| 1:D:960:THR:O    | 1:D:963:THR:OG1  | 2.24                     | 0.45              |
| 1:F:726:PHE:O    | 1:F:730:LEU:HG   | 2.17                     | 0.45              |
| 1:F:758:LEU:HD21 | 1:F:772:LEU:HD11 | 1.97                     | 0.45              |
| 1:G:138:ARG:CD   | 1:G:141:ARG:HH21 | 2.30                     | 0.45              |
| 1:G:167:LEU:HB2  | 1:G:366:ILE:HD11 | 1.98                     | 0.45              |
| 1:G:374:ARG:NE   | 1:G:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:A:443:LEU:HD22 | 1:A:524:PHE:CE2  | 2.44                     | 0.45              |
| 1:A:828:LYS:HD3  | 1:A:856:ARG:HG2  | 1.99                     | 0.45              |
| 1:B:601:GLN:O    | 1:B:605:GLU:HG2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:219:VAL:HG13 | 1:C:344:ILE:HG13 | 1.98                     | 0.45              |
| 1:C:369:PHE:HA   | 1:C:373:LYS:HZ2  | 1.82                     | 0.45              |
| 1:C:1007:LEU:HB2 | 1:C:1012:LYS:HZ1 | 1.81                     | 0.45              |
| 1:D:138:ARG:CD   | 1:D:141:ARG:HH21 | 2.30                     | 0.45              |
| 1:D:374:ARG:NE   | 1:D:405:CYS:HB2  | 2.32                     | 0.45              |
| 1:E:601:GLN:O    | 1:E:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:726:PHE:O    | 1:E:730:LEU:HG   | 2.17                     | 0.45              |
| 1:F:601:GLN:O    | 1:F:605:GLU:HG2  | 2.16                     | 0.45              |
| 1:F:649:PRO:HA   | 1:F:674:VAL:HA   | 1.99                     | 0.45              |
| 1:H:370:SER:H    | 1:H:373:LYS:HE3  | 1.82                     | 0.45              |
| 1:H:968:LEU:HD13 | 1:H:970:LYS:O    | 2.17                     | 0.45              |
| 1:K:828:LYS:HD3  | 1:K:856:ARG:HG2  | 1.99                     | 0.45              |
| 1:L:219:VAL:HG13 | 1:L:344:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:221:GLN:O    | 1:A:366:ILE:N    | 2.45                     | 0.44              |
| 1:A:901:LEU:HA   | 1:A:904:VAL:HG12 | 1.98                     | 0.44              |
| 1:B:388:ALA:HB3  | 1:B:389:ARG:NH1  | 2.32                     | 0.44              |
| 1:B:1017:ALA:O   | 1:B:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:C:968:LEU:HD13 | 1:C:970:LYS:O    | 2.17                     | 0.44              |
| 1:E:332:ILE:HA   | 1:E:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:E:649:PRO:HA   | 1:E:674:VAL:HA   | 1.99                     | 0.44              |
| 1:G:968:LEU:HD13 | 1:G:970:LYS:O    | 2.17                     | 0.44              |
| 1:I:138:ARG:CD   | 1:I:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:J:221:GLN:O    | 1:J:366:ILE:N    | 2.45                     | 0.44              |
| 1:J:369:PHE:HA   | 1:J:373:LYS:HZ2  | 1.82                     | 0.44              |
| 1:J:374:ARG:NE   | 1:J:405:CYS:HB2  | 2.32                     | 0.44              |
| 1:J:388:ALA:HB3  | 1:J:389:ARG:NH1  | 2.32                     | 0.44              |
| 1:J:726:PHE:O    | 1:J:730:LEU:HG   | 2.17                     | 0.44              |
| 1:J:828:LYS:HD3  | 1:J:856:ARG:HG2  | 1.99                     | 0.44              |
| 1:L:828:LYS:HD3  | 1:L:856:ARG:HG2  | 1.99                     | 0.44              |
| 1:L:894:THR:HG23 | 1:L:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:A:726:PHE:O    | 1:A:730:LEU:HG   | 2.17                     | 0.44              |
| 1:B:138:ARG:CD   | 1:B:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:B:291:SER:HA   | 1:B:339:LYS:HZ3  | 1.82                     | 0.44              |
| 1:C:370:SER:H    | 1:C:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:F:732:SER:O    | 1:F:735:SER:OG   | 2.20                     | 0.44              |
| 1:F:784:CYS:SG   | 1:F:811:GLY:HA3  | 2.58                     | 0.44              |
| 1:H:219:VAL:HG13 | 1:H:344:ILE:HG13 | 1.98                     | 0.44              |
| 1:H:830:TRP:HZ3  | 1:I:1009:ARG:NE  | 2.15                     | 0.44              |
| 1:I:784:CYS:SG   | 1:I:811:GLY:HA3  | 2.57                     | 0.44              |
| 1:J:900:ALA:O    | 1:J:903:SER:OG   | 2.26                     | 0.44              |
| 1:K:132:TYR:OH   | 1:K:278:ASP:OD1  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:894:THR:HG23 | 1:K:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:L:968:LEU:HD13 | 1:L:970:LYS:O    | 2.17                     | 0.44              |
| 1:A:219:VAL:HG13 | 1:A:344:ILE:HG13 | 1.98                     | 0.44              |
| 1:A:228:LYS:HZ2  | 1:A:299:GLY:H    | 1.64                     | 0.44              |
| 1:A:374:ARG:NE   | 1:A:405:CYS:HB2  | 2.32                     | 0.44              |
| 1:A:469:ALA:HA   | 1:A:480:PHE:HZ   | 1.82                     | 0.44              |
| 1:A:564:GLY:HA2  | 1:A:570:TYR:O    | 2.18                     | 0.44              |
| 1:A:1017:ALA:O   | 1:A:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:B:784:CYS:SG   | 1:B:811:GLY:HA3  | 2.57                     | 0.44              |
| 1:C:247:ASP:O    | 1:C:292:ARG:NH2  | 2.31                     | 0.44              |
| 1:C:443:LEU:HD22 | 1:C:524:PHE:CE2  | 2.44                     | 0.44              |
| 1:C:828:LYS:HD3  | 1:C:856:ARG:HG2  | 1.99                     | 0.44              |
| 1:D:968:LEU:HD13 | 1:D:970:LYS:O    | 2.17                     | 0.44              |
| 1:G:258:ARG:HH22 | 1:G:515:SER:HB2  | 1.82                     | 0.44              |
| 1:G:726:PHE:O    | 1:G:730:LEU:HG   | 2.17                     | 0.44              |
| 1:G:894:THR:HG23 | 1:G:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:H:649:PRO:HA   | 1:H:674:VAL:HA   | 1.99                     | 0.44              |
| 1:I:250:ASP:N    | 1:I:292:ARG:O    | 2.46                     | 0.44              |
| 1:I:388:ALA:HB3  | 1:I:389:ARG:NH1  | 2.32                     | 0.44              |
| 1:I:601:GLN:O    | 1:I:605:GLU:HG2  | 2.16                     | 0.44              |
| 1:J:271:LEU:HD21 | 1:J:277:PRO:HA   | 1.98                     | 0.44              |
| 1:J:901:LEU:HA   | 1:J:904:VAL:HG12 | 1.98                     | 0.44              |
| 1:K:332:ILE:HA   | 1:K:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:K:564:GLY:HA2  | 1:K:570:TYR:O    | 2.18                     | 0.44              |
| 1:K:968:LEU:HD13 | 1:K:970:LYS:O    | 2.17                     | 0.44              |
| 1:L:332:ILE:HA   | 1:L:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:L:813:ARG:NH1  | 1:L:843:ASP:OD2  | 2.50                     | 0.44              |
| 1:A:369:PHE:HA   | 1:A:373:LYS:HZ2  | 1.82                     | 0.44              |
| 1:B:167:LEU:HB2  | 1:B:366:ILE:HD11 | 1.99                     | 0.44              |
| 1:B:228:LYS:HZ2  | 1:B:299:GLY:H    | 1.62                     | 0.44              |
| 1:B:734:LEU:HD23 | 1:B:737:ASN:ND2  | 2.30                     | 0.44              |
| 1:B:884:GLN:C    | 1:B:912:THR:HG22 | 2.38                     | 0.44              |
| 1:C:901:LEU:HA   | 1:C:904:VAL:HG12 | 1.98                     | 0.44              |
| 1:C:955:CYS:HA   | 1:C:958:LEU:HG   | 2.00                     | 0.44              |
| 1:D:258:ARG:HH22 | 1:D:515:SER:HB2  | 1.82                     | 0.44              |
| 1:D:726:PHE:O    | 1:D:730:LEU:HG   | 2.17                     | 0.44              |
| 1:D:894:THR:HG23 | 1:D:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:F:935:HIS:ND1  | 1:F:936:PRO:O    | 2.43                     | 0.44              |
| 1:G:511:GLU:HG3  | 1:G:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:G:564:GLY:HA2  | 1:G:570:TYR:O    | 2.18                     | 0.44              |
| 1:H:828:LYS:HD3  | 1:H:856:ARG:HG2  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:1017:ALA:O   | 1:I:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:J:469:ALA:HA   | 1:J:480:PHE:HZ   | 1.81                     | 0.44              |
| 1:J:564:GLY:HA2  | 1:J:570:TYR:O    | 2.18                     | 0.44              |
| 1:J:1017:ALA:O   | 1:J:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:K:258:ARG:HH22 | 1:K:515:SER:HB2  | 1.82                     | 0.44              |
| 1:K:579:PHE:HD2  | 1:K:635:MET:HG2  | 1.83                     | 0.44              |
| 1:K:1017:ALA:O   | 1:K:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:L:132:TYR:OH   | 1:L:278:ASP:OD1  | 2.33                     | 0.44              |
| 1:L:564:GLY:HA2  | 1:L:570:TYR:O    | 2.18                     | 0.44              |
| 1:L:579:PHE:HD2  | 1:L:635:MET:HG2  | 1.83                     | 0.44              |
| 1:L:1017:ALA:O   | 1:L:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:A:900:ALA:O    | 1:A:903:SER:OG   | 2.26                     | 0.44              |
| 1:B:872:LEU:HD23 | 1:B:875:LYS:HZ1  | 1.83                     | 0.44              |
| 1:D:511:GLU:HG3  | 1:D:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:D:1017:ALA:O   | 1:D:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:E:911:PHE:HZ   | 1:E:914:LEU:HD13 | 1.83                     | 0.44              |
| 1:F:894:THR:HG23 | 1:F:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:G:1017:ALA:O   | 1:G:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:H:443:LEU:HD22 | 1:H:524:PHE:CE2  | 2.44                     | 0.44              |
| 1:H:901:LEU:HA   | 1:H:904:VAL:HG12 | 1.98                     | 0.44              |
| 1:H:911:PHE:HZ   | 1:H:914:LEU:HD13 | 1.83                     | 0.44              |
| 1:I:167:LEU:HB2  | 1:I:366:ILE:HD11 | 1.99                     | 0.44              |
| 1:I:649:PRO:HA   | 1:I:674:VAL:HA   | 1.99                     | 0.44              |
| 1:I:1007:LEU:HB2 | 1:I:1012:LYS:HZ1 | 1.81                     | 0.44              |
| 1:J:590:LEU:HA   | 1:J:590:LEU:HD23 | 1.79                     | 0.44              |
| 1:L:258:ARG:HH22 | 1:L:515:SER:HB2  | 1.82                     | 0.44              |
| 1:A:884:GLN:C    | 1:A:912:THR:HG22 | 2.38                     | 0.44              |
| 1:B:579:PHE:HD2  | 1:B:635:MET:HG2  | 1.83                     | 0.44              |
| 1:B:649:PRO:HA   | 1:B:674:VAL:HA   | 1.99                     | 0.44              |
| 1:B:968:LEU:HD13 | 1:B:970:LYS:O    | 2.17                     | 0.44              |
| 1:B:1007:LEU:HB2 | 1:B:1012:LYS:HZ1 | 1.81                     | 0.44              |
| 1:C:138:ARG:CD   | 1:C:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:C:167:LEU:HB2  | 1:C:366:ILE:HD11 | 1.99                     | 0.44              |
| 1:D:564:GLY:HA2  | 1:D:570:TYR:O    | 2.18                     | 0.44              |
| 1:D:601:GLN:O    | 1:D:605:GLU:HG2  | 2.16                     | 0.44              |
| 1:D:784:CYS:SG   | 1:D:811:GLY:HA3  | 2.58                     | 0.44              |
| 1:E:132:TYR:OH   | 1:E:278:ASP:OD1  | 2.33                     | 0.44              |
| 1:E:138:ARG:CD   | 1:E:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:E:167:LEU:HB2  | 1:E:366:ILE:HD11 | 1.98                     | 0.44              |
| 1:E:564:GLY:HA2  | 1:E:570:TYR:O    | 2.18                     | 0.44              |
| 1:E:784:CYS:SG   | 1:E:811:GLY:HA3  | 2.58                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:889:VAL:O    | 1:E:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:E:894:THR:HG23 | 1:E:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:F:564:GLY:HA2  | 1:F:570:TYR:O    | 2.18                     | 0.44              |
| 1:G:601:GLN:O    | 1:G:605:GLU:HG2  | 2.16                     | 0.44              |
| 1:G:784:CYS:SG   | 1:G:811:GLY:HA3  | 2.58                     | 0.44              |
| 1:G:889:VAL:O    | 1:G:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:H:332:ILE:HA   | 1:H:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:H:369:PHE:CE2  | 1:H:408:PRO:HA   | 2.53                     | 0.44              |
| 1:H:889:VAL:O    | 1:H:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:I:171:LYS:HE3  | 1:I:364:VAL:HB   | 2.00                     | 0.44              |
| 1:I:889:VAL:O    | 1:I:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:J:219:VAL:HG13 | 1:J:344:ILE:HG13 | 1.98                     | 0.44              |
| 1:J:884:GLN:C    | 1:J:912:THR:HG22 | 2.38                     | 0.44              |
| 1:J:1007:LEU:HB2 | 1:J:1012:LYS:HZ1 | 1.81                     | 0.44              |
| 1:K:813:ARG:NH1  | 1:K:843:ASP:OD2  | 2.50                     | 0.44              |
| 1:B:171:LYS:HE3  | 1:B:364:VAL:HB   | 2.00                     | 0.44              |
| 1:B:889:VAL:O    | 1:B:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:C:469:ALA:HA   | 1:C:480:PHE:HZ   | 1.81                     | 0.44              |
| 1:C:649:PRO:HA   | 1:C:674:VAL:HA   | 1.99                     | 0.44              |
| 1:C:911:PHE:HZ   | 1:C:914:LEU:HD13 | 1.83                     | 0.44              |
| 1:D:889:VAL:O    | 1:D:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:E:1017:ALA:O   | 1:E:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:F:138:ARG:CD   | 1:F:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:F:889:VAL:O    | 1:F:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:H:469:ALA:HA   | 1:H:480:PHE:HZ   | 1.81                     | 0.44              |
| 1:H:955:CYS:HA   | 1:H:958:LEU:HG   | 2.00                     | 0.44              |
| 1:H:1017:ALA:O   | 1:H:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:I:579:PHE:HD2  | 1:I:635:MET:HG2  | 1.83                     | 0.44              |
| 1:I:884:GLN:C    | 1:I:912:THR:HG22 | 2.38                     | 0.44              |
| 1:I:900:ALA:O    | 1:I:903:SER:OG   | 2.26                     | 0.44              |
| 1:I:968:LEU:HD13 | 1:I:970:LYS:O    | 2.17                     | 0.44              |
| 1:J:138:ARG:CD   | 1:J:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:J:579:PHE:HD2  | 1:J:635:MET:HG2  | 1.83                     | 0.44              |
| 1:K:138:ARG:CD   | 1:K:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:L:138:ARG:CD   | 1:L:141:ARG:HH21 | 2.30                     | 0.44              |
| 1:A:579:PHE:HD2  | 1:A:635:MET:HG2  | 1.83                     | 0.44              |
| 1:B:726:PHE:O    | 1:B:730:LEU:HG   | 2.17                     | 0.44              |
| 1:C:352:GLU:OE1  | 1:C:352:GLU:N    | 2.46                     | 0.44              |
| 1:C:369:PHE:CE2  | 1:C:408:PRO:HA   | 2.53                     | 0.44              |
| 1:D:221:GLN:O    | 1:D:366:ILE:N    | 2.45                     | 0.44              |
| 1:E:369:PHE:CE2  | 1:E:408:PRO:HA   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:370:SER:H    | 1:E:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:F:352:GLU:OE1  | 1:F:352:GLU:N    | 2.46                     | 0.44              |
| 1:F:369:PHE:CE2  | 1:F:408:PRO:HA   | 2.53                     | 0.44              |
| 1:F:370:SER:H    | 1:F:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:G:956:TRP:O    | 1:G:960:THR:HG23 | 2.18                     | 0.44              |
| 1:I:511:GLU:HG3  | 1:I:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:I:726:PHE:O    | 1:I:730:LEU:HG   | 2.17                     | 0.44              |
| 1:J:1009:ARG:NE  | 1:K:830:TRP:CZ3  | 2.84                     | 0.44              |
| 1:K:370:SER:H    | 1:K:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:K:511:GLU:HG3  | 1:K:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:K:784:CYS:SG   | 1:K:811:GLY:HA3  | 2.57                     | 0.44              |
| 1:K:884:GLN:C    | 1:K:912:THR:HG22 | 2.38                     | 0.44              |
| 1:A:332:ILE:HA   | 1:A:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:A:889:VAL:O    | 1:A:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:B:511:GLU:HG3  | 1:B:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:B:817:VAL:HG12 | 1:B:820:LYS:NZ   | 2.33                     | 0.44              |
| 1:C:726:PHE:O    | 1:C:730:LEU:HG   | 2.17                     | 0.44              |
| 1:C:734:LEU:HD23 | 1:C:737:ASN:ND2  | 2.30                     | 0.44              |
| 1:C:872:LEU:HA   | 1:C:875:LYS:HZ3  | 1.83                     | 0.44              |
| 1:C:889:VAL:O    | 1:C:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:C:894:THR:HG23 | 1:C:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:1017:ALA:O   | 1:C:1020:GLU:HG2 | 2.18                     | 0.44              |
| 1:D:956:TRP:O    | 1:D:960:THR:HG23 | 2.18                     | 0.44              |
| 1:E:884:GLN:C    | 1:E:912:THR:HG22 | 2.38                     | 0.44              |
| 1:F:511:GLU:HG3  | 1:F:512:ARG:HG3  | 2.00                     | 0.44              |
| 1:F:911:PHE:HZ   | 1:F:914:LEU:HD13 | 1.83                     | 0.44              |
| 1:H:894:THR:HG23 | 1:H:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:I:370:SER:H    | 1:I:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:I:734:LEU:HD23 | 1:I:737:ASN:ND2  | 2.30                     | 0.44              |
| 1:I:905:LEU:HD11 | 1:I:914:LEU:HD22 | 2.00                     | 0.44              |
| 1:J:332:ILE:HA   | 1:J:335:LYS:HB2  | 1.98                     | 0.44              |
| 1:J:369:PHE:CE2  | 1:J:408:PRO:HA   | 2.53                     | 0.44              |
| 1:J:443:LEU:HD22 | 1:J:524:PHE:CE2  | 2.44                     | 0.44              |
| 1:J:889:VAL:O    | 1:J:919:ASN:ND2  | 2.51                     | 0.44              |
| 1:J:894:THR:HG23 | 1:J:921:LEU:HD22 | 1.99                     | 0.44              |
| 1:K:813:ARG:HG2  | 1:K:843:ASP:OD2  | 2.18                     | 0.44              |
| 1:L:370:SER:H    | 1:L:373:LYS:HE3  | 1.82                     | 0.44              |
| 1:L:784:CYS:SG   | 1:L:811:GLY:HA3  | 2.58                     | 0.44              |
| 1:A:258:ARG:HH22 | 1:A:515:SER:HB2  | 1.82                     | 0.43              |
| 1:A:369:PHE:CE2  | 1:A:408:PRO:HA   | 2.53                     | 0.43              |
| 1:B:564:GLY:HA2  | 1:B:570:TYR:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:900:ALA:O    | 1:B:903:SER:OG   | 2.26                     | 0.43              |
| 1:D:987:CYS:HA   | 1:D:990:LEU:HG   | 2.00                     | 0.43              |
| 1:F:167:LEU:HB2  | 1:F:366:ILE:HD11 | 1.99                     | 0.43              |
| 1:F:291:SER:HA   | 1:F:339:LYS:HZ3  | 1.83                     | 0.43              |
| 1:F:518:HIS:O    | 1:F:520:THR:HG23 | 2.19                     | 0.43              |
| 1:F:884:GLN:C    | 1:F:912:THR:HG22 | 2.38                     | 0.43              |
| 1:F:968:LEU:HD13 | 1:F:970:LYS:O    | 2.17                     | 0.43              |
| 1:F:1017:ALA:O   | 1:F:1020:GLU:HG2 | 2.18                     | 0.43              |
| 1:G:221:GLN:O    | 1:G:366:ILE:N    | 2.45                     | 0.43              |
| 1:H:138:ARG:CD   | 1:H:141:ARG:HH21 | 2.30                     | 0.43              |
| 1:H:167:LEU:HB2  | 1:H:366:ILE:HD11 | 1.99                     | 0.43              |
| 1:H:258:ARG:HH22 | 1:H:515:SER:HB2  | 1.82                     | 0.43              |
| 1:H:726:PHE:O    | 1:H:730:LEU:HG   | 2.17                     | 0.43              |
| 1:H:830:TRP:HZ3  | 1:I:1009:ARG:HE  | 1.62                     | 0.43              |
| 1:I:228:LYS:HZ2  | 1:I:299:GLY:H    | 1.62                     | 0.43              |
| 1:I:564:GLY:HA2  | 1:I:570:TYR:O    | 2.18                     | 0.43              |
| 1:I:817:VAL:HG12 | 1:I:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:J:649:PRO:HA   | 1:J:674:VAL:HA   | 1.99                     | 0.43              |
| 1:J:911:PHE:HZ   | 1:J:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:K:665:SER:C    | 1:K:669:LYS:HZ2  | 2.21                     | 0.43              |
| 1:L:511:GLU:HG3  | 1:L:512:ARG:HG3  | 2.00                     | 0.43              |
| 1:L:813:ARG:HG2  | 1:L:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:L:884:GLN:C    | 1:L:912:THR:HG22 | 2.38                     | 0.43              |
| 1:A:649:PRO:HA   | 1:A:674:VAL:HA   | 1.99                     | 0.43              |
| 1:B:828:LYS:HD3  | 1:B:856:ARG:HG2  | 1.99                     | 0.43              |
| 1:B:905:LEU:HD11 | 1:B:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:956:TRP:O    | 1:C:960:THR:HG23 | 2.18                     | 0.43              |
| 1:D:369:PHE:CE2  | 1:D:408:PRO:HA   | 2.53                     | 0.43              |
| 1:D:884:GLN:C    | 1:D:912:THR:HG22 | 2.38                     | 0.43              |
| 1:E:511:GLU:HG3  | 1:E:512:ARG:HG3  | 2.00                     | 0.43              |
| 1:E:518:HIS:O    | 1:E:520:THR:HG23 | 2.19                     | 0.43              |
| 1:E:556:VAL:O    | 1:E:559:LEU:HG   | 2.19                     | 0.43              |
| 1:E:830:TRP:CD1  | 1:E:830:TRP:N    | 2.86                     | 0.43              |
| 1:E:968:LEU:HD13 | 1:E:970:LYS:O    | 2.17                     | 0.43              |
| 1:G:884:GLN:C    | 1:G:912:THR:HG22 | 2.38                     | 0.43              |
| 1:G:987:CYS:HA   | 1:G:990:LEU:HG   | 2.00                     | 0.43              |
| 1:I:369:PHE:CE2  | 1:I:408:PRO:HA   | 2.53                     | 0.43              |
| 1:I:665:SER:C    | 1:I:669:LYS:HZ2  | 2.21                     | 0.43              |
| 1:I:872:LEU:HA   | 1:I:875:LYS:HZ3  | 1.83                     | 0.43              |
| 1:J:905:LEU:HD11 | 1:J:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:J:956:TRP:O    | 1:J:960:THR:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:665:SER:C    | 1:L:669:LYS:HZ2  | 2.21                     | 0.43              |
| 1:A:138:ARG:CD   | 1:A:141:ARG:HH21 | 2.30                     | 0.43              |
| 1:A:813:ARG:HG2  | 1:A:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:A:894:THR:HG23 | 1:A:921:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:911:PHE:HZ   | 1:A:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:A:956:TRP:O    | 1:A:960:THR:HG23 | 2.18                     | 0.43              |
| 1:B:369:PHE:CE2  | 1:B:408:PRO:HA   | 2.53                     | 0.43              |
| 1:B:370:SER:H    | 1:B:373:LYS:HE3  | 1.82                     | 0.43              |
| 1:B:911:PHE:HZ   | 1:B:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:B:935:HIS:ND1  | 1:B:936:PRO:O    | 2.43                     | 0.43              |
| 1:C:258:ARG:HH22 | 1:C:515:SER:HB2  | 1.82                     | 0.43              |
| 1:C:332:ILE:HA   | 1:C:335:LYS:HB2  | 1.98                     | 0.43              |
| 1:C:830:TRP:CD1  | 1:C:830:TRP:N    | 2.86                     | 0.43              |
| 1:C:944:GLU:CG   | 1:C:972:ASN:HB2  | 2.46                     | 0.43              |
| 1:D:579:PHE:HD2  | 1:D:635:MET:HG2  | 1.83                     | 0.43              |
| 1:E:171:LYS:HE3  | 1:E:364:VAL:HB   | 2.00                     | 0.43              |
| 1:F:171:LYS:HE3  | 1:F:364:VAL:HB   | 2.00                     | 0.43              |
| 1:F:828:LYS:HD3  | 1:F:856:ARG:HG2  | 1.99                     | 0.43              |
| 1:F:955:CYS:HA   | 1:F:958:LEU:HG   | 2.00                     | 0.43              |
| 1:G:369:PHE:CE2  | 1:G:408:PRO:HA   | 2.53                     | 0.43              |
| 1:G:400:VAL:HG22 | 1:G:404:MET:HE1  | 1.99                     | 0.43              |
| 1:G:771:ARG:HG3  | 1:G:771:ARG:O    | 2.19                     | 0.43              |
| 1:G:911:PHE:HZ   | 1:G:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:J:401:LEU:HD21 | 1:J:432:SER:HB2  | 2.00                     | 0.43              |
| 1:K:369:PHE:CE2  | 1:K:408:PRO:HA   | 2.53                     | 0.43              |
| 1:K:817:VAL:HG12 | 1:K:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:L:911:PHE:HZ   | 1:L:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:L:956:TRP:O    | 1:L:960:THR:HG23 | 2.18                     | 0.43              |
| 1:B:661:HIS:ND1  | 1:B:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:B:956:TRP:O    | 1:B:960:THR:HG23 | 2.18                     | 0.43              |
| 1:B:987:CYS:HA   | 1:B:990:LEU:HG   | 2.00                     | 0.43              |
| 1:C:564:GLY:HA2  | 1:C:570:TYR:O    | 2.18                     | 0.43              |
| 1:E:987:CYS:HA   | 1:E:990:LEU:HG   | 2.00                     | 0.43              |
| 1:F:556:VAL:O    | 1:F:559:LEU:HG   | 2.19                     | 0.43              |
| 1:G:370:SER:H    | 1:G:373:LYS:HE3  | 1.82                     | 0.43              |
| 1:G:518:HIS:O    | 1:G:520:THR:HG23 | 2.19                     | 0.43              |
| 1:G:905:LEU:HD11 | 1:G:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:H:388:ALA:HB3  | 1:H:389:ARG:NH1  | 2.32                     | 0.43              |
| 1:H:784:CYS:SG   | 1:H:811:GLY:HA3  | 2.58                     | 0.43              |
| 1:H:905:LEU:HD11 | 1:H:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:H:956:TRP:O    | 1:H:960:THR:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:955:CYS:HA   | 1:I:958:LEU:HG   | 2.00                     | 0.43              |
| 1:I:956:TRP:O    | 1:I:960:THR:HG23 | 2.18                     | 0.43              |
| 1:J:813:ARG:HG2  | 1:J:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:K:987:CYS:HA   | 1:K:990:LEU:HG   | 2.01                     | 0.43              |
| 1:L:267:SER:HB2  | 1:L:323:ARG:HA   | 2.01                     | 0.43              |
| 1:L:369:PHE:CE2  | 1:L:408:PRO:HA   | 2.53                     | 0.43              |
| 1:A:905:LEU:HD11 | 1:A:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:579:PHE:HD2  | 1:C:635:MET:HG2  | 1.83                     | 0.43              |
| 1:D:464:GLY:HA3  | 1:D:490:LEU:HG   | 2.01                     | 0.43              |
| 1:D:771:ARG:O    | 1:D:771:ARG:HG3  | 2.19                     | 0.43              |
| 1:D:905:LEU:HD11 | 1:D:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:D:955:CYS:HA   | 1:D:958:LEU:HG   | 2.00                     | 0.43              |
| 1:E:509:ASP:CB   | 1:E:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:E:771:ARG:HG3  | 1:E:771:ARG:O    | 2.19                     | 0.43              |
| 1:E:828:LYS:HD3  | 1:E:856:ARG:HG2  | 1.99                     | 0.43              |
| 1:E:955:CYS:HA   | 1:E:958:LEU:HG   | 2.00                     | 0.43              |
| 1:F:579:PHE:HD2  | 1:F:635:MET:HG2  | 1.83                     | 0.43              |
| 1:F:955:CYS:O    | 1:F:958:LEU:HG   | 2.19                     | 0.43              |
| 1:G:407:ILE:HA   | 1:G:408:PRO:HD3  | 1.92                     | 0.43              |
| 1:G:464:GLY:HA3  | 1:G:490:LEU:HG   | 2.01                     | 0.43              |
| 1:H:884:GLN:C    | 1:H:912:THR:HG22 | 2.38                     | 0.43              |
| 1:I:661:HIS:ND1  | 1:I:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:I:987:CYS:HA   | 1:I:990:LEU:HG   | 2.00                     | 0.43              |
| 1:K:267:SER:HB2  | 1:K:323:ARG:HA   | 2.01                     | 0.43              |
| 1:K:649:PRO:HA   | 1:K:674:VAL:HA   | 1.99                     | 0.43              |
| 1:K:661:HIS:ND1  | 1:K:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:K:911:PHE:HZ   | 1:K:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:L:661:HIS:ND1  | 1:L:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:L:817:VAL:HG12 | 1:L:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:A:267:SER:HB2  | 1:A:323:ARG:HA   | 2.01                     | 0.43              |
| 1:A:784:CYS:SG   | 1:A:811:GLY:HA3  | 2.58                     | 0.43              |
| 1:B:283:VAL:HA   | 1:B:286:ILE:HG12 | 2.01                     | 0.43              |
| 1:B:665:SER:C    | 1:B:669:LYS:HZ2  | 2.22                     | 0.43              |
| 1:B:813:ARG:HG2  | 1:B:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:C:771:ARG:HG3  | 1:C:771:ARG:O    | 2.19                     | 0.43              |
| 1:C:898:CYS:O    | 1:C:902:THR:HG23 | 2.19                     | 0.43              |
| 1:C:905:LEU:HD11 | 1:C:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:955:CYS:O    | 1:C:958:LEU:HG   | 2.19                     | 0.43              |
| 1:D:267:SER:HB2  | 1:D:323:ARG:HA   | 2.01                     | 0.43              |
| 1:D:370:SER:H    | 1:D:373:LYS:HE3  | 1.82                     | 0.43              |
| 1:D:518:HIS:O    | 1:D:520:THR:HG23 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:911:PHE:HZ   | 1:D:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:E:980:ASP:O    | 1:E:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:G:267:SER:HB2  | 1:G:323:ARG:HA   | 2.01                     | 0.43              |
| 1:G:579:PHE:HD2  | 1:G:635:MET:HG2  | 1.83                     | 0.43              |
| 1:G:955:CYS:HA   | 1:G:958:LEU:HG   | 2.00                     | 0.43              |
| 1:H:579:PHE:HA   | 1:H:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:H:771:ARG:HG3  | 1:H:771:ARG:O    | 2.19                     | 0.43              |
| 1:H:955:CYS:O    | 1:H:958:LEU:HG   | 2.19                     | 0.43              |
| 1:I:464:GLY:HA3  | 1:I:490:LEU:HG   | 2.01                     | 0.43              |
| 1:I:828:LYS:HD3  | 1:I:856:ARG:HG2  | 1.99                     | 0.43              |
| 1:I:911:PHE:HZ   | 1:I:914:LEU:HD13 | 1.83                     | 0.43              |
| 1:J:258:ARG:HH22 | 1:J:515:SER:HB2  | 1.82                     | 0.43              |
| 1:J:556:VAL:O    | 1:J:559:LEU:HG   | 2.19                     | 0.43              |
| 1:J:784:CYS:SG   | 1:J:811:GLY:HA3  | 2.58                     | 0.43              |
| 1:J:898:CYS:O    | 1:J:902:THR:HG23 | 2.19                     | 0.43              |
| 1:K:590:LEU:HA   | 1:K:590:LEU:HD23 | 1.79                     | 0.43              |
| 1:K:956:TRP:O    | 1:K:960:THR:HG23 | 2.18                     | 0.43              |
| 1:L:987:CYS:HA   | 1:L:990:LEU:HG   | 2.01                     | 0.43              |
| 1:A:401:LEU:HD21 | 1:A:432:SER:HB2  | 2.00                     | 0.43              |
| 1:A:661:HIS:ND1  | 1:A:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:A:898:CYS:O    | 1:A:902:THR:HG23 | 2.19                     | 0.43              |
| 1:A:953:HIS:NE2  | 1:L:617:LYS:HB2  | 2.33                     | 0.43              |
| 1:B:464:GLY:HA3  | 1:B:490:LEU:HG   | 2.01                     | 0.43              |
| 1:C:171:LYS:HE3  | 1:C:364:VAL:HB   | 2.00                     | 0.43              |
| 1:C:388:ALA:HB3  | 1:C:389:ARG:NH1  | 2.32                     | 0.43              |
| 1:C:401:LEU:HD21 | 1:C:432:SER:HB2  | 2.00                     | 0.43              |
| 1:C:813:ARG:HG2  | 1:C:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:D:898:CYS:O    | 1:D:902:THR:HG23 | 2.19                     | 0.43              |
| 1:E:400:VAL:C    | 1:E:402:PHE:H    | 2.22                     | 0.43              |
| 1:E:579:PHE:HD2  | 1:E:635:MET:HG2  | 1.83                     | 0.43              |
| 1:E:734:LEU:HD23 | 1:E:737:ASN:ND2  | 2.30                     | 0.43              |
| 1:E:955:CYS:O    | 1:E:958:LEU:HG   | 2.19                     | 0.43              |
| 1:F:255:ILE:HD11 | 1:F:295:PHE:HB3  | 2.00                     | 0.43              |
| 1:F:987:CYS:HA   | 1:F:990:LEU:HG   | 2.01                     | 0.43              |
| 1:G:734:LEU:HD23 | 1:G:737:ASN:ND2  | 2.30                     | 0.43              |
| 1:G:898:CYS:O    | 1:G:902:THR:HG23 | 2.19                     | 0.43              |
| 1:H:217:THR:HG23 | 1:H:361:PRO:HB3  | 2.01                     | 0.43              |
| 1:H:291:SER:HA   | 1:H:339:LYS:HZ3  | 1.83                     | 0.43              |
| 1:H:813:ARG:HG2  | 1:H:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:I:283:VAL:HA   | 1:I:286:ILE:HG12 | 2.01                     | 0.43              |
| 1:J:661:HIS:ND1  | 1:J:726:PHE:HB3  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:649:PRO:HA   | 1:L:674:VAL:HA   | 1.99                     | 0.43              |
| 1:L:889:VAL:O    | 1:L:919:ASN:ND2  | 2.51                     | 0.43              |
| 1:A:250:ASP:CG   | 1:A:292:ARG:HE   | 2.21                     | 0.43              |
| 1:A:556:VAL:O    | 1:A:559:LEU:HG   | 2.19                     | 0.43              |
| 1:A:579:PHE:HA   | 1:A:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:A:590:LEU:HD23 | 1:A:590:LEU:HA   | 1.80                     | 0.43              |
| 1:A:943:LEU:O    | 1:A:971:LEU:HA   | 2.19                     | 0.43              |
| 1:B:955:CYS:O    | 1:B:958:LEU:HG   | 2.19                     | 0.43              |
| 1:C:217:THR:HG23 | 1:C:361:PRO:HB3  | 2.01                     | 0.43              |
| 1:C:224:ALA:HB1  | 1:C:573:PHE:CE2  | 2.54                     | 0.43              |
| 1:C:250:ASP:N    | 1:C:292:ARG:O    | 2.46                     | 0.43              |
| 1:C:884:GLN:C    | 1:C:912:THR:HG22 | 2.38                     | 0.43              |
| 1:D:509:ASP:CB   | 1:D:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:D:817:VAL:HG12 | 1:D:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:E:898:CYS:O    | 1:E:902:THR:HG23 | 2.19                     | 0.43              |
| 1:F:509:ASP:CB   | 1:F:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:F:956:TRP:O    | 1:F:960:THR:HG23 | 2.18                     | 0.43              |
| 1:F:980:ASP:O    | 1:F:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:G:388:ALA:HB3  | 1:G:389:ARG:NH1  | 2.32                     | 0.43              |
| 1:G:509:ASP:CB   | 1:G:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:G:817:VAL:HG12 | 1:G:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:H:401:LEU:HD21 | 1:H:432:SER:HB2  | 2.00                     | 0.43              |
| 1:H:564:GLY:HA2  | 1:H:570:TYR:O    | 2.18                     | 0.43              |
| 1:H:830:TRP:N    | 1:H:830:TRP:CD1  | 2.86                     | 0.43              |
| 1:H:898:CYS:O    | 1:H:902:THR:HG23 | 2.19                     | 0.43              |
| 1:H:980:ASP:O    | 1:H:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:I:255:ILE:HD11 | 1:I:295:PHE:HB3  | 2.00                     | 0.43              |
| 1:I:401:LEU:HD21 | 1:I:432:SER:HB2  | 2.00                     | 0.43              |
| 1:I:955:CYS:O    | 1:I:958:LEU:HG   | 2.19                     | 0.43              |
| 1:J:250:ASP:CG   | 1:J:292:ARG:HE   | 2.21                     | 0.43              |
| 1:J:267:SER:HB2  | 1:J:323:ARG:HA   | 2.01                     | 0.43              |
| 1:J:943:LEU:O    | 1:J:971:LEU:HA   | 2.19                     | 0.43              |
| 1:K:624:SER:OG   | 1:K:627:GLU:OE2  | 2.30                     | 0.43              |
| 1:K:834:CYS:O    | 1:K:836:LEU:N    | 2.52                     | 0.43              |
| 1:K:889:VAL:O    | 1:K:919:ASN:ND2  | 2.51                     | 0.43              |
| 1:K:905:LEU:HD11 | 1:K:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:L:556:VAL:O    | 1:L:559:LEU:HG   | 2.19                     | 0.43              |
| 1:L:590:LEU:HA   | 1:L:590:LEU:HD23 | 1.80                     | 0.43              |
| 1:L:834:CYS:O    | 1:L:836:LEU:N    | 2.52                     | 0.43              |
| 1:A:224:ALA:HB1  | 1:A:573:PHE:CE2  | 2.54                     | 0.43              |
| 1:A:511:GLU:HG3  | 1:A:512:ARG:HG3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:771:ARG:HG3  | 1:A:771:ARG:O    | 2.19                     | 0.43              |
| 1:A:955:CYS:HA   | 1:A:958:LEU:HG   | 2.00                     | 0.43              |
| 1:B:579:PHE:HA   | 1:B:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:B:771:ARG:HG3  | 1:B:771:ARG:O    | 2.19                     | 0.43              |
| 1:B:955:CYS:HA   | 1:B:958:LEU:HG   | 2.00                     | 0.43              |
| 1:C:556:VAL:O    | 1:C:559:LEU:HG   | 2.19                     | 0.43              |
| 1:C:579:PHE:HA   | 1:C:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:C:980:ASP:O    | 1:C:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:D:579:PHE:HA   | 1:D:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:D:980:ASP:O    | 1:D:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:E:255:ILE:HD11 | 1:E:295:PHE:HB3  | 2.00                     | 0.43              |
| 1:E:417:GLY:O    | 1:E:420:GLN:NE2  | 2.52                     | 0.43              |
| 1:F:315:CYS:HA   | 1:F:332:ILE:HG21 | 2.01                     | 0.43              |
| 1:F:388:ALA:HB3  | 1:F:389:ARG:NH1  | 2.32                     | 0.43              |
| 1:F:771:ARG:HG3  | 1:F:771:ARG:O    | 2.19                     | 0.43              |
| 1:F:830:TRP:CD1  | 1:F:830:TRP:N    | 2.86                     | 0.43              |
| 1:G:171:LYS:HE3  | 1:G:364:VAL:HB   | 2.00                     | 0.43              |
| 1:G:283:VAL:HA   | 1:G:286:ILE:HG12 | 2.01                     | 0.43              |
| 1:G:291:SER:HA   | 1:G:339:LYS:HZ3  | 1.84                     | 0.43              |
| 1:G:955:CYS:O    | 1:G:958:LEU:HG   | 2.19                     | 0.43              |
| 1:G:980:ASP:O    | 1:G:984:VAL:HG23 | 2.19                     | 0.43              |
| 1:H:224:ALA:HB1  | 1:H:573:PHE:CE2  | 2.54                     | 0.43              |
| 1:H:400:VAL:C    | 1:H:402:PHE:H    | 2.22                     | 0.43              |
| 1:H:511:GLU:HG3  | 1:H:512:ARG:HG3  | 2.00                     | 0.43              |
| 1:H:518:HIS:O    | 1:H:520:THR:HG23 | 2.18                     | 0.43              |
| 1:I:267:SER:HB2  | 1:I:323:ARG:HA   | 2.01                     | 0.43              |
| 1:I:509:ASP:CB   | 1:I:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:I:579:PHE:HA   | 1:I:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:I:771:ARG:HG3  | 1:I:771:ARG:O    | 2.19                     | 0.43              |
| 1:I:813:ARG:HG2  | 1:I:843:ASP:OD2  | 2.18                     | 0.43              |
| 1:J:224:ALA:HB1  | 1:J:573:PHE:CE2  | 2.54                     | 0.43              |
| 1:J:509:ASP:CB   | 1:J:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:J:771:ARG:HG3  | 1:J:771:ARG:O    | 2.19                     | 0.43              |
| 1:K:556:VAL:O    | 1:K:559:LEU:HG   | 2.19                     | 0.43              |
| 1:L:905:LEU:HD11 | 1:L:914:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:217:THR:HG23 | 1:A:361:PRO:HB3  | 2.01                     | 0.43              |
| 1:A:400:VAL:C    | 1:A:402:PHE:H    | 2.22                     | 0.43              |
| 1:A:509:ASP:CB   | 1:A:513:PHE:HB3  | 2.49                     | 0.43              |
| 1:A:955:CYS:O    | 1:A:958:LEU:HG   | 2.19                     | 0.43              |
| 1:B:250:ASP:CG   | 1:B:292:ARG:HE   | 2.21                     | 0.43              |
| 1:B:401:LEU:HD21 | 1:B:432:SER:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:943:LEU:O    | 1:B:971:LEU:HA   | 2.19                     | 0.43              |
| 1:C:400:VAL:C    | 1:C:402:PHE:H    | 2.22                     | 0.43              |
| 1:C:661:HIS:ND1  | 1:C:726:PHE:HB3  | 2.34                     | 0.43              |
| 1:C:784:CYS:SG   | 1:C:811:GLY:HA3  | 2.58                     | 0.43              |
| 1:D:171:LYS:HE3  | 1:D:364:VAL:HB   | 2.00                     | 0.43              |
| 1:D:283:VAL:HA   | 1:D:286:ILE:HG12 | 2.01                     | 0.43              |
| 1:D:291:SER:HA   | 1:D:339:LYS:HZ3  | 1.84                     | 0.43              |
| 1:D:388:ALA:HB3  | 1:D:389:ARG:NH1  | 2.32                     | 0.43              |
| 1:D:407:ILE:HA   | 1:D:408:PRO:HD3  | 1.92                     | 0.43              |
| 1:D:734:LEU:HD23 | 1:D:737:ASN:ND2  | 2.30                     | 0.43              |
| 1:D:773:TRP:HH2  | 1:E:1013:ARG:HG2 | 1.83                     | 0.43              |
| 1:D:828:LYS:HD3  | 1:D:856:ARG:HG2  | 1.99                     | 0.43              |
| 1:E:217:THR:HG23 | 1:E:361:PRO:HB3  | 2.01                     | 0.43              |
| 1:E:817:VAL:HG12 | 1:E:820:LYS:NZ   | 2.33                     | 0.43              |
| 1:F:258:ARG:HH22 | 1:F:515:SER:HB2  | 1.82                     | 0.43              |
| 1:F:579:PHE:HA   | 1:F:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:F:871:VAL:HG12 | 1:F:875:LYS:HZ2  | 1.81                     | 0.43              |
| 1:G:579:PHE:HA   | 1:G:582:VAL:HG22 | 2.01                     | 0.43              |
| 1:H:417:GLY:O    | 1:H:420:GLN:NE2  | 2.52                     | 0.43              |
| 1:H:579:PHE:HD2  | 1:H:635:MET:HG2  | 1.83                     | 0.43              |
| 1:I:369:PHE:HA   | 1:I:373:LYS:HZ2  | 1.83                     | 0.43              |
| 1:I:943:LEU:O    | 1:I:971:LEU:HA   | 2.19                     | 0.43              |
| 1:J:217:THR:HG23 | 1:J:361:PRO:HB3  | 2.01                     | 0.43              |
| 1:J:400:VAL:C    | 1:J:402:PHE:H    | 2.22                     | 0.43              |
| 1:J:955:CYS:HA   | 1:J:958:LEU:HG   | 2.00                     | 0.43              |
| 1:K:955:CYS:HA   | 1:K:958:LEU:HG   | 2.00                     | 0.43              |
| 1:L:943:LEU:O    | 1:L:971:LEU:HA   | 2.19                     | 0.43              |
| 1:L:955:CYS:HA   | 1:L:958:LEU:HG   | 2.00                     | 0.43              |
| 1:A:665:SER:C    | 1:A:669:LYS:HZ2  | 2.22                     | 0.42              |
| 1:B:255:ILE:HD11 | 1:B:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:B:267:SER:HB2  | 1:B:323:ARG:HA   | 2.01                     | 0.42              |
| 1:B:400:VAL:C    | 1:B:402:PHE:H    | 2.22                     | 0.42              |
| 1:B:509:ASP:CB   | 1:B:513:PHE:HB3  | 2.49                     | 0.42              |
| 1:B:528:MET:HE2  | 1:B:531:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:518:HIS:O    | 1:C:520:THR:HG23 | 2.19                     | 0.42              |
| 1:D:256:HIS:NE2  | 1:D:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:D:955:CYS:O    | 1:D:958:LEU:HG   | 2.19                     | 0.42              |
| 1:E:256:HIS:NE2  | 1:E:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:E:315:CYS:HA   | 1:E:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:E:905:LEU:HD11 | 1:E:914:LEU:HD22 | 2.00                     | 0.42              |
| 1:F:217:THR:HG23 | 1:F:361:PRO:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:256:HIS:NE2  | 1:G:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:G:315:CYS:HA   | 1:G:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:H:171:LYS:HE3  | 1:H:364:VAL:HB   | 2.00                     | 0.42              |
| 1:H:315:CYS:HA   | 1:H:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:H:734:LEU:HD23 | 1:H:737:ASN:ND2  | 2.30                     | 0.42              |
| 1:H:828:LYS:CD   | 1:H:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:I:400:VAL:C    | 1:I:402:PHE:H    | 2.22                     | 0.42              |
| 1:I:834:CYS:O    | 1:I:836:LEU:N    | 2.52                     | 0.42              |
| 1:I:970:LYS:HD2  | 1:I:1001:GLN:NE2 | 2.32                     | 0.42              |
| 1:J:511:GLU:HG3  | 1:J:512:ARG:HG3  | 2.00                     | 0.42              |
| 1:J:579:PHE:HA   | 1:J:582:VAL:HG22 | 2.01                     | 0.42              |
| 1:J:970:LYS:HD2  | 1:J:1001:GLN:NE2 | 2.32                     | 0.42              |
| 1:K:955:CYS:O    | 1:K:958:LEU:HG   | 2.19                     | 0.42              |
| 1:L:579:PHE:HA   | 1:L:582:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:987:CYS:HA   | 1:A:990:LEU:HG   | 2.01                     | 0.42              |
| 1:C:417:GLY:O    | 1:C:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:D:315:CYS:HA   | 1:D:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:E:250:ASP:N    | 1:E:292:ARG:O    | 2.46                     | 0.42              |
| 1:E:464:GLY:HA3  | 1:E:490:LEU:HG   | 2.01                     | 0.42              |
| 1:E:956:TRP:O    | 1:E:960:THR:HG23 | 2.18                     | 0.42              |
| 1:F:256:HIS:NE2  | 1:F:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:F:417:GLY:O    | 1:F:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:G:661:HIS:ND1  | 1:G:726:PHE:HB3  | 2.34                     | 0.42              |
| 1:G:828:LYS:HD3  | 1:G:856:ARG:HG2  | 1.99                     | 0.42              |
| 1:H:256:HIS:NE2  | 1:H:258:ARG:HB3  | 2.35                     | 0.42              |
| 1:H:509:ASP:CB   | 1:H:513:PHE:HB3  | 2.49                     | 0.42              |
| 1:H:556:VAL:O    | 1:H:559:LEU:HG   | 2.19                     | 0.42              |
| 1:H:925:GLY:O    | 1:H:928:LEU:HG   | 2.19                     | 0.42              |
| 1:J:955:CYS:O    | 1:J:958:LEU:HG   | 2.19                     | 0.42              |
| 1:K:579:PHE:HA   | 1:K:582:VAL:HG22 | 2.01                     | 0.42              |
| 1:K:943:LEU:O    | 1:K:971:LEU:HA   | 2.19                     | 0.42              |
| 1:L:224:ALA:HB1  | 1:L:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:L:283:VAL:HA   | 1:L:286:ILE:HG12 | 2.01                     | 0.42              |
| 1:L:955:CYS:O    | 1:L:958:LEU:HG   | 2.19                     | 0.42              |
| 1:B:256:HIS:NE2  | 1:B:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:B:518:HIS:O    | 1:B:520:THR:HG23 | 2.18                     | 0.42              |
| 1:C:511:GLU:HG3  | 1:C:512:ARG:HG3  | 2.00                     | 0.42              |
| 1:D:400:VAL:HG22 | 1:D:404:MET:HE1  | 2.00                     | 0.42              |
| 1:D:661:HIS:ND1  | 1:D:726:PHE:HB3  | 2.34                     | 0.42              |
| 1:E:224:ALA:HB1  | 1:E:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:258:ARG:HH22 | 1:E:515:SER:HB2  | 1.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:267:SER:HB2  | 1:E:323:ARG:HA   | 2.01                     | 0.42              |
| 1:E:579:PHE:HA   | 1:E:582:VAL:HG22 | 2.01                     | 0.42              |
| 1:F:464:GLY:HA3  | 1:F:490:LEU:HG   | 2.01                     | 0.42              |
| 1:F:817:VAL:HG12 | 1:F:820:LYS:NZ   | 2.33                     | 0.42              |
| 1:F:898:CYS:O    | 1:F:902:THR:HG23 | 2.19                     | 0.42              |
| 1:F:925:GLY:O    | 1:F:928:LEU:HG   | 2.20                     | 0.42              |
| 1:G:255:ILE:HD11 | 1:G:295:PHE:HB3  | 2.01                     | 0.42              |
| 1:H:255:ILE:HD11 | 1:H:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:I:250:ASP:CG   | 1:I:292:ARG:HE   | 2.21                     | 0.42              |
| 1:I:256:HIS:NE2  | 1:I:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:I:291:SER:HA   | 1:I:339:LYS:HZ3  | 1.84                     | 0.42              |
| 1:I:315:CYS:HA   | 1:I:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:I:828:LYS:CD   | 1:I:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:J:171:LYS:HE3  | 1:J:364:VAL:HB   | 2.00                     | 0.42              |
| 1:J:987:CYS:HA   | 1:J:990:LEU:HG   | 2.00                     | 0.42              |
| 1:K:171:LYS:HE3  | 1:K:364:VAL:HB   | 2.00                     | 0.42              |
| 1:K:283:VAL:HA   | 1:K:286:ILE:HG12 | 2.01                     | 0.42              |
| 1:K:400:VAL:C    | 1:K:402:PHE:H    | 2.22                     | 0.42              |
| 1:K:464:GLY:HA3  | 1:K:490:LEU:HG   | 2.01                     | 0.42              |
| 1:K:509:ASP:CB   | 1:K:513:PHE:HB3  | 2.49                     | 0.42              |
| 1:L:400:VAL:C    | 1:L:402:PHE:H    | 2.23                     | 0.42              |
| 1:L:509:ASP:CB   | 1:L:513:PHE:HB3  | 2.49                     | 0.42              |
| 1:L:518:HIS:O    | 1:L:520:THR:HG23 | 2.18                     | 0.42              |
| 1:A:134:LYS:HG3  | 1:A:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:171:LYS:HE3  | 1:A:364:VAL:HB   | 2.00                     | 0.42              |
| 1:B:632:LEU:HD12 | 1:B:641:VAL:HG22 | 2.02                     | 0.42              |
| 1:B:828:LYS:CD   | 1:B:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:C:256:HIS:NE2  | 1:C:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:C:267:SER:HB2  | 1:C:323:ARG:HA   | 2.01                     | 0.42              |
| 1:C:294:LEU:HD12 | 1:C:295:PHE:N    | 2.35                     | 0.42              |
| 1:C:632:LEU:HD12 | 1:C:641:VAL:HG22 | 2.01                     | 0.42              |
| 1:C:828:LYS:CD   | 1:C:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:C:925:GLY:O    | 1:C:928:LEU:HG   | 2.19                     | 0.42              |
| 1:D:224:ALA:HB1  | 1:D:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:D:255:ILE:HD11 | 1:D:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:D:391:ALA:HA   | 1:D:394:LEU:HG   | 2.02                     | 0.42              |
| 1:D:925:GLY:O    | 1:D:928:LEU:HG   | 2.19                     | 0.42              |
| 1:D:943:LEU:O    | 1:D:971:LEU:HA   | 2.19                     | 0.42              |
| 1:E:294:LEU:HD12 | 1:E:295:PHE:N    | 2.34                     | 0.42              |
| 1:E:925:GLY:O    | 1:E:928:LEU:HG   | 2.19                     | 0.42              |
| 1:E:944:GLU:CG   | 1:E:972:ASN:HB2  | 2.46                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:267:SER:HB2  | 1:F:323:ARG:HA   | 2.01                     | 0.42              |
| 1:F:813:ARG:HG2  | 1:F:843:ASP:OD2  | 2.18                     | 0.42              |
| 1:F:998:GLN:O    | 1:F:1026:THR:OG1 | 2.26                     | 0.42              |
| 1:G:391:ALA:HA   | 1:G:394:LEU:HG   | 2.02                     | 0.42              |
| 1:G:401:LEU:HD21 | 1:G:432:SER:HB2  | 2.00                     | 0.42              |
| 1:G:813:ARG:HG2  | 1:G:843:ASP:OD2  | 2.18                     | 0.42              |
| 1:G:925:GLY:O    | 1:G:928:LEU:HG   | 2.19                     | 0.42              |
| 1:G:970:LYS:HD2  | 1:G:1001:GLN:NE2 | 2.32                     | 0.42              |
| 1:H:284:CYS:HA   | 1:H:287:LEU:HG   | 2.02                     | 0.42              |
| 1:H:294:LEU:HD12 | 1:H:295:PHE:N    | 2.34                     | 0.42              |
| 1:H:987:CYS:HA   | 1:H:990:LEU:HG   | 2.00                     | 0.42              |
| 1:J:366:ILE:HD12 | 1:J:366:ILE:HA   | 1.94                     | 0.42              |
| 1:J:484:ASP:OD1  | 1:J:485:LEU:N    | 2.53                     | 0.42              |
| 1:J:665:SER:C    | 1:J:669:LYS:HZ2  | 2.22                     | 0.42              |
| 1:K:224:ALA:HB1  | 1:K:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:K:506:LYS:HG3  | 1:K:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:K:632:LEU:HD12 | 1:K:641:VAL:HG22 | 2.02                     | 0.42              |
| 1:L:171:LYS:HE3  | 1:L:364:VAL:HB   | 2.00                     | 0.42              |
| 1:L:464:GLY:HA3  | 1:L:490:LEU:HG   | 2.01                     | 0.42              |
| 1:L:484:ASP:OD1  | 1:L:485:LEU:N    | 2.53                     | 0.42              |
| 1:A:473:ILE:HB   | 1:A:568:LYS:O    | 2.20                     | 0.42              |
| 1:A:484:ASP:OD1  | 1:A:485:LEU:N    | 2.53                     | 0.42              |
| 1:A:518:HIS:O    | 1:A:520:THR:HG23 | 2.19                     | 0.42              |
| 1:B:315:CYS:HA   | 1:B:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:B:506:LYS:HG3  | 1:B:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:B:556:VAL:O    | 1:B:559:LEU:HG   | 2.19                     | 0.42              |
| 1:B:834:CYS:O    | 1:B:836:LEU:N    | 2.52                     | 0.42              |
| 1:B:970:LYS:HD2  | 1:B:1001:GLN:NE2 | 2.32                     | 0.42              |
| 1:C:509:ASP:CB   | 1:C:513:PHE:HB3  | 2.49                     | 0.42              |
| 1:C:624:SER:OG   | 1:C:627:GLU:OE2  | 2.30                     | 0.42              |
| 1:C:987:CYS:HA   | 1:C:990:LEU:HG   | 2.00                     | 0.42              |
| 1:D:556:VAL:O    | 1:D:559:LEU:HG   | 2.19                     | 0.42              |
| 1:D:813:ARG:HG2  | 1:D:843:ASP:OD2  | 2.18                     | 0.42              |
| 1:D:828:LYS:CD   | 1:D:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:D:970:LYS:HD2  | 1:D:1001:GLN:NE2 | 2.32                     | 0.42              |
| 1:F:230:ILE:HG23 | 1:F:234:LYS:NZ   | 2.35                     | 0.42              |
| 1:F:473:ILE:HB   | 1:F:568:LYS:O    | 2.20                     | 0.42              |
| 1:F:828:LYS:CD   | 1:F:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:G:390:GLU:HG2  | 1:G:391:ALA:N    | 2.35                     | 0.42              |
| 1:G:828:LYS:CD   | 1:G:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:H:632:LEU:HD12 | 1:H:641:VAL:HG22 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:400:VAL:HG22 | 1:I:404:MET:HE1  | 2.01                     | 0.42              |
| 1:I:632:LEU:HD12 | 1:I:641:VAL:HG22 | 2.01                     | 0.42              |
| 1:J:134:LYS:HG3  | 1:J:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:J:473:ILE:HB   | 1:J:568:LYS:O    | 2.20                     | 0.42              |
| 1:J:518:HIS:O    | 1:J:520:THR:HG23 | 2.18                     | 0.42              |
| 1:K:484:ASP:OD1  | 1:K:485:LEU:N    | 2.53                     | 0.42              |
| 1:K:518:HIS:O    | 1:K:520:THR:HG23 | 2.19                     | 0.42              |
| 1:L:632:LEU:HD12 | 1:L:641:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:464:GLY:HA3  | 1:A:490:LEU:HG   | 2.01                     | 0.42              |
| 1:C:284:CYS:HA   | 1:C:287:LEU:HG   | 2.02                     | 0.42              |
| 1:E:230:ILE:HG23 | 1:E:234:LYS:NZ   | 2.35                     | 0.42              |
| 1:E:473:ILE:HB   | 1:E:568:LYS:O    | 2.20                     | 0.42              |
| 1:E:768:ASN:N    | 1:E:796:LYS:HZ2  | 2.16                     | 0.42              |
| 1:E:813:ARG:HG2  | 1:E:843:ASP:OD2  | 2.18                     | 0.42              |
| 1:E:828:LYS:CD   | 1:E:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:F:905:LEU:HD11 | 1:F:914:LEU:HD22 | 2.00                     | 0.42              |
| 1:G:224:ALA:HB1  | 1:G:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:G:834:CYS:O    | 1:G:836:LEU:N    | 2.52                     | 0.42              |
| 1:G:943:LEU:O    | 1:G:971:LEU:HA   | 2.19                     | 0.42              |
| 1:H:661:HIS:ND1  | 1:H:726:PHE:HB3  | 2.34                     | 0.42              |
| 1:H:834:CYS:O    | 1:H:836:LEU:N    | 2.52                     | 0.42              |
| 1:I:134:LYS:HG3  | 1:I:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:I:391:ALA:HA   | 1:I:394:LEU:HG   | 2.02                     | 0.42              |
| 1:I:518:HIS:O    | 1:I:520:THR:HG23 | 2.18                     | 0.42              |
| 1:I:925:GLY:O    | 1:I:928:LEU:HG   | 2.19                     | 0.42              |
| 1:J:132:TYR:OH   | 1:J:278:ASP:OD1  | 2.33                     | 0.42              |
| 1:J:417:GLY:O    | 1:J:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:J:980:ASP:O    | 1:J:984:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:401:LEU:HD21 | 1:K:432:SER:HB2  | 2.01                     | 0.42              |
| 1:L:506:LYS:HG3  | 1:L:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:L:898:CYS:O    | 1:L:902:THR:HG23 | 2.19                     | 0.42              |
| 1:A:256:HIS:NE2  | 1:A:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:A:284:CYS:HA   | 1:A:287:LEU:HG   | 2.02                     | 0.42              |
| 1:A:980:ASP:O    | 1:A:984:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:224:ALA:HB1  | 1:B:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:B:284:CYS:HA   | 1:B:287:LEU:HG   | 2.02                     | 0.42              |
| 1:B:391:ALA:HA   | 1:B:394:LEU:HG   | 2.02                     | 0.42              |
| 1:B:925:GLY:O    | 1:B:928:LEU:HG   | 2.19                     | 0.42              |
| 1:C:255:ILE:HD11 | 1:C:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:C:315:CYS:HA   | 1:C:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:390:GLU:HG2  | 1:C:391:ALA:N    | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:834:CYS:O    | 1:C:836:LEU:N    | 2.52                     | 0.42              |
| 1:C:943:LEU:O    | 1:C:971:LEU:HA   | 2.19                     | 0.42              |
| 1:D:284:CYS:HA   | 1:D:287:LEU:HG   | 2.02                     | 0.42              |
| 1:D:390:GLU:HG2  | 1:D:391:ALA:N    | 2.35                     | 0.42              |
| 1:D:401:LEU:HD21 | 1:D:432:SER:HB2  | 2.00                     | 0.42              |
| 1:D:506:LYS:HG3  | 1:D:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:D:834:CYS:O    | 1:D:836:LEU:N    | 2.52                     | 0.42              |
| 1:D:893:LEU:HD22 | 1:D:896:ILE:HG13 | 2.02                     | 0.42              |
| 1:F:294:LEU:HD12 | 1:F:295:PHE:N    | 2.35                     | 0.42              |
| 1:G:134:LYS:HG3  | 1:G:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:G:417:GLY:O    | 1:G:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:G:506:LYS:HG3  | 1:G:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:G:556:VAL:O    | 1:G:559:LEU:HG   | 2.19                     | 0.42              |
| 1:H:267:SER:HB2  | 1:H:323:ARG:HA   | 2.01                     | 0.42              |
| 1:H:390:GLU:HG2  | 1:H:391:ALA:N    | 2.35                     | 0.42              |
| 1:I:284:CYS:HA   | 1:I:287:LEU:HG   | 2.02                     | 0.42              |
| 1:I:370:SER:O    | 1:I:374:ARG:HB2  | 2.20                     | 0.42              |
| 1:I:390:GLU:HG2  | 1:I:391:ALA:N    | 2.35                     | 0.42              |
| 1:I:556:VAL:O    | 1:I:559:LEU:HG   | 2.19                     | 0.42              |
| 1:I:898:CYS:O    | 1:I:902:THR:HG23 | 2.19                     | 0.42              |
| 1:J:255:ILE:HD11 | 1:J:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:J:256:HIS:NE2  | 1:J:258:ARG:HB3  | 2.35                     | 0.42              |
| 1:J:284:CYS:HA   | 1:J:287:LEU:HG   | 2.02                     | 0.42              |
| 1:K:284:CYS:HA   | 1:K:287:LEU:HG   | 2.02                     | 0.42              |
| 1:K:391:ALA:HA   | 1:K:394:LEU:HG   | 2.02                     | 0.42              |
| 1:K:473:ILE:HB   | 1:K:568:LYS:O    | 2.20                     | 0.42              |
| 1:L:134:LYS:HG3  | 1:L:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:L:284:CYS:HA   | 1:L:287:LEU:HG   | 2.02                     | 0.42              |
| 1:L:391:ALA:HA   | 1:L:394:LEU:HG   | 2.02                     | 0.42              |
| 1:L:473:ILE:HB   | 1:L:568:LYS:O    | 2.20                     | 0.42              |
| 1:A:132:TYR:OH   | 1:A:278:ASP:OD1  | 2.32                     | 0.42              |
| 1:A:315:CYS:HA   | 1:A:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:417:GLY:O    | 1:A:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:A:925:GLY:O    | 1:A:928:LEU:HG   | 2.20                     | 0.42              |
| 1:A:952:SER:HB3  | 1:A:982:CYS:HA   | 2.02                     | 0.42              |
| 1:B:370:SER:O    | 1:B:374:ARG:HB2  | 2.20                     | 0.42              |
| 1:B:893:LEU:HD22 | 1:B:896:ILE:HG13 | 2.02                     | 0.42              |
| 1:B:898:CYS:O    | 1:B:902:THR:HG23 | 2.19                     | 0.42              |
| 1:C:134:LYS:HG3  | 1:C:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:C:464:GLY:HA3  | 1:C:490:LEU:HG   | 2.01                     | 0.42              |
| 1:C:952:SER:HB3  | 1:C:982:CYS:HA   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:230:ILE:HG23 | 1:D:234:LYS:NZ   | 2.35                     | 0.42              |
| 1:D:417:GLY:O    | 1:D:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:D:794:SER:HB2  | 1:D:797:LEU:HD23 | 2.02                     | 0.42              |
| 1:D:952:SER:HB3  | 1:D:982:CYS:HA   | 2.02                     | 0.42              |
| 1:E:284:CYS:HA   | 1:E:287:LEU:HG   | 2.02                     | 0.42              |
| 1:E:661:HIS:ND1  | 1:E:726:PHE:HB3  | 2.34                     | 0.42              |
| 1:F:224:ALA:HB1  | 1:F:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:F:250:ASP:N    | 1:F:292:ARG:O    | 2.46                     | 0.42              |
| 1:F:284:CYS:HA   | 1:F:287:LEU:HG   | 2.02                     | 0.42              |
| 1:F:400:VAL:C    | 1:F:402:PHE:H    | 2.23                     | 0.42              |
| 1:G:230:ILE:HG23 | 1:G:234:LYS:NZ   | 2.35                     | 0.42              |
| 1:G:284:CYS:HA   | 1:G:287:LEU:HG   | 2.02                     | 0.42              |
| 1:G:893:LEU:HD22 | 1:G:896:ILE:HG13 | 2.02                     | 0.42              |
| 1:G:952:SER:HB3  | 1:G:982:CYS:HA   | 2.02                     | 0.42              |
| 1:H:250:ASP:CG   | 1:H:292:ARG:HE   | 2.21                     | 0.42              |
| 1:H:484:ASP:OD1  | 1:H:485:LEU:N    | 2.53                     | 0.42              |
| 1:I:506:LYS:HG3  | 1:I:514:TYR:CZ   | 2.55                     | 0.42              |
| 1:J:315:CYS:HA   | 1:J:332:ILE:HG21 | 2.01                     | 0.42              |
| 1:J:828:LYS:CD   | 1:J:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:K:134:LYS:HG3  | 1:K:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:K:230:ILE:HG23 | 1:K:234:LYS:NZ   | 2.35                     | 0.42              |
| 1:K:256:HIS:NE2  | 1:K:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:K:898:CYS:O    | 1:K:902:THR:HG23 | 2.19                     | 0.42              |
| 1:K:925:GLY:O    | 1:K:928:LEU:HG   | 2.20                     | 0.42              |
| 1:L:256:HIS:NE2  | 1:L:258:ARG:HB3  | 2.34                     | 0.42              |
| 1:L:401:LEU:HD21 | 1:L:432:SER:HB2  | 2.01                     | 0.42              |
| 1:A:283:VAL:HA   | 1:A:286:ILE:HG12 | 2.01                     | 0.42              |
| 1:B:387:GLN:NE2  | 1:B:422:MET:HG2  | 2.35                     | 0.42              |
| 1:B:390:GLU:HG2  | 1:B:391:ALA:N    | 2.35                     | 0.42              |
| 1:C:250:ASP:CG   | 1:C:292:ARG:HE   | 2.21                     | 0.42              |
| 1:C:484:ASP:OD1  | 1:C:485:LEU:N    | 2.53                     | 0.42              |
| 1:D:217:THR:HG23 | 1:D:361:PRO:HB3  | 2.01                     | 0.42              |
| 1:D:400:VAL:C    | 1:D:402:PHE:H    | 2.22                     | 0.42              |
| 1:E:283:VAL:HA   | 1:E:286:ILE:HG12 | 2.01                     | 0.42              |
| 1:E:794:SER:HB2  | 1:E:797:LEU:HD23 | 2.02                     | 0.42              |
| 1:E:943:LEU:O    | 1:E:971:LEU:HA   | 2.19                     | 0.42              |
| 1:F:283:VAL:HA   | 1:F:286:ILE:HG12 | 2.01                     | 0.42              |
| 1:F:390:GLU:HG2  | 1:F:391:ALA:N    | 2.35                     | 0.42              |
| 1:F:401:LEU:HD21 | 1:F:432:SER:HB2  | 2.00                     | 0.42              |
| 1:F:734:LEU:HD23 | 1:F:737:ASN:ND2  | 2.30                     | 0.42              |
| 1:G:217:THR:HG23 | 1:G:361:PRO:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:794:SER:HB2  | 1:G:797:LEU:HD23 | 2.02                     | 0.42              |
| 1:H:250:ASP:N    | 1:H:292:ARG:O    | 2.46                     | 0.42              |
| 1:H:334:LYS:CG   | 1:H:342:LEU:HD11 | 2.48                     | 0.42              |
| 1:H:464:GLY:HA3  | 1:H:490:LEU:HG   | 2.01                     | 0.42              |
| 1:I:224:ALA:HB1  | 1:I:573:PHE:CE2  | 2.54                     | 0.42              |
| 1:I:473:ILE:HB   | 1:I:568:LYS:O    | 2.20                     | 0.42              |
| 1:I:579:PHE:CE1  | 1:I:606:LEU:HD22 | 2.55                     | 0.42              |
| 1:I:893:LEU:HD22 | 1:I:896:ILE:HG13 | 2.02                     | 0.42              |
| 1:I:952:SER:HB3  | 1:I:982:CYS:HA   | 2.02                     | 0.42              |
| 1:J:464:GLY:HA3  | 1:J:490:LEU:HG   | 2.01                     | 0.42              |
| 1:J:579:PHE:CE1  | 1:J:606:LEU:HD22 | 2.55                     | 0.42              |
| 1:J:732:SER:O    | 1:J:735:SER:OG   | 2.20                     | 0.42              |
| 1:J:925:GLY:O    | 1:J:928:LEU:HG   | 2.20                     | 0.42              |
| 1:J:952:SER:HB3  | 1:J:982:CYS:HA   | 2.02                     | 0.42              |
| 1:K:352:GLU:OE1  | 1:K:352:GLU:N    | 2.46                     | 0.42              |
| 1:K:387:GLN:NE2  | 1:K:422:MET:HG2  | 2.35                     | 0.42              |
| 1:K:828:LYS:CD   | 1:K:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:L:387:GLN:NE2  | 1:L:422:MET:HG2  | 2.35                     | 0.42              |
| 1:L:925:GLY:O    | 1:L:928:LEU:HG   | 2.19                     | 0.42              |
| 1:A:255:ILE:HD11 | 1:A:295:PHE:HB3  | 2.00                     | 0.42              |
| 1:A:294:LEU:HD12 | 1:A:295:PHE:N    | 2.34                     | 0.42              |
| 1:A:579:PHE:CE1  | 1:A:606:LEU:HD22 | 2.55                     | 0.42              |
| 1:A:794:SER:HB2  | 1:A:797:LEU:HD23 | 2.02                     | 0.42              |
| 1:A:828:LYS:CD   | 1:A:856:ARG:HG2  | 2.49                     | 0.42              |
| 1:A:978:LEU:HB3  | 1:A:982:CYS:SG   | 2.60                     | 0.42              |
| 1:B:473:ILE:HB   | 1:B:568:LYS:O    | 2.20                     | 0.42              |
| 1:B:579:PHE:CD2  | 1:B:631:CYS:HB3  | 2.55                     | 0.42              |
| 1:B:952:SER:HB3  | 1:B:982:CYS:HA   | 2.02                     | 0.42              |
| 1:D:134:LYS:HG3  | 1:D:137:ARG:NH2  | 2.34                     | 0.42              |
| 1:D:579:PHE:CD2  | 1:D:631:CYS:HB3  | 2.55                     | 0.42              |
| 1:E:401:LEU:O    | 1:E:405:CYS:HB3  | 2.20                     | 0.42              |
| 1:E:484:ASP:OD1  | 1:E:485:LEU:N    | 2.53                     | 0.42              |
| 1:F:400:VAL:HG13 | 1:F:401:LEU:CD2  | 2.50                     | 0.42              |
| 1:F:401:LEU:O    | 1:F:405:CYS:HB3  | 2.20                     | 0.42              |
| 1:F:978:LEU:HB3  | 1:F:982:CYS:SG   | 2.60                     | 0.42              |
| 1:I:387:GLN:NE2  | 1:I:422:MET:HG2  | 2.35                     | 0.42              |
| 1:I:484:ASP:OD1  | 1:I:485:LEU:N    | 2.53                     | 0.42              |
| 1:J:390:GLU:HG2  | 1:J:391:ALA:N    | 2.35                     | 0.42              |
| 1:K:952:SER:HB3  | 1:K:982:CYS:HA   | 2.02                     | 0.42              |
| 1:L:217:THR:HG23 | 1:L:361:PRO:HB3  | 2.01                     | 0.42              |
| 1:L:230:ILE:HG23 | 1:L:234:LYS:NZ   | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:417:GLY:O    | 1:L:420:GLN:NE2  | 2.52                     | 0.42              |
| 1:L:952:SER:HB3  | 1:L:982:CYS:HA   | 2.02                     | 0.42              |
| 1:A:390:GLU:HG2  | 1:A:391:ALA:N    | 2.35                     | 0.41              |
| 1:A:506:LYS:HG3  | 1:A:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:B:400:VAL:HG22 | 1:B:404:MET:HE1  | 2.02                     | 0.41              |
| 1:B:637:GLU:OE2  | 1:B:640:PHE:N    | 2.28                     | 0.41              |
| 1:E:239:TRP:CD1  | 1:E:245:PHE:CD2  | 3.08                     | 0.41              |
| 1:E:388:ALA:HB3  | 1:E:389:ARG:NH1  | 2.32                     | 0.41              |
| 1:E:390:GLU:HG2  | 1:E:391:ALA:N    | 2.35                     | 0.41              |
| 1:E:401:LEU:HD21 | 1:E:432:SER:HB2  | 2.00                     | 0.41              |
| 1:E:871:VAL:HG12 | 1:E:875:LYS:HZ2  | 1.81                     | 0.41              |
| 1:E:952:SER:HB3  | 1:E:982:CYS:HA   | 2.02                     | 0.41              |
| 1:E:978:LEU:HB3  | 1:E:982:CYS:SG   | 2.60                     | 0.41              |
| 1:G:579:PHE:CD2  | 1:G:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:H:134:LYS:HG3  | 1:H:137:ARG:NH2  | 2.34                     | 0.41              |
| 1:H:943:LEU:O    | 1:H:971:LEU:HA   | 2.19                     | 0.41              |
| 1:I:794:SER:HB2  | 1:I:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:J:294:LEU:HD12 | 1:J:295:PHE:N    | 2.35                     | 0.41              |
| 1:J:574:VAL:O    | 1:J:578:LEU:HG   | 2.20                     | 0.41              |
| 1:J:978:LEU:HB3  | 1:J:982:CYS:SG   | 2.60                     | 0.41              |
| 1:K:255:ILE:HD11 | 1:K:295:PHE:HB3  | 2.00                     | 0.41              |
| 1:K:579:PHE:CE1  | 1:K:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:K:768:ASN:N    | 1:K:796:LYS:HZ3  | 2.18                     | 0.41              |
| 1:K:769:ILE:HG22 | 1:K:771:ARG:N    | 2.32                     | 0.41              |
| 1:L:579:PHE:CE1  | 1:L:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:L:579:PHE:CD2  | 1:L:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:L:768:ASN:N    | 1:L:796:LYS:HZ3  | 2.18                     | 0.41              |
| 1:L:828:LYS:CD   | 1:L:856:ARG:HG2  | 2.50                     | 0.41              |
| 1:A:391:ALA:HA   | 1:A:394:LEU:HG   | 2.02                     | 0.41              |
| 1:B:417:GLY:O    | 1:B:420:GLN:NE2  | 2.52                     | 0.41              |
| 1:B:484:ASP:OD1  | 1:B:485:LEU:N    | 2.53                     | 0.41              |
| 1:B:579:PHE:CE1  | 1:B:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:B:622:GLN:HB3  | 1:B:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:978:LEU:HB3  | 1:C:982:CYS:SG   | 2.60                     | 0.41              |
| 1:D:132:TYR:OH   | 1:D:278:ASP:OD1  | 2.33                     | 0.41              |
| 1:D:622:GLN:HB3  | 1:D:623:PRO:HD2  | 2.03                     | 0.41              |
| 1:D:944:GLU:CG   | 1:D:972:ASN:HB2  | 2.46                     | 0.41              |
| 1:E:400:VAL:HG13 | 1:E:401:LEU:CD2  | 2.50                     | 0.41              |
| 1:F:239:TRP:CD1  | 1:F:245:PHE:CD2  | 3.08                     | 0.41              |
| 1:F:370:SER:O    | 1:F:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:F:419:LYS:HA   | 1:F:419:LYS:HE2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:400:VAL:C    | 1:G:402:PHE:H    | 2.22                     | 0.41              |
| 1:G:574:VAL:O    | 1:G:578:LEU:HG   | 2.20                     | 0.41              |
| 1:G:622:GLN:HB3  | 1:G:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:H:230:ILE:HG23 | 1:H:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:H:952:SER:HB3  | 1:H:982:CYS:HA   | 2.02                     | 0.41              |
| 1:I:574:VAL:O    | 1:I:578:LEU:HG   | 2.20                     | 0.41              |
| 1:I:622:GLN:HB3  | 1:I:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:I:980:ASP:O    | 1:I:984:VAL:HG23 | 2.19                     | 0.41              |
| 1:J:283:VAL:HA   | 1:J:286:ILE:HG12 | 2.01                     | 0.41              |
| 1:J:579:PHE:CD2  | 1:J:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:J:734:LEU:HD23 | 1:J:737:ASN:ND2  | 2.30                     | 0.41              |
| 1:J:794:SER:HB2  | 1:J:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:K:217:THR:HG23 | 1:K:361:PRO:HB3  | 2.01                     | 0.41              |
| 1:K:417:GLY:O    | 1:K:420:GLN:NE2  | 2.52                     | 0.41              |
| 1:K:579:PHE:CD2  | 1:K:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:K:632:LEU:HA   | 1:K:635:MET:HG3  | 2.03                     | 0.41              |
| 1:K:771:ARG:HG3  | 1:K:771:ARG:O    | 2.19                     | 0.41              |
| 1:K:893:LEU:HD22 | 1:K:896:ILE:HG13 | 2.02                     | 0.41              |
| 1:L:769:ILE:HG22 | 1:L:771:ARG:N    | 2.32                     | 0.41              |
| 1:L:830:TRP:N    | 1:L:830:TRP:CD1  | 2.86                     | 0.41              |
| 1:A:407:ILE:HA   | 1:A:408:PRO:HD3  | 1.92                     | 0.41              |
| 1:A:579:PHE:CD2  | 1:A:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:A:622:GLN:HB3  | 1:A:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:734:LEU:HD23 | 1:A:737:ASN:ND2  | 2.30                     | 0.41              |
| 1:A:817:VAL:HG12 | 1:A:820:LYS:NZ   | 2.33                     | 0.41              |
| 1:A:834:CYS:O    | 1:A:836:LEU:N    | 2.52                     | 0.41              |
| 1:B:574:VAL:O    | 1:B:578:LEU:HG   | 2.21                     | 0.41              |
| 1:B:632:LEU:HA   | 1:B:635:MET:HG3  | 2.03                     | 0.41              |
| 1:C:230:ILE:HG23 | 1:C:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:C:866:ASP:HA   | 1:C:869:VAL:HG13 | 2.03                     | 0.41              |
| 1:D:250:ASP:CG   | 1:D:292:ARG:HE   | 2.21                     | 0.41              |
| 1:D:401:LEU:O    | 1:D:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:D:574:VAL:O    | 1:D:578:LEU:HG   | 2.20                     | 0.41              |
| 1:E:370:SER:O    | 1:E:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:E:579:PHE:CD2  | 1:E:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:F:391:ALA:HA   | 1:F:394:LEU:HG   | 2.02                     | 0.41              |
| 1:F:661:HIS:ND1  | 1:F:726:PHE:HB3  | 2.34                     | 0.41              |
| 1:F:952:SER:HB3  | 1:F:982:CYS:HA   | 2.02                     | 0.41              |
| 1:I:417:GLY:O    | 1:I:420:GLN:NE2  | 2.52                     | 0.41              |
| 1:I:579:PHE:CD2  | 1:I:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:I:632:LEU:HA   | 1:I:635:MET:HG3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:506:LYS:HG3  | 1:J:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:J:834:CYS:O    | 1:J:836:LEU:N    | 2.52                     | 0.41              |
| 1:K:401:LEU:O    | 1:K:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:K:574:VAL:O    | 1:K:578:LEU:HG   | 2.20                     | 0.41              |
| 1:L:159:ASP:HB3  | 1:L:160:LEU:H    | 1.63                     | 0.41              |
| 1:L:771:ARG:O    | 1:L:771:ARG:HG3  | 2.19                     | 0.41              |
| 1:L:893:LEU:HD22 | 1:L:896:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:574:VAL:O    | 1:A:578:LEU:HG   | 2.20                     | 0.41              |
| 1:A:830:TRP:N    | 1:A:830:TRP:CD1  | 2.86                     | 0.41              |
| 1:B:230:ILE:HG23 | 1:B:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:B:401:LEU:O    | 1:B:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:B:794:SER:HB2  | 1:B:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:B:819:LEU:HB2  | 1:B:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:980:ASP:O    | 1:B:984:VAL:HG23 | 2.19                     | 0.41              |
| 1:B:985:THR:HA   | 1:B:988:GLU:HG3  | 2.03                     | 0.41              |
| 1:C:283:VAL:HA   | 1:C:286:ILE:HG12 | 2.01                     | 0.41              |
| 1:C:579:PHE:CE1  | 1:C:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:C:622:GLN:HB3  | 1:C:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:959:SER:O    | 1:C:963:THR:HG23 | 2.21                     | 0.41              |
| 1:D:473:ILE:HB   | 1:D:568:LYS:O    | 2.20                     | 0.41              |
| 1:D:484:ASP:OD1  | 1:D:485:LEU:N    | 2.53                     | 0.41              |
| 1:E:419:LYS:HE2  | 1:E:419:LYS:HA   | 2.02                     | 0.41              |
| 1:E:574:VAL:O    | 1:E:578:LEU:HG   | 2.20                     | 0.41              |
| 1:F:334:LYS:CG   | 1:F:342:LEU:HD11 | 2.48                     | 0.41              |
| 1:F:484:ASP:OD1  | 1:F:485:LEU:N    | 2.53                     | 0.41              |
| 1:F:632:LEU:HD12 | 1:F:641:VAL:HG22 | 2.02                     | 0.41              |
| 1:F:794:SER:HB2  | 1:F:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:G:250:ASP:CG   | 1:G:292:ARG:HE   | 2.21                     | 0.41              |
| 1:G:370:SER:O    | 1:G:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:G:401:LEU:O    | 1:G:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:G:999:SER:OG   | 1:G:1000:LEU:N   | 2.54                     | 0.41              |
| 1:H:283:VAL:HA   | 1:H:286:ILE:HG12 | 2.01                     | 0.41              |
| 1:H:866:ASP:HA   | 1:H:869:VAL:HG13 | 2.03                     | 0.41              |
| 1:I:819:LEU:HB2  | 1:I:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:J:391:ALA:HA   | 1:J:394:LEU:HG   | 2.02                     | 0.41              |
| 1:J:622:GLN:HB3  | 1:J:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:J:819:LEU:HB2  | 1:J:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:K:315:CYS:HA   | 1:K:332:ILE:HG21 | 2.01                     | 0.41              |
| 1:K:622:GLN:HB3  | 1:K:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:K:819:LEU:HB2  | 1:K:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:K:830:TRP:N    | 1:K:830:TRP:CD1  | 2.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:255:ILE:HD11 | 1:L:295:PHE:HB3  | 2.00                     | 0.41              |
| 1:L:352:GLU:OE1  | 1:L:352:GLU:N    | 2.46                     | 0.41              |
| 1:L:401:LEU:O    | 1:L:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:L:574:VAL:O    | 1:L:578:LEU:HG   | 2.20                     | 0.41              |
| 1:L:622:GLN:HB3  | 1:L:623:PRO:HD2  | 2.03                     | 0.41              |
| 1:A:278:ASP:O    | 1:A:280:ASN:N    | 2.53                     | 0.41              |
| 1:A:387:GLN:NE2  | 1:A:422:MET:HG2  | 2.35                     | 0.41              |
| 1:B:217:THR:HG23 | 1:B:361:PRO:HB3  | 2.01                     | 0.41              |
| 1:D:370:SER:O    | 1:D:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:D:959:SER:O    | 1:D:963:THR:HG23 | 2.21                     | 0.41              |
| 1:D:978:LEU:HB3  | 1:D:982:CYS:SG   | 2.60                     | 0.41              |
| 1:D:999:SER:OG   | 1:D:1000:LEU:N   | 2.54                     | 0.41              |
| 1:E:391:ALA:HA   | 1:E:394:LEU:HG   | 2.02                     | 0.41              |
| 1:E:506:LYS:HG3  | 1:E:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:E:893:LEU:HD22 | 1:E:896:ILE:HG13 | 2.02                     | 0.41              |
| 1:E:959:SER:O    | 1:E:963:THR:HG23 | 2.21                     | 0.41              |
| 1:F:834:CYS:O    | 1:F:836:LEU:N    | 2.52                     | 0.41              |
| 1:F:893:LEU:HD22 | 1:F:896:ILE:HG13 | 2.02                     | 0.41              |
| 1:F:943:LEU:O    | 1:F:971:LEU:HA   | 2.19                     | 0.41              |
| 1:G:484:ASP:OD1  | 1:G:485:LEU:N    | 2.53                     | 0.41              |
| 1:H:239:TRP:CD1  | 1:H:245:PHE:CD2  | 3.08                     | 0.41              |
| 1:H:401:LEU:O    | 1:H:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:H:419:LYS:HE2  | 1:H:419:LYS:HA   | 2.02                     | 0.41              |
| 1:H:554:ARG:HB3  | 1:H:555:ASP:H    | 1.62                     | 0.41              |
| 1:H:579:PHE:CE1  | 1:H:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:H:617:LYS:HB2  | 1:I:953:HIS:NE2  | 2.36                     | 0.41              |
| 1:H:622:GLN:HB3  | 1:H:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:H:959:SER:O    | 1:H:963:THR:HG23 | 2.21                     | 0.41              |
| 1:H:978:LEU:HB3  | 1:H:982:CYS:SG   | 2.60                     | 0.41              |
| 1:I:217:THR:HB   | 1:I:342:LEU:HB3  | 2.03                     | 0.41              |
| 1:I:985:THR:HA   | 1:I:988:GLU:HG3  | 2.03                     | 0.41              |
| 1:J:278:ASP:O    | 1:J:280:ASN:N    | 2.53                     | 0.41              |
| 1:J:830:TRP:N    | 1:J:830:TRP:CD1  | 2.86                     | 0.41              |
| 1:K:159:ASP:HB3  | 1:K:160:LEU:H    | 1.63                     | 0.41              |
| 1:K:390:GLU:HG2  | 1:K:391:ALA:N    | 2.35                     | 0.41              |
| 1:L:278:ASP:O    | 1:L:280:ASN:N    | 2.53                     | 0.41              |
| 1:L:315:CYS:HA   | 1:L:332:ILE:HG21 | 2.01                     | 0.41              |
| 1:L:632:LEU:HA   | 1:L:635:MET:HG3  | 2.03                     | 0.41              |
| 1:L:794:SER:HB2  | 1:L:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:A:632:LEU:HD12 | 1:A:641:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:732:SER:O    | 1:A:735:SER:OG   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:217:THR:HB   | 1:B:342:LEU:HB3  | 2.03                     | 0.41              |
| 1:C:334:LYS:CG   | 1:C:342:LEU:HD11 | 2.48                     | 0.41              |
| 1:C:817:VAL:HG12 | 1:C:820:LYS:NZ   | 2.33                     | 0.41              |
| 1:E:632:LEU:HD12 | 1:E:641:VAL:HG22 | 2.02                     | 0.41              |
| 1:F:506:LYS:HG3  | 1:F:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:F:872:LEU:HA   | 1:F:875:LYS:HZ3  | 1.86                     | 0.41              |
| 1:F:959:SER:O    | 1:F:963:THR:HG23 | 2.21                     | 0.41              |
| 1:G:294:LEU:HD12 | 1:G:295:PHE:N    | 2.35                     | 0.41              |
| 1:G:871:VAL:HG12 | 1:G:875:LYS:HZ2  | 1.83                     | 0.41              |
| 1:G:959:SER:O    | 1:G:963:THR:HG23 | 2.21                     | 0.41              |
| 1:G:978:LEU:HB3  | 1:G:982:CYS:SG   | 2.60                     | 0.41              |
| 1:H:769:ILE:HG22 | 1:H:771:ARG:N    | 2.32                     | 0.41              |
| 1:H:817:VAL:HG12 | 1:H:820:LYS:NZ   | 2.33                     | 0.41              |
| 1:I:637:GLU:OE2  | 1:I:640:PHE:N    | 2.28                     | 0.41              |
| 1:J:370:SER:O    | 1:J:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:J:387:GLN:NE2  | 1:J:422:MET:HG2  | 2.35                     | 0.41              |
| 1:J:632:LEU:HD12 | 1:J:641:VAL:HG22 | 2.01                     | 0.41              |
| 1:K:278:ASP:O    | 1:K:280:ASN:N    | 2.53                     | 0.41              |
| 1:K:370:SER:O    | 1:K:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:K:794:SER:HB2  | 1:K:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:K:911:PHE:CZ   | 1:K:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:L:390:GLU:HG2  | 1:L:391:ALA:N    | 2.35                     | 0.41              |
| 1:L:911:PHE:CZ   | 1:L:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:A:250:ASP:N    | 1:A:292:ARG:O    | 2.46                     | 0.41              |
| 1:A:819:LEU:HB2  | 1:A:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:274:SER:O    | 1:B:274:SER:OG   | 2.36                     | 0.41              |
| 1:B:369:PHE:HA   | 1:B:373:LYS:HE3  | 2.03                     | 0.41              |
| 1:B:769:ILE:HG22 | 1:B:771:ARG:N    | 2.32                     | 0.41              |
| 1:C:239:TRP:CD1  | 1:C:245:PHE:CD2  | 3.08                     | 0.41              |
| 1:C:473:ILE:HB   | 1:C:568:LYS:O    | 2.20                     | 0.41              |
| 1:D:294:LEU:HD12 | 1:D:295:PHE:N    | 2.35                     | 0.41              |
| 1:E:250:ASP:CG   | 1:E:292:ARG:HE   | 2.21                     | 0.41              |
| 1:E:579:PHE:CE1  | 1:E:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:F:250:ASP:CG   | 1:F:292:ARG:HE   | 2.21                     | 0.41              |
| 1:F:579:PHE:CD2  | 1:F:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:F:836:LEU:HD13 | 1:F:840:CYS:SG   | 2.61                     | 0.41              |
| 1:G:473:ILE:HB   | 1:G:568:LYS:O    | 2.20                     | 0.41              |
| 1:H:794:SER:HB2  | 1:H:797:LEU:HD23 | 2.02                     | 0.41              |
| 1:I:217:THR:HG23 | 1:I:361:PRO:HB3  | 2.01                     | 0.41              |
| 1:I:230:ILE:HG23 | 1:I:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:I:401:LEU:O    | 1:I:405:CYS:HB3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:769:ILE:HG22 | 1:I:771:ARG:N    | 2.32                     | 0.41              |
| 1:I:999:SER:OG   | 1:I:1000:LEU:N   | 2.54                     | 0.41              |
| 1:J:280:ASN:HB2  | 1:J:281:PRO:HD3  | 2.03                     | 0.41              |
| 1:K:980:ASP:O    | 1:K:984:VAL:HG23 | 2.19                     | 0.41              |
| 1:L:294:LEU:HD12 | 1:L:295:PHE:N    | 2.34                     | 0.41              |
| 1:L:819:LEU:HB2  | 1:L:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:L:1019:GLN:N   | 1:L:1019:GLN:OE1 | 2.46                     | 0.41              |
| 1:A:370:SER:O    | 1:A:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:400:VAL:HG13 | 1:A:401:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:632:LEU:HA   | 1:A:635:MET:HG3  | 2.03                     | 0.41              |
| 1:A:893:LEU:HD22 | 1:A:896:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:959:SER:O    | 1:A:963:THR:HG23 | 2.21                     | 0.41              |
| 1:B:294:LEU:HD12 | 1:B:295:PHE:N    | 2.34                     | 0.41              |
| 1:B:768:ASN:N    | 1:B:796:LYS:HZ3  | 2.18                     | 0.41              |
| 1:B:974:GLY:N    | 1:B:976:ASN:OD1  | 2.54                     | 0.41              |
| 1:B:999:SER:OG   | 1:B:1000:LEU:N   | 2.54                     | 0.41              |
| 1:C:280:ASN:HB2  | 1:C:281:PRO:HD3  | 2.03                     | 0.41              |
| 1:C:370:SER:O    | 1:C:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:C:506:LYS:HG3  | 1:C:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:C:579:PHE:CD2  | 1:C:631:CYS:HB3  | 2.55                     | 0.41              |
| 1:D:579:PHE:CE1  | 1:D:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:D:830:TRP:N    | 1:D:830:TRP:CD1  | 2.86                     | 0.41              |
| 1:E:387:GLN:NE2  | 1:E:422:MET:HG2  | 2.35                     | 0.41              |
| 1:E:622:GLN:HB3  | 1:E:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:E:834:CYS:O    | 1:E:836:LEU:N    | 2.52                     | 0.41              |
| 1:E:836:LEU:HD13 | 1:E:840:CYS:SG   | 2.61                     | 0.41              |
| 1:E:872:LEU:HA   | 1:E:875:LYS:HZ3  | 1.86                     | 0.41              |
| 1:F:1019:GLN:N   | 1:F:1019:GLN:OE1 | 2.46                     | 0.41              |
| 1:G:132:TYR:OH   | 1:G:278:ASP:OD1  | 2.33                     | 0.41              |
| 1:G:830:TRP:N    | 1:G:830:TRP:CD1  | 2.86                     | 0.41              |
| 1:G:944:GLU:CG   | 1:G:972:ASN:HB2  | 2.46                     | 0.41              |
| 1:H:370:SER:O    | 1:H:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:H:391:ALA:HA   | 1:H:394:LEU:HG   | 2.02                     | 0.41              |
| 1:H:473:ILE:HB   | 1:H:568:LYS:O    | 2.20                     | 0.41              |
| 1:H:624:SER:OG   | 1:H:627:GLU:OE2  | 2.30                     | 0.41              |
| 1:H:830:TRP:CD1  | 1:H:858:TYR:HD2  | 2.39                     | 0.41              |
| 1:I:959:SER:O    | 1:I:963:THR:HG23 | 2.21                     | 0.41              |
| 1:J:199:LEU:HB3  | 1:J:200:LYS:H    | 1.68                     | 0.41              |
| 1:J:230:ILE:HG23 | 1:J:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:J:400:VAL:HG13 | 1:J:401:LEU:CD2  | 2.50                     | 0.41              |
| 1:J:817:VAL:HG12 | 1:J:820:LYS:NZ   | 2.33                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:959:SER:O    | 1:J:963:THR:HG23 | 2.21                     | 0.41              |
| 1:K:294:LEU:HD12 | 1:K:295:PHE:N    | 2.35                     | 0.41              |
| 1:L:370:SER:O    | 1:L:374:ARG:HB2  | 2.20                     | 0.41              |
| 1:L:866:ASP:HA   | 1:L:869:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:230:ILE:HG23 | 1:A:234:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:280:ASN:HB2  | 1:A:281:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:494:ASP:OD1  | 1:A:495:VAL:N    | 2.54                     | 0.41              |
| 1:A:911:PHE:CZ   | 1:A:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:B:959:SER:O    | 1:B:963:THR:HG23 | 2.21                     | 0.41              |
| 1:C:391:ALA:HA   | 1:C:394:LEU:HG   | 2.02                     | 0.41              |
| 1:C:400:VAL:O    | 1:C:401:LEU:HB2  | 2.21                     | 0.41              |
| 1:C:401:LEU:O    | 1:C:405:CYS:HB3  | 2.20                     | 0.41              |
| 1:C:419:LYS:HA   | 1:C:419:LYS:HE2  | 2.02                     | 0.41              |
| 1:C:632:LEU:HA   | 1:C:635:MET:HG3  | 2.03                     | 0.41              |
| 1:C:769:ILE:HG22 | 1:C:771:ARG:N    | 2.32                     | 0.41              |
| 1:C:830:TRP:CD1  | 1:C:858:TYR:HD2  | 2.39                     | 0.41              |
| 1:D:632:LEU:HA   | 1:D:635:MET:HG3  | 2.03                     | 0.41              |
| 1:D:911:PHE:CZ   | 1:D:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:E:227:GLY:O    | 1:E:230:ILE:HG22 | 2.21                     | 0.41              |
| 1:E:280:ASN:HB2  | 1:E:281:PRO:HD3  | 2.03                     | 0.41              |
| 1:E:366:ILE:HD12 | 1:E:366:ILE:HA   | 1.94                     | 0.41              |
| 1:E:911:PHE:CZ   | 1:E:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:E:1019:GLN:N   | 1:E:1019:GLN:OE1 | 2.46                     | 0.41              |
| 1:F:366:ILE:HD12 | 1:F:366:ILE:HA   | 1.94                     | 0.41              |
| 1:F:387:GLN:NE2  | 1:F:422:MET:HG2  | 2.35                     | 0.41              |
| 1:F:574:VAL:O    | 1:F:578:LEU:HG   | 2.20                     | 0.41              |
| 1:F:622:GLN:HB3  | 1:F:623:PRO:HD2  | 2.02                     | 0.41              |
| 1:F:837:THR:OG1  | 1:F:838:SER:N    | 2.54                     | 0.41              |
| 1:F:866:ASP:HA   | 1:F:869:VAL:HG13 | 2.03                     | 0.41              |
| 1:F:876:MET:HB3  | 1:F:908:ASN:HB2  | 2.03                     | 0.41              |
| 1:G:239:TRP:CD1  | 1:G:245:PHE:CD2  | 3.08                     | 0.41              |
| 1:G:419:LYS:HE2  | 1:G:419:LYS:HA   | 2.02                     | 0.41              |
| 1:G:579:PHE:CE1  | 1:G:606:LEU:HD22 | 2.55                     | 0.41              |
| 1:G:632:LEU:HA   | 1:G:635:MET:HG3  | 2.03                     | 0.41              |
| 1:G:785:PHE:HB3  | 1:H:810:PHE:HZ   | 1.85                     | 0.41              |
| 1:G:911:PHE:CZ   | 1:G:914:LEU:HD13 | 2.56                     | 0.41              |
| 1:H:227:GLY:O    | 1:H:230:ILE:HG22 | 2.21                     | 0.41              |
| 1:H:280:ASN:HB2  | 1:H:281:PRO:HD3  | 2.03                     | 0.41              |
| 1:H:400:VAL:O    | 1:H:401:LEU:HB2  | 2.21                     | 0.41              |
| 1:H:506:LYS:HG3  | 1:H:514:TYR:CZ   | 2.55                     | 0.41              |
| 1:H:837:THR:OG1  | 1:H:838:SER:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:893:LEU:HD22 | 1:H:896:ILE:HG13  | 2.02                     | 0.41              |
| 1:I:369:PHE:HA   | 1:I:373:LYS:HE3   | 2.03                     | 0.41              |
| 1:I:974:GLY:N    | 1:I:976:ASN:OD1   | 2.54                     | 0.41              |
| 1:J:239:TRP:CD1  | 1:J:245:PHE:CD2   | 3.08                     | 0.41              |
| 1:J:407:ILE:HA   | 1:J:408:PRO:HD3   | 1.92                     | 0.41              |
| 1:J:474:TRP:CD1  | 1:J:568:LYS:HE2   | 2.56                     | 0.41              |
| 1:J:828:LYS:HB3  | 1:J:830:TRP:NE1   | 2.36                     | 0.41              |
| 1:J:893:LEU:HD22 | 1:J:896:ILE:HG13  | 2.02                     | 0.41              |
| 1:J:911:PHE:CZ   | 1:J:914:LEU:HD13  | 2.56                     | 0.41              |
| 1:K:199:LEU:HB3  | 1:K:200:LYS:H     | 1.68                     | 0.41              |
| 1:K:217:THR:HB   | 1:K:342:LEU:HB3   | 2.03                     | 0.41              |
| 1:K:280:ASN:HB2  | 1:K:281:PRO:HD3   | 2.03                     | 0.41              |
| 1:K:836:LEU:HD13 | 1:K:840:CYS:SG    | 2.61                     | 0.41              |
| 1:K:866:ASP:HA   | 1:K:869:VAL:HG13  | 2.03                     | 0.41              |
| 1:K:978:LEU:HB3  | 1:K:982:CYS:SG    | 2.60                     | 0.41              |
| 1:L:280:ASN:HB2  | 1:L:281:PRO:HD3   | 2.03                     | 0.41              |
| 1:L:828:LYS:HB3  | 1:L:830:TRP:NE1   | 2.36                     | 0.41              |
| 1:L:836:LEU:HD13 | 1:L:840:CYS:SG    | 2.61                     | 0.41              |
| 1:L:978:LEU:HB3  | 1:L:982:CYS:SG    | 2.60                     | 0.41              |
| 1:L:980:ASP:O    | 1:L:984:VAL:HG23  | 2.19                     | 0.41              |
| 1:A:239:TRP:CD1  | 1:A:245:PHE:CD2   | 3.08                     | 0.41              |
| 1:A:268:LEU:O    | 1:A:268:LEU:HD12  | 2.21                     | 0.41              |
| 1:A:474:TRP:CD1  | 1:A:568:LYS:HE2   | 2.56                     | 0.41              |
| 1:A:828:LYS:HB3  | 1:A:830:TRP:NE1   | 2.36                     | 0.41              |
| 1:B:830:TRP:CD1  | 1:B:858:TYR:HD2   | 2.39                     | 0.41              |
| 1:B:1005:MET:O   | 1:B:1031:ILE:HG21 | 2.21                     | 0.41              |
| 1:C:278:ASP:O    | 1:C:280:ASN:N     | 2.53                     | 0.41              |
| 1:C:387:GLN:NE2  | 1:C:422:MET:HG2   | 2.35                     | 0.41              |
| 1:C:415:CYS:SG   | 1:C:416:THR:N     | 2.94                     | 0.41              |
| 1:C:819:LEU:HB2  | 1:C:847:VAL:HG21  | 2.02                     | 0.41              |
| 1:D:168:GLN:O    | 1:D:366:ILE:HA    | 2.21                     | 0.41              |
| 1:D:239:TRP:CD1  | 1:D:245:PHE:CD2   | 3.08                     | 0.41              |
| 1:D:369:PHE:HA   | 1:D:373:LYS:HE3   | 2.03                     | 0.41              |
| 1:D:419:LYS:HE2  | 1:D:419:LYS:HA    | 2.02                     | 0.41              |
| 1:D:836:LEU:HD13 | 1:D:840:CYS:SG    | 2.61                     | 0.41              |
| 1:E:400:VAL:O    | 1:E:401:LEU:HB2   | 2.21                     | 0.41              |
| 1:E:866:ASP:HA   | 1:E:869:VAL:HG13  | 2.03                     | 0.41              |
| 1:F:579:PHE:CE1  | 1:F:606:LEU:HD22  | 2.55                     | 0.41              |
| 1:F:911:PHE:CZ   | 1:F:914:LEU:HD13  | 2.56                     | 0.41              |
| 1:G:168:GLN:O    | 1:G:366:ILE:HA    | 2.21                     | 0.41              |
| 1:H:366:ILE:HD12 | 1:H:366:ILE:HA    | 1.94                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:387:GLN:NE2  | 1:H:422:MET:HG2  | 2.35                     | 0.41              |
| 1:H:400:VAL:HG22 | 1:H:404:MET:CE   | 2.51                     | 0.41              |
| 1:H:574:VAL:O    | 1:H:578:LEU:HG   | 2.20                     | 0.41              |
| 1:H:819:LEU:HB2  | 1:H:847:VAL:HG21 | 2.02                     | 0.41              |
| 1:H:836:LEU:HD13 | 1:H:840:CYS:SG   | 2.61                     | 0.41              |
| 1:H:876:MET:HB3  | 1:H:908:ASN:HB2  | 2.03                     | 0.41              |
| 1:I:830:TRP:CD1  | 1:I:858:TYR:HD2  | 2.39                     | 0.41              |
| 1:J:250:ASP:N    | 1:J:292:ARG:O    | 2.46                     | 0.41              |
| 1:J:494:ASP:OD1  | 1:J:495:VAL:N    | 2.54                     | 0.41              |
| 1:K:419:LYS:HE2  | 1:K:419:LYS:HA   | 2.02                     | 0.41              |
| 1:K:828:LYS:HB3  | 1:K:830:TRP:NE1  | 2.36                     | 0.41              |
| 1:K:974:GLY:N    | 1:K:976:ASN:OD1  | 2.54                     | 0.41              |
| 1:K:1019:GLN:N   | 1:K:1019:GLN:OE1 | 2.46                     | 0.41              |
| 1:L:974:GLY:N    | 1:L:976:ASN:OD1  | 2.54                     | 0.41              |
| 1:A:400:VAL:HG22 | 1:A:404:MET:CE   | 2.51                     | 0.40              |
| 1:A:837:THR:OG1  | 1:A:838:SER:N    | 2.54                     | 0.40              |
| 1:B:911:PHE:CZ   | 1:B:914:LEU:HD13 | 2.56                     | 0.40              |
| 1:B:978:LEU:HB3  | 1:B:982:CYS:SG   | 2.60                     | 0.40              |
| 1:C:227:GLY:O    | 1:C:230:ILE:HG22 | 2.21                     | 0.40              |
| 1:C:400:VAL:HG22 | 1:C:404:MET:CE   | 2.51                     | 0.40              |
| 1:C:836:LEU:HD13 | 1:C:840:CYS:SG   | 2.61                     | 0.40              |
| 1:C:876:MET:HB3  | 1:C:908:ASN:HB2  | 2.03                     | 0.40              |
| 1:C:893:LEU:HD22 | 1:C:896:ILE:HG13 | 2.02                     | 0.40              |
| 1:D:400:VAL:HG13 | 1:D:401:LEU:CD2  | 2.50                     | 0.40              |
| 1:D:632:LEU:HD12 | 1:D:641:VAL:HG22 | 2.02                     | 0.40              |
| 1:D:829:LEU:C    | 1:D:830:TRP:HD1  | 2.25                     | 0.40              |
| 1:D:830:TRP:CD1  | 1:D:858:TYR:HD2  | 2.39                     | 0.40              |
| 1:E:494:ASP:OD1  | 1:E:495:VAL:N    | 2.54                     | 0.40              |
| 1:E:632:LEU:HA   | 1:E:635:MET:HG3  | 2.03                     | 0.40              |
| 1:F:280:ASN:HB2  | 1:F:281:PRO:HD3  | 2.03                     | 0.40              |
| 1:F:400:VAL:O    | 1:F:401:LEU:HB2  | 2.21                     | 0.40              |
| 1:F:819:LEU:HB2  | 1:F:847:VAL:HG21 | 2.02                     | 0.40              |
| 1:F:829:LEU:C    | 1:F:830:TRP:HD1  | 2.25                     | 0.40              |
| 1:G:382:PHE:CE1  | 1:G:419:LYS:HE3  | 2.57                     | 0.40              |
| 1:G:836:LEU:HD13 | 1:G:840:CYS:SG   | 2.61                     | 0.40              |
| 1:G:974:GLY:N    | 1:G:976:ASN:OD1  | 2.54                     | 0.40              |
| 1:H:407:ILE:HA   | 1:H:408:PRO:HD3  | 1.92                     | 0.40              |
| 1:H:415:CYS:SG   | 1:H:416:THR:N    | 2.95                     | 0.40              |
| 1:H:474:TRP:CD1  | 1:H:568:LYS:HE2  | 2.56                     | 0.40              |
| 1:H:579:PHE:CD2  | 1:H:631:CYS:HB3  | 2.55                     | 0.40              |
| 1:I:159:ASP:HB3  | 1:I:160:LEU:H    | 1.63                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:274:SER:O    | 1:I:274:SER:OG    | 2.36                     | 0.40              |
| 1:I:294:LEU:HD12 | 1:I:295:PHE:N     | 2.35                     | 0.40              |
| 1:I:419:LYS:HE2  | 1:I:419:LYS:HA    | 2.02                     | 0.40              |
| 1:I:785:PHE:HB3  | 1:J:810:PHE:CZ    | 2.54                     | 0.40              |
| 1:J:400:VAL:HG22 | 1:J:404:MET:CE    | 2.51                     | 0.40              |
| 1:J:632:LEU:HA   | 1:J:635:MET:HG3   | 2.03                     | 0.40              |
| 1:J:837:THR:OG1  | 1:J:838:SER:N     | 2.54                     | 0.40              |
| 1:K:247:ASP:O    | 1:K:292:ARG:NH2   | 2.31                     | 0.40              |
| 1:K:369:PHE:HA   | 1:K:373:LYS:HE3   | 2.03                     | 0.40              |
| 1:K:970:LYS:HD2  | 1:K:1001:GLN:NE2  | 2.32                     | 0.40              |
| 1:L:400:VAL:HG22 | 1:L:404:MET:HE1   | 2.03                     | 0.40              |
| 1:L:419:LYS:HE2  | 1:L:419:LYS:HA    | 2.02                     | 0.40              |
| 1:A:227:GLY:O    | 1:A:230:ILE:HG22  | 2.21                     | 0.40              |
| 1:A:415:CYS:SG   | 1:A:416:THR:N     | 2.95                     | 0.40              |
| 1:B:419:LYS:HA   | 1:B:419:LYS:HE2   | 2.02                     | 0.40              |
| 1:B:885:LYS:HG2  | 1:B:913:HIS:ND1   | 2.37                     | 0.40              |
| 1:C:366:ILE:HD12 | 1:C:366:ILE:HA    | 1.95                     | 0.40              |
| 1:C:474:TRP:CD1  | 1:C:568:LYS:HE2   | 2.56                     | 0.40              |
| 1:C:837:THR:OG1  | 1:C:838:SER:N     | 2.54                     | 0.40              |
| 1:D:217:THR:HB   | 1:D:342:LEU:HB3   | 2.03                     | 0.40              |
| 1:D:382:PHE:CE1  | 1:D:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:D:400:VAL:O    | 1:D:401:LEU:HB2   | 2.21                     | 0.40              |
| 1:D:885:LYS:HG2  | 1:D:913:HIS:ND1   | 2.37                     | 0.40              |
| 1:D:974:GLY:N    | 1:D:976:ASN:OD1   | 2.54                     | 0.40              |
| 1:E:334:LYS:CG   | 1:E:342:LEU:HD11  | 2.48                     | 0.40              |
| 1:E:829:LEU:C    | 1:E:830:TRP:HD1   | 2.25                     | 0.40              |
| 1:E:876:MET:HB3  | 1:E:908:ASN:HB2   | 2.03                     | 0.40              |
| 1:F:227:GLY:O    | 1:F:230:ILE:HG22  | 2.21                     | 0.40              |
| 1:F:985:THR:HA   | 1:F:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:G:199:LEU:HB3  | 1:G:200:LYS:H     | 1.68                     | 0.40              |
| 1:G:217:THR:HB   | 1:G:342:LEU:HB3   | 2.03                     | 0.40              |
| 1:G:369:PHE:HA   | 1:G:373:LYS:HE3   | 2.03                     | 0.40              |
| 1:G:400:VAL:O    | 1:G:401:LEU:HB2   | 2.21                     | 0.40              |
| 1:G:632:LEU:HD12 | 1:G:641:VAL:HG22  | 2.01                     | 0.40              |
| 1:G:829:LEU:C    | 1:G:830:TRP:HD1   | 2.25                     | 0.40              |
| 1:G:830:TRP:CD1  | 1:G:858:TYR:HD2   | 2.39                     | 0.40              |
| 1:G:896:ILE:O    | 1:G:899:SER:OG    | 2.27                     | 0.40              |
| 1:H:632:LEU:HA   | 1:H:635:MET:HG3   | 2.03                     | 0.40              |
| 1:I:885:LYS:HG2  | 1:I:913:HIS:ND1   | 2.37                     | 0.40              |
| 1:I:978:LEU:HB3  | 1:I:982:CYS:SG    | 2.60                     | 0.40              |
| 1:I:1005:MET:O   | 1:I:1031:ILE:HG21 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:227:GLY:O    | 1:J:230:ILE:HG22  | 2.21                     | 0.40              |
| 1:J:268:LEU:HD12 | 1:J:268:LEU:O     | 2.21                     | 0.40              |
| 1:J:415:CYS:SG   | 1:J:416:THR:N     | 2.94                     | 0.40              |
| 1:L:217:THR:HB   | 1:L:342:LEU:HB3   | 2.03                     | 0.40              |
| 1:L:239:TRP:CD1  | 1:L:245:PHE:CD2   | 3.08                     | 0.40              |
| 1:L:247:ASP:O    | 1:L:292:ARG:NH2   | 2.31                     | 0.40              |
| 1:L:369:PHE:HA   | 1:L:373:LYS:HE3   | 2.03                     | 0.40              |
| 1:L:400:VAL:HG22 | 1:L:404:MET:CE    | 2.52                     | 0.40              |
| 1:L:970:LYS:HD2  | 1:L:1001:GLN:NE2  | 2.32                     | 0.40              |
| 1:A:614:ALA:HA   | 1:A:648:PHE:CE1   | 2.57                     | 0.40              |
| 1:B:382:PHE:CE1  | 1:B:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:C:268:LEU:HD12 | 1:C:268:LEU:O     | 2.21                     | 0.40              |
| 1:E:134:LYS:HG3  | 1:E:137:ARG:NH2   | 2.34                     | 0.40              |
| 1:E:415:CYS:SG   | 1:E:416:THR:N     | 2.95                     | 0.40              |
| 1:E:828:LYS:HB3  | 1:E:830:TRP:NE1   | 2.36                     | 0.40              |
| 1:F:217:THR:HB   | 1:F:342:LEU:HB3   | 2.03                     | 0.40              |
| 1:F:944:GLU:CG   | 1:F:972:ASN:HB2   | 2.46                     | 0.40              |
| 1:G:400:VAL:HG13 | 1:G:401:LEU:CD2   | 2.50                     | 0.40              |
| 1:G:885:LYS:HG2  | 1:G:913:HIS:ND1   | 2.37                     | 0.40              |
| 1:G:1005:MET:O   | 1:G:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:H:168:GLN:O    | 1:H:366:ILE:HA    | 2.21                     | 0.40              |
| 1:H:278:ASP:O    | 1:H:280:ASN:N     | 2.53                     | 0.40              |
| 1:I:382:PHE:CE1  | 1:I:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:I:614:ALA:HA   | 1:I:648:PHE:CE1   | 2.57                     | 0.40              |
| 1:I:911:PHE:CZ   | 1:I:914:LEU:HD13  | 2.56                     | 0.40              |
| 1:J:401:LEU:O    | 1:J:405:CYS:HB3   | 2.20                     | 0.40              |
| 1:J:614:ALA:HA   | 1:J:648:PHE:CE1   | 2.57                     | 0.40              |
| 1:K:168:GLN:O    | 1:K:366:ILE:HA    | 2.21                     | 0.40              |
| 1:K:239:TRP:CD1  | 1:K:245:PHE:CD2   | 3.08                     | 0.40              |
| 1:K:382:PHE:CE1  | 1:K:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:K:792:SER:HB2  | 1:K:822:LEU:HD22  | 2.04                     | 0.40              |
| 1:L:199:LEU:HB3  | 1:L:200:LYS:H     | 1.68                     | 0.40              |
| 1:L:830:TRP:CD1  | 1:L:858:TYR:HD2   | 2.39                     | 0.40              |
| 1:A:258:ARG:NH2  | 1:A:515:SER:HB2   | 2.37                     | 0.40              |
| 1:A:401:LEU:O    | 1:A:405:CYS:HB3   | 2.20                     | 0.40              |
| 1:A:528:MET:HE2  | 1:A:531:LEU:HD12  | 2.04                     | 0.40              |
| 1:A:769:ILE:HG22 | 1:A:771:ARG:N     | 2.32                     | 0.40              |
| 1:B:134:LYS:HG3  | 1:B:137:ARG:NH2   | 2.34                     | 0.40              |
| 1:B:159:ASP:HB3  | 1:B:160:LEU:H     | 1.63                     | 0.40              |
| 1:B:828:LYS:HB3  | 1:B:830:TRP:NE1   | 2.36                     | 0.40              |
| 1:C:554:ARG:HB3  | 1:C:555:ASP:H     | 1.63                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:574:VAL:O    | 1:C:578:LEU:HG    | 2.20                     | 0.40              |
| 1:C:590:LEU:HD23 | 1:C:590:LEU:HA    | 1.80                     | 0.40              |
| 1:C:1005:MET:O   | 1:C:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:D:415:CYS:SG   | 1:D:416:THR:N     | 2.94                     | 0.40              |
| 1:D:474:TRP:CD1  | 1:D:568:LYS:HE2   | 2.56                     | 0.40              |
| 1:D:578:LEU:O    | 1:D:582:VAL:HG13  | 2.22                     | 0.40              |
| 1:D:819:LEU:HB2  | 1:D:847:VAL:HG21  | 2.02                     | 0.40              |
| 1:D:1005:MET:O   | 1:D:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:E:400:VAL:HG22 | 1:E:404:MET:CE    | 2.52                     | 0.40              |
| 1:E:483:CYS:HB3  | 1:E:486:ARG:NE    | 2.37                     | 0.40              |
| 1:E:819:LEU:HB2  | 1:E:847:VAL:HG21  | 2.02                     | 0.40              |
| 1:E:837:THR:OG1  | 1:E:838:SER:N     | 2.54                     | 0.40              |
| 1:F:134:LYS:HG3  | 1:F:137:ARG:NH2   | 2.34                     | 0.40              |
| 1:F:268:LEU:O    | 1:F:268:LEU:HD12  | 2.21                     | 0.40              |
| 1:F:400:VAL:HG22 | 1:F:404:MET:CE    | 2.52                     | 0.40              |
| 1:F:483:CYS:HB3  | 1:F:486:ARG:NE    | 2.37                     | 0.40              |
| 1:F:494:ASP:OD1  | 1:F:495:VAL:N     | 2.54                     | 0.40              |
| 1:F:885:LYS:HG2  | 1:F:913:HIS:ND1   | 2.37                     | 0.40              |
| 1:F:970:LYS:HE2  | 1:G:1027:ILE:HD13 | 2.02                     | 0.40              |
| 1:G:387:GLN:NE2  | 1:G:422:MET:HG2   | 2.35                     | 0.40              |
| 1:G:474:TRP:CD1  | 1:G:568:LYS:HE2   | 2.56                     | 0.40              |
| 1:G:578:LEU:O    | 1:G:582:VAL:HG13  | 2.22                     | 0.40              |
| 1:G:792:SER:HB2  | 1:G:822:LEU:HD22  | 2.04                     | 0.40              |
| 1:G:985:THR:HA   | 1:G:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:H:1005:MET:O   | 1:H:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:I:876:MET:HB3  | 1:I:908:ASN:HB2   | 2.03                     | 0.40              |
| 1:J:419:LYS:HE2  | 1:J:419:LYS:HA    | 2.02                     | 0.40              |
| 1:J:836:LEU:HD13 | 1:J:840:CYS:SG    | 2.61                     | 0.40              |
| 1:J:866:ASP:HA   | 1:J:869:VAL:HG13  | 2.03                     | 0.40              |
| 1:K:268:LEU:O    | 1:K:268:LEU:HD12  | 2.21                     | 0.40              |
| 1:K:830:TRP:CD1  | 1:K:858:TYR:HD2   | 2.39                     | 0.40              |
| 1:K:1005:MET:O   | 1:K:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:L:268:LEU:O    | 1:L:268:LEU:HD12  | 2.21                     | 0.40              |
| 1:L:382:PHE:CE1  | 1:L:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:L:474:TRP:CD1  | 1:L:568:LYS:HE2   | 2.56                     | 0.40              |
| 1:A:400:VAL:O    | 1:A:401:LEU:HB2   | 2.21                     | 0.40              |
| 1:A:836:LEU:HD13 | 1:A:840:CYS:SG    | 2.61                     | 0.40              |
| 1:A:985:THR:HA   | 1:A:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:B:239:TRP:CD1  | 1:B:245:PHE:CD2   | 3.08                     | 0.40              |
| 1:B:415:CYS:SG   | 1:B:416:THR:N     | 2.95                     | 0.40              |
| 1:B:494:ASP:OD1  | 1:B:495:VAL:N     | 2.55                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:578:LEU:O    | 1:B:582:VAL:HG13  | 2.22                     | 0.40              |
| 1:B:614:ALA:HA   | 1:B:648:PHE:CE1   | 2.57                     | 0.40              |
| 1:B:830:TRP:CD1  | 1:B:830:TRP:N     | 2.86                     | 0.40              |
| 1:C:794:SER:HB2  | 1:C:797:LEU:HD23  | 2.02                     | 0.40              |
| 1:C:985:THR:HA   | 1:C:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:D:369:PHE:HA   | 1:D:373:LYS:CE    | 2.51                     | 0.40              |
| 1:D:792:SER:HB2  | 1:D:822:LEU:HD22  | 2.04                     | 0.40              |
| 1:E:369:PHE:HA   | 1:E:373:LYS:HE3   | 2.03                     | 0.40              |
| 1:E:382:PHE:CE1  | 1:E:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:E:573:PHE:HA   | 1:E:576:ARG:HB2   | 2.04                     | 0.40              |
| 1:E:830:TRP:CD1  | 1:E:858:TYR:HD2   | 2.39                     | 0.40              |
| 1:F:382:PHE:CE1  | 1:F:419:LYS:HE3   | 2.57                     | 0.40              |
| 1:F:415:CYS:SG   | 1:F:416:THR:N     | 2.94                     | 0.40              |
| 1:F:474:TRP:CD1  | 1:F:568:LYS:HE2   | 2.56                     | 0.40              |
| 1:F:578:LEU:O    | 1:F:582:VAL:HG13  | 2.22                     | 0.40              |
| 1:F:632:LEU:HA   | 1:F:635:MET:HG3   | 2.03                     | 0.40              |
| 1:F:730:LEU:C    | 1:F:733:SER:HG    | 2.19                     | 0.40              |
| 1:F:1005:MET:O   | 1:F:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:G:250:ASP:N    | 1:G:292:ARG:O     | 2.46                     | 0.40              |
| 1:G:369:PHE:HA   | 1:G:373:LYS:CE    | 2.52                     | 0.40              |
| 1:G:415:CYS:SG   | 1:G:416:THR:N     | 2.95                     | 0.40              |
| 1:G:819:LEU:HB2  | 1:G:847:VAL:HG21  | 2.02                     | 0.40              |
| 1:G:876:MET:HB3  | 1:G:908:ASN:HB2   | 2.03                     | 0.40              |
| 1:H:768:ASN:N    | 1:H:796:LYS:HZ3   | 2.18                     | 0.40              |
| 1:H:829:LEU:C    | 1:H:830:TRP:HD1   | 2.25                     | 0.40              |
| 1:H:985:THR:HA   | 1:H:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:I:239:TRP:CD1  | 1:I:245:PHE:CD2   | 3.08                     | 0.40              |
| 1:I:415:CYS:SG   | 1:I:416:THR:N     | 2.95                     | 0.40              |
| 1:I:578:LEU:O    | 1:I:582:VAL:HG13  | 2.22                     | 0.40              |
| 1:I:836:LEU:HD13 | 1:I:840:CYS:SG    | 2.61                     | 0.40              |
| 1:I:944:GLU:CG   | 1:I:972:ASN:HB2   | 2.46                     | 0.40              |
| 1:J:168:GLN:O    | 1:J:366:ILE:HA    | 2.21                     | 0.40              |
| 1:J:258:ARG:NH2  | 1:J:515:SER:HB2   | 2.37                     | 0.40              |
| 1:J:400:VAL:O    | 1:J:401:LEU:HB2   | 2.21                     | 0.40              |
| 1:J:999:SER:OG   | 1:J:1000:LEU:N    | 2.54                     | 0.40              |
| 1:J:1005:MET:O   | 1:J:1031:ILE:HG21 | 2.21                     | 0.40              |
| 1:K:985:THR:HA   | 1:K:988:GLU:HG3   | 2.03                     | 0.40              |
| 1:L:168:GLN:O    | 1:L:366:ILE:HA    | 2.21                     | 0.40              |
| 1:L:415:CYS:SG   | 1:L:416:THR:N     | 2.94                     | 0.40              |
| 1:L:792:SER:HB2  | 1:L:822:LEU:HD22  | 2.04                     | 0.40              |
| 1:L:985:THR:HA   | 1:L:988:GLU:HG3   | 2.03                     | 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     | 794/1037 (77%)   | 688 (87%)  | 105 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | B     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | C     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | D     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | E     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | F     | 794/1037 (77%)   | 688 (87%)  | 105 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | G     | 794/1037 (77%)   | 688 (87%)  | 105 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | H     | 794/1037 (77%)   | 690 (87%)  | 103 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | I     | 794/1037 (77%)   | 690 (87%)  | 103 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | J     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | K     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| 1   | L     | 794/1037 (77%)   | 689 (87%)  | 104 (13%)  | 1 (0%)   | 51          | 85 |
| All | All   | 9528/12444 (77%) | 8267 (87%) | 1249 (13%) | 12 (0%)  | 54          | 85 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 571 | LEU  |
| 1   | B     | 571 | LEU  |
| 1   | C     | 571 | LEU  |
| 1   | D     | 571 | LEU  |
| 1   | E     | 571 | LEU  |
| 1   | F     | 571 | LEU  |
| 1   | G     | 571 | LEU  |
| 1   | H     | 571 | LEU  |
| 1   | I     | 571 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 571 | LEU  |
| 1   | K     | 571 | LEU  |
| 1   | L     | 571 | LEU  |

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

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | A     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | B     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | C     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | D     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | E     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | F     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | G     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | H     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | I     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | J     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | K     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| 1   | L     | 720/937 (77%)    | 716 (99%)  | 4 (1%)   | 86          | 92 |
| All | All   | 8640/11244 (77%) | 8592 (99%) | 48 (1%)  | 86          | 92 |

All (48) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 228  | LYS  |
| 1   | A     | 373  | LYS  |
| 1   | A     | 389  | ARG  |
| 1   | A     | 1009 | ARG  |
| 1   | B     | 228  | LYS  |
| 1   | B     | 373  | LYS  |
| 1   | B     | 389  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1009 | ARG  |
| 1   | C     | 228  | LYS  |
| 1   | C     | 373  | LYS  |
| 1   | C     | 389  | ARG  |
| 1   | C     | 1009 | ARG  |
| 1   | D     | 228  | LYS  |
| 1   | D     | 373  | LYS  |
| 1   | D     | 389  | ARG  |
| 1   | D     | 1009 | ARG  |
| 1   | E     | 228  | LYS  |
| 1   | E     | 373  | LYS  |
| 1   | E     | 389  | ARG  |
| 1   | E     | 1009 | ARG  |
| 1   | F     | 228  | LYS  |
| 1   | F     | 373  | LYS  |
| 1   | F     | 389  | ARG  |
| 1   | F     | 1009 | ARG  |
| 1   | G     | 228  | LYS  |
| 1   | G     | 373  | LYS  |
| 1   | G     | 389  | ARG  |
| 1   | G     | 1009 | ARG  |
| 1   | H     | 228  | LYS  |
| 1   | H     | 373  | LYS  |
| 1   | H     | 389  | ARG  |
| 1   | H     | 1009 | ARG  |
| 1   | I     | 228  | LYS  |
| 1   | I     | 373  | LYS  |
| 1   | I     | 389  | ARG  |
| 1   | I     | 1009 | ARG  |
| 1   | J     | 228  | LYS  |
| 1   | J     | 373  | LYS  |
| 1   | J     | 389  | ARG  |
| 1   | J     | 1009 | ARG  |
| 1   | K     | 228  | LYS  |
| 1   | K     | 373  | LYS  |
| 1   | K     | 389  | ARG  |
| 1   | K     | 1009 | ARG  |
| 1   | L     | 228  | LYS  |
| 1   | L     | 373  | LYS  |
| 1   | L     | 389  | ARG  |
| 1   | L     | 1009 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)



such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 670 | ASN  |
| 1   | A     | 737 | ASN  |
| 1   | A     | 884 | GLN  |
| 1   | A     | 976 | ASN  |
| 1   | B     | 670 | ASN  |
| 1   | B     | 737 | ASN  |
| 1   | B     | 890 | ASN  |
| 1   | B     | 976 | ASN  |
| 1   | C     | 670 | ASN  |
| 1   | C     | 737 | ASN  |
| 1   | C     | 890 | ASN  |
| 1   | C     | 976 | ASN  |
| 1   | D     | 670 | ASN  |
| 1   | D     | 737 | ASN  |
| 1   | D     | 890 | ASN  |
| 1   | D     | 976 | ASN  |
| 1   | E     | 670 | ASN  |
| 1   | E     | 737 | ASN  |
| 1   | E     | 890 | ASN  |
| 1   | E     | 976 | ASN  |
| 1   | F     | 670 | ASN  |
| 1   | F     | 737 | ASN  |
| 1   | F     | 890 | ASN  |
| 1   | F     | 976 | ASN  |
| 1   | G     | 670 | ASN  |
| 1   | G     | 737 | ASN  |
| 1   | G     | 890 | ASN  |
| 1   | G     | 976 | ASN  |
| 1   | H     | 670 | ASN  |
| 1   | H     | 737 | ASN  |
| 1   | H     | 890 | ASN  |
| 1   | H     | 976 | ASN  |
| 1   | I     | 670 | ASN  |
| 1   | I     | 737 | ASN  |
| 1   | I     | 890 | ASN  |
| 1   | I     | 976 | ASN  |
| 1   | J     | 670 | ASN  |
| 1   | J     | 737 | ASN  |
| 1   | J     | 890 | ASN  |
| 1   | J     | 976 | ASN  |
| 1   | K     | 670 | ASN  |
| 1   | K     | 737 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 890 | ASN  |
| 1   | K     | 976 | ASN  |
| 1   | L     | 670 | ASN  |
| 1   | L     | 737 | ASN  |
| 1   | L     | 890 | ASN  |
| 1   | L     | 976 | 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 monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

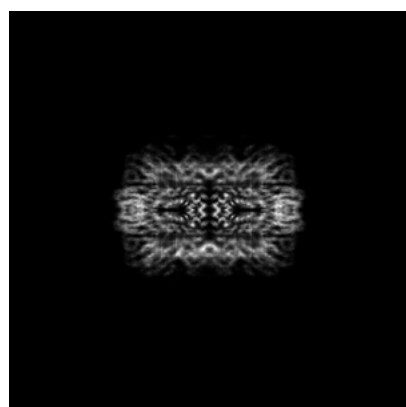
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23302. These allow visual inspection of the internal detail of the map and identification of artifacts.

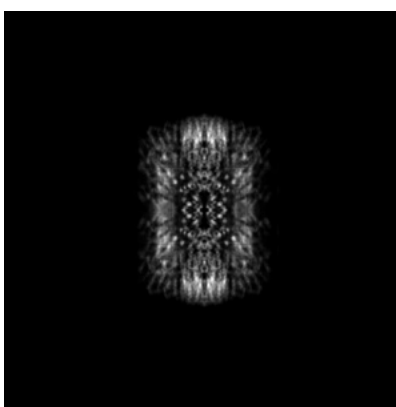
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

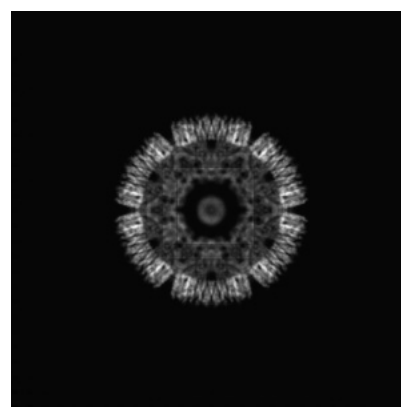
#### 6.1.1 Primary map



X



Y



Z

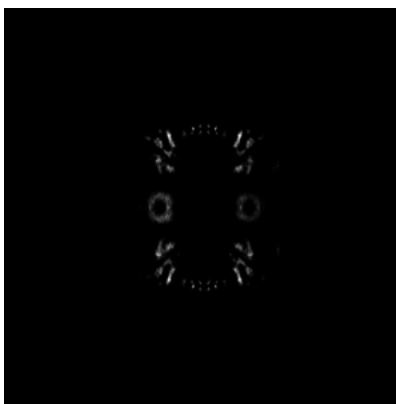
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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

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

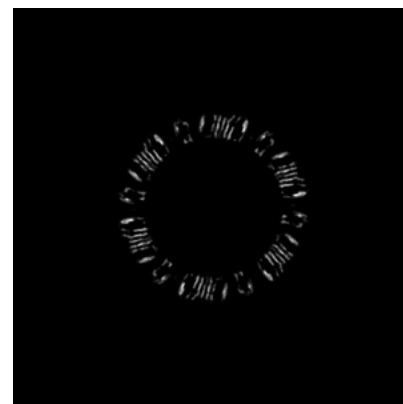
### 6.3.1 Primary map



X Index: 348



Y Index: 323

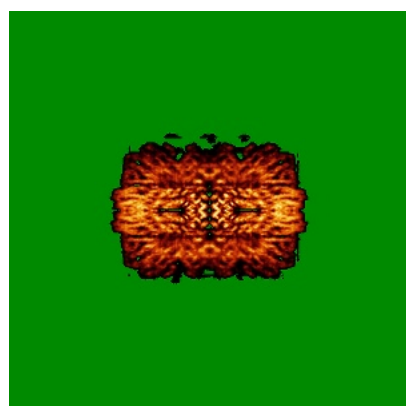


Z Index: 266

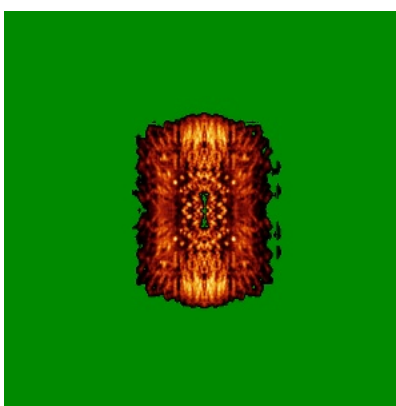
The images above show the largest variance slices of the map in three orthogonal directions.

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

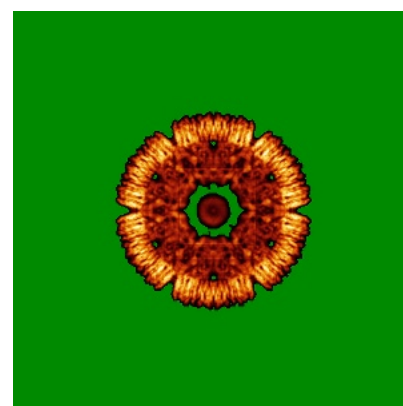
### 6.4.1 Primary map



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 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

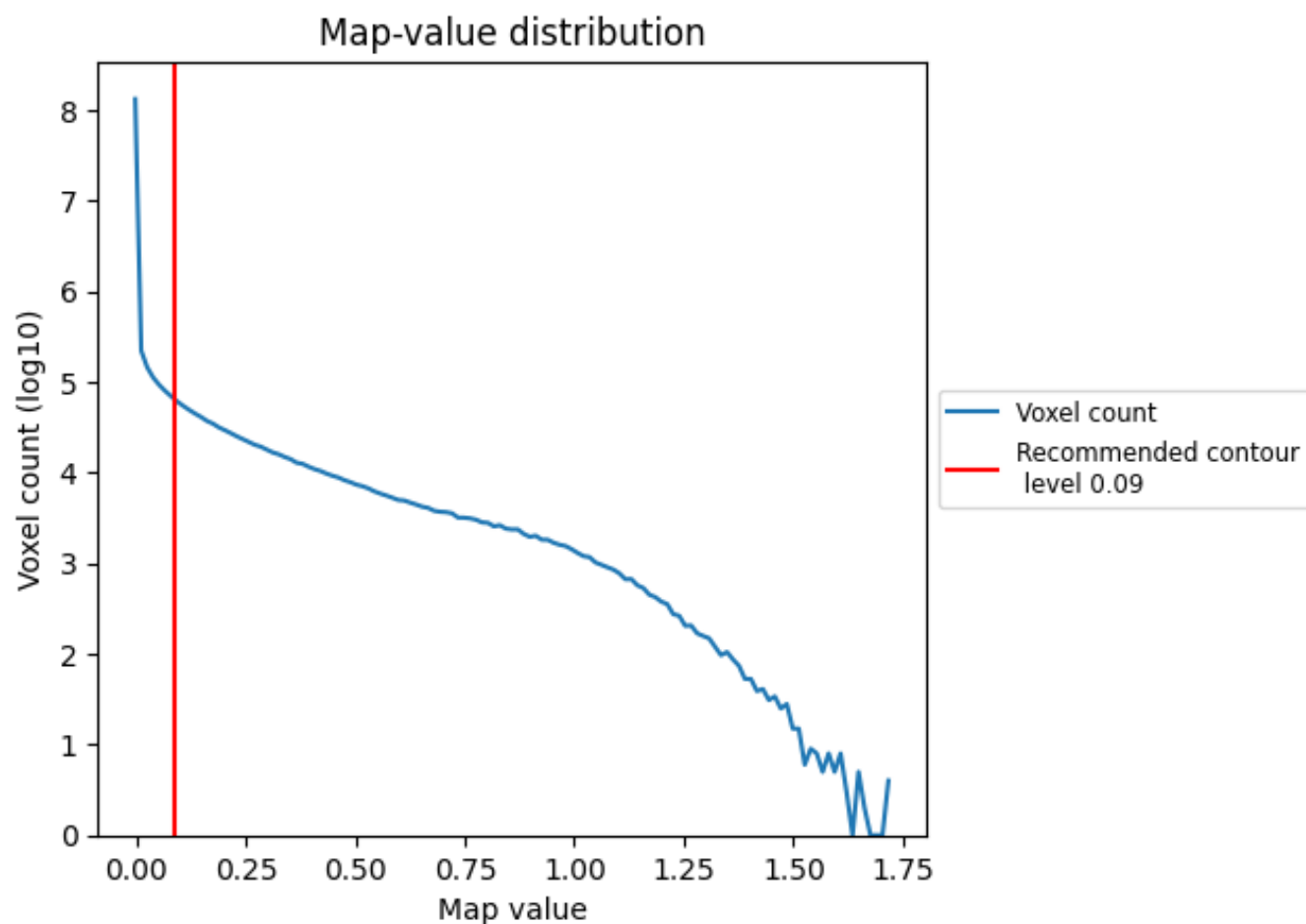
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

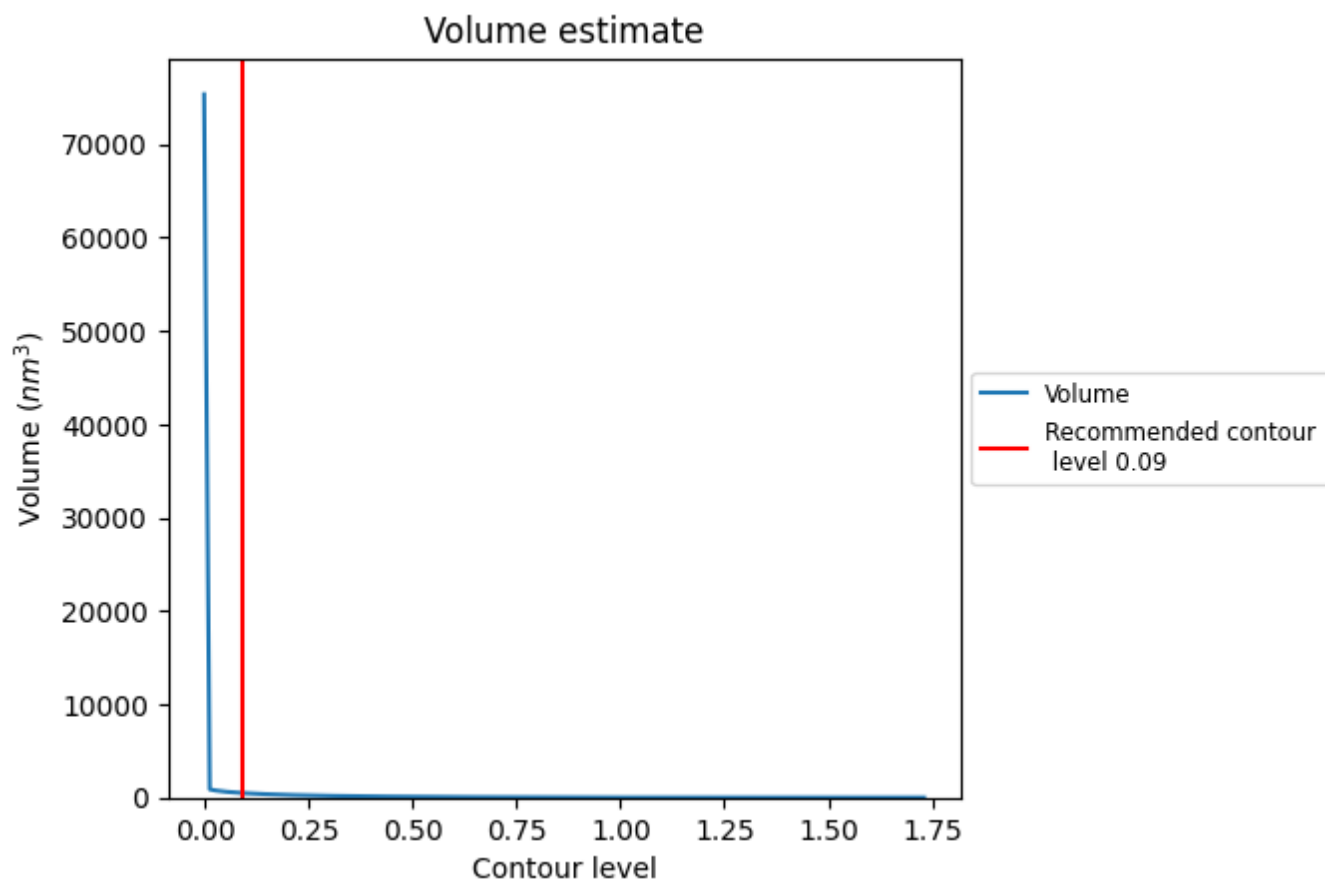
This section contains the results of statistical analysis of the map.

### 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](#)

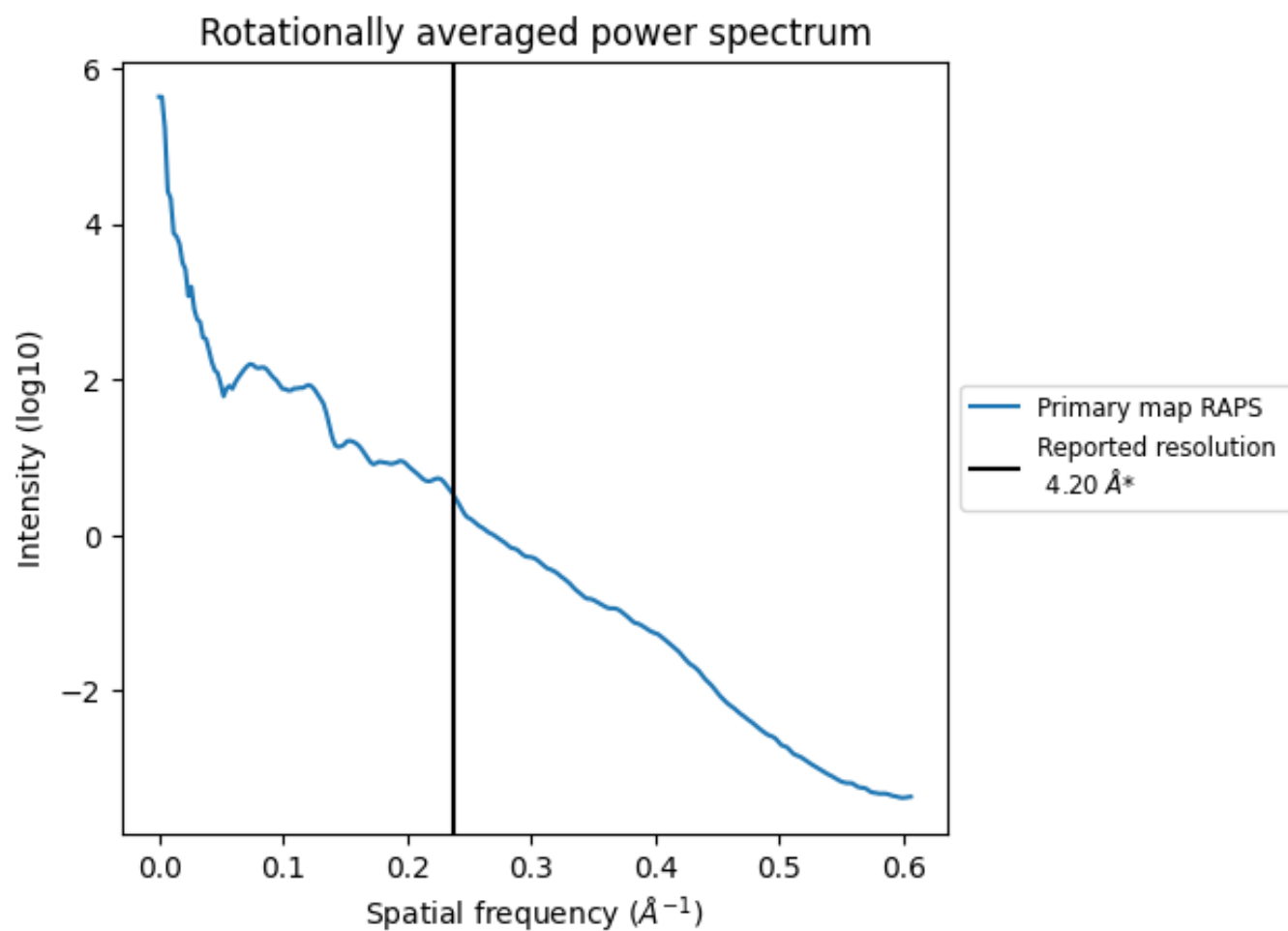


The volume at the recommended contour level is 489  $\text{nm}^3$ ; this corresponds to an approximate mass of 442 kDa.

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 ⓘ

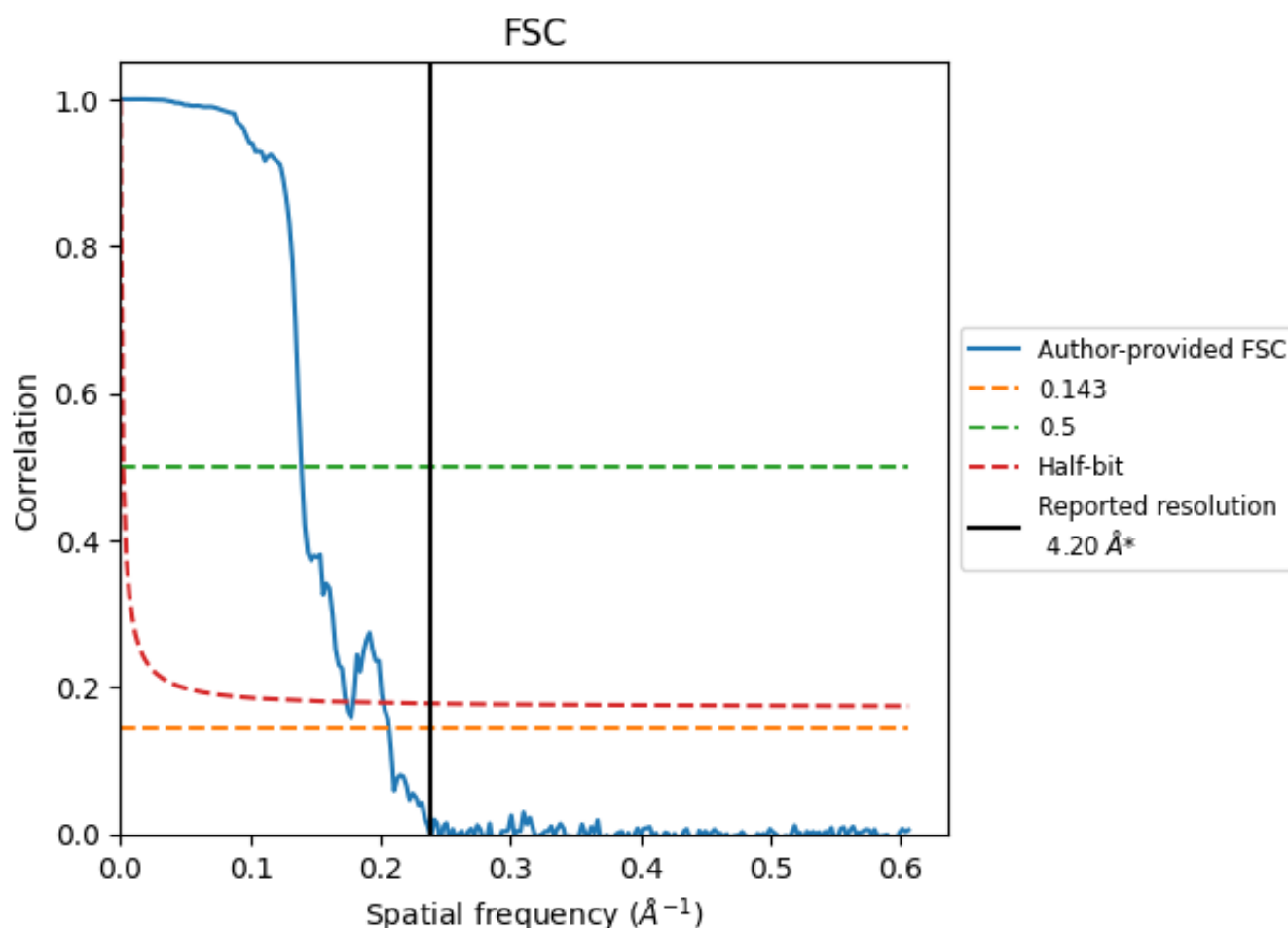


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

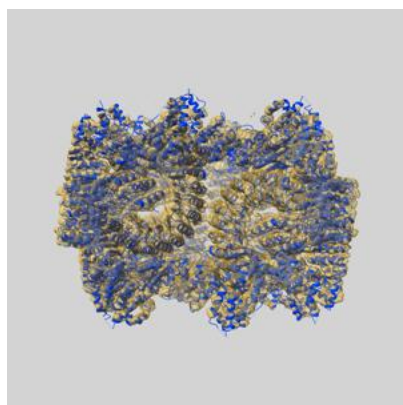
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.20                               | -    | -        |
| Author-provided FSC curve | 4.84                               | 7.17 | 5.76     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.84 differs from the reported value 4.2 by more than 10 %

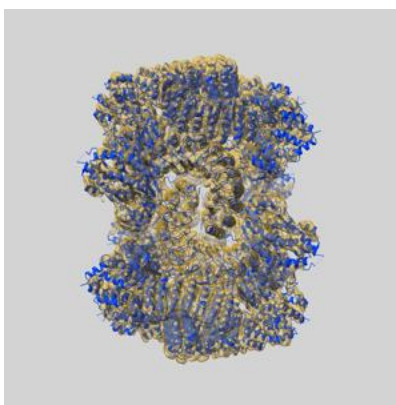
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23302 and PDB model 7LFH. Per-residue inclusion information can be found in section 3 on page 6.

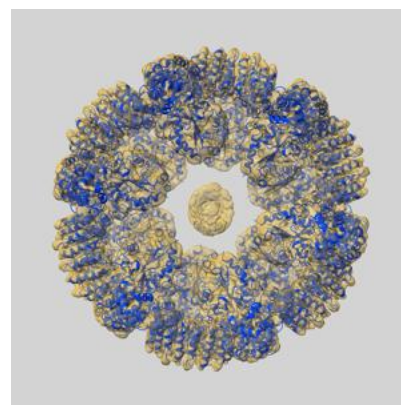
### 9.1 Map-model overlay [i](#)



X



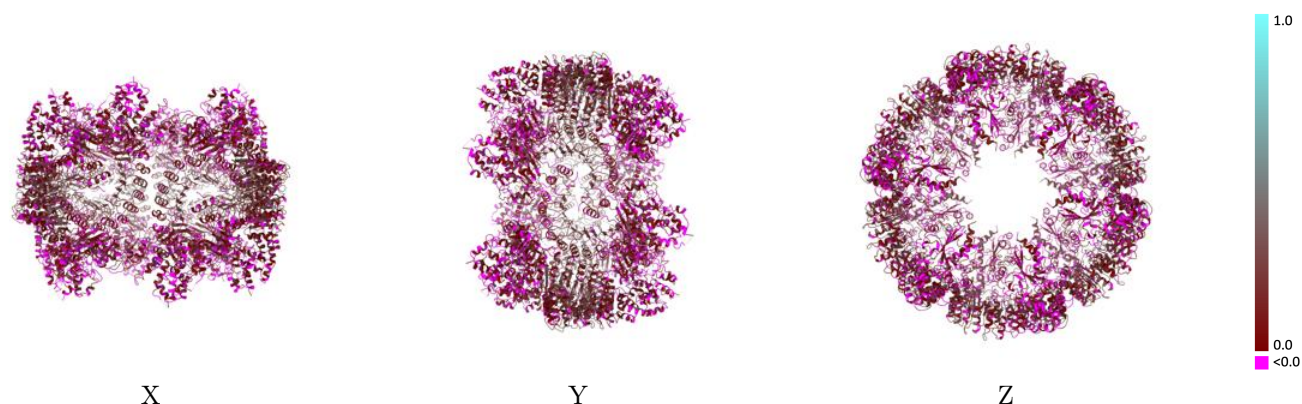
Y



Z

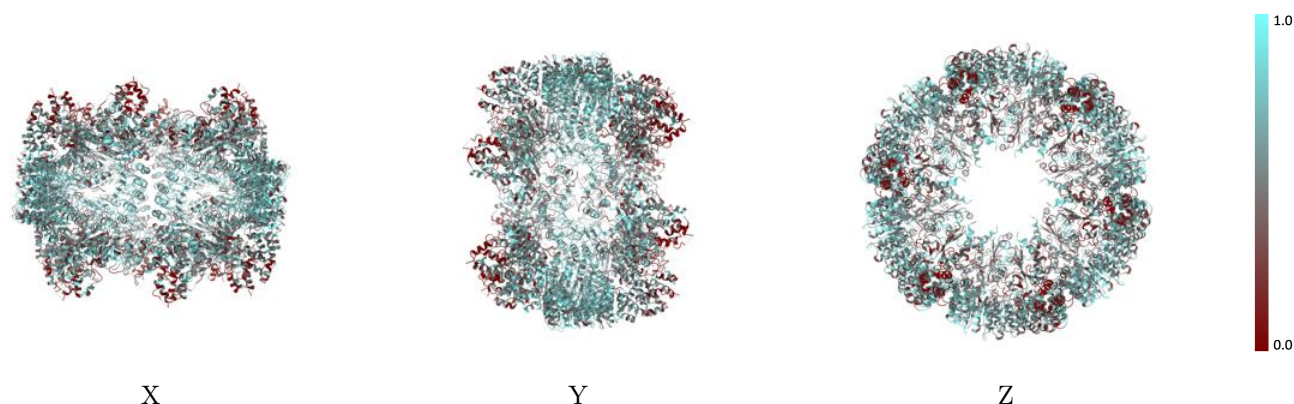
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



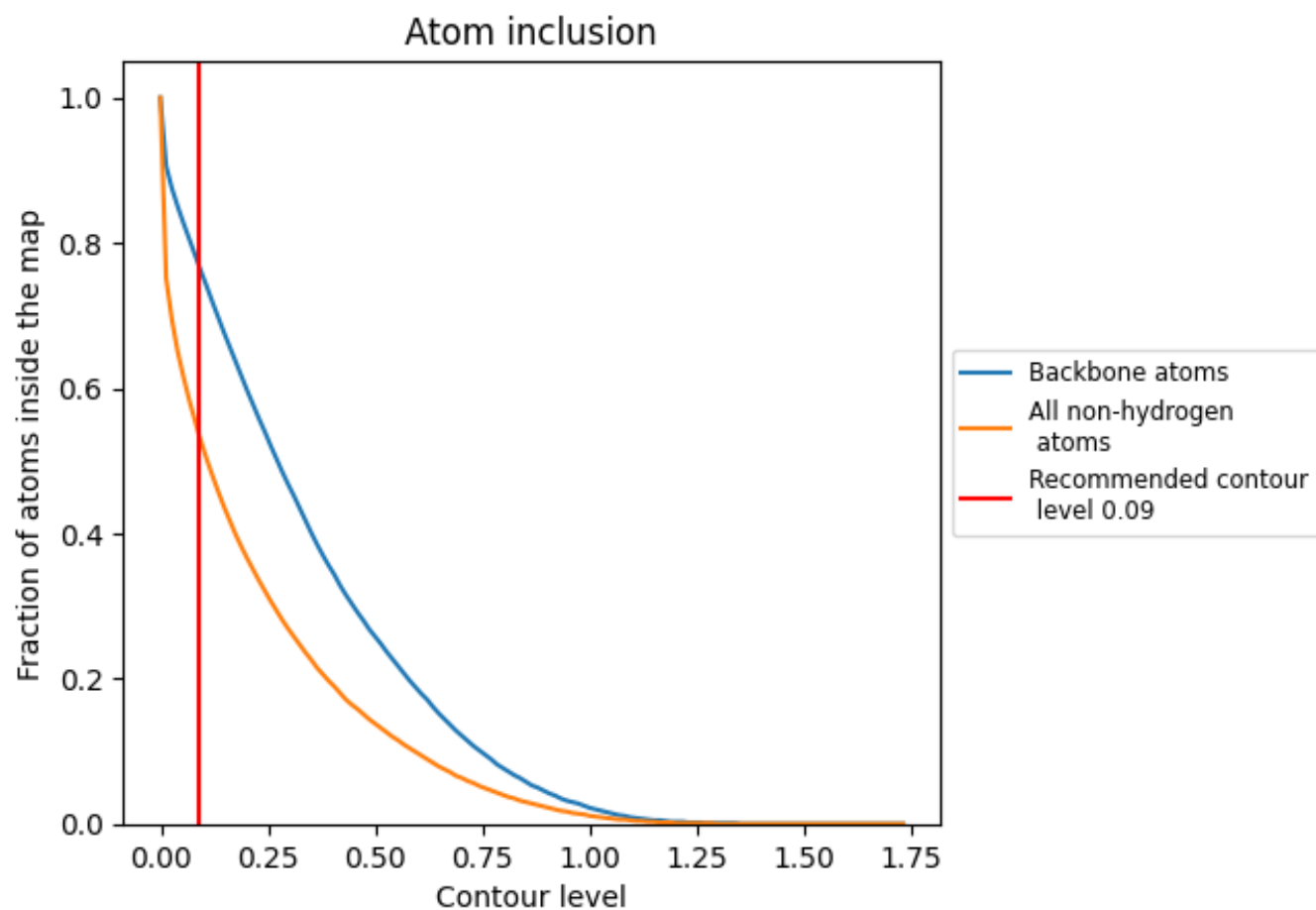
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.5320 | <div><div></div></div> 0.1150 |
| A     | <div><div></div></div> 0.5310 | <div><div></div></div> 0.1180 |
| B     | <div><div></div></div> 0.5360 | <div><div></div></div> 0.1150 |
| C     | <div><div></div></div> 0.5020 | <div><div></div></div> 0.1070 |
| D     | <div><div></div></div> 0.5540 | <div><div></div></div> 0.1190 |
| E     | <div><div></div></div> 0.5160 | <div><div></div></div> 0.1140 |
| F     | <div><div></div></div> 0.5430 | <div><div></div></div> 0.1160 |
| G     | <div><div></div></div> 0.5200 | <div><div></div></div> 0.1120 |
| H     | <div><div></div></div> 0.5280 | <div><div></div></div> 0.1140 |
| I     | <div><div></div></div> 0.5180 | <div><div></div></div> 0.1140 |
| J     | <div><div></div></div> 0.5430 | <div><div></div></div> 0.1160 |
| K     | <div><div></div></div> 0.5370 | <div><div></div></div> 0.1180 |
| L     | <div><div></div></div> 0.5600 | <div><div></div></div> 0.1170 |

1.0

0.0

<0.0