



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:55 PM BST

PDB ID : 4AOD  
EMDB ID: : EMD-2055  
Title : Biomphalaria glabrata Acetylcholine-binding protein type 1 (BgAChBP1)  
Authors : Saur, M.; Moeller, V.; Kapetanopoulos, K.; Braukmann, S.; Gebauer, W.;  
Tenzer, S.; Markl, J.  
Deposited on : 2012-03-26  
Resolution : 6.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

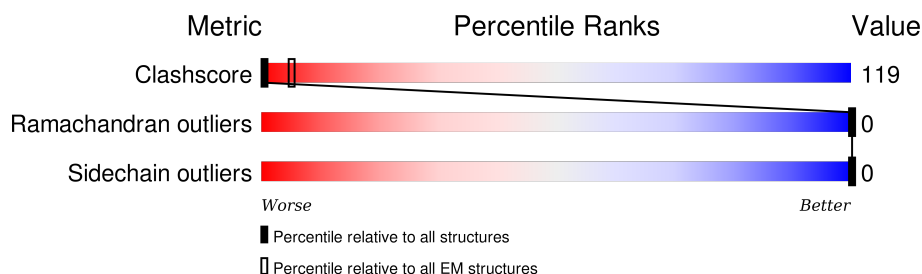
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 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            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |     |
|-----|-------|--------|------------------|-----|
| 1   | A     | 205    | 27%              | 72% |
| 1   | B     | 205    | 28%              | 71% |
| 1   | C     | 205    | 27%              | 73% |
| 1   | D     | 205    | 29%              | 70% |
| 1   | E     | 205    | 29%              | 71% |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8265 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.

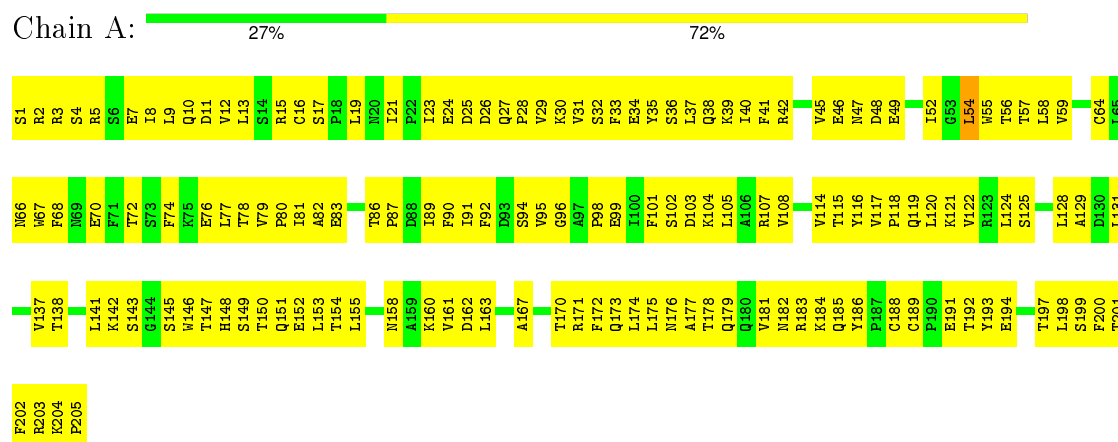
- Molecule 1 is a protein called ACETYLCHOLINE-BINDING PROTEIN TYPE 1.

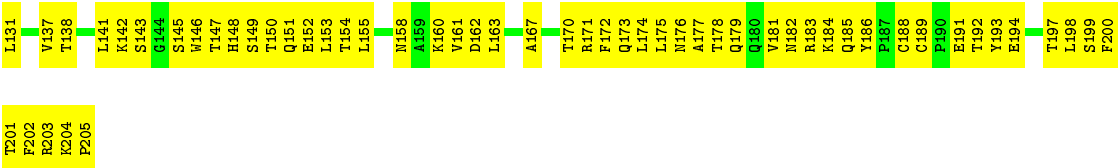
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1050 | 273 | 324 | 6 |         |       |
| 1   | B     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1050 | 273 | 324 | 6 |         |       |
| 1   | C     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1050 | 273 | 324 | 6 |         |       |
| 1   | D     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1050 | 273 | 324 | 6 |         |       |
| 1   | E     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1050 | 273 | 324 | 6 |         |       |

### 3 Residue-property plots

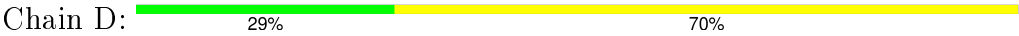
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: ACETYLCHOLINE-BINDING PROTEIN TYPE 1





● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN TYPE 1



## 4 Experimental information

| Property                             | Value           | Source    |
|--------------------------------------|-----------------|-----------|
| Reconstruction method                | SINGLE PARTICLE | Depositor |
| Imposed symmetry                     | POINT, T        | Depositor |
| Number of images                     | Not provided    | Depositor |
| Resolution determination method      | Not provided    | Depositor |
| CTF correction method                | PER MICROGRAPH  | Depositor |
| Microscope                           | FEI TECNAI F20  | Depositor |
| Voltage (kV)                         | 200             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30              | Depositor |
| Minimum defocus (nm)                 | 2000            | Depositor |
| Maximum defocus (nm)                 | 5000            | Depositor |
| Magnification                        | 50000           | Depositor |
| Image detector                       | KODAK SO163     | 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         | $\# Z  > 2$   | RMSZ        | $\# Z  > 2$     |
| 1   | A     | 0.91         | 1/1689 (0.1%) | 1.22        | 2/2297 (0.1%)   |
| 1   | B     | 0.91         | 1/1689 (0.1%) | 1.22        | 2/2297 (0.1%)   |
| 1   | C     | 0.91         | 1/1689 (0.1%) | 1.22        | 2/2297 (0.1%)   |
| 1   | D     | 0.91         | 1/1689 (0.1%) | 1.22        | 2/2297 (0.1%)   |
| 1   | E     | 0.91         | 1/1689 (0.1%) | 1.22        | 2/2297 (0.1%)   |
| All | All   | 0.91         | 5/8445 (0.1%) | 1.22        | 10/11485 (0.1%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 67  | TRP  | CD2-CE2 | -6.55 | 1.33        | 1.41     |
| 1   | A     | 67  | TRP  | CD2-CE2 | -6.52 | 1.33        | 1.41     |
| 1   | D     | 67  | TRP  | CD2-CE2 | -6.51 | 1.33        | 1.41     |
| 1   | B     | 67  | TRP  | CD2-CE2 | -6.51 | 1.33        | 1.41     |
| 1   | C     | 67  | TRP  | CD2-CE2 | -6.51 | 1.33        | 1.41     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 54  | LEU  | CB-CA-C    | -7.54 | 95.86       | 110.20   |
| 1   | D     | 54  | LEU  | CB-CA-C    | -7.54 | 95.88       | 110.20   |
| 1   | C     | 54  | LEU  | CB-CA-C    | -7.53 | 95.90       | 110.20   |
| 1   | A     | 54  | LEU  | CB-CA-C    | -7.52 | 95.91       | 110.20   |
| 1   | B     | 54  | LEU  | CB-CA-C    | -7.52 | 95.91       | 110.20   |
| 1   | E     | 67  | TRP  | CG-CD2-CE3 | -5.03 | 129.38      | 133.90   |
| 1   | B     | 67  | TRP  | CG-CD2-CE3 | -5.03 | 129.38      | 133.90   |
| 1   | A     | 67  | TRP  | CG-CD2-CE3 | -5.01 | 129.39      | 133.90   |
| 1   | D     | 67  | TRP  | CG-CD2-CE3 | -5.00 | 129.40      | 133.90   |
| 1   | C     | 67  | TRP  | CG-CD2-CE3 | -5.00 | 129.40      | 133.90   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1653  | 0        | 1613     | 533     | 0            |
| 1   | B     | 1653  | 0        | 1613     | 529     | 0            |
| 1   | C     | 1653  | 0        | 1613     | 538     | 0            |
| 1   | D     | 1653  | 0        | 1613     | 531     | 0            |
| 1   | E     | 1653  | 0        | 1613     | 531     | 0            |
| All | All   | 8265  | 0        | 8065     | 1944    | 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 119.

All (1944) 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:D:47:ASN:HB3  | 1:E:41:PHE:CZ    | 1.25                     | 1.68              |
| 1:B:47:ASN:HB3  | 1:C:41:PHE:CZ    | 1.25                     | 1.64              |
| 1:C:47:ASN:HB3  | 1:D:41:PHE:CZ    | 1.25                     | 1.62              |
| 1:A:47:ASN:HB3  | 1:B:41:PHE:CZ    | 1.25                     | 1.61              |
| 1:A:105:LEU:HB3 | 1:E:147:THR:CB   | 1.25                     | 1.61              |
| 1:A:41:PHE:CZ   | 1:E:47:ASN:HB3   | 1.25                     | 1.61              |
| 1:D:147:THR:CB  | 1:E:105:LEU:HB3  | 1.25                     | 1.59              |
| 1:D:147:THR:HB  | 1:E:105:LEU:CB   | 1.16                     | 1.59              |
| 1:A:147:THR:HB  | 1:B:105:LEU:CB   | 1.16                     | 1.59              |
| 1:C:147:THR:CB  | 1:D:105:LEU:HB3  | 1.25                     | 1.58              |
| 1:A:105:LEU:CB  | 1:E:147:THR:HB   | 1.16                     | 1.58              |
| 1:A:147:THR:CB  | 1:B:105:LEU:HB3  | 1.25                     | 1.57              |
| 1:B:147:THR:CB  | 1:C:105:LEU:HB3  | 1.25                     | 1.57              |
| 1:C:147:THR:HB  | 1:D:105:LEU:CB   | 1.16                     | 1.56              |
| 1:B:147:THR:H   | 1:C:105:LEU:CD1  | 1.18                     | 1.56              |
| 1:A:147:THR:H   | 1:B:105:LEU:CD1  | 1.18                     | 1.55              |
| 1:B:147:THR:HB  | 1:C:105:LEU:CB   | 1.16                     | 1.54              |
| 1:B:147:THR:CG2 | 1:C:105:LEU:HD13 | 1.39                     | 1.52              |
| 1:A:147:THR:CG2 | 1:B:105:LEU:HD13 | 1.39                     | 1.52              |
| 1:A:47:ASN:CB   | 1:B:41:PHE:CZ    | 1.93                     | 1.51              |
| 1:A:105:LEU:CD1 | 1:E:147:THR:H    | 1.18                     | 1.51              |
| 1:C:47:ASN:CB   | 1:D:41:PHE:CZ    | 1.93                     | 1.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:147:THR:CG2  | 1:E:105:LEU:HD13 | 1.39                     | 1.50              |
| 1:C:147:THR:H    | 1:D:105:LEU:CD1  | 1.18                     | 1.50              |
| 1:A:41:PHE:CZ    | 1:E:47:ASN:CB    | 1.93                     | 1.50              |
| 1:D:147:THR:H    | 1:E:105:LEU:CD1  | 1.18                     | 1.50              |
| 1:C:147:THR:CG2  | 1:D:105:LEU:HD13 | 1.39                     | 1.50              |
| 1:B:147:THR:HG22 | 1:C:105:LEU:CD1  | 1.43                     | 1.49              |
| 1:B:47:ASN:CB    | 1:C:41:PHE:CZ    | 1.93                     | 1.49              |
| 1:C:147:THR:HG22 | 1:D:105:LEU:CD1  | 1.43                     | 1.49              |
| 1:A:105:LEU:HD13 | 1:E:147:THR:CG2  | 1.39                     | 1.48              |
| 1:D:47:ASN:CB    | 1:E:41:PHE:CZ    | 1.93                     | 1.48              |
| 1:A:147:THR:HG22 | 1:B:105:LEU:CD1  | 1.43                     | 1.47              |
| 1:A:105:LEU:CD1  | 1:E:147:THR:HG22 | 1.43                     | 1.47              |
| 1:D:47:ASN:CB    | 1:E:41:PHE:HZ    | 1.25                     | 1.45              |
| 1:D:147:THR:HG22 | 1:E:105:LEU:CD1  | 1.43                     | 1.45              |
| 1:C:47:ASN:CB    | 1:D:41:PHE:HZ    | 1.25                     | 1.44              |
| 1:A:41:PHE:HZ    | 1:E:47:ASN:CB    | 1.25                     | 1.44              |
| 1:B:47:ASN:CB    | 1:C:41:PHE:HZ    | 1.25                     | 1.43              |
| 1:B:74:PHE:CE2   | 1:B:76:GLU:O     | 1.74                     | 1.40              |
| 1:C:74:PHE:CE2   | 1:C:76:GLU:O     | 1.74                     | 1.40              |
| 1:A:47:ASN:CB    | 1:B:41:PHE:HZ    | 1.25                     | 1.40              |
| 1:D:147:THR:N    | 1:E:105:LEU:HD12 | 1.35                     | 1.39              |
| 1:B:147:THR:N    | 1:C:105:LEU:HD12 | 1.35                     | 1.39              |
| 1:D:74:PHE:CE2   | 1:D:76:GLU:O     | 1.74                     | 1.39              |
| 1:A:74:PHE:CE2   | 1:A:76:GLU:O     | 1.74                     | 1.39              |
| 1:E:74:PHE:CE2   | 1:E:76:GLU:O     | 1.74                     | 1.39              |
| 1:B:81:ILE:CD1   | 1:B:104:LYS:HE3  | 1.38                     | 1.38              |
| 1:C:147:THR:N    | 1:D:105:LEU:HD12 | 1.35                     | 1.38              |
| 1:E:81:ILE:CD1   | 1:E:104:LYS:HE3  | 1.38                     | 1.38              |
| 1:A:81:ILE:CD1   | 1:A:104:LYS:HE3  | 1.38                     | 1.37              |
| 1:A:105:LEU:HD12 | 1:E:147:THR:N    | 1.35                     | 1.37              |
| 1:A:147:THR:N    | 1:B:105:LEU:HD12 | 1.35                     | 1.35              |
| 1:C:81:ILE:CD1   | 1:C:104:LYS:HE3  | 1.38                     | 1.34              |
| 1:C:125:SER:CB   | 1:D:39:LYS:HZ2   | 1.40                     | 1.34              |
| 1:C:24:GLU:CB    | 1:D:3:ARG:HB3    | 1.60                     | 1.32              |
| 1:D:24:GLU:CB    | 1:E:3:ARG:HB3    | 1.60                     | 1.31              |
| 1:B:24:GLU:CB    | 1:C:3:ARG:HB3    | 1.60                     | 1.30              |
| 1:A:3:ARG:HB3    | 1:E:24:GLU:CB    | 1.60                     | 1.30              |
| 1:A:125:SER:CB   | 1:B:39:LYS:NZ    | 1.95                     | 1.30              |
| 1:C:125:SER:CB   | 1:D:39:LYS:NZ    | 1.95                     | 1.30              |
| 1:A:125:SER:HB2  | 1:B:39:LYS:NZ    | 1.47                     | 1.30              |
| 1:B:125:SER:CB   | 1:C:39:LYS:NZ    | 1.95                     | 1.30              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:24:GLU:CB   | 1:B:3:ARG:HB3   | 1.60                     | 1.29              |
| 1:A:39:LYS:NZ   | 1:E:125:SER:HB2 | 1.47                     | 1.29              |
| 1:D:125:SER:CB  | 1:E:39:LYS:NZ   | 1.95                     | 1.29              |
| 1:B:125:SER:HB2 | 1:C:39:LYS:NZ   | 1.47                     | 1.28              |
| 1:A:39:LYS:NZ   | 1:E:125:SER:CB  | 1.95                     | 1.28              |
| 1:D:81:ILE:CD1  | 1:D:104:LYS:HE3 | 1.38                     | 1.27              |
| 1:A:125:SER:CB  | 1:B:39:LYS:HZ2  | 1.44                     | 1.27              |
| 1:D:24:GLU:HB3  | 1:E:3:ARG:CB    | 1.65                     | 1.26              |
| 1:B:125:SER:CB  | 1:C:39:LYS:HZ2  | 1.48                     | 1.26              |
| 1:D:125:SER:HB2 | 1:E:39:LYS:NZ   | 1.47                     | 1.26              |
| 1:A:74:PHE:CZ   | 1:A:76:GLU:O    | 1.89                     | 1.25              |
| 1:C:24:GLU:HB3  | 1:D:3:ARG:CB    | 1.66                     | 1.25              |
| 1:B:24:GLU:HB3  | 1:C:3:ARG:CB    | 1.65                     | 1.25              |
| 1:E:74:PHE:CZ   | 1:E:76:GLU:O    | 1.89                     | 1.25              |
| 1:C:125:SER:HB2 | 1:D:39:LYS:NZ   | 1.47                     | 1.25              |
| 1:C:74:PHE:CZ   | 1:C:76:GLU:O    | 1.89                     | 1.24              |
| 1:A:3:ARG:CB    | 1:E:24:GLU:HB3  | 1.65                     | 1.24              |
| 1:D:74:PHE:CZ   | 1:D:76:GLU:O    | 1.89                     | 1.24              |
| 1:B:76:GLU:OE1  | 1:B:107:ARG:HG2 | 1.35                     | 1.24              |
| 1:B:74:PHE:CZ   | 1:B:76:GLU:O    | 1.89                     | 1.24              |
| 1:A:41:PHE:HE2  | 1:E:47:ASN:ND2  | 1.35                     | 1.24              |
| 1:A:24:GLU:HB3  | 1:B:3:ARG:CB    | 1.65                     | 1.24              |
| 1:A:76:GLU:OE1  | 1:A:107:ARG:HG2 | 1.35                     | 1.23              |
| 1:C:47:ASN:ND2  | 1:D:41:PHE:HE2  | 1.35                     | 1.23              |
| 1:D:47:ASN:ND2  | 1:E:41:PHE:HE2  | 1.35                     | 1.22              |
| 1:C:76:GLU:OE1  | 1:C:107:ARG:HG2 | 1.35                     | 1.21              |
| 1:A:47:ASN:ND2  | 1:B:41:PHE:HE2  | 1.35                     | 1.21              |
| 1:C:81:ILE:CD1  | 1:C:104:LYS:CE  | 2.15                     | 1.21              |
| 1:A:78:THR:HG21 | 1:E:148:HIS:CD2 | 1.76                     | 1.21              |
| 1:C:81:ILE:HD13 | 1:C:104:LYS:CE  | 1.69                     | 1.21              |
| 1:B:47:ASN:ND2  | 1:C:41:PHE:HE2  | 1.35                     | 1.21              |
| 1:E:81:ILE:HD13 | 1:E:104:LYS:CE  | 1.69                     | 1.21              |
| 1:E:76:GLU:OE1  | 1:E:107:ARG:HG2 | 1.35                     | 1.21              |
| 1:B:47:ASN:CA   | 1:C:41:PHE:CZ   | 2.17                     | 1.21              |
| 1:A:148:HIS:CD2 | 1:B:78:THR:HG21 | 1.76                     | 1.21              |
| 1:D:81:ILE:HD13 | 1:D:104:LYS:CE  | 1.69                     | 1.20              |
| 1:D:148:HIS:CD2 | 1:E:78:THR:HG21 | 1.76                     | 1.20              |
| 1:C:47:ASN:CA   | 1:D:41:PHE:CZ   | 2.17                     | 1.20              |
| 1:A:81:ILE:HD13 | 1:A:104:LYS:CE  | 1.69                     | 1.20              |
| 1:B:148:HIS:CD2 | 1:C:78:THR:HG21 | 1.76                     | 1.20              |
| 1:D:76:GLU:OE1  | 1:D:107:ARG:HG2 | 1.35                     | 1.19              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:96:GLY:HA2  | 1:C:99:GLU:OE2  | 1.02                     | 1.19              |
| 1:C:148:HIS:CD2 | 1:D:78:THR:HG21 | 1.76                     | 1.19              |
| 1:A:99:GLU:OE2  | 1:E:96:GLY:CA   | 1.91                     | 1.19              |
| 1:D:96:GLY:CA   | 1:E:99:GLU:OE2  | 1.91                     | 1.19              |
| 1:C:96:GLY:CA   | 1:D:99:GLU:OE2  | 1.91                     | 1.19              |
| 1:B:96:GLY:CA   | 1:C:99:GLU:OE2  | 1.91                     | 1.18              |
| 1:A:96:GLY:HA2  | 1:B:99:GLU:OE2  | 1.02                     | 1.18              |
| 1:D:146:TRP:CE3 | 1:E:102:SER:HB2 | 1.78                     | 1.18              |
| 1:A:102:SER:HB2 | 1:E:146:TRP:CE3 | 1.78                     | 1.18              |
| 1:A:39:LYS:HZ2  | 1:E:125:SER:CB  | 1.52                     | 1.18              |
| 1:A:47:ASN:CA   | 1:B:41:PHE:CZ   | 2.17                     | 1.18              |
| 1:A:95:VAL:CA   | 1:B:101:PHE:CE1 | 2.26                     | 1.18              |
| 1:A:96:GLY:CA   | 1:B:99:GLU:OE2  | 1.91                     | 1.18              |
| 1:D:95:VAL:CA   | 1:E:101:PHE:CE1 | 2.26                     | 1.17              |
| 1:B:81:ILE:HD13 | 1:B:104:LYS:CE  | 1.69                     | 1.17              |
| 1:E:76:GLU:HB3  | 1:E:107:ARG:HD2 | 1.18                     | 1.17              |
| 1:C:146:TRP:CE3 | 1:D:102:SER:HB2 | 1.78                     | 1.17              |
| 1:C:96:GLY:HA2  | 1:D:99:GLU:OE2  | 1.02                     | 1.17              |
| 1:D:152:GLU:OE2 | 1:E:107:ARG:NH1 | 1.78                     | 1.17              |
| 1:C:152:GLU:OE2 | 1:D:107:ARG:NH1 | 1.78                     | 1.17              |
| 1:C:95:VAL:CA   | 1:D:101:PHE:CE1 | 2.26                     | 1.17              |
| 1:D:96:GLY:HA2  | 1:E:99:GLU:OE2  | 1.02                     | 1.16              |
| 1:A:146:TRP:CE3 | 1:B:102:SER:HB2 | 1.79                     | 1.16              |
| 1:B:146:TRP:CE3 | 1:C:102:SER:HB2 | 1.78                     | 1.16              |
| 1:D:47:ASN:CA   | 1:E:41:PHE:CZ   | 2.17                     | 1.16              |
| 1:A:101:PHE:CE1 | 1:E:95:VAL:CA   | 2.26                     | 1.15              |
| 1:E:81:ILE:CD1  | 1:E:104:LYS:CE  | 2.15                     | 1.15              |
| 1:A:99:GLU:OE2  | 1:E:96:GLY:HA2  | 1.02                     | 1.15              |
| 1:A:152:GLU:OE2 | 1:B:107:ARG:NH1 | 1.78                     | 1.14              |
| 1:D:125:SER:CB  | 1:E:39:LYS:HZ2  | 1.52                     | 1.14              |
| 1:B:152:GLU:OE2 | 1:C:107:ARG:NH1 | 1.78                     | 1.14              |
| 1:A:107:ARG:NH1 | 1:E:152:GLU:OE2 | 1.78                     | 1.14              |
| 1:D:47:ASN:HB3  | 1:E:41:PHE:CE2  | 1.83                     | 1.14              |
| 1:C:47:ASN:HB3  | 1:D:41:PHE:CE2  | 1.83                     | 1.14              |
| 1:A:41:PHE:CZ   | 1:E:47:ASN:CA   | 2.17                     | 1.14              |
| 1:A:47:ASN:HB3  | 1:B:41:PHE:CE2  | 1.83                     | 1.12              |
| 1:C:24:GLU:HA   | 1:D:3:ARG:HA    | 1.32                     | 1.12              |
| 1:B:95:VAL:CA   | 1:C:101:PHE:CE1 | 2.26                     | 1.12              |
| 1:A:41:PHE:CE2  | 1:E:47:ASN:HB3  | 1.83                     | 1.11              |
| 1:B:47:ASN:HB3  | 1:C:41:PHE:CE2  | 1.83                     | 1.11              |
| 1:D:21:ILE:HD12 | 1:E:5:ARG:HH22  | 1.15                     | 1.11              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:183:ARG:HG2 | 1:E:194:GLU:HG2  | 1.11                     | 1.10              |
| 1:A:21:ILE:HD12 | 1:B:5:ARG:HH22   | 1.16                     | 1.10              |
| 1:B:76:GLU:HB3  | 1:B:107:ARG:HD2  | 1.18                     | 1.09              |
| 1:A:105:LEU:CD1 | 1:E:147:THR:N    | 2.02                     | 1.09              |
| 1:A:3:ARG:HA    | 1:E:24:GLU:HA    | 1.32                     | 1.09              |
| 1:C:183:ARG:HG2 | 1:C:194:GLU:HG2  | 1.11                     | 1.09              |
| 1:C:76:GLU:HB3  | 1:C:107:ARG:HD2  | 1.18                     | 1.09              |
| 1:C:47:ASN:CB   | 1:D:41:PHE:CE2   | 2.36                     | 1.09              |
| 1:D:24:GLU:HA   | 1:E:3:ARG:HA     | 1.32                     | 1.09              |
| 1:B:95:VAL:O    | 1:C:99:GLU:OE2   | 1.71                     | 1.08              |
| 1:B:183:ARG:HG2 | 1:B:194:GLU:HG2  | 1.11                     | 1.08              |
| 1:C:95:VAL:O    | 1:D:99:GLU:OE2   | 1.71                     | 1.08              |
| 1:A:24:GLU:HA   | 1:B:3:ARG:HA     | 1.32                     | 1.08              |
| 1:D:47:ASN:CB   | 1:E:41:PHE:CE2   | 2.36                     | 1.08              |
| 1:D:76:GLU:HB3  | 1:D:107:ARG:HD2  | 1.18                     | 1.08              |
| 1:A:76:GLU:HB3  | 1:A:107:ARG:HD2  | 1.18                     | 1.08              |
| 1:A:1:SER:HA    | 1:E:27:GLN:O     | 1.53                     | 1.08              |
| 1:A:47:ASN:CB   | 1:B:41:PHE:CE2   | 2.36                     | 1.08              |
| 1:A:95:VAL:O    | 1:B:99:GLU:OE2   | 1.71                     | 1.08              |
| 1:D:183:ARG:HG2 | 1:D:194:GLU:HG2  | 1.11                     | 1.07              |
| 1:E:33:PHE:CE1  | 1:E:35:TYR:CZ    | 2.43                     | 1.07              |
| 1:B:27:GLN:O    | 1:C:1:SER:HA     | 1.53                     | 1.07              |
| 1:B:21:ILE:HD12 | 1:C:5:ARG:HH22   | 1.16                     | 1.07              |
| 1:C:21:ILE:HD12 | 1:D:5:ARG:HH22   | 1.16                     | 1.07              |
| 1:A:27:GLN:O    | 1:B:1:SER:HA     | 1.53                     | 1.07              |
| 1:A:46:GLU:OE1  | 1:B:42:ARG:NH2   | 1.88                     | 1.07              |
| 1:B:47:ASN:CB   | 1:C:41:PHE:CE2   | 2.36                     | 1.07              |
| 1:A:99:GLU:OE2  | 1:E:95:VAL:O     | 1.71                     | 1.07              |
| 1:D:27:GLN:O    | 1:E:1:SER:HA     | 1.53                     | 1.07              |
| 1:B:33:PHE:CE1  | 1:B:35:TYR:CZ    | 2.43                     | 1.07              |
| 1:A:33:PHE:CE1  | 1:A:35:TYR:CZ    | 2.43                     | 1.07              |
| 1:A:42:ARG:NH2  | 1:E:46:GLU:OE1   | 1.88                     | 1.07              |
| 1:C:33:PHE:CE1  | 1:C:35:TYR:CZ    | 2.43                     | 1.06              |
| 1:C:31:VAL:HG23 | 1:C:153:LEU:HD11 | 1.36                     | 1.06              |
| 1:D:95:VAL:O    | 1:E:99:GLU:OE2   | 1.71                     | 1.06              |
| 1:B:24:GLU:HA   | 1:C:3:ARG:HA     | 1.32                     | 1.06              |
| 1:D:31:VAL:HG23 | 1:D:153:LEU:HD11 | 1.36                     | 1.06              |
| 1:D:33:PHE:CE1  | 1:D:35:TYR:CZ    | 2.43                     | 1.06              |
| 1:E:31:VAL:HG23 | 1:E:153:LEU:HD11 | 1.36                     | 1.06              |
| 1:B:148:HIS:HD2 | 1:C:78:THR:HG21  | 1.09                     | 1.06              |
| 1:A:183:ARG:HG2 | 1:A:194:GLU:HG2  | 1.11                     | 1.06              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:147:THR:N   | 1:E:105:LEU:CD1  | 2.02                     | 1.06              |
| 1:B:46:GLU:OE1  | 1:C:42:ARG:NH2   | 1.88                     | 1.06              |
| 1:C:27:GLN:O    | 1:D:1:SER:HA     | 1.53                     | 1.05              |
| 1:A:41:PHE:CE2  | 1:E:47:ASN:CB    | 2.36                     | 1.05              |
| 1:A:5:ARG:HH22  | 1:E:21:ILE:HD12  | 1.16                     | 1.05              |
| 1:C:46:GLU:OE1  | 1:D:42:ARG:NH2   | 1.88                     | 1.05              |
| 1:D:46:GLU:OE1  | 1:E:42:ARG:NH2   | 1.88                     | 1.04              |
| 1:C:16:CYS:C    | 1:C:17:SER:N     | 2.11                     | 1.04              |
| 1:A:49:GLU:HG3  | 1:B:41:PHE:CE1   | 1.92                     | 1.04              |
| 1:B:49:GLU:HG3  | 1:C:41:PHE:CE1   | 1.92                     | 1.04              |
| 1:C:148:HIS:HD2 | 1:D:78:THR:CG2   | 1.70                     | 1.04              |
| 1:C:147:THR:N   | 1:D:105:LEU:CD1  | 2.02                     | 1.04              |
| 1:B:25:ASP:O    | 1:C:1:SER:O      | 1.76                     | 1.03              |
| 1:A:148:HIS:HD2 | 1:B:78:THR:HG21  | 1.10                     | 1.03              |
| 1:B:74:PHE:HE2  | 1:B:77:LEU:HA    | 1.23                     | 1.03              |
| 1:A:1:SER:O     | 1:E:25:ASP:O     | 1.76                     | 1.03              |
| 1:E:16:CYS:C    | 1:E:17:SER:N     | 2.11                     | 1.03              |
| 1:B:66:ASN:OD1  | 1:B:70:GLU:OE1   | 1.77                     | 1.03              |
| 1:E:74:PHE:HE2  | 1:E:77:LEU:HA    | 1.23                     | 1.03              |
| 1:B:148:HIS:HD2 | 1:C:78:THR:CG2   | 1.70                     | 1.03              |
| 1:D:49:GLU:HG3  | 1:E:41:PHE:CE1   | 1.92                     | 1.03              |
| 1:C:49:GLU:HG3  | 1:D:41:PHE:CE1   | 1.92                     | 1.03              |
| 1:A:66:ASN:OD1  | 1:A:70:GLU:OE1   | 1.77                     | 1.03              |
| 1:A:16:CYS:C    | 1:A:17:SER:N     | 2.11                     | 1.03              |
| 1:D:25:ASP:O    | 1:E:1:SER:O      | 1.76                     | 1.03              |
| 1:D:148:HIS:HD2 | 1:E:78:THR:CG2   | 1.71                     | 1.03              |
| 1:A:41:PHE:CE1  | 1:E:49:GLU:HG3   | 1.92                     | 1.03              |
| 1:C:66:ASN:OD1  | 1:C:70:GLU:OE1   | 1.77                     | 1.03              |
| 1:D:16:CYS:C    | 1:D:17:SER:N     | 2.11                     | 1.03              |
| 1:B:74:PHE:HE2  | 1:B:77:LEU:CA    | 1.71                     | 1.03              |
| 1:B:74:PHE:CE2  | 1:B:77:LEU:HA    | 1.94                     | 1.03              |
| 1:E:66:ASN:OD1  | 1:E:70:GLU:OE1   | 1.76                     | 1.03              |
| 1:B:16:CYS:C    | 1:B:17:SER:N     | 2.11                     | 1.03              |
| 1:E:74:PHE:CE2  | 1:E:77:LEU:HA    | 1.94                     | 1.02              |
| 1:B:142:LYS:HG2 | 1:B:197:THR:HG22 | 1.03                     | 1.02              |
| 1:A:95:VAL:HA   | 1:B:101:PHE:CZ   | 1.95                     | 1.02              |
| 1:D:66:ASN:OD1  | 1:D:70:GLU:OE1   | 1.76                     | 1.02              |
| 1:D:95:VAL:HA   | 1:E:101:PHE:CZ   | 1.94                     | 1.02              |
| 1:D:21:ILE:HD12 | 1:E:5:ARG:NH2    | 1.74                     | 1.02              |
| 1:B:31:VAL:HG23 | 1:B:153:LEU:HD11 | 1.37                     | 1.02              |
| 1:C:142:LYS:HG2 | 1:C:197:THR:HG22 | 1.03                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:21:ILE:HD12  | 1:D:5:ARG:NH2    | 1.75                     | 1.02              |
| 1:D:142:LYS:HG2  | 1:D:197:THR:HG22 | 1.03                     | 1.02              |
| 1:C:25:ASP:O     | 1:D:1:SER:O      | 1.76                     | 1.02              |
| 1:A:147:THR:N    | 1:B:105:LEU:CD1  | 2.02                     | 1.02              |
| 1:E:142:LYS:HG2  | 1:E:197:THR:HG22 | 1.03                     | 1.02              |
| 1:B:21:ILE:HD12  | 1:C:5:ARG:NH2    | 1.75                     | 1.02              |
| 1:C:74:PHE:HE2   | 1:C:77:LEU:CA    | 1.71                     | 1.02              |
| 1:A:31:VAL:HG23  | 1:A:153:LEU:HD11 | 1.36                     | 1.02              |
| 1:A:74:PHE:HE2   | 1:A:77:LEU:CA    | 1.71                     | 1.02              |
| 1:A:74:PHE:CE2   | 1:A:77:LEU:HA    | 1.94                     | 1.02              |
| 1:A:21:ILE:HD12  | 1:B:5:ARG:NH2    | 1.74                     | 1.02              |
| 1:D:96:GLY:HA2   | 1:E:99:GLU:CD    | 1.80                     | 1.01              |
| 1:A:148:HIS:HD2  | 1:B:78:THR:CG2   | 1.71                     | 1.01              |
| 1:A:141:LEU:HD21 | 1:A:198:LEU:HB3  | 1.42                     | 1.01              |
| 1:E:74:PHE:HE2   | 1:E:77:LEU:CA    | 1.71                     | 1.01              |
| 1:A:142:LYS:HG2  | 1:A:197:THR:HG22 | 1.03                     | 1.01              |
| 1:A:25:ASP:O     | 1:B:1:SER:O      | 1.76                     | 1.01              |
| 1:A:5:ARG:NH2    | 1:E:21:ILE:HD12  | 1.75                     | 1.01              |
| 1:E:141:LEU:HD21 | 1:E:198:LEU:HB3  | 1.42                     | 1.01              |
| 1:C:74:PHE:CE2   | 1:C:77:LEU:HA    | 1.94                     | 1.01              |
| 1:D:74:PHE:CE2   | 1:D:77:LEU:HA    | 1.94                     | 1.01              |
| 1:D:74:PHE:HE2   | 1:D:77:LEU:CA    | 1.71                     | 1.01              |
| 1:A:78:THR:CG2   | 1:E:148:HIS:HD2  | 1.70                     | 1.01              |
| 1:B:95:VAL:HA    | 1:C:101:PHE:CZ   | 1.95                     | 1.01              |
| 1:B:76:GLU:OE1   | 1:B:107:ARG:CG   | 2.09                     | 1.01              |
| 1:E:76:GLU:OE1   | 1:E:107:ARG:CG   | 2.09                     | 1.00              |
| 1:B:96:GLY:HA2   | 1:C:99:GLU:CD    | 1.80                     | 1.00              |
| 1:C:76:GLU:OE1   | 1:C:107:ARG:CG   | 2.09                     | 1.00              |
| 1:C:96:GLY:HA2   | 1:D:99:GLU:CD    | 1.80                     | 1.00              |
| 1:A:76:GLU:OE1   | 1:A:107:ARG:CG   | 2.09                     | 1.00              |
| 1:C:95:VAL:HA    | 1:D:101:PHE:CZ   | 1.95                     | 1.00              |
| 1:A:78:THR:HG21  | 1:E:148:HIS:HD2  | 1.10                     | 1.00              |
| 1:D:76:GLU:OE1   | 1:D:107:ARG:CG   | 2.09                     | 1.00              |
| 1:C:200:PHE:HE2  | 1:C:202:PHE:HB3  | 1.27                     | 1.00              |
| 1:A:95:VAL:HA    | 1:B:101:PHE:CE1  | 1.97                     | 0.99              |
| 1:A:74:PHE:HE2   | 1:A:77:LEU:HA    | 1.23                     | 0.99              |
| 1:A:101:PHE:CZ   | 1:E:95:VAL:HA    | 1.95                     | 0.99              |
| 1:A:99:GLU:CD    | 1:E:96:GLY:HA2   | 1.80                     | 0.99              |
| 1:B:148:HIS:CD2  | 1:C:78:THR:CG2   | 2.44                     | 0.99              |
| 1:A:200:PHE:HE2  | 1:A:202:PHE:HB3  | 1.27                     | 0.99              |
| 1:B:200:PHE:CE2  | 1:B:202:PHE:HB3  | 1.98                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:200:PHE:CE2  | 1:E:202:PHE:HB3  | 1.98                     | 0.99              |
| 1:C:200:PHE:CE2  | 1:C:202:PHE:HB3  | 1.98                     | 0.99              |
| 1:D:200:PHE:CE2  | 1:D:202:PHE:HB3  | 1.98                     | 0.99              |
| 1:A:1:SER:OG     | 1:E:21:ILE:HG21  | 1.63                     | 0.99              |
| 1:B:32:SER:HB2   | 1:B:59:VAL:HG12  | 1.44                     | 0.99              |
| 1:C:148:HIS:CD2  | 1:D:78:THR:CG2   | 2.44                     | 0.99              |
| 1:A:96:GLY:HA2   | 1:B:99:GLU:CD    | 1.80                     | 0.99              |
| 1:B:147:THR:N    | 1:C:105:LEU:CD1  | 2.02                     | 0.98              |
| 1:A:148:HIS:CD2  | 1:B:78:THR:CG2   | 2.45                     | 0.98              |
| 1:C:95:VAL:HA    | 1:D:101:PHE:CE1  | 1.97                     | 0.98              |
| 1:C:32:SER:HB2   | 1:C:59:VAL:HG12  | 1.44                     | 0.98              |
| 1:D:21:ILE:HG21  | 1:E:1:SER:OG     | 1.63                     | 0.98              |
| 1:D:200:PHE:HE2  | 1:D:202:PHE:HB3  | 1.27                     | 0.98              |
| 1:A:21:ILE:HG21  | 1:B:1:SER:OG     | 1.63                     | 0.98              |
| 1:C:141:LEU:HD21 | 1:C:198:LEU:HB3  | 1.42                     | 0.98              |
| 1:B:95:VAL:HA    | 1:C:101:PHE:CE1  | 1.97                     | 0.98              |
| 1:E:33:PHE:HE1   | 1:E:35:TYR:CZ    | 1.82                     | 0.98              |
| 1:D:141:LEU:HD21 | 1:D:198:LEU:HB3  | 1.42                     | 0.98              |
| 1:A:101:PHE:CE1  | 1:E:95:VAL:HA    | 1.97                     | 0.98              |
| 1:A:200:PHE:CE2  | 1:A:202:PHE:HB3  | 1.98                     | 0.97              |
| 1:A:78:THR:CG2   | 1:E:148:HIS:CD2  | 2.44                     | 0.97              |
| 1:E:182:ASN:HD21 | 1:E:197:THR:HG23 | 1.28                     | 0.97              |
| 1:B:33:PHE:HE1   | 1:B:35:TYR:CZ    | 1.82                     | 0.97              |
| 1:C:21:ILE:CD1   | 1:D:5:ARG:HH22   | 1.77                     | 0.97              |
| 1:D:46:GLU:CD    | 1:E:42:ARG:HE    | 1.67                     | 0.97              |
| 1:A:32:SER:HB2   | 1:A:59:VAL:HG12  | 1.44                     | 0.97              |
| 1:E:32:SER:HB2   | 1:E:59:VAL:HG12  | 1.44                     | 0.97              |
| 1:D:182:ASN:HD21 | 1:D:197:THR:HG23 | 1.28                     | 0.97              |
| 1:D:146:TRP:HB2  | 1:E:103:ASP:HB2  | 1.47                     | 0.97              |
| 1:E:200:PHE:HE2  | 1:E:202:PHE:HB3  | 1.27                     | 0.97              |
| 1:C:46:GLU:CD    | 1:D:42:ARG:HE    | 1.67                     | 0.97              |
| 1:B:141:LEU:HD21 | 1:B:198:LEU:HB3  | 1.42                     | 0.97              |
| 1:B:46:GLU:CD    | 1:C:42:ARG:HE    | 1.67                     | 0.97              |
| 1:D:33:PHE:HE1   | 1:D:35:TYR:CZ    | 1.82                     | 0.97              |
| 1:B:21:ILE:CD1   | 1:C:5:ARG:HH22   | 1.77                     | 0.96              |
| 1:A:21:ILE:CD1   | 1:B:5:ARG:HH22   | 1.77                     | 0.96              |
| 1:A:33:PHE:HE1   | 1:A:35:TYR:CZ    | 1.82                     | 0.96              |
| 1:D:146:TRP:CZ3  | 1:E:102:SER:CB   | 2.49                     | 0.96              |
| 1:C:146:TRP:HB2  | 1:D:103:ASP:HB2  | 1.47                     | 0.96              |
| 1:D:32:SER:HB2   | 1:D:59:VAL:HG12  | 1.44                     | 0.96              |
| 1:A:5:ARG:HH22   | 1:E:21:ILE:CD1   | 1.77                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:95:VAL:HA    | 1:E:101:PHE:CE1  | 1.97                     | 0.96              |
| 1:A:46:GLU:CD    | 1:B:42:ARG:HE    | 1.67                     | 0.96              |
| 1:A:146:TRP:HB2  | 1:B:103:ASP:HB2  | 1.47                     | 0.96              |
| 1:C:182:ASN:HD21 | 1:C:197:THR:HG23 | 1.28                     | 0.96              |
| 1:C:21:ILE:HG21  | 1:D:1:SER:OG     | 1.63                     | 0.96              |
| 1:D:21:ILE:CD1   | 1:E:5:ARG:HH22   | 1.77                     | 0.96              |
| 1:C:33:PHE:HE1   | 1:C:35:TYR:CZ    | 1.81                     | 0.96              |
| 1:A:146:TRP:CZ3  | 1:B:102:SER:CB   | 2.49                     | 0.96              |
| 1:A:103:ASP:HB2  | 1:E:146:TRP:HB2  | 1.47                     | 0.96              |
| 1:B:182:ASN:HD21 | 1:B:197:THR:HG23 | 1.28                     | 0.96              |
| 1:A:42:ARG:HE    | 1:E:46:GLU:CD    | 1.67                     | 0.95              |
| 1:B:146:TRP:HB2  | 1:C:103:ASP:HB2  | 1.47                     | 0.95              |
| 1:B:21:ILE:HG21  | 1:C:1:SER:OG     | 1.63                     | 0.95              |
| 1:A:102:SER:CB   | 1:E:146:TRP:CZ3  | 2.49                     | 0.95              |
| 1:B:146:TRP:CZ3  | 1:C:102:SER:CB   | 2.49                     | 0.95              |
| 1:C:146:TRP:CZ3  | 1:D:102:SER:CB   | 2.49                     | 0.95              |
| 1:B:200:PHE:HE2  | 1:B:202:PHE:HB3  | 1.27                     | 0.95              |
| 1:A:182:ASN:HD21 | 1:A:197:THR:HG23 | 1.28                     | 0.95              |
| 1:D:148:HIS:CD2  | 1:E:78:THR:CG2   | 2.44                     | 0.95              |
| 1:A:24:GLU:HA    | 1:B:3:ARG:CA     | 1.97                     | 0.95              |
| 1:A:42:ARG:HD2   | 1:E:47:ASN:ND2   | 1.82                     | 0.94              |
| 1:A:47:ASN:ND2   | 1:B:42:ARG:HD2   | 1.82                     | 0.94              |
| 1:C:74:PHE:HE2   | 1:C:77:LEU:HA    | 1.23                     | 0.94              |
| 1:D:74:PHE:HE2   | 1:D:77:LEU:HA    | 1.23                     | 0.94              |
| 1:B:47:ASN:ND2   | 1:C:42:ARG:HD2   | 1.82                     | 0.94              |
| 1:D:24:GLU:HA    | 1:E:3:ARG:CA     | 1.97                     | 0.94              |
| 1:C:47:ASN:ND2   | 1:D:42:ARG:HD2   | 1.81                     | 0.93              |
| 1:C:95:VAL:C     | 1:D:101:PHE:CE1  | 2.42                     | 0.93              |
| 1:D:148:HIS:HD2  | 1:E:78:THR:HG21  | 1.10                     | 0.93              |
| 1:D:95:VAL:C     | 1:E:101:PHE:CE1  | 2.42                     | 0.93              |
| 1:B:95:VAL:C     | 1:C:101:PHE:CE1  | 2.42                     | 0.93              |
| 1:D:47:ASN:ND2   | 1:E:42:ARG:HD2   | 1.82                     | 0.93              |
| 1:A:76:GLU:CB    | 1:A:107:ARG:HD2  | 1.98                     | 0.93              |
| 1:A:101:PHE:CE1  | 1:E:95:VAL:C     | 2.42                     | 0.93              |
| 1:C:25:ASP:O     | 1:D:2:ARG:HA     | 1.69                     | 0.92              |
| 1:C:148:HIS:HD2  | 1:D:78:THR:HG21  | 1.10                     | 0.92              |
| 1:B:25:ASP:O     | 1:C:2:ARG:HA     | 1.69                     | 0.92              |
| 1:D:81:ILE:CD1   | 1:D:104:LYS:CE   | 2.15                     | 0.92              |
| 1:E:76:GLU:CB    | 1:E:107:ARG:HD2  | 1.98                     | 0.92              |
| 1:C:76:GLU:CB    | 1:C:107:ARG:HD2  | 1.98                     | 0.92              |
| 1:A:95:VAL:C     | 1:B:101:PHE:CE1  | 2.42                     | 0.92              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:76:GLU:CB   | 1:D:107:ARG:HD2 | 1.99                     | 0.92              |
| 1:B:24:GLU:HA   | 1:C:3:ARG:CA    | 1.96                     | 0.92              |
| 1:A:2:ARG:HA    | 1:E:25:ASP:O    | 1.69                     | 0.91              |
| 1:D:25:ASP:O    | 1:E:2:ARG:HA    | 1.69                     | 0.91              |
| 1:D:125:SER:CB  | 1:E:39:LYS:HZ3  | 1.79                     | 0.91              |
| 1:D:146:TRP:CB  | 1:E:103:ASP:HB2 | 2.01                     | 0.91              |
| 1:A:25:ASP:O    | 1:B:2:ARG:HA    | 1.69                     | 0.91              |
| 1:A:3:ARG:CA    | 1:E:24:GLU:HA   | 1.96                     | 0.91              |
| 1:D:76:GLU:HB3  | 1:D:107:ARG:CD  | 2.01                     | 0.91              |
| 1:B:76:GLU:CB   | 1:B:107:ARG:HD2 | 1.98                     | 0.91              |
| 1:C:146:TRP:CB  | 1:D:103:ASP:HB2 | 2.01                     | 0.91              |
| 1:C:76:GLU:HB3  | 1:C:107:ARG:CD  | 2.01                     | 0.90              |
| 1:A:41:PHE:CZ   | 1:E:49:GLU:HG3  | 2.06                     | 0.90              |
| 1:D:146:TRP:CZ3 | 1:E:102:SER:HB2 | 2.06                     | 0.90              |
| 1:A:103:ASP:HB2 | 1:E:146:TRP:CB  | 2.01                     | 0.90              |
| 1:B:146:TRP:CZ3 | 1:C:102:SER:HB2 | 2.06                     | 0.90              |
| 1:C:49:GLU:HG3  | 1:D:41:PHE:CZ   | 2.06                     | 0.90              |
| 1:D:49:GLU:HG3  | 1:E:41:PHE:CZ   | 2.06                     | 0.90              |
| 1:A:49:GLU:HG3  | 1:B:41:PHE:CZ   | 2.06                     | 0.90              |
| 1:A:76:GLU:HB3  | 1:A:107:ARG:CD  | 2.01                     | 0.90              |
| 1:B:49:GLU:HG3  | 1:C:41:PHE:CZ   | 2.06                     | 0.90              |
| 1:B:146:TRP:CB  | 1:C:103:ASP:HB2 | 2.01                     | 0.90              |
| 1:A:146:TRP:CB  | 1:B:103:ASP:HB2 | 2.01                     | 0.90              |
| 1:C:146:TRP:CZ3 | 1:D:102:SER:HB2 | 2.06                     | 0.90              |
| 1:A:39:LYS:HZ3  | 1:E:125:SER:CB  | 1.79                     | 0.90              |
| 1:A:102:SER:HB2 | 1:E:146:TRP:CZ3 | 2.06                     | 0.90              |
| 1:A:146:TRP:CZ3 | 1:B:102:SER:HB2 | 2.06                     | 0.89              |
| 1:B:76:GLU:HB3  | 1:B:107:ARG:CD  | 2.01                     | 0.89              |
| 1:C:81:ILE:HD12 | 1:C:116:TYR:CZ  | 2.08                     | 0.89              |
| 1:D:47:ASN:ND2  | 1:E:41:PHE:CE2  | 2.27                     | 0.89              |
| 1:B:81:ILE:HD12 | 1:B:116:TYR:CZ  | 2.08                     | 0.89              |
| 1:E:76:GLU:HB3  | 1:E:107:ARG:CD  | 2.01                     | 0.89              |
| 1:C:40:ILE:HD11 | 1:C:200:PHE:CE2 | 2.08                     | 0.89              |
| 1:E:81:ILE:HD12 | 1:E:116:TYR:CZ  | 2.08                     | 0.89              |
| 1:B:125:SER:CB  | 1:C:39:LYS:HZ3  | 1.83                     | 0.89              |
| 1:D:81:ILE:HD12 | 1:D:116:TYR:CZ  | 2.08                     | 0.89              |
| 1:B:40:ILE:HD11 | 1:B:200:PHE:CE2 | 2.08                     | 0.88              |
| 1:E:92:PHE:HD2  | 1:E:142:LYS:HB2 | 1.38                     | 0.88              |
| 1:D:40:ILE:HD11 | 1:D:200:PHE:CE2 | 2.08                     | 0.88              |
| 1:A:81:ILE:HD12 | 1:A:116:TYR:CZ  | 2.08                     | 0.88              |
| 1:B:81:ILE:CD1  | 1:B:104:LYS:CE  | 2.15                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:24:GLU:HA    | 1:D:3:ARG:CA     | 1.97                     | 0.88              |
| 1:A:142:LYS:HG2  | 1:A:197:THR:CG2  | 1.99                     | 0.88              |
| 1:C:147:THR:CB   | 1:D:105:LEU:CB   | 2.08                     | 0.87              |
| 1:D:142:LYS:CG   | 1:D:197:THR:HG22 | 1.99                     | 0.87              |
| 1:C:92:PHE:HD2   | 1:C:142:LYS:HB2  | 1.38                     | 0.87              |
| 1:B:183:ARG:HG2  | 1:B:194:GLU:CG   | 2.02                     | 0.87              |
| 1:D:94:SER:HG    | 1:E:101:PHE:HD1  | 0.89                     | 0.87              |
| 1:E:40:ILE:HD11  | 1:E:200:PHE:CE2  | 2.08                     | 0.87              |
| 1:D:92:PHE:HD2   | 1:D:142:LYS:HB2  | 1.38                     | 0.87              |
| 1:B:147:THR:CB   | 1:C:105:LEU:CB   | 2.08                     | 0.87              |
| 1:C:141:LEU:CD2  | 1:C:198:LEU:HB3  | 2.05                     | 0.87              |
| 1:A:47:ASN:ND2   | 1:B:41:PHE:CE2   | 2.27                     | 0.87              |
| 1:B:92:PHE:HD2   | 1:B:142:LYS:HB2  | 1.38                     | 0.86              |
| 1:A:141:LEU:CD2  | 1:A:198:LEU:HB3  | 2.05                     | 0.86              |
| 1:E:141:LEU:CD2  | 1:E:198:LEU:HB3  | 2.05                     | 0.86              |
| 1:A:40:ILE:HD11  | 1:A:200:PHE:CE2  | 2.08                     | 0.86              |
| 1:C:46:GLU:CD    | 1:D:42:ARG:NE    | 2.29                     | 0.86              |
| 1:D:175:LEU:HD23 | 1:D:202:PHE:HA   | 1.58                     | 0.86              |
| 1:A:94:SER:HG    | 1:B:101:PHE:HD1  | 0.89                     | 0.86              |
| 1:A:42:ARG:NE    | 1:E:46:GLU:CD    | 2.29                     | 0.86              |
| 1:D:46:GLU:CD    | 1:E:42:ARG:NE    | 2.29                     | 0.86              |
| 1:D:141:LEU:CD2  | 1:D:198:LEU:HB3  | 2.05                     | 0.86              |
| 1:D:183:ARG:HG2  | 1:D:194:GLU:CG   | 2.02                     | 0.86              |
| 1:B:147:THR:CB   | 1:C:105:LEU:HD13 | 2.06                     | 0.86              |
| 1:C:125:SER:HB3  | 1:D:39:LYS:NZ    | 1.91                     | 0.85              |
| 1:B:46:GLU:CD    | 1:C:42:ARG:NE    | 2.29                     | 0.85              |
| 1:B:141:LEU:CD2  | 1:B:198:LEU:HB3  | 2.05                     | 0.85              |
| 1:A:92:PHE:HD2   | 1:A:142:LYS:HB2  | 1.38                     | 0.85              |
| 1:A:147:THR:CB   | 1:B:105:LEU:HD13 | 2.06                     | 0.85              |
| 1:B:175:LEU:HD23 | 1:B:202:PHE:HA   | 1.58                     | 0.85              |
| 1:A:101:PHE:HD1  | 1:E:94:SER:HG    | 0.88                     | 0.85              |
| 1:B:142:LYS:HG2  | 1:B:197:THR:CG2  | 1.99                     | 0.85              |
| 1:A:105:LEU:HD13 | 1:E:147:THR:CB   | 2.06                     | 0.85              |
| 1:A:39:LYS:NZ    | 1:E:125:SER:HB3  | 1.91                     | 0.85              |
| 1:A:142:LYS:CG   | 1:A:197:THR:HG22 | 1.99                     | 0.85              |
| 1:C:183:ARG:HG2  | 1:C:194:GLU:CG   | 2.02                     | 0.85              |
| 1:D:147:THR:CB   | 1:E:105:LEU:HD13 | 2.06                     | 0.85              |
| 1:B:94:SER:HG    | 1:C:101:PHE:HD1  | 0.88                     | 0.85              |
| 1:B:142:LYS:CG   | 1:B:197:THR:HG22 | 1.99                     | 0.84              |
| 1:C:142:LYS:CG   | 1:C:197:THR:HG22 | 1.99                     | 0.84              |
| 1:C:94:SER:HG    | 1:D:101:PHE:HD1  | 0.86                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:LEU:HD23 | 1:A:202:PHE:HA   | 1.58                     | 0.84              |
| 1:A:41:PHE:CE2   | 1:E:47:ASN:ND2   | 2.27                     | 0.84              |
| 1:C:147:THR:CB   | 1:D:105:LEU:HD13 | 2.06                     | 0.84              |
| 1:E:175:LEU:HD23 | 1:E:202:PHE:HA   | 1.58                     | 0.84              |
| 1:E:183:ARG:HG2  | 1:E:194:GLU:CG   | 2.02                     | 0.84              |
| 1:A:183:ARG:HG2  | 1:A:194:GLU:CG   | 2.02                     | 0.84              |
| 1:B:24:GLU:CA    | 1:C:3:ARG:CA     | 2.56                     | 0.84              |
| 1:C:175:LEU:HD23 | 1:C:202:PHE:HA   | 1.58                     | 0.84              |
| 1:A:125:SER:CB   | 1:B:39:LYS:HZ3   | 1.88                     | 0.84              |
| 1:A:125:SER:HB3  | 1:B:39:LYS:NZ    | 1.91                     | 0.84              |
| 1:A:46:GLU:CD    | 1:B:42:ARG:NE    | 2.29                     | 0.84              |
| 1:B:24:GLU:HB3   | 1:C:3:ARG:HB3    | 0.84                     | 0.84              |
| 1:D:125:SER:HB3  | 1:E:39:LYS:NZ    | 1.91                     | 0.84              |
| 1:B:125:SER:HB3  | 1:C:39:LYS:NZ    | 1.91                     | 0.83              |
| 1:B:146:TRP:CZ3  | 1:C:102:SER:HB3  | 2.13                     | 0.83              |
| 1:A:49:GLU:HG2   | 1:A:95:VAL:HG21  | 1.60                     | 0.83              |
| 1:A:24:GLU:HB3   | 1:B:3:ARG:HB3    | 0.84                     | 0.83              |
| 1:C:24:GLU:HB3   | 1:D:3:ARG:HB3    | 0.84                     | 0.83              |
| 1:D:24:GLU:CA    | 1:E:3:ARG:CA     | 2.56                     | 0.83              |
| 1:B:49:GLU:HG2   | 1:B:95:VAL:HG21  | 1.60                     | 0.83              |
| 1:C:146:TRP:CZ3  | 1:D:102:SER:HB3  | 2.13                     | 0.83              |
| 1:D:24:GLU:CA    | 1:E:3:ARG:HB3    | 2.09                     | 0.83              |
| 1:E:163:LEU:HD22 | 1:E:174:LEU:HD11 | 1.61                     | 0.83              |
| 1:A:42:ARG:NE    | 1:E:46:GLU:OE1   | 2.12                     | 0.83              |
| 1:D:125:SER:HB3  | 1:E:39:LYS:HZ3   | 1.42                     | 0.83              |
| 1:C:24:GLU:CA    | 1:D:3:ARG:CA     | 2.56                     | 0.83              |
| 1:C:46:GLU:OE1   | 1:D:42:ARG:NE    | 2.12                     | 0.82              |
| 1:A:3:ARG:HB3    | 1:E:24:GLU:CA    | 2.09                     | 0.82              |
| 1:C:142:LYS:HG2  | 1:C:197:THR:CG2  | 1.99                     | 0.82              |
| 1:C:49:GLU:HG2   | 1:C:95:VAL:HG21  | 1.60                     | 0.82              |
| 1:B:163:LEU:HD22 | 1:B:174:LEU:HD11 | 1.61                     | 0.82              |
| 1:A:24:GLU:CA    | 1:B:3:ARG:HB3    | 2.09                     | 0.82              |
| 1:D:21:ILE:CD1   | 1:E:5:ARG:NH2    | 2.40                     | 0.82              |
| 1:D:142:LYS:HG2  | 1:D:197:THR:CG2  | 1.99                     | 0.82              |
| 1:A:3:ARG:HB3    | 1:E:24:GLU:HB3   | 0.84                     | 0.82              |
| 1:D:49:GLU:HG2   | 1:D:95:VAL:HG21  | 1.60                     | 0.82              |
| 1:E:131:LEU:HD21 | 1:E:172:PHE:CE1  | 2.15                     | 0.82              |
| 1:E:163:LEU:HD22 | 1:E:174:LEU:CD1  | 2.09                     | 0.82              |
| 1:C:163:LEU:HD22 | 1:C:174:LEU:CD1  | 2.09                     | 0.82              |
| 1:D:74:PHE:CE2   | 1:D:77:LEU:CA    | 2.59                     | 0.82              |
| 1:E:142:LYS:CG   | 1:E:197:THR:HG22 | 1.99                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:3:ARG:CA     | 1:E:24:GLU:CA    | 2.56                     | 0.82              |
| 1:C:24:GLU:CA    | 1:D:3:ARG:HB3    | 2.09                     | 0.82              |
| 1:D:24:GLU:HB3   | 1:E:3:ARG:HB3    | 0.84                     | 0.82              |
| 1:D:163:LEU:HD22 | 1:D:174:LEU:CD1  | 2.09                     | 0.81              |
| 1:B:131:LEU:HD21 | 1:B:172:PHE:CE1  | 2.15                     | 0.81              |
| 1:D:147:THR:CB   | 1:E:105:LEU:CB   | 2.08                     | 0.81              |
| 1:D:46:GLU:OE1   | 1:E:42:ARG:NE    | 2.12                     | 0.81              |
| 1:A:46:GLU:OE1   | 1:B:42:ARG:NE    | 2.12                     | 0.81              |
| 1:C:163:LEU:HD22 | 1:C:174:LEU:HD11 | 1.61                     | 0.81              |
| 1:D:163:LEU:HD22 | 1:D:174:LEU:HD11 | 1.61                     | 0.81              |
| 1:C:21:ILE:CD1   | 1:D:5:ARG:NH2    | 2.40                     | 0.81              |
| 1:A:45:VAL:HG23  | 1:A:128:LEU:HD21 | 1.62                     | 0.81              |
| 1:B:173:GLN:H    | 1:B:205:PRO:HD3  | 1.46                     | 0.81              |
| 1:A:102:SER:HB3  | 1:E:146:TRP:CZ3  | 2.13                     | 0.81              |
| 1:A:163:LEU:HD22 | 1:A:174:LEU:CD1  | 2.09                     | 0.81              |
| 1:A:39:LYS:HZ3   | 1:E:125:SER:HB3  | 1.42                     | 0.81              |
| 1:E:49:GLU:HG2   | 1:E:95:VAL:HG21  | 1.60                     | 0.81              |
| 1:B:163:LEU:HD22 | 1:B:174:LEU:CD1  | 2.09                     | 0.81              |
| 1:A:183:ARG:HB3  | 1:A:192:THR:CG2  | 2.11                     | 0.81              |
| 1:D:131:LEU:HD21 | 1:D:172:PHE:CE1  | 2.15                     | 0.81              |
| 1:B:24:GLU:CA    | 1:C:3:ARG:HB3    | 2.09                     | 0.81              |
| 1:D:183:ARG:HB3  | 1:D:192:THR:CG2  | 2.11                     | 0.81              |
| 1:E:32:SER:HB2   | 1:E:59:VAL:CG1   | 2.11                     | 0.81              |
| 1:A:146:TRP:CZ3  | 1:B:102:SER:HB3  | 2.13                     | 0.81              |
| 1:B:183:ARG:HB3  | 1:B:192:THR:CG2  | 2.11                     | 0.81              |
| 1:B:32:SER:HB2   | 1:B:59:VAL:CG1   | 2.11                     | 0.81              |
| 1:D:146:TRP:CZ3  | 1:E:102:SER:HB3  | 2.13                     | 0.81              |
| 1:C:173:GLN:H    | 1:C:205:PRO:HD3  | 1.46                     | 0.81              |
| 1:B:46:GLU:OE1   | 1:C:42:ARG:NE    | 2.12                     | 0.81              |
| 1:D:32:SER:HB2   | 1:D:59:VAL:CG1   | 2.11                     | 0.81              |
| 1:A:131:LEU:HD21 | 1:A:172:PHE:CE1  | 2.15                     | 0.81              |
| 1:C:92:PHE:O     | 1:D:119:GLN:NE2  | 2.14                     | 0.81              |
| 1:A:173:GLN:H    | 1:A:205:PRO:HD3  | 1.46                     | 0.81              |
| 1:E:45:VAL:HG23  | 1:E:128:LEU:HD21 | 1.62                     | 0.80              |
| 1:E:173:GLN:H    | 1:E:205:PRO:HD3  | 1.46                     | 0.80              |
| 1:B:92:PHE:O     | 1:C:119:GLN:NE2  | 2.14                     | 0.80              |
| 1:C:131:LEU:HD21 | 1:C:172:PHE:CE1  | 2.15                     | 0.80              |
| 1:A:147:THR:HB   | 1:B:105:LEU:CG   | 2.11                     | 0.80              |
| 1:D:147:THR:HB   | 1:E:105:LEU:CG   | 2.11                     | 0.80              |
| 1:A:21:ILE:CD1   | 1:B:5:ARG:NH2    | 2.40                     | 0.80              |
| 1:C:183:ARG:HB3  | 1:C:192:THR:CG2  | 2.11                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:32:SER:HB2   | 1:A:59:VAL:CG1   | 2.11                     | 0.80              |
| 1:D:47:ASN:CA    | 1:E:41:PHE:CE2   | 2.64                     | 0.80              |
| 1:C:147:THR:HB   | 1:D:105:LEU:CG   | 2.11                     | 0.80              |
| 1:D:173:GLN:H    | 1:D:205:PRO:HD3  | 1.46                     | 0.80              |
| 1:A:119:GLN:NE2  | 1:E:92:PHE:O     | 2.14                     | 0.80              |
| 1:A:163:LEU:HD22 | 1:A:174:LEU:HD11 | 1.61                     | 0.80              |
| 1:A:42:ARG:CZ    | 1:E:46:GLU:OE1   | 2.30                     | 0.80              |
| 1:E:183:ARG:HB3  | 1:E:192:THR:CG2  | 2.11                     | 0.80              |
| 1:D:149:SER:OG   | 1:D:152:GLU:OE1  | 2.00                     | 0.80              |
| 1:B:149:SER:OG   | 1:B:152:GLU:OE1  | 2.00                     | 0.80              |
| 1:B:21:ILE:CD1   | 1:C:5:ARG:NH2    | 2.40                     | 0.80              |
| 1:A:92:PHE:O     | 1:B:119:GLN:NE2  | 2.14                     | 0.80              |
| 1:D:46:GLU:OE1   | 1:E:42:ARG:CZ    | 2.29                     | 0.79              |
| 1:E:77:LEU:HD12  | 1:E:78:THR:H     | 1.48                     | 0.79              |
| 1:B:47:ASN:ND2   | 1:C:41:PHE:CE2   | 2.27                     | 0.79              |
| 1:C:45:VAL:HG23  | 1:C:128:LEU:HD21 | 1.62                     | 0.79              |
| 1:C:47:ASN:CA    | 1:D:41:PHE:CE2   | 2.64                     | 0.79              |
| 1:E:149:SER:OG   | 1:E:152:GLU:OE1  | 2.00                     | 0.79              |
| 1:A:24:GLU:CA    | 1:B:3:ARG:CA     | 2.56                     | 0.79              |
| 1:C:32:SER:HB2   | 1:C:59:VAL:CG1   | 2.11                     | 0.79              |
| 1:A:46:GLU:OE1   | 1:B:42:ARG:CZ    | 2.30                     | 0.79              |
| 1:D:45:VAL:HG23  | 1:D:128:LEU:HD21 | 1.62                     | 0.79              |
| 1:D:92:PHE:O     | 1:E:119:GLN:NE2  | 2.14                     | 0.79              |
| 1:B:45:VAL:HG23  | 1:B:128:LEU:HD21 | 1.62                     | 0.79              |
| 1:C:46:GLU:OE1   | 1:D:42:ARG:CZ    | 2.30                     | 0.79              |
| 1:D:77:LEU:HD12  | 1:D:78:THR:H     | 1.48                     | 0.79              |
| 1:A:31:VAL:CG2   | 1:A:153:LEU:HD11 | 2.12                     | 0.79              |
| 1:A:147:THR:CB   | 1:B:105:LEU:CB   | 2.08                     | 0.79              |
| 1:A:105:LEU:CG   | 1:E:147:THR:HB   | 2.11                     | 0.79              |
| 1:E:31:VAL:CG2   | 1:E:153:LEU:HD11 | 2.12                     | 0.79              |
| 1:C:77:LEU:HD12  | 1:C:78:THR:H     | 1.48                     | 0.79              |
| 1:C:31:VAL:CG2   | 1:C:153:LEU:HD11 | 2.12                     | 0.79              |
| 1:B:31:VAL:CG2   | 1:B:153:LEU:HD11 | 2.12                     | 0.79              |
| 1:B:46:GLU:OE1   | 1:C:42:ARG:CZ    | 2.30                     | 0.79              |
| 1:D:95:VAL:CA    | 1:E:101:PHE:HE1  | 1.54                     | 0.78              |
| 1:E:74:PHE:CE2   | 1:E:77:LEU:CA    | 2.59                     | 0.78              |
| 1:D:31:VAL:CG2   | 1:D:153:LEU:HD11 | 2.12                     | 0.78              |
| 1:C:47:ASN:ND2   | 1:D:41:PHE:CE2   | 2.27                     | 0.78              |
| 1:A:77:LEU:HD12  | 1:A:78:THR:H     | 1.48                     | 0.78              |
| 1:C:149:SER:OG   | 1:C:152:GLU:OE1  | 2.00                     | 0.78              |
| 1:A:149:SER:OG   | 1:A:152:GLU:OE1  | 2.00                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:PHE:HE1   | 1:A:35:TYR:CE1   | 2.02                     | 0.78              |
| 1:B:47:ASN:CA    | 1:C:41:PHE:CE2   | 2.64                     | 0.78              |
| 1:A:41:PHE:CE2   | 1:E:47:ASN:CA    | 2.64                     | 0.78              |
| 1:B:95:VAL:CA    | 1:C:101:PHE:CZ   | 2.61                     | 0.78              |
| 1:A:5:ARG:NH2    | 1:E:21:ILE:CD1   | 2.40                     | 0.78              |
| 1:D:147:THR:H    | 1:E:105:LEU:HD13 | 1.43                     | 0.78              |
| 1:B:147:THR:HB   | 1:C:105:LEU:CG   | 2.11                     | 0.78              |
| 1:A:5:ARG:HD2    | 1:A:77:LEU:HD13  | 1.65                     | 0.78              |
| 1:A:74:PHE:CE2   | 1:A:76:GLU:C     | 2.58                     | 0.77              |
| 1:C:125:SER:CB   | 1:D:39:LYS:HZ3   | 1.94                     | 0.77              |
| 1:E:33:PHE:HE1   | 1:E:35:TYR:CE1   | 2.02                     | 0.77              |
| 1:D:33:PHE:HE1   | 1:D:35:TYR:CE1   | 2.02                     | 0.77              |
| 1:D:5:ARG:HD2    | 1:D:77:LEU:HD13  | 1.65                     | 0.77              |
| 1:A:29:VAL:O     | 1:A:153:LEU:HD12 | 1.85                     | 0.77              |
| 1:E:74:PHE:CE2   | 1:E:76:GLU:C     | 2.58                     | 0.77              |
| 1:C:74:PHE:CE2   | 1:C:76:GLU:C     | 2.58                     | 0.77              |
| 1:D:74:PHE:CE2   | 1:D:76:GLU:C     | 2.58                     | 0.77              |
| 1:B:5:ARG:HD2    | 1:B:77:LEU:HD13  | 1.65                     | 0.77              |
| 1:A:74:PHE:HE2   | 1:A:77:LEU:CB    | 1.97                     | 0.77              |
| 1:A:105:LEU:CD1  | 1:E:147:THR:CG2  | 2.26                     | 0.77              |
| 1:D:29:VAL:O     | 1:D:153:LEU:HD12 | 1.85                     | 0.77              |
| 1:A:95:VAL:CA    | 1:B:101:PHE:CZ   | 2.61                     | 0.77              |
| 1:C:33:PHE:HE1   | 1:C:35:TYR:CE1   | 2.02                     | 0.77              |
| 1:B:74:PHE:CE2   | 1:B:77:LEU:CA    | 2.59                     | 0.77              |
| 1:B:33:PHE:HE1   | 1:B:35:TYR:CE1   | 2.02                     | 0.77              |
| 1:B:77:LEU:HD12  | 1:B:78:THR:H     | 1.48                     | 0.77              |
| 1:D:74:PHE:HE2   | 1:D:77:LEU:CB    | 1.97                     | 0.77              |
| 1:B:74:PHE:CE2   | 1:B:76:GLU:C     | 2.58                     | 0.77              |
| 1:A:47:ASN:CA    | 1:B:41:PHE:CE2   | 2.64                     | 0.77              |
| 1:E:74:PHE:HE2   | 1:E:77:LEU:CB    | 1.97                     | 0.77              |
| 1:B:74:PHE:HE2   | 1:B:77:LEU:CB    | 1.97                     | 0.77              |
| 1:C:131:LEU:HD12 | 1:C:203:ARG:HA   | 1.68                     | 0.76              |
| 1:C:125:SER:HB2  | 1:D:39:LYS:HZ1   | 1.49                     | 0.76              |
| 1:B:29:VAL:O     | 1:B:153:LEU:HD12 | 1.85                     | 0.76              |
| 1:C:29:VAL:O     | 1:C:153:LEU:HD12 | 1.85                     | 0.76              |
| 1:C:74:PHE:HE2   | 1:C:77:LEU:CB    | 1.97                     | 0.76              |
| 1:D:119:GLN:C    | 1:D:120:LEU:HD12 | 2.06                     | 0.76              |
| 1:E:5:ARG:HD2    | 1:E:77:LEU:HD13  | 1.65                     | 0.76              |
| 1:B:131:LEU:HD12 | 1:B:203:ARG:HA   | 1.68                     | 0.76              |
| 1:E:119:GLN:C    | 1:E:120:LEU:HD12 | 2.06                     | 0.76              |
| 1:C:119:GLN:C    | 1:C:120:LEU:HD12 | 2.06                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:131:LEU:HD12 | 1:D:203:ARG:HA   | 1.68                     | 0.76              |
| 1:A:105:LEU:CB   | 1:E:147:THR:CB   | 2.08                     | 0.76              |
| 1:B:119:GLN:C    | 1:B:120:LEU:HD12 | 2.06                     | 0.76              |
| 1:B:174:LEU:HG   | 1:B:200:PHE:CE1  | 2.21                     | 0.76              |
| 1:B:171:ARG:O    | 1:B:204:LYS:HD2  | 1.86                     | 0.76              |
| 1:D:147:THR:CG2  | 1:E:105:LEU:CD1  | 2.26                     | 0.75              |
| 1:E:171:ARG:O    | 1:E:204:LYS:HD2  | 1.86                     | 0.75              |
| 1:C:74:PHE:CE2   | 1:C:77:LEU:CA    | 2.59                     | 0.75              |
| 1:D:174:LEU:HG   | 1:D:200:PHE:CE1  | 2.21                     | 0.75              |
| 1:B:174:LEU:HG   | 1:B:200:PHE:CZ   | 2.21                     | 0.75              |
| 1:E:131:LEU:HD12 | 1:E:203:ARG:HA   | 1.68                     | 0.75              |
| 1:C:5:ARG:HD2    | 1:C:77:LEU:HD13  | 1.65                     | 0.75              |
| 1:A:119:GLN:C    | 1:A:120:LEU:HD12 | 2.06                     | 0.75              |
| 1:E:142:LYS:HG2  | 1:E:197:THR:CG2  | 1.99                     | 0.75              |
| 1:E:174:LEU:HG   | 1:E:200:PHE:CE1  | 2.21                     | 0.75              |
| 1:A:174:LEU:HG   | 1:A:200:PHE:CZ   | 2.21                     | 0.75              |
| 1:E:174:LEU:HG   | 1:E:200:PHE:CZ   | 2.22                     | 0.75              |
| 1:A:105:LEU:CD1  | 1:E:147:THR:CB   | 2.64                     | 0.75              |
| 1:C:174:LEU:HG   | 1:C:200:PHE:CE1  | 2.21                     | 0.75              |
| 1:B:175:LEU:HD23 | 1:B:202:PHE:CA   | 2.17                     | 0.75              |
| 1:A:175:LEU:HD23 | 1:A:202:PHE:CA   | 2.17                     | 0.75              |
| 1:E:29:VAL:O     | 1:E:153:LEU:HD12 | 1.85                     | 0.75              |
| 1:C:174:LEU:HG   | 1:C:200:PHE:CZ   | 2.21                     | 0.75              |
| 1:C:171:ARG:O    | 1:C:204:LYS:HD2  | 1.86                     | 0.75              |
| 1:C:147:THR:CG2  | 1:D:105:LEU:CD1  | 2.26                     | 0.75              |
| 1:D:174:LEU:HG   | 1:D:200:PHE:CZ   | 2.21                     | 0.75              |
| 1:E:16:CYS:O     | 1:E:17:SER:N     | 2.20                     | 0.75              |
| 1:E:175:LEU:HD23 | 1:E:202:PHE:CA   | 2.17                     | 0.74              |
| 1:C:175:LEU:HD23 | 1:C:202:PHE:CA   | 2.17                     | 0.74              |
| 1:C:147:THR:H    | 1:D:105:LEU:HD13 | 1.43                     | 0.74              |
| 1:D:94:SER:OG    | 1:E:101:PHE:HD1  | 1.69                     | 0.74              |
| 1:C:94:SER:OG    | 1:D:101:PHE:HD1  | 1.69                     | 0.74              |
| 1:D:175:LEU:HD23 | 1:D:202:PHE:CA   | 2.17                     | 0.74              |
| 1:A:131:LEU:HD12 | 1:A:203:ARG:HA   | 1.68                     | 0.74              |
| 1:C:81:ILE:HD13  | 1:C:104:LYS:HE3  | 0.74                     | 0.74              |
| 1:A:171:ARG:O    | 1:A:204:LYS:HD2  | 1.86                     | 0.74              |
| 1:B:24:GLU:CA    | 1:C:3:ARG:HA     | 2.14                     | 0.74              |
| 1:D:81:ILE:HD12  | 1:D:116:TYR:CE2  | 2.23                     | 0.74              |
| 1:B:70:GLU:HG2   | 1:B:70:GLU:O     | 1.87                     | 0.74              |
| 1:C:48:ASP:OD1   | 1:D:171:ARG:NH2  | 2.21                     | 0.74              |
| 1:D:171:ARG:O    | 1:D:204:LYS:HD2  | 1.86                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:THR:H    | 1:B:105:LEU:HD12 | 0.57                     | 0.74              |
| 1:D:81:ILE:HD13  | 1:D:104:LYS:HE3  | 0.74                     | 0.74              |
| 1:C:147:THR:CB   | 1:D:105:LEU:CD1  | 2.64                     | 0.74              |
| 1:A:74:PHE:CE2   | 1:A:77:LEU:CA    | 2.59                     | 0.74              |
| 1:A:16:CYS:O     | 1:A:17:SER:N     | 2.20                     | 0.74              |
| 1:D:147:THR:CB   | 1:E:105:LEU:CD1  | 2.64                     | 0.74              |
| 1:B:81:ILE:HD13  | 1:B:104:LYS:HE3  | 0.74                     | 0.74              |
| 1:B:81:ILE:HD12  | 1:B:116:TYR:CE2  | 2.23                     | 0.74              |
| 1:E:81:ILE:HD13  | 1:E:104:LYS:HE3  | 0.74                     | 0.74              |
| 1:A:81:ILE:HD13  | 1:A:104:LYS:HE3  | 0.74                     | 0.74              |
| 1:B:147:THR:H    | 1:C:105:LEU:HD12 | 0.57                     | 0.74              |
| 1:A:171:ARG:NH2  | 1:E:48:ASP:OD1   | 2.21                     | 0.74              |
| 1:A:101:PHE:CZ   | 1:E:95:VAL:CA    | 2.61                     | 0.74              |
| 1:E:81:ILE:HD12  | 1:E:116:TYR:CE2  | 2.23                     | 0.74              |
| 1:E:70:GLU:HG2   | 1:E:70:GLU:O     | 1.87                     | 0.74              |
| 1:C:161:VAL:HG11 | 1:C:177:ALA:HB1  | 1.70                     | 0.73              |
| 1:A:174:LEU:HG   | 1:A:200:PHE:CE1  | 2.21                     | 0.73              |
| 1:D:70:GLU:HG2   | 1:D:70:GLU:O     | 1.87                     | 0.73              |
| 1:C:147:THR:H    | 1:D:105:LEU:HD12 | 0.57                     | 0.73              |
| 1:B:142:LYS:HE2  | 1:B:184:LYS:HZ3  | 1.52                     | 0.73              |
| 1:C:146:TRP:CE3  | 1:D:102:SER:CB   | 2.64                     | 0.73              |
| 1:A:48:ASP:OD1   | 1:B:171:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:161:VAL:HG11 | 1:A:177:ALA:HB1  | 1.70                     | 0.73              |
| 1:A:81:ILE:HD12  | 1:A:116:TYR:CE2  | 2.23                     | 0.73              |
| 1:D:16:CYS:O     | 1:D:17:SER:N     | 2.20                     | 0.73              |
| 1:A:125:SER:HB2  | 1:B:39:LYS:HZ1   | 1.50                     | 0.73              |
| 1:D:48:ASP:OD1   | 1:E:171:ARG:NH2  | 2.21                     | 0.73              |
| 1:B:48:ASP:OD1   | 1:C:171:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:147:THR:H    | 1:B:105:LEU:HD13 | 1.43                     | 0.73              |
| 1:C:81:ILE:HD12  | 1:C:116:TYR:CE2  | 2.23                     | 0.73              |
| 1:C:24:GLU:CB    | 1:D:3:ARG:CB     | 2.44                     | 0.73              |
| 1:D:161:VAL:HG11 | 1:D:177:ALA:HB1  | 1.70                     | 0.73              |
| 1:A:142:LYS:HE2  | 1:A:184:LYS:HZ3  | 1.53                     | 0.73              |
| 1:A:105:LEU:HD12 | 1:E:147:THR:H    | 0.57                     | 0.73              |
| 1:C:57:THR:HA    | 1:C:117:VAL:HG12 | 1.71                     | 0.72              |
| 1:A:70:GLU:O     | 1:A:70:GLU:HG2   | 1.87                     | 0.72              |
| 1:C:70:GLU:HG2   | 1:C:70:GLU:O     | 1.87                     | 0.72              |
| 1:D:147:THR:H    | 1:E:105:LEU:HD12 | 0.57                     | 0.72              |
| 1:A:57:THR:HA    | 1:A:117:VAL:HG12 | 1.71                     | 0.72              |
| 1:D:24:GLU:CB    | 1:E:3:ARG:CB     | 2.44                     | 0.72              |
| 1:B:95:VAL:C     | 1:C:101:PHE:HE1  | 1.88                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:95:VAL:CA    | 1:D:101:PHE:CZ   | 2.61                     | 0.72              |
| 1:C:24:GLU:CA    | 1:D:3:ARG:HA     | 2.14                     | 0.72              |
| 1:A:3:ARG:CB     | 1:E:24:GLU:CB    | 2.44                     | 0.72              |
| 1:B:101:PHE:CE2  | 1:B:121:LYS:HB2  | 2.24                     | 0.72              |
| 1:A:101:PHE:HD1  | 1:E:94:SER:OG    | 1.69                     | 0.72              |
| 1:A:101:PHE:CE2  | 1:A:121:LYS:HB2  | 2.24                     | 0.72              |
| 1:B:94:SER:OG    | 1:C:101:PHE:HD1  | 1.69                     | 0.72              |
| 1:A:39:LYS:HZ1   | 1:E:125:SER:HB2  | 1.51                     | 0.72              |
| 1:B:16:CYS:O     | 1:B:17:SER:N     | 2.20                     | 0.72              |
| 1:E:161:VAL:HG11 | 1:E:177:ALA:HB1  | 1.70                     | 0.72              |
| 1:D:142:LYS:HE2  | 1:D:184:LYS:HZ3  | 1.54                     | 0.72              |
| 1:D:101:PHE:CE2  | 1:D:121:LYS:HB2  | 2.24                     | 0.72              |
| 1:B:57:THR:HA    | 1:B:117:VAL:HG12 | 1.71                     | 0.71              |
| 1:E:101:PHE:CE2  | 1:E:121:LYS:HB2  | 2.24                     | 0.71              |
| 1:C:16:CYS:O     | 1:C:17:SER:N     | 2.20                     | 0.71              |
| 1:B:182:ASN:HD21 | 1:B:197:THR:CG2  | 2.03                     | 0.71              |
| 1:B:91:ILE:HD11  | 1:B:122:VAL:HG11 | 1.73                     | 0.71              |
| 1:A:171:ARG:O    | 1:A:205:PRO:HD2  | 1.91                     | 0.71              |
| 1:C:171:ARG:O    | 1:C:205:PRO:HD2  | 1.90                     | 0.71              |
| 1:A:94:SER:OG    | 1:B:101:PHE:HD1  | 1.69                     | 0.71              |
| 1:B:171:ARG:O    | 1:B:205:PRO:HD2  | 1.91                     | 0.71              |
| 1:B:3:ARG:HD2    | 1:B:4:SER:N      | 2.06                     | 0.71              |
| 1:D:171:ARG:O    | 1:D:205:PRO:HD2  | 1.91                     | 0.71              |
| 1:A:91:ILE:HD11  | 1:A:122:VAL:HG11 | 1.73                     | 0.71              |
| 1:D:95:VAL:CA    | 1:E:101:PHE:CZ   | 2.61                     | 0.71              |
| 1:E:57:THR:HA    | 1:E:117:VAL:HG12 | 1.71                     | 0.71              |
| 1:C:101:PHE:CE2  | 1:C:121:LYS:HB2  | 2.24                     | 0.71              |
| 1:C:91:ILE:HD11  | 1:C:122:VAL:HG11 | 1.73                     | 0.71              |
| 1:C:182:ASN:HD21 | 1:C:197:THR:CG2  | 2.03                     | 0.71              |
| 1:B:161:VAL:HG11 | 1:B:177:ALA:HB1  | 1.70                     | 0.71              |
| 1:A:147:THR:CG2  | 1:B:105:LEU:CD1  | 2.26                     | 0.71              |
| 1:A:171:ARG:HH12 | 1:E:46:GLU:HA    | 1.56                     | 0.71              |
| 1:D:46:GLU:HA    | 1:E:171:ARG:HH12 | 1.56                     | 0.71              |
| 1:A:46:GLU:HA    | 1:B:171:ARG:HH12 | 1.56                     | 0.71              |
| 1:B:183:ARG:HB3  | 1:B:192:THR:HG21 | 1.73                     | 0.71              |
| 1:D:91:ILE:HD11  | 1:D:122:VAL:HG11 | 1.73                     | 0.70              |
| 1:C:56:THR:HG22  | 1:C:118:PRO:HG2  | 1.73                     | 0.70              |
| 1:D:57:THR:HA    | 1:D:117:VAL:HG12 | 1.71                     | 0.70              |
| 1:A:56:THR:HG22  | 1:A:118:PRO:HG2  | 1.73                     | 0.70              |
| 1:C:46:GLU:HA    | 1:D:171:ARG:HH12 | 1.56                     | 0.70              |
| 1:E:33:PHE:CE1   | 1:E:35:TYR:CE2   | 2.80                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:46:GLU:HA    | 1:C:171:ARG:HH12 | 1.56                     | 0.70              |
| 1:A:3:ARG:HD2    | 1:A:4:SER:N      | 2.06                     | 0.70              |
| 1:D:125:SER:HB2  | 1:E:39:LYS:HZ1   | 1.51                     | 0.70              |
| 1:E:171:ARG:O    | 1:E:205:PRO:HD2  | 1.91                     | 0.70              |
| 1:C:24:GLU:CA    | 1:D:3:ARG:CB     | 2.70                     | 0.70              |
| 1:C:3:ARG:HD2    | 1:C:4:SER:N      | 2.06                     | 0.70              |
| 1:D:183:ARG:HB3  | 1:D:192:THR:HG21 | 1.73                     | 0.70              |
| 1:C:176:ASN:OD1  | 1:C:201:THR:HB   | 1.92                     | 0.70              |
| 1:E:91:ILE:HD11  | 1:E:122:VAL:HG11 | 1.73                     | 0.70              |
| 1:A:3:ARG:CB     | 1:E:24:GLU:CA    | 2.70                     | 0.70              |
| 1:D:33:PHE:CE1   | 1:D:35:TYR:CE2   | 2.80                     | 0.70              |
| 1:B:176:ASN:OD1  | 1:B:201:THR:HB   | 1.92                     | 0.70              |
| 1:D:3:ARG:HD2    | 1:D:4:SER:N      | 2.06                     | 0.70              |
| 1:B:147:THR:CB   | 1:C:105:LEU:CD1  | 2.64                     | 0.70              |
| 1:C:183:ARG:HB3  | 1:C:192:THR:HG21 | 1.72                     | 0.70              |
| 1:E:124:LEU:HD22 | 1:E:141:LEU:HB3  | 1.74                     | 0.70              |
| 1:B:125:SER:HB2  | 1:C:39:LYS:HZ1   | 1.51                     | 0.70              |
| 1:E:56:THR:HG22  | 1:E:118:PRO:HG2  | 1.73                     | 0.70              |
| 1:C:47:ASN:HA    | 1:D:41:PHE:CE2   | 2.27                     | 0.70              |
| 1:D:176:ASN:OD1  | 1:D:201:THR:HB   | 1.92                     | 0.69              |
| 1:A:147:THR:CB   | 1:B:105:LEU:CD1  | 2.64                     | 0.69              |
| 1:E:3:ARG:HD2    | 1:E:4:SER:N      | 2.06                     | 0.69              |
| 1:C:95:VAL:C     | 1:D:101:PHE:HE1  | 1.88                     | 0.69              |
| 1:A:183:ARG:HB3  | 1:A:192:THR:HG21 | 1.73                     | 0.69              |
| 1:D:146:TRP:CE3  | 1:E:102:SER:CB   | 2.64                     | 0.69              |
| 1:B:56:THR:HG22  | 1:B:118:PRO:HG2  | 1.73                     | 0.69              |
| 1:A:33:PHE:CE1   | 1:A:35:TYR:CE2   | 2.80                     | 0.69              |
| 1:A:176:ASN:OD1  | 1:A:201:THR:HB   | 1.92                     | 0.69              |
| 1:D:92:PHE:CD2   | 1:D:142:LYS:HB2  | 2.27                     | 0.69              |
| 1:B:24:GLU:CB    | 1:C:3:ARG:CB     | 2.44                     | 0.69              |
| 1:D:47:ASN:HA    | 1:E:41:PHE:CE2   | 2.27                     | 0.69              |
| 1:B:146:TRP:CD2  | 1:C:102:SER:HB2  | 2.28                     | 0.69              |
| 1:D:56:THR:HG22  | 1:D:118:PRO:HG2  | 1.73                     | 0.69              |
| 1:D:24:GLU:CA    | 1:E:3:ARG:CB     | 2.70                     | 0.69              |
| 1:B:49:GLU:OE2   | 1:B:95:VAL:HG11  | 1.93                     | 0.69              |
| 1:C:33:PHE:CE1   | 1:C:35:TYR:CE2   | 2.80                     | 0.69              |
| 1:C:49:GLU:OE2   | 1:C:95:VAL:HG11  | 1.93                     | 0.69              |
| 1:C:146:TRP:CD2  | 1:D:102:SER:HB2  | 2.28                     | 0.69              |
| 1:B:124:LEU:HD22 | 1:B:141:LEU:HB3  | 1.74                     | 0.69              |
| 1:B:33:PHE:CE1   | 1:B:35:TYR:CE2   | 2.80                     | 0.69              |
| 1:A:47:ASN:HA    | 1:B:41:PHE:CE2   | 2.27                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:24:GLU:CB    | 1:B:3:ARG:CB     | 2.44                     | 0.69              |
| 1:E:183:ARG:HB3  | 1:E:192:THR:HG21 | 1.73                     | 0.69              |
| 1:C:30:LYS:HG3   | 1:C:154:THR:HB   | 1.75                     | 0.69              |
| 1:D:147:THR:HG21 | 1:E:105:LEU:HD22 | 1.75                     | 0.69              |
| 1:E:56:THR:CG2   | 1:E:118:PRO:HG2  | 2.23                     | 0.69              |
| 1:B:147:THR:CG2  | 1:C:105:LEU:CD1  | 2.26                     | 0.69              |
| 1:B:125:SER:HB3  | 1:C:39:LYS:HZ3   | 1.49                     | 0.69              |
| 1:D:146:TRP:CD2  | 1:E:102:SER:HB2  | 2.28                     | 0.69              |
| 1:E:176:ASN:OD1  | 1:E:201:THR:HB   | 1.92                     | 0.69              |
| 1:A:146:TRP:CD2  | 1:B:102:SER:HB2  | 2.28                     | 0.69              |
| 1:A:41:PHE:CE2   | 1:E:47:ASN:HA    | 2.27                     | 0.69              |
| 1:D:147:THR:CG2  | 1:E:105:LEU:CG   | 2.71                     | 0.68              |
| 1:C:147:THR:CG2  | 1:D:105:LEU:CG   | 2.71                     | 0.68              |
| 1:E:182:ASN:HD21 | 1:E:197:THR:CG2  | 2.03                     | 0.68              |
| 1:B:92:PHE:CD2   | 1:B:142:LYS:HB2  | 2.27                     | 0.68              |
| 1:A:49:GLU:OE2   | 1:A:95:VAL:HG11  | 1.93                     | 0.68              |
| 1:D:49:GLU:OE2   | 1:D:95:VAL:HG11  | 1.93                     | 0.68              |
| 1:C:125:SER:HB3  | 1:D:39:LYS:HZ2   | 1.50                     | 0.68              |
| 1:C:56:THR:CG2   | 1:C:118:PRO:HG2  | 2.23                     | 0.68              |
| 1:D:56:THR:CG2   | 1:D:118:PRO:HG2  | 2.23                     | 0.68              |
| 1:A:24:GLU:CA    | 1:B:3:ARG:CB     | 2.70                     | 0.68              |
| 1:C:147:THR:CB   | 1:D:105:LEU:CG   | 2.71                     | 0.68              |
| 1:A:147:THR:CG2  | 1:B:105:LEU:CG   | 2.71                     | 0.68              |
| 1:D:31:VAL:HG23  | 1:D:153:LEU:CD1  | 2.20                     | 0.68              |
| 1:D:45:VAL:HB    | 1:D:128:LEU:HD11 | 1.76                     | 0.68              |
| 1:B:147:THR:CG2  | 1:C:105:LEU:CG   | 2.71                     | 0.68              |
| 1:A:105:LEU:CG   | 1:E:147:THR:CG2  | 2.71                     | 0.68              |
| 1:A:105:LEU:HD22 | 1:E:147:THR:HG21 | 1.75                     | 0.68              |
| 1:B:47:ASN:HA    | 1:C:41:PHE:CE2   | 2.27                     | 0.68              |
| 1:B:56:THR:CG2   | 1:B:118:PRO:HG2  | 2.23                     | 0.68              |
| 1:A:1:SER:CA     | 1:E:27:GLN:O     | 2.38                     | 0.68              |
| 1:E:30:LYS:HG3   | 1:E:154:THR:HB   | 1.75                     | 0.68              |
| 1:C:124:LEU:HD22 | 1:C:141:LEU:HB3  | 1.74                     | 0.68              |
| 1:B:45:VAL:HB    | 1:B:128:LEU:HD11 | 1.76                     | 0.68              |
| 1:C:147:THR:HG22 | 1:D:105:LEU:CG   | 2.22                     | 0.68              |
| 1:C:31:VAL:HG23  | 1:C:153:LEU:CD1  | 2.20                     | 0.68              |
| 1:A:56:THR:CG2   | 1:A:118:PRO:HG2  | 2.23                     | 0.68              |
| 1:C:125:SER:HB2  | 1:D:39:LYS:HZ3   | 1.51                     | 0.68              |
| 1:B:147:THR:H    | 1:C:105:LEU:HD13 | 1.43                     | 0.68              |
| 1:A:147:THR:HG21 | 1:B:105:LEU:HD22 | 1.75                     | 0.68              |
| 1:B:24:GLU:CA    | 1:C:3:ARG:CB     | 2.70                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:45:VAL:HA    | 1:B:128:LEU:HD22 | 1.76                     | 0.67              |
| 1:D:124:LEU:HD22 | 1:D:141:LEU:HB3  | 1.74                     | 0.67              |
| 1:E:31:VAL:HG23  | 1:E:153:LEU:CD1  | 2.20                     | 0.67              |
| 1:D:76:GLU:OE1   | 1:D:107:ARG:CD   | 2.43                     | 0.67              |
| 1:C:45:VAL:HA    | 1:C:128:LEU:HD22 | 1.76                     | 0.67              |
| 1:A:124:LEU:HD22 | 1:A:141:LEU:HB3  | 1.74                     | 0.67              |
| 1:D:24:GLU:CA    | 1:E:3:ARG:HA     | 2.14                     | 0.67              |
| 1:A:125:SER:HB2  | 1:B:39:LYS:HZ3   | 1.50                     | 0.67              |
| 1:C:45:VAL:HB    | 1:C:128:LEU:HD11 | 1.76                     | 0.67              |
| 1:D:163:LEU:HD21 | 1:D:177:ALA:HB3  | 1.76                     | 0.67              |
| 1:A:47:ASN:HA    | 1:B:41:PHE:CZ    | 2.28                     | 0.67              |
| 1:A:76:GLU:OE1   | 1:A:107:ARG:CD   | 2.43                     | 0.67              |
| 1:E:49:GLU:OE2   | 1:E:95:VAL:HG11  | 1.93                     | 0.67              |
| 1:E:45:VAL:HA    | 1:E:128:LEU:HD22 | 1.76                     | 0.67              |
| 1:D:95:VAL:C     | 1:E:101:PHE:HE1  | 1.88                     | 0.67              |
| 1:B:147:THR:HG21 | 1:C:105:LEU:HD22 | 1.75                     | 0.67              |
| 1:A:182:ASN:HD21 | 1:A:197:THR:CG2  | 2.03                     | 0.67              |
| 1:B:76:GLU:OE1   | 1:B:107:ARG:CD   | 2.43                     | 0.67              |
| 1:A:90:PHE:CE2   | 1:B:103:ASP:HA   | 2.30                     | 0.67              |
| 1:B:131:LEU:HD21 | 1:B:172:PHE:CD1  | 2.30                     | 0.67              |
| 1:B:37:LEU:CD1   | 1:B:52:ILE:HG23  | 2.25                     | 0.67              |
| 1:E:178:THR:O    | 1:E:198:LEU:HD22 | 1.95                     | 0.67              |
| 1:A:163:LEU:HD21 | 1:A:177:ALA:HB3  | 1.76                     | 0.67              |
| 1:E:45:VAL:HB    | 1:E:128:LEU:HD11 | 1.76                     | 0.67              |
| 1:A:30:LYS:HG3   | 1:A:154:THR:HB   | 1.75                     | 0.67              |
| 1:D:30:LYS:HG3   | 1:D:154:THR:HB   | 1.75                     | 0.67              |
| 1:E:131:LEU:HD21 | 1:E:172:PHE:CD1  | 2.30                     | 0.67              |
| 1:E:76:GLU:OE1   | 1:E:107:ARG:CD   | 2.43                     | 0.67              |
| 1:C:90:PHE:CE2   | 1:D:103:ASP:HA   | 2.30                     | 0.67              |
| 1:A:178:THR:O    | 1:A:198:LEU:HD22 | 1.95                     | 0.67              |
| 1:D:131:LEU:HD21 | 1:D:172:PHE:CD1  | 2.30                     | 0.66              |
| 1:B:30:LYS:HG3   | 1:B:154:THR:HB   | 1.75                     | 0.66              |
| 1:B:147:THR:HG22 | 1:C:105:LEU:CG   | 2.22                     | 0.66              |
| 1:C:37:LEU:CD1   | 1:C:52:ILE:HG23  | 2.25                     | 0.66              |
| 1:C:147:THR:HG21 | 1:D:105:LEU:HD22 | 1.75                     | 0.66              |
| 1:A:27:GLN:O     | 1:B:1:SER:CA     | 2.38                     | 0.66              |
| 1:A:101:PHE:HZ   | 1:E:95:VAL:HA    | 1.58                     | 0.66              |
| 1:D:182:ASN:HD21 | 1:D:197:THR:CG2  | 2.03                     | 0.66              |
| 1:D:45:VAL:HA    | 1:D:128:LEU:HD22 | 1.76                     | 0.66              |
| 1:E:163:LEU:HD21 | 1:E:177:ALA:HB3  | 1.76                     | 0.66              |
| 1:B:163:LEU:HD21 | 1:B:177:ALA:HB3  | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:37:LEU:CD1   | 1:A:52:ILE:HG23  | 2.25                     | 0.66              |
| 1:B:45:VAL:HA    | 1:B:128:LEU:CD2  | 2.26                     | 0.66              |
| 1:C:178:THR:O    | 1:C:198:LEU:HD22 | 1.95                     | 0.66              |
| 1:C:76:GLU:OE1   | 1:C:107:ARG:CD   | 2.43                     | 0.66              |
| 1:A:103:ASP:HA   | 1:E:90:PHE:CE2   | 2.30                     | 0.66              |
| 1:D:90:PHE:CE2   | 1:E:103:ASP:HA   | 2.30                     | 0.66              |
| 1:D:178:THR:O    | 1:D:198:LEU:HD22 | 1.95                     | 0.66              |
| 1:D:37:LEU:CD1   | 1:D:52:ILE:HG23  | 2.25                     | 0.66              |
| 1:D:45:VAL:HA    | 1:D:128:LEU:CD2  | 2.26                     | 0.66              |
| 1:B:95:VAL:HA    | 1:C:101:PHE:HZ   | 1.58                     | 0.66              |
| 1:C:45:VAL:HA    | 1:C:128:LEU:CD2  | 2.26                     | 0.66              |
| 1:A:45:VAL:HB    | 1:A:128:LEU:HD11 | 1.76                     | 0.66              |
| 1:D:147:THR:CB   | 1:E:105:LEU:CG   | 2.71                     | 0.66              |
| 1:A:45:VAL:HA    | 1:A:128:LEU:CD2  | 2.26                     | 0.66              |
| 1:A:102:SER:HB2  | 1:E:146:TRP:CD2  | 2.28                     | 0.66              |
| 1:A:99:GLU:OE2   | 1:E:95:VAL:C     | 2.34                     | 0.66              |
| 1:A:105:LEU:CG   | 1:E:147:THR:CB   | 2.71                     | 0.66              |
| 1:D:147:THR:HG22 | 1:E:105:LEU:CG   | 2.22                     | 0.66              |
| 1:C:5:ARG:HA     | 1:C:8:ILE:HD12   | 1.78                     | 0.66              |
| 1:A:147:THR:CB   | 1:B:105:LEU:CG   | 2.71                     | 0.66              |
| 1:A:45:VAL:HA    | 1:A:128:LEU:HD22 | 1.76                     | 0.66              |
| 1:E:5:ARG:HA     | 1:E:8:ILE:HD12   | 1.78                     | 0.66              |
| 1:D:95:VAL:C     | 1:E:99:GLU:OE2   | 2.34                     | 0.66              |
| 1:E:37:LEU:CD1   | 1:E:52:ILE:HG23  | 2.25                     | 0.65              |
| 1:B:95:VAL:O     | 1:C:101:PHE:CZ   | 2.49                     | 0.65              |
| 1:A:95:VAL:HA    | 1:B:101:PHE:HZ   | 1.58                     | 0.65              |
| 1:A:131:LEU:HD21 | 1:A:172:PHE:CD1  | 2.30                     | 0.65              |
| 1:A:5:ARG:HA     | 1:A:8:ILE:HD12   | 1.78                     | 0.65              |
| 1:B:90:PHE:CE2   | 1:C:103:ASP:HA   | 2.30                     | 0.65              |
| 1:B:178:THR:O    | 1:B:198:LEU:HD22 | 1.95                     | 0.65              |
| 1:B:5:ARG:HA     | 1:B:8:ILE:HD12   | 1.78                     | 0.65              |
| 1:D:27:GLN:O     | 1:E:1:SER:CA     | 2.38                     | 0.65              |
| 1:A:95:VAL:C     | 1:B:99:GLU:OE2   | 2.34                     | 0.65              |
| 1:B:24:GLU:O     | 1:C:3:ARG:CG     | 2.45                     | 0.65              |
| 1:C:131:LEU:HD21 | 1:C:172:PHE:CD1  | 2.30                     | 0.65              |
| 1:D:5:ARG:HA     | 1:D:8:ILE:HD12   | 1.78                     | 0.65              |
| 1:A:101:PHE:CZ   | 1:E:95:VAL:O     | 2.49                     | 0.65              |
| 1:B:95:VAL:C     | 1:C:99:GLU:OE2   | 2.34                     | 0.65              |
| 1:C:142:LYS:HE2  | 1:C:184:LYS:HZ3  | 1.61                     | 0.65              |
| 1:C:23:ILE:O     | 1:D:1:SER:C      | 2.35                     | 0.65              |
| 1:A:147:THR:HG22 | 1:B:105:LEU:CG   | 2.22                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:PHE:HA   | 1:A:205:PRO:HD2  | 1.79                     | 0.65              |
| 1:A:105:LEU:HD13 | 1:E:147:THR:H    | 1.43                     | 0.65              |
| 1:E:45:VAL:HA    | 1:E:128:LEU:CD2  | 2.26                     | 0.65              |
| 1:B:31:VAL:HG23  | 1:B:153:LEU:CD1  | 2.20                     | 0.65              |
| 1:B:23:ILE:O     | 1:C:1:SER:C      | 2.35                     | 0.65              |
| 1:A:173:GLN:N    | 1:A:205:PRO:HD3  | 2.12                     | 0.65              |
| 1:C:183:ARG:CG   | 1:C:194:GLU:HG2  | 2.07                     | 0.65              |
| 1:C:163:LEU:HD21 | 1:C:177:ALA:HB3  | 1.76                     | 0.65              |
| 1:D:173:GLN:N    | 1:D:205:PRO:HD3  | 2.12                     | 0.65              |
| 1:A:92:PHE:CD2   | 1:A:142:LYS:HB2  | 2.27                     | 0.65              |
| 1:B:172:PHE:HA   | 1:B:205:PRO:HD2  | 1.79                     | 0.65              |
| 1:C:161:VAL:HG22 | 1:C:179:GLN:HG3  | 1.79                     | 0.65              |
| 1:C:95:VAL:O     | 1:D:101:PHE:CZ   | 2.49                     | 0.65              |
| 1:A:41:PHE:HE2   | 1:E:47:ASN:CG    | 1.99                     | 0.65              |
| 1:D:95:VAL:O     | 1:E:101:PHE:CZ   | 2.49                     | 0.65              |
| 1:C:92:PHE:CD2   | 1:C:142:LYS:HB2  | 2.27                     | 0.65              |
| 1:C:95:VAL:C     | 1:D:99:GLU:OE2   | 2.34                     | 0.65              |
| 1:B:173:GLN:N    | 1:B:205:PRO:HD3  | 2.12                     | 0.65              |
| 1:A:161:VAL:HG22 | 1:A:179:GLN:HG3  | 1.79                     | 0.65              |
| 1:C:173:GLN:N    | 1:C:205:PRO:HD3  | 2.12                     | 0.65              |
| 1:A:95:VAL:O     | 1:B:101:PHE:CZ   | 2.49                     | 0.65              |
| 1:D:24:GLU:O     | 1:E:3:ARG:CG     | 2.45                     | 0.65              |
| 1:A:24:GLU:O     | 1:B:3:ARG:CG     | 2.45                     | 0.65              |
| 1:D:47:ASN:CG    | 1:E:41:PHE:HE2   | 1.99                     | 0.64              |
| 1:E:161:VAL:HG22 | 1:E:179:GLN:HG3  | 1.79                     | 0.64              |
| 1:E:172:PHE:HA   | 1:E:205:PRO:HD2  | 1.79                     | 0.64              |
| 1:B:161:VAL:HG22 | 1:B:179:GLN:HG3  | 1.79                     | 0.64              |
| 1:A:1:SER:C      | 1:E:23:ILE:O     | 2.35                     | 0.64              |
| 1:D:161:VAL:HG22 | 1:D:179:GLN:HG3  | 1.79                     | 0.64              |
| 1:A:31:VAL:HG23  | 1:A:153:LEU:CD1  | 2.20                     | 0.64              |
| 1:A:23:ILE:O     | 1:B:1:SER:C      | 2.35                     | 0.64              |
| 1:B:147:THR:CB   | 1:C:105:LEU:CG   | 2.71                     | 0.64              |
| 1:B:147:THR:CA   | 1:C:105:LEU:CD1  | 2.76                     | 0.64              |
| 1:D:47:ASN:HA    | 1:E:41:PHE:CZ    | 2.28                     | 0.64              |
| 1:C:25:ASP:OD1   | 1:C:26:ASP:N     | 2.28                     | 0.64              |
| 1:C:147:THR:CA   | 1:D:105:LEU:CD1  | 2.76                     | 0.64              |
| 1:C:146:TRP:C    | 1:D:105:LEU:HD12 | 2.16                     | 0.64              |
| 1:A:147:THR:CA   | 1:B:105:LEU:CD1  | 2.76                     | 0.64              |
| 1:A:105:LEU:HD12 | 1:E:146:TRP:C    | 2.16                     | 0.64              |
| 1:D:146:TRP:C    | 1:E:105:LEU:HD12 | 2.16                     | 0.64              |
| 1:A:141:LEU:HD23 | 1:A:141:LEU:H    | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:141:LEU:H    | 1:E:141:LEU:HD23 | 1.63                     | 0.64              |
| 1:D:23:ILE:O     | 1:E:1:SER:C      | 2.35                     | 0.64              |
| 1:A:33:PHE:CE1   | 1:A:35:TYR:CE1   | 2.83                     | 0.64              |
| 1:C:24:GLU:O     | 1:D:3:ARG:CG     | 2.45                     | 0.64              |
| 1:D:172:PHE:HA   | 1:D:205:PRO:HD2  | 1.79                     | 0.63              |
| 1:B:141:LEU:H    | 1:B:141:LEU:HD23 | 1.63                     | 0.63              |
| 1:C:47:ASN:HD22  | 1:D:41:PHE:HE2   | 0.69                     | 0.63              |
| 1:A:146:TRP:C    | 1:B:105:LEU:HD12 | 2.16                     | 0.63              |
| 1:E:173:GLN:N    | 1:E:205:PRO:HD3  | 2.12                     | 0.63              |
| 1:D:47:ASN:CG    | 1:E:41:PHE:CE2   | 2.71                     | 0.63              |
| 1:B:25:ASP:OD1   | 1:B:26:ASP:N     | 2.28                     | 0.63              |
| 1:C:141:LEU:H    | 1:C:141:LEU:HD23 | 1.63                     | 0.63              |
| 1:A:102:SER:CB   | 1:E:146:TRP:CE3  | 2.64                     | 0.63              |
| 1:D:25:ASP:OD1   | 1:D:26:ASP:N     | 2.28                     | 0.63              |
| 1:D:74:PHE:CE2   | 1:D:77:LEU:HB2   | 2.34                     | 0.63              |
| 1:A:125:SER:HB3  | 1:B:39:LYS:HZ3   | 1.56                     | 0.63              |
| 1:C:172:PHE:HA   | 1:C:205:PRO:HD2  | 1.79                     | 0.63              |
| 1:C:47:ASN:CG    | 1:D:41:PHE:CE2   | 2.71                     | 0.63              |
| 1:D:146:TRP:HB3  | 1:E:103:ASP:HB2  | 1.80                     | 0.63              |
| 1:D:47:ASN:HD22  | 1:E:41:PHE:HE2   | 0.68                     | 0.63              |
| 1:B:27:GLN:O     | 1:C:1:SER:CA     | 2.38                     | 0.63              |
| 1:C:74:PHE:CE2   | 1:C:77:LEU:HB2   | 2.34                     | 0.63              |
| 1:A:103:ASP:HB2  | 1:E:146:TRP:HB3  | 1.80                     | 0.63              |
| 1:A:105:LEU:CD1  | 1:E:147:THR:CA   | 2.76                     | 0.63              |
| 1:C:163:LEU:CD2  | 1:C:174:LEU:HD11 | 2.29                     | 0.63              |
| 1:C:27:GLN:O     | 1:D:1:SER:CA     | 2.38                     | 0.63              |
| 1:D:76:GLU:CD    | 1:D:107:ARG:HG2  | 2.17                     | 0.63              |
| 1:C:47:ASN:CG    | 1:D:41:PHE:HE2   | 1.99                     | 0.63              |
| 1:A:3:ARG:CG     | 1:E:24:GLU:O     | 2.45                     | 0.63              |
| 1:B:147:THR:CA   | 1:C:105:LEU:CB   | 2.77                     | 0.62              |
| 1:B:47:ASN:HD22  | 1:C:41:PHE:HE2   | 0.68                     | 0.62              |
| 1:A:47:ASN:CG    | 1:B:41:PHE:CE2   | 2.71                     | 0.62              |
| 1:D:141:LEU:HD23 | 1:D:141:LEU:H    | 1.63                     | 0.62              |
| 1:E:92:PHE:CD2   | 1:E:142:LYS:HB2  | 2.27                     | 0.62              |
| 1:E:161:VAL:HG11 | 1:E:177:ALA:CB   | 2.29                     | 0.62              |
| 1:B:47:ASN:CG    | 1:C:41:PHE:HE2   | 1.99                     | 0.62              |
| 1:D:147:THR:CA   | 1:E:105:LEU:CB   | 2.77                     | 0.62              |
| 1:B:47:ASN:CG    | 1:C:41:PHE:CE2   | 2.72                     | 0.62              |
| 1:B:47:ASN:HD21  | 1:C:42:ARG:HD2   | 1.65                     | 0.62              |
| 1:A:41:PHE:CE2   | 1:E:47:ASN:CG    | 2.71                     | 0.62              |
| 1:A:74:PHE:CE2   | 1:A:77:LEU:HB2   | 2.34                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:146:TRP:HB3  | 1:C:103:ASP:HB2  | 1.80                     | 0.62              |
| 1:C:95:VAL:HA    | 1:D:101:PHE:HZ   | 1.58                     | 0.62              |
| 1:A:76:GLU:CD    | 1:A:107:ARG:HG2  | 2.17                     | 0.62              |
| 1:A:161:VAL:HG11 | 1:A:177:ALA:CB   | 2.29                     | 0.62              |
| 1:A:183:ARG:CG   | 1:A:194:GLU:HG2  | 2.07                     | 0.62              |
| 1:B:76:GLU:CD    | 1:B:107:ARG:HG2  | 2.17                     | 0.62              |
| 1:A:41:PHE:HE2   | 1:E:47:ASN:HD22  | 0.68                     | 0.62              |
| 1:D:147:THR:CA   | 1:E:105:LEU:CD1  | 2.76                     | 0.62              |
| 1:A:147:THR:CA   | 1:B:105:LEU:CB   | 2.77                     | 0.62              |
| 1:A:47:ASN:HD22  | 1:B:41:PHE:HE2   | 0.68                     | 0.62              |
| 1:B:163:LEU:CD2  | 1:B:174:LEU:HD11 | 2.29                     | 0.62              |
| 1:B:74:PHE:CE2   | 1:B:77:LEU:HB2   | 2.34                     | 0.62              |
| 1:D:24:GLU:C     | 1:E:3:ARG:HB3    | 2.19                     | 0.62              |
| 1:D:95:VAL:C     | 1:E:101:PHE:CZ   | 2.73                     | 0.62              |
| 1:B:95:VAL:C     | 1:C:101:PHE:CZ   | 2.73                     | 0.62              |
| 1:A:47:ASN:CG    | 1:B:41:PHE:HE2   | 1.99                     | 0.62              |
| 1:D:95:VAL:HA    | 1:E:101:PHE:HZ   | 1.58                     | 0.62              |
| 1:C:161:VAL:HG11 | 1:C:177:ALA:CB   | 2.29                     | 0.62              |
| 1:C:74:PHE:HE2   | 1:C:77:LEU:HB2   | 1.65                     | 0.62              |
| 1:A:105:LEU:CG   | 1:E:147:THR:HG22 | 2.22                     | 0.62              |
| 1:E:163:LEU:CD2  | 1:E:174:LEU:HD11 | 2.29                     | 0.61              |
| 1:E:74:PHE:CE2   | 1:E:77:LEU:HB2   | 2.34                     | 0.61              |
| 1:C:124:LEU:HD23 | 1:C:141:LEU:HD13 | 1.82                     | 0.61              |
| 1:D:161:VAL:HG11 | 1:D:177:ALA:CB   | 2.29                     | 0.61              |
| 1:B:124:LEU:HD23 | 1:B:141:LEU:HD13 | 1.82                     | 0.61              |
| 1:E:76:GLU:CD    | 1:E:107:ARG:HG2  | 2.17                     | 0.61              |
| 1:A:42:ARG:HD2   | 1:E:47:ASN:HD21  | 1.65                     | 0.61              |
| 1:D:142:LYS:HE2  | 1:D:184:LYS:NZ   | 2.16                     | 0.61              |
| 1:A:101:PHE:CZ   | 1:E:95:VAL:C     | 2.73                     | 0.61              |
| 1:C:24:GLU:C     | 1:D:3:ARG:HB3    | 2.19                     | 0.61              |
| 1:A:3:ARG:HB3    | 1:E:24:GLU:C     | 2.19                     | 0.61              |
| 1:B:146:TRP:CE3  | 1:C:102:SER:CB   | 2.64                     | 0.61              |
| 1:A:105:LEU:CB   | 1:E:147:THR:CA   | 2.77                     | 0.61              |
| 1:D:24:GLU:O     | 1:E:3:ARG:HG3    | 2.01                     | 0.61              |
| 1:B:24:GLU:O     | 1:C:3:ARG:HG3    | 2.01                     | 0.61              |
| 1:C:33:PHE:CE1   | 1:C:35:TYR:CE1   | 2.83                     | 0.61              |
| 1:C:95:VAL:C     | 1:D:101:PHE:CZ   | 2.73                     | 0.61              |
| 1:C:146:TRP:HB3  | 1:D:103:ASP:HB2  | 1.80                     | 0.61              |
| 1:C:47:ASN:HA    | 1:D:41:PHE:CZ    | 2.28                     | 0.61              |
| 1:A:146:TRP:HB3  | 1:B:103:ASP:HB2  | 1.80                     | 0.61              |
| 1:B:161:VAL:HG11 | 1:B:177:ALA:CB   | 2.30                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:146:TRP:CE3  | 1:B:102:SER:CB   | 2.64                     | 0.61              |
| 1:A:24:GLU:CA    | 1:B:3:ARG:HA     | 2.14                     | 0.61              |
| 1:A:101:PHE:HB2  | 1:A:119:GLN:HB3  | 1.83                     | 0.60              |
| 1:A:131:LEU:CD1  | 1:A:203:ARG:HA   | 2.31                     | 0.60              |
| 1:E:33:PHE:CE1   | 1:E:35:TYR:CE1   | 2.83                     | 0.60              |
| 1:A:142:LYS:HE2  | 1:A:184:LYS:NZ   | 2.16                     | 0.60              |
| 1:A:24:GLU:C     | 1:B:3:ARG:HB3    | 2.19                     | 0.60              |
| 1:B:142:LYS:HE2  | 1:B:184:LYS:NZ   | 2.16                     | 0.60              |
| 1:B:149:SER:HA   | 1:B:193:TYR:CD2  | 2.36                     | 0.60              |
| 1:E:131:LEU:CD1  | 1:E:203:ARG:HA   | 2.31                     | 0.60              |
| 1:C:23:ILE:HD11  | 1:C:29:VAL:HG13  | 1.83                     | 0.60              |
| 1:C:24:GLU:O     | 1:D:3:ARG:HG3    | 2.01                     | 0.60              |
| 1:D:147:THR:CA   | 1:E:105:LEU:HD13 | 2.31                     | 0.60              |
| 1:C:101:PHE:HB2  | 1:C:119:GLN:HB3  | 1.83                     | 0.60              |
| 1:D:163:LEU:CD2  | 1:D:174:LEU:HD11 | 2.29                     | 0.60              |
| 1:A:102:SER:CB   | 1:E:146:TRP:CH2  | 2.85                     | 0.60              |
| 1:E:149:SER:HA   | 1:E:193:TYR:CD2  | 2.37                     | 0.60              |
| 1:E:142:LYS:HE2  | 1:E:184:LYS:NZ   | 2.16                     | 0.60              |
| 1:A:25:ASP:OD1   | 1:A:26:ASP:N     | 2.28                     | 0.60              |
| 1:E:124:LEU:HD23 | 1:E:141:LEU:HD13 | 1.82                     | 0.60              |
| 1:C:41:PHE:CD2   | 1:C:42:ARG:HB2   | 2.37                     | 0.60              |
| 1:E:142:LYS:HE2  | 1:E:184:LYS:HZ3  | 1.66                     | 0.60              |
| 1:E:25:ASP:OD1   | 1:E:26:ASP:N     | 2.28                     | 0.60              |
| 1:D:146:TRP:CH2  | 1:E:102:SER:CB   | 2.85                     | 0.60              |
| 1:D:23:ILE:HD11  | 1:D:29:VAL:HG13  | 1.83                     | 0.60              |
| 1:B:147:THR:CA   | 1:C:105:LEU:HD13 | 2.31                     | 0.60              |
| 1:A:41:PHE:CD2   | 1:A:42:ARG:HB2   | 2.37                     | 0.60              |
| 1:A:3:ARG:HG3    | 1:E:24:GLU:O     | 2.01                     | 0.60              |
| 1:C:149:SER:HA   | 1:C:193:TYR:CD2  | 2.37                     | 0.60              |
| 1:D:124:LEU:HD23 | 1:D:141:LEU:HD13 | 1.82                     | 0.60              |
| 1:A:149:SER:HA   | 1:A:193:TYR:CD2  | 2.37                     | 0.60              |
| 1:A:95:VAL:C     | 1:B:101:PHE:CZ   | 2.73                     | 0.60              |
| 1:A:24:GLU:O     | 1:B:3:ARG:HG3    | 2.01                     | 0.60              |
| 1:C:76:GLU:CD    | 1:C:107:ARG:HG2  | 2.17                     | 0.60              |
| 1:C:142:LYS:HE2  | 1:C:184:LYS:NZ   | 2.16                     | 0.60              |
| 1:A:163:LEU:CD2  | 1:A:174:LEU:HD11 | 2.29                     | 0.60              |
| 1:A:39:LYS:HZ3   | 1:E:125:SER:HB2  | 1.48                     | 0.60              |
| 1:D:41:PHE:CD2   | 1:D:42:ARG:HB2   | 2.37                     | 0.59              |
| 1:A:146:TRP:CH2  | 1:B:102:SER:CB   | 2.85                     | 0.59              |
| 1:B:131:LEU:CD1  | 1:B:203:ARG:HA   | 2.31                     | 0.59              |
| 1:B:23:ILE:HD11  | 1:B:29:VAL:HG13  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:101:PHE:HB2  | 1:D:119:GLN:HB3  | 1.83                     | 0.59              |
| 1:C:147:THR:CA   | 1:D:105:LEU:HD13 | 2.31                     | 0.59              |
| 1:A:131:LEU:HD13 | 1:A:202:PHE:CE2  | 2.38                     | 0.59              |
| 1:D:149:SER:HA   | 1:D:193:TYR:CD2  | 2.37                     | 0.59              |
| 1:C:131:LEU:CD1  | 1:C:203:ARG:HA   | 2.31                     | 0.59              |
| 1:B:131:LEU:HD13 | 1:B:202:PHE:CE2  | 2.38                     | 0.59              |
| 1:B:33:PHE:CE1   | 1:B:35:TYR:CE1   | 2.83                     | 0.59              |
| 1:B:146:TRP:CH2  | 1:C:102:SER:CB   | 2.85                     | 0.59              |
| 1:B:101:PHE:HB2  | 1:B:119:GLN:HB3  | 1.83                     | 0.59              |
| 1:A:124:LEU:HD23 | 1:A:141:LEU:HD13 | 1.82                     | 0.59              |
| 1:D:74:PHE:HE2   | 1:D:77:LEU:HB2   | 1.65                     | 0.59              |
| 1:A:47:ASN:HD21  | 1:B:42:ARG:HD2   | 1.65                     | 0.59              |
| 1:A:105:LEU:HD13 | 1:E:147:THR:CA   | 2.32                     | 0.59              |
| 1:C:147:THR:CA   | 1:D:105:LEU:CB   | 2.77                     | 0.59              |
| 1:A:147:THR:CG2  | 1:B:105:LEU:HD22 | 2.33                     | 0.59              |
| 1:E:41:PHE:CD2   | 1:E:42:ARG:HB2   | 2.37                     | 0.59              |
| 1:C:170:THR:HG22 | 1:C:171:ARG:N    | 2.18                     | 0.59              |
| 1:A:23:ILE:HD11  | 1:A:29:VAL:HG13  | 1.83                     | 0.59              |
| 1:B:41:PHE:CD2   | 1:B:42:ARG:HB2   | 2.37                     | 0.59              |
| 1:E:101:PHE:HB2  | 1:E:119:GLN:HB3  | 1.83                     | 0.59              |
| 1:E:170:THR:HG22 | 1:E:171:ARG:N    | 2.18                     | 0.59              |
| 1:E:131:LEU:HD13 | 1:E:202:PHE:CE2  | 2.38                     | 0.59              |
| 1:D:47:ASN:HD21  | 1:E:42:ARG:HD2   | 1.65                     | 0.59              |
| 1:C:131:LEU:HD13 | 1:C:202:PHE:CE2  | 2.38                     | 0.59              |
| 1:C:146:TRP:CH2  | 1:D:102:SER:CB   | 2.85                     | 0.59              |
| 1:A:105:LEU:HD22 | 1:E:147:THR:CG2  | 2.33                     | 0.59              |
| 1:D:147:THR:CG2  | 1:E:105:LEU:HD22 | 2.33                     | 0.59              |
| 1:E:117:VAL:HG23 | 1:E:117:VAL:O    | 2.03                     | 0.59              |
| 1:E:52:ILE:CG2   | 1:E:54:LEU:HG    | 2.33                     | 0.59              |
| 1:B:147:THR:CG2  | 1:C:105:LEU:HD22 | 2.33                     | 0.59              |
| 1:D:77:LEU:CD1   | 1:D:78:THR:H     | 2.16                     | 0.59              |
| 1:A:21:ILE:HD12  | 1:B:5:ARG:CZ     | 2.33                     | 0.59              |
| 1:A:147:THR:CA   | 1:B:105:LEU:HD13 | 2.32                     | 0.59              |
| 1:B:117:VAL:O    | 1:B:117:VAL:HG23 | 2.03                     | 0.59              |
| 1:C:21:ILE:HD12  | 1:D:5:ARG:CZ     | 2.33                     | 0.58              |
| 1:A:170:THR:HG22 | 1:A:171:ARG:N    | 2.18                     | 0.58              |
| 1:C:147:THR:CG2  | 1:D:105:LEU:HD22 | 2.33                     | 0.58              |
| 1:D:131:LEU:HD13 | 1:D:202:PHE:CE2  | 2.38                     | 0.58              |
| 1:D:33:PHE:CE1   | 1:D:35:TYR:CE1   | 2.83                     | 0.58              |
| 1:C:74:PHE:CE2   | 1:C:77:LEU:CB    | 2.84                     | 0.58              |
| 1:A:117:VAL:O    | 1:A:117:VAL:HG23 | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:7:GLU:HG2    | 1:B:11:ASP:OD2   | 2.04                     | 0.58              |
| 1:D:95:VAL:HG13  | 1:E:121:LYS:HD2  | 1.85                     | 0.58              |
| 1:D:117:VAL:O    | 1:D:117:VAL:HG23 | 2.03                     | 0.58              |
| 1:D:170:THR:HG22 | 1:D:171:ARG:N    | 2.18                     | 0.58              |
| 1:E:23:ILE:HD11  | 1:E:29:VAL:HG13  | 1.83                     | 0.58              |
| 1:A:79:VAL:HG22  | 1:A:80:PRO:N     | 2.19                     | 0.58              |
| 1:E:77:LEU:CD1   | 1:E:78:THR:H     | 2.16                     | 0.58              |
| 1:C:95:VAL:HG13  | 1:D:121:LYS:HD2  | 1.85                     | 0.58              |
| 1:D:52:ILE:CG2   | 1:D:54:LEU:HG    | 2.33                     | 0.58              |
| 1:B:120:LEU:HD12 | 1:B:120:LEU:N    | 2.19                     | 0.58              |
| 1:A:74:PHE:CZ    | 1:A:77:LEU:HA    | 2.39                     | 0.58              |
| 1:B:24:GLU:C     | 1:C:3:ARG:HB3    | 2.19                     | 0.58              |
| 1:C:7:GLU:HG2    | 1:C:11:ASP:OD2   | 2.04                     | 0.58              |
| 1:A:7:GLU:HG2    | 1:A:11:ASP:OD2   | 2.04                     | 0.58              |
| 1:D:146:TRP:CZ2  | 1:E:117:VAL:O    | 2.57                     | 0.58              |
| 1:C:47:ASN:HD21  | 1:D:42:ARG:HD2   | 1.65                     | 0.58              |
| 1:B:170:THR:HG22 | 1:B:171:ARG:N    | 2.18                     | 0.58              |
| 1:B:52:ILE:CG2   | 1:B:54:LEU:HG    | 2.33                     | 0.58              |
| 1:D:79:VAL:HG22  | 1:D:80:PRO:N     | 2.19                     | 0.58              |
| 1:C:117:VAL:O    | 1:C:117:VAL:HG23 | 2.04                     | 0.58              |
| 1:C:120:LEU:N    | 1:C:120:LEU:HD12 | 2.19                     | 0.58              |
| 1:C:52:ILE:CG2   | 1:C:54:LEU:HG    | 2.33                     | 0.58              |
| 1:C:146:TRP:CZ2  | 1:D:117:VAL:O    | 2.57                     | 0.58              |
| 1:D:131:LEU:CD1  | 1:D:203:ARG:HA   | 2.31                     | 0.58              |
| 1:A:95:VAL:HG13  | 1:B:121:LYS:HD2  | 1.85                     | 0.58              |
| 1:B:146:TRP:CZ2  | 1:C:117:VAL:O    | 2.57                     | 0.58              |
| 1:C:179:GLN:HG2  | 1:C:198:LEU:HD23 | 1.86                     | 0.58              |
| 1:B:183:ARG:CG   | 1:B:194:GLU:HG2  | 2.07                     | 0.58              |
| 1:B:66:ASN:CG    | 1:B:70:GLU:OE1   | 2.43                     | 0.58              |
| 1:B:21:ILE:HD12  | 1:C:5:ARG:CZ     | 2.33                     | 0.57              |
| 1:E:79:VAL:HG22  | 1:E:80:PRO:N     | 2.19                     | 0.57              |
| 1:C:66:ASN:CG    | 1:C:70:GLU:OE1   | 2.43                     | 0.57              |
| 1:B:79:VAL:HG22  | 1:B:80:PRO:N     | 2.19                     | 0.57              |
| 1:D:161:VAL:HB   | 1:D:177:ALA:HB3  | 1.87                     | 0.57              |
| 1:D:7:GLU:HG2    | 1:D:11:ASP:OD2   | 2.04                     | 0.57              |
| 1:D:21:ILE:HD12  | 1:E:5:ARG:CZ     | 2.33                     | 0.57              |
| 1:D:124:LEU:CD2  | 1:D:141:LEU:HD13 | 2.35                     | 0.57              |
| 1:A:52:ILE:CG2   | 1:A:54:LEU:HG    | 2.33                     | 0.57              |
| 1:A:117:VAL:O    | 1:E:146:TRP:CZ2  | 2.57                     | 0.57              |
| 1:E:7:GLU:HG2    | 1:E:11:ASP:OD2   | 2.04                     | 0.57              |
| 1:C:124:LEU:CD2  | 1:C:141:LEU:HD13 | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:179:GLN:HG2  | 1:D:198:LEU:HD23 | 1.86                     | 0.57              |
| 1:D:66:ASN:CG    | 1:D:70:GLU:OE1   | 2.43                     | 0.57              |
| 1:D:120:LEU:N    | 1:D:120:LEU:HD12 | 2.19                     | 0.57              |
| 1:A:146:TRP:CZ2  | 1:B:117:VAL:O    | 2.57                     | 0.57              |
| 1:A:45:VAL:HG13  | 1:A:46:GLU:N     | 2.20                     | 0.57              |
| 1:E:45:VAL:HG13  | 1:E:46:GLU:N     | 2.20                     | 0.57              |
| 1:E:66:ASN:CG    | 1:E:70:GLU:OE1   | 2.42                     | 0.57              |
| 1:C:161:VAL:HB   | 1:C:177:ALA:HB3  | 1.87                     | 0.57              |
| 1:A:161:VAL:HB   | 1:A:177:ALA:HB3  | 1.87                     | 0.57              |
| 1:A:77:LEU:CD1   | 1:A:78:THR:H     | 2.16                     | 0.57              |
| 1:B:77:LEU:CD1   | 1:B:78:THR:H     | 2.16                     | 0.57              |
| 1:A:179:GLN:HG2  | 1:A:198:LEU:HD23 | 1.86                     | 0.57              |
| 1:D:125:SER:HB2  | 1:E:39:LYS:HZ3   | 1.48                     | 0.57              |
| 1:E:161:VAL:HB   | 1:E:177:ALA:HB3  | 1.87                     | 0.56              |
| 1:B:95:VAL:HG13  | 1:C:121:LYS:HD2  | 1.85                     | 0.56              |
| 1:C:45:VAL:HG13  | 1:C:46:GLU:N     | 2.20                     | 0.56              |
| 1:B:124:LEU:CD2  | 1:B:141:LEU:HD13 | 2.35                     | 0.56              |
| 1:A:120:LEU:N    | 1:A:120:LEU:HD12 | 2.19                     | 0.56              |
| 1:A:121:LYS:HD2  | 1:E:95:VAL:HG13  | 1.85                     | 0.56              |
| 1:A:5:ARG:CZ     | 1:E:21:ILE:HD12  | 2.33                     | 0.56              |
| 1:A:81:ILE:CD1   | 1:A:104:LYS:CE   | 2.15                     | 0.56              |
| 1:C:79:VAL:HG22  | 1:C:80:PRO:N     | 2.19                     | 0.56              |
| 1:E:120:LEU:HD12 | 1:E:120:LEU:N    | 2.19                     | 0.56              |
| 1:E:74:PHE:CE2   | 1:E:77:LEU:CB    | 2.84                     | 0.56              |
| 1:B:146:TRP:C    | 1:C:105:LEU:HD12 | 2.16                     | 0.56              |
| 1:A:163:LEU:HD13 | 1:A:174:LEU:HD22 | 1.87                     | 0.56              |
| 1:C:77:LEU:CD1   | 1:C:78:THR:H     | 2.16                     | 0.56              |
| 1:C:147:THR:HG23 | 1:C:148:HIS:N    | 2.20                     | 0.56              |
| 1:B:179:GLN:HG2  | 1:B:198:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:149:SER:H    | 1:B:107:ARG:HH22 | 1.54                     | 0.56              |
| 1:B:12:VAL:HG23  | 1:B:13:LEU:N     | 2.20                     | 0.56              |
| 1:B:161:VAL:HB   | 1:B:177:ALA:HB3  | 1.87                     | 0.56              |
| 1:C:12:VAL:HG23  | 1:C:13:LEU:N     | 2.20                     | 0.56              |
| 1:E:124:LEU:CD2  | 1:E:141:LEU:HD13 | 2.35                     | 0.56              |
| 1:B:163:LEU:HD13 | 1:B:174:LEU:HD22 | 1.87                     | 0.56              |
| 1:A:12:VAL:HG23  | 1:A:13:LEU:N     | 2.20                     | 0.56              |
| 1:D:147:THR:HG22 | 1:E:105:LEU:HD13 | 0.63                     | 0.56              |
| 1:B:33:PHE:HE1   | 1:B:35:TYR:CE2   | 2.22                     | 0.56              |
| 1:D:12:VAL:HG23  | 1:D:13:LEU:N     | 2.20                     | 0.56              |
| 1:E:12:VAL:HG23  | 1:E:13:LEU:N     | 2.20                     | 0.56              |
| 1:B:147:THR:HG23 | 1:B:148:HIS:N    | 2.20                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:149:SER:H    | 1:C:107:ARG:HH22 | 1.54                     | 0.56              |
| 1:A:107:ARG:HH22 | 1:E:149:SER:H    | 1.54                     | 0.56              |
| 1:E:147:THR:HG23 | 1:E:148:HIS:N    | 2.20                     | 0.56              |
| 1:E:179:GLN:HG2  | 1:E:198:LEU:HD23 | 1.86                     | 0.56              |
| 1:C:74:PHE:CZ    | 1:C:77:LEU:HA    | 2.39                     | 0.56              |
| 1:A:124:LEU:CD2  | 1:A:141:LEU:HD13 | 2.35                     | 0.56              |
| 1:D:46:GLU:HG3   | 1:D:47:ASN:N     | 2.21                     | 0.56              |
| 1:B:45:VAL:HG13  | 1:B:46:GLU:N     | 2.20                     | 0.56              |
| 1:B:46:GLU:HG3   | 1:B:47:ASN:N     | 2.21                     | 0.56              |
| 1:D:163:LEU:HD13 | 1:D:174:LEU:HD22 | 1.87                     | 0.56              |
| 1:A:46:GLU:HG3   | 1:A:47:ASN:N     | 2.21                     | 0.56              |
| 1:A:105:LEU:HD13 | 1:E:147:THR:HG22 | 0.63                     | 0.56              |
| 1:D:147:THR:HG23 | 1:D:148:HIS:N    | 2.20                     | 0.55              |
| 1:E:163:LEU:HD13 | 1:E:174:LEU:HD22 | 1.87                     | 0.55              |
| 1:B:21:ILE:CG2   | 1:C:1:SER:OG     | 2.49                     | 0.55              |
| 1:D:74:PHE:CZ    | 1:D:77:LEU:HA    | 2.39                     | 0.55              |
| 1:E:86:THR:CG2   | 1:E:87:PRO:HD2   | 2.37                     | 0.55              |
| 1:A:66:ASN:CG    | 1:A:70:GLU:OE1   | 2.42                     | 0.55              |
| 1:E:170:THR:HG22 | 1:E:172:PHE:H    | 1.72                     | 0.55              |
| 1:B:170:THR:HG22 | 1:B:172:PHE:H    | 1.72                     | 0.55              |
| 1:A:74:PHE:CE2   | 1:A:77:LEU:CB    | 2.84                     | 0.55              |
| 1:D:45:VAL:HG13  | 1:D:46:GLU:N     | 2.20                     | 0.55              |
| 1:C:163:LEU:HD23 | 1:C:163:LEU:N    | 2.22                     | 0.55              |
| 1:C:46:GLU:HG3   | 1:C:47:ASN:N     | 2.21                     | 0.55              |
| 1:D:131:LEU:HD21 | 1:D:172:PHE:HE1  | 1.70                     | 0.55              |
| 1:A:147:THR:HG23 | 1:A:148:HIS:N    | 2.20                     | 0.55              |
| 1:B:86:THR:CG2   | 1:B:87:PRO:HD2   | 2.37                     | 0.55              |
| 1:E:74:PHE:CZ    | 1:E:77:LEU:HA    | 2.39                     | 0.55              |
| 1:C:108:VAL:HG12 | 1:C:114:VAL:HG22 | 1.89                     | 0.55              |
| 1:D:86:THR:CG2   | 1:D:87:PRO:HD2   | 2.37                     | 0.55              |
| 1:E:200:PHE:HD2  | 1:E:202:PHE:HD1  | 1.55                     | 0.55              |
| 1:D:170:THR:HG22 | 1:D:172:PHE:H    | 1.72                     | 0.55              |
| 1:A:86:THR:CG2   | 1:A:87:PRO:HD2   | 2.37                     | 0.55              |
| 1:E:163:LEU:N    | 1:E:163:LEU:HD23 | 2.22                     | 0.55              |
| 1:C:149:SER:H    | 1:D:107:ARG:HH22 | 1.53                     | 0.55              |
| 1:D:124:LEU:HD12 | 1:D:124:LEU:C    | 2.27                     | 0.55              |
| 1:D:33:PHE:HE1   | 1:D:35:TYR:CE2   | 2.22                     | 0.55              |
| 1:B:108:VAL:HG12 | 1:B:114:VAL:HG22 | 1.89                     | 0.55              |
| 1:D:183:ARG:CG   | 1:D:194:GLU:HG2  | 2.07                     | 0.55              |
| 1:C:147:THR:HG22 | 1:D:105:LEU:HD13 | 0.63                     | 0.55              |
| 1:A:98:PRO:HB3   | 1:A:122:VAL:HG12 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:200:PHE:HD2  | 1:B:202:PHE:HD1  | 1.55                     | 0.55              |
| 1:C:124:LEU:C    | 1:C:124:LEU:HD12 | 2.27                     | 0.54              |
| 1:C:163:LEU:HD13 | 1:C:174:LEU:HD22 | 1.87                     | 0.54              |
| 1:C:98:PRO:HB3   | 1:C:122:VAL:HG12 | 1.89                     | 0.54              |
| 1:D:108:VAL:HG12 | 1:D:114:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:163:LEU:N    | 1:B:163:LEU:HD23 | 2.22                     | 0.54              |
| 1:A:108:VAL:HG12 | 1:A:114:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:170:THR:HG22 | 1:A:172:PHE:H    | 1.72                     | 0.54              |
| 1:D:149:SER:H    | 1:E:107:ARG:HH22 | 1.54                     | 0.54              |
| 1:C:86:THR:CG2   | 1:C:87:PRO:HD2   | 2.37                     | 0.54              |
| 1:A:49:GLU:CG    | 1:B:41:PHE:CE1   | 2.82                     | 0.54              |
| 1:B:74:PHE:CZ    | 1:B:77:LEU:HA    | 2.39                     | 0.54              |
| 1:E:98:PRO:HB3   | 1:E:122:VAL:HG12 | 1.89                     | 0.54              |
| 1:E:46:GLU:HG3   | 1:E:47:ASN:N     | 2.21                     | 0.54              |
| 1:C:24:GLU:C     | 1:D:3:ARG:CB     | 2.74                     | 0.54              |
| 1:E:108:VAL:HG12 | 1:E:114:VAL:HG22 | 1.89                     | 0.54              |
| 1:E:124:LEU:C    | 1:E:124:LEU:HD12 | 2.27                     | 0.54              |
| 1:E:34:GLU:OE2   | 1:E:158:ASN:HB2  | 2.08                     | 0.54              |
| 1:C:174:LEU:C    | 1:C:174:LEU:HD23 | 2.28                     | 0.54              |
| 1:B:174:LEU:C    | 1:B:174:LEU:HD23 | 2.28                     | 0.54              |
| 1:B:9:LEU:O      | 1:B:12:VAL:HG22  | 2.07                     | 0.54              |
| 1:E:9:LEU:O      | 1:E:12:VAL:HG22  | 2.07                     | 0.54              |
| 1:D:200:PHE:HD2  | 1:D:202:PHE:HD1  | 1.55                     | 0.54              |
| 1:B:124:LEU:C    | 1:B:124:LEU:HD12 | 2.27                     | 0.54              |
| 1:A:163:LEU:N    | 1:A:163:LEU:HD23 | 2.22                     | 0.54              |
| 1:D:24:GLU:C     | 1:E:3:ARG:CB     | 2.74                     | 0.54              |
| 1:C:9:LEU:O      | 1:C:12:VAL:HG22  | 2.07                     | 0.54              |
| 1:C:170:THR:HG22 | 1:C:172:PHE:H    | 1.72                     | 0.54              |
| 1:B:49:GLU:CG    | 1:C:41:PHE:CE1   | 2.82                     | 0.54              |
| 1:D:77:LEU:HG    | 1:D:78:THR:N     | 2.23                     | 0.54              |
| 1:B:175:LEU:CD2  | 1:B:202:PHE:HA   | 2.36                     | 0.54              |
| 1:D:11:ASP:CG    | 1:D:68:PHE:CE2   | 2.81                     | 0.54              |
| 1:D:34:GLU:OE2   | 1:D:158:ASN:HB2  | 2.08                     | 0.54              |
| 1:A:200:PHE:HD2  | 1:A:202:PHE:HD1  | 1.55                     | 0.54              |
| 1:A:41:PHE:CZ    | 1:E:47:ASN:HA    | 2.28                     | 0.54              |
| 1:D:163:LEU:N    | 1:D:163:LEU:HD23 | 2.22                     | 0.54              |
| 1:D:175:LEU:CD2  | 1:D:202:PHE:HA   | 2.36                     | 0.54              |
| 1:A:3:ARG:HA     | 1:E:24:GLU:CA    | 2.14                     | 0.54              |
| 1:C:56:THR:HG23  | 1:C:56:THR:O     | 2.08                     | 0.54              |
| 1:A:174:LEU:HD23 | 1:A:174:LEU:C    | 2.28                     | 0.54              |
| 1:B:77:LEU:HG    | 1:B:78:THR:N     | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:11:ASP:CG    | 1:B:68:PHE:CE2   | 2.81                     | 0.54              |
| 1:E:11:ASP:CG    | 1:E:68:PHE:CE2   | 2.81                     | 0.54              |
| 1:D:9:LEU:O      | 1:D:12:VAL:HG22  | 2.07                     | 0.54              |
| 1:D:98:PRO:HB3   | 1:D:122:VAL:HG12 | 1.89                     | 0.54              |
| 1:E:174:LEU:HD23 | 1:E:174:LEU:C    | 2.28                     | 0.54              |
| 1:A:147:THR:HG22 | 1:B:105:LEU:HD13 | 0.63                     | 0.54              |
| 1:A:77:LEU:HG    | 1:A:78:THR:N     | 2.23                     | 0.54              |
| 1:A:9:LEU:O      | 1:A:12:VAL:HG22  | 2.07                     | 0.54              |
| 1:D:174:LEU:C    | 1:D:174:LEU:HD23 | 2.28                     | 0.53              |
| 1:A:11:ASP:CG    | 1:A:68:PHE:CE2   | 2.81                     | 0.53              |
| 1:B:98:PRO:HB3   | 1:B:122:VAL:HG12 | 1.89                     | 0.53              |
| 1:D:56:THR:HG23  | 1:D:56:THR:O     | 2.08                     | 0.53              |
| 1:A:124:LEU:HD12 | 1:A:124:LEU:C    | 2.27                     | 0.53              |
| 1:C:34:GLU:OE2   | 1:C:158:ASN:HB2  | 2.08                     | 0.53              |
| 1:B:47:ASN:HA    | 1:C:41:PHE:CZ    | 2.28                     | 0.53              |
| 1:B:56:THR:HG23  | 1:B:56:THR:O     | 2.08                     | 0.53              |
| 1:B:74:PHE:CE2   | 1:B:77:LEU:CB    | 2.84                     | 0.53              |
| 1:A:42:ARG:CD    | 1:E:47:ASN:ND2   | 2.66                     | 0.53              |
| 1:A:137:VAL:HG22 | 1:A:138:THR:N    | 2.24                     | 0.53              |
| 1:C:77:LEU:HG    | 1:C:78:THR:N     | 2.23                     | 0.53              |
| 1:C:149:SER:N    | 1:D:107:ARG:HH22 | 2.07                     | 0.53              |
| 1:D:86:THR:HG23  | 1:D:87:PRO:HD2   | 1.91                     | 0.53              |
| 1:A:34:GLU:OE2   | 1:A:158:ASN:HB2  | 2.08                     | 0.53              |
| 1:D:185:GLN:HG2  | 1:D:186:TYR:N    | 2.24                     | 0.53              |
| 1:A:115:THR:HG23 | 1:A:115:THR:O    | 2.09                     | 0.53              |
| 1:E:185:GLN:HG2  | 1:E:186:TYR:N    | 2.24                     | 0.53              |
| 1:D:137:VAL:HG22 | 1:D:138:THR:N    | 2.24                     | 0.53              |
| 1:C:185:GLN:HG2  | 1:C:186:TYR:N    | 2.24                     | 0.53              |
| 1:E:183:ARG:CG   | 1:E:194:GLU:HG2  | 2.07                     | 0.53              |
| 1:B:147:THR:HG22 | 1:C:105:LEU:HD13 | 0.63                     | 0.53              |
| 1:C:35:TYR:HD2   | 1:C:179:GLN:CD   | 2.12                     | 0.53              |
| 1:C:200:PHE:HD2  | 1:C:202:PHE:HD1  | 1.55                     | 0.53              |
| 1:E:37:LEU:HD11  | 1:E:52:ILE:HG23  | 1.91                     | 0.53              |
| 1:D:37:LEU:HD11  | 1:D:52:ILE:HG23  | 1.91                     | 0.53              |
| 1:B:34:GLU:OE2   | 1:B:158:ASN:HB2  | 2.07                     | 0.53              |
| 1:A:185:GLN:HG2  | 1:A:186:TYR:N    | 2.24                     | 0.53              |
| 1:E:33:PHE:HE1   | 1:E:35:TYR:CE2   | 2.22                     | 0.53              |
| 1:E:86:THR:HG23  | 1:E:87:PRO:HD2   | 1.91                     | 0.53              |
| 1:C:87:PRO:HB2   | 1:C:89:ILE:HD13  | 1.90                     | 0.53              |
| 1:B:137:VAL:HG22 | 1:B:138:THR:N    | 2.24                     | 0.53              |
| 1:A:19:LEU:HD22  | 1:A:19:LEU:H     | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:19:LEU:H     | 1:C:19:LEU:HD22  | 1.74                     | 0.53              |
| 1:C:131:LEU:HD21 | 1:C:172:PHE:HE1  | 1.70                     | 0.53              |
| 1:A:3:ARG:HD2    | 1:A:3:ARG:C      | 2.29                     | 0.53              |
| 1:E:77:LEU:HG    | 1:E:78:THR:N     | 2.23                     | 0.52              |
| 1:D:141:LEU:N    | 1:D:141:LEU:HD23 | 2.24                     | 0.52              |
| 1:D:35:TYR:HD2   | 1:D:179:GLN:CD   | 2.12                     | 0.52              |
| 1:B:35:TYR:HD2   | 1:B:179:GLN:CD   | 2.12                     | 0.52              |
| 1:C:11:ASP:CG    | 1:C:68:PHE:CE2   | 2.81                     | 0.52              |
| 1:D:19:LEU:H     | 1:D:19:LEU:HD22  | 1.74                     | 0.52              |
| 1:B:185:GLN:HG2  | 1:B:186:TYR:N    | 2.24                     | 0.52              |
| 1:D:149:SER:N    | 1:E:107:ARG:HH22 | 2.07                     | 0.52              |
| 1:B:149:SER:N    | 1:C:107:ARG:HH22 | 2.07                     | 0.52              |
| 1:A:102:SER:HB3  | 1:E:146:TRP:CH2  | 2.44                     | 0.52              |
| 1:A:37:LEU:HD11  | 1:A:52:ILE:HG23  | 1.91                     | 0.52              |
| 1:A:72:THR:HG23  | 1:A:72:THR:O     | 2.10                     | 0.52              |
| 1:B:115:THR:HG23 | 1:B:115:THR:O    | 2.09                     | 0.52              |
| 1:B:72:THR:HG23  | 1:B:72:THR:O     | 2.10                     | 0.52              |
| 1:C:72:THR:O     | 1:C:72:THR:HG23  | 2.09                     | 0.52              |
| 1:D:115:THR:HG23 | 1:D:115:THR:O    | 2.09                     | 0.52              |
| 1:E:35:TYR:HD2   | 1:E:179:GLN:CD   | 2.12                     | 0.52              |
| 1:A:35:TYR:HD2   | 1:A:179:GLN:CD   | 2.12                     | 0.52              |
| 1:A:87:PRO:HB2   | 1:A:89:ILE:HD13  | 1.90                     | 0.52              |
| 1:C:137:VAL:HG22 | 1:C:138:THR:N    | 2.24                     | 0.52              |
| 1:E:19:LEU:HD22  | 1:E:19:LEU:H     | 1.74                     | 0.52              |
| 1:C:174:LEU:CD1  | 1:C:200:PHE:HE1  | 2.23                     | 0.52              |
| 1:C:37:LEU:HD11  | 1:C:52:ILE:HG23  | 1.91                     | 0.52              |
| 1:D:174:LEU:CD1  | 1:D:200:PHE:HE1  | 2.23                     | 0.52              |
| 1:A:131:LEU:HD21 | 1:A:172:PHE:HE1  | 1.70                     | 0.52              |
| 1:E:115:THR:HG23 | 1:E:115:THR:O    | 2.09                     | 0.52              |
| 1:C:101:PHE:HE2  | 1:C:121:LYS:HB2  | 1.74                     | 0.52              |
| 1:B:37:LEU:HD11  | 1:B:52:ILE:HG23  | 1.91                     | 0.52              |
| 1:B:86:THR:HG23  | 1:B:87:PRO:HD2   | 1.91                     | 0.52              |
| 1:A:174:LEU:CD1  | 1:A:200:PHE:HE1  | 2.23                     | 0.52              |
| 1:B:7:GLU:O      | 1:B:10:GLN:HG2   | 2.10                     | 0.52              |
| 1:E:137:VAL:HG22 | 1:E:138:THR:N    | 2.24                     | 0.52              |
| 1:D:72:THR:O     | 1:D:72:THR:HG23  | 2.10                     | 0.52              |
| 1:C:141:LEU:HD23 | 1:C:141:LEU:N    | 2.25                     | 0.52              |
| 1:B:33:PHE:CE2   | 1:B:58:LEU:HD21  | 2.45                     | 0.52              |
| 1:A:56:THR:HG23  | 1:A:56:THR:O     | 2.08                     | 0.52              |
| 1:A:86:THR:HG23  | 1:A:87:PRO:HD2   | 1.91                     | 0.52              |
| 1:E:91:ILE:CD1   | 1:E:122:VAL:HG11 | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:174:LEU:CD1  | 1:E:200:PHE:HE1  | 2.23                     | 0.52              |
| 1:E:87:PRO:HB2   | 1:E:89:ILE:HD13  | 1.90                     | 0.52              |
| 1:D:74:PHE:CE2   | 1:D:77:LEU:CB    | 2.84                     | 0.52              |
| 1:D:87:PRO:HB2   | 1:D:89:ILE:HD13  | 1.90                     | 0.52              |
| 1:B:174:LEU:CD1  | 1:B:200:PHE:HE1  | 2.23                     | 0.52              |
| 1:E:56:THR:O     | 1:E:56:THR:HG23  | 2.08                     | 0.52              |
| 1:D:33:PHE:CE2   | 1:D:58:LEU:HD21  | 2.45                     | 0.52              |
| 1:A:146:TRP:CA   | 1:B:105:LEU:HD12 | 2.40                     | 0.52              |
| 1:A:141:LEU:N    | 1:A:141:LEU:HD23 | 2.24                     | 0.52              |
| 1:C:7:GLU:O      | 1:C:10:GLN:HG2   | 2.10                     | 0.52              |
| 1:A:7:GLU:O      | 1:A:10:GLN:HG2   | 2.10                     | 0.52              |
| 1:A:149:SER:N    | 1:B:107:ARG:HH22 | 2.07                     | 0.52              |
| 1:E:3:ARG:HD2    | 1:E:3:ARG:C      | 2.29                     | 0.52              |
| 1:E:33:PHE:CE2   | 1:E:58:LEU:HD21  | 2.45                     | 0.51              |
| 1:C:118:PRO:HB2  | 1:C:120:LEU:HD11 | 1.92                     | 0.51              |
| 1:C:33:PHE:HE1   | 1:C:35:TYR:CE2   | 2.22                     | 0.51              |
| 1:E:7:GLU:O      | 1:E:10:GLN:HG2   | 2.10                     | 0.51              |
| 1:B:19:LEU:H     | 1:B:19:LEU:HD22  | 1.74                     | 0.51              |
| 1:E:118:PRO:HB2  | 1:E:120:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:175:LEU:CD2  | 1:C:202:PHE:HA   | 2.36                     | 0.51              |
| 1:A:118:PRO:HB2  | 1:A:120:LEU:HD11 | 1.93                     | 0.51              |
| 1:A:107:ARG:HH22 | 1:E:149:SER:N    | 2.07                     | 0.51              |
| 1:D:7:GLU:O      | 1:D:10:GLN:HG2   | 2.10                     | 0.51              |
| 1:E:175:LEU:CD2  | 1:E:202:PHE:HA   | 2.36                     | 0.51              |
| 1:C:146:TRP:CA   | 1:D:105:LEU:HD12 | 2.40                     | 0.51              |
| 1:D:118:PRO:HB2  | 1:D:120:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:131:LEU:HD21 | 1:B:172:PHE:HE1  | 1.70                     | 0.51              |
| 1:B:160:LYS:HD2  | 1:B:160:LYS:N    | 2.26                     | 0.51              |
| 1:A:21:ILE:CG2   | 1:B:1:SER:OG     | 2.49                     | 0.51              |
| 1:B:87:PRO:HB2   | 1:B:89:ILE:HD13  | 1.90                     | 0.51              |
| 1:D:3:ARG:HD2    | 1:D:3:ARG:C      | 2.29                     | 0.51              |
| 1:B:3:ARG:HD2    | 1:B:3:ARG:C      | 2.30                     | 0.51              |
| 1:B:9:LEU:N      | 1:B:9:LEU:HD12   | 2.26                     | 0.51              |
| 1:E:131:LEU:HD21 | 1:E:172:PHE:HE1  | 1.70                     | 0.51              |
| 1:B:47:ASN:ND2   | 1:C:42:ARG:CD    | 2.66                     | 0.51              |
| 1:B:146:TRP:CA   | 1:C:105:LEU:HD12 | 2.40                     | 0.51              |
| 1:C:146:TRP:CH2  | 1:D:102:SER:HB3  | 2.44                     | 0.51              |
| 1:D:160:LYS:HD2  | 1:D:160:LYS:N    | 2.26                     | 0.51              |
| 1:A:146:TRP:CH2  | 1:B:102:SER:HB3  | 2.44                     | 0.51              |
| 1:B:24:GLU:C     | 1:C:3:ARG:CB     | 2.74                     | 0.51              |
| 1:C:3:ARG:C      | 1:C:3:ARG:HD2    | 2.29                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:72:THR:O     | 1:E:72:THR:HG23  | 2.10                     | 0.51              |
| 1:A:9:LEU:N      | 1:A:9:LEU:HD12   | 2.26                     | 0.51              |
| 1:C:115:THR:O    | 1:C:115:THR:HG23 | 2.09                     | 0.51              |
| 1:B:118:PRO:HB2  | 1:B:120:LEU:HD11 | 1.93                     | 0.51              |
| 1:A:160:LYS:N    | 1:A:160:LYS:HD2  | 2.26                     | 0.51              |
| 1:A:77:LEU:CG    | 1:A:78:THR:N     | 2.74                     | 0.51              |
| 1:C:77:LEU:CG    | 1:C:78:THR:N     | 2.74                     | 0.51              |
| 1:C:86:THR:HG23  | 1:C:87:PRO:HD2   | 1.91                     | 0.51              |
| 1:A:33:PHE:CE2   | 1:A:58:LEU:HD21  | 2.45                     | 0.51              |
| 1:D:146:TRP:CA   | 1:E:105:LEU:HD12 | 2.40                     | 0.51              |
| 1:B:146:TRP:CH2  | 1:C:102:SER:HB3  | 2.44                     | 0.51              |
| 1:B:174:LEU:CG   | 1:B:200:PHE:CZ   | 2.94                     | 0.51              |
| 1:D:26:ASP:OD1   | 1:E:2:ARG:CZ     | 2.59                     | 0.51              |
| 1:C:33:PHE:CE2   | 1:C:58:LEU:HD21  | 2.45                     | 0.51              |
| 1:A:105:LEU:HD12 | 1:E:146:TRP:CA   | 2.40                     | 0.51              |
| 1:A:33:PHE:HE1   | 1:A:35:TYR:CE2   | 2.22                     | 0.51              |
| 1:A:2:ARG:CZ     | 1:E:26:ASP:OD1   | 2.59                     | 0.51              |
| 1:D:49:GLU:CD    | 1:D:95:VAL:HG11  | 2.31                     | 0.51              |
| 1:A:91:ILE:CD1   | 1:A:122:VAL:HG11 | 2.40                     | 0.51              |
| 1:C:9:LEU:N      | 1:C:9:LEU:HD12   | 2.26                     | 0.51              |
| 1:D:9:LEU:N      | 1:D:9:LEU:HD12   | 2.26                     | 0.51              |
| 1:A:117:VAL:O    | 1:E:146:TRP:HZ2  | 1.94                     | 0.50              |
| 1:D:128:LEU:HD23 | 1:D:129:ALA:N    | 2.27                     | 0.50              |
| 1:B:26:ASP:OD1   | 1:C:2:ARG:CZ     | 2.59                     | 0.50              |
| 1:D:146:TRP:HZ2  | 1:E:117:VAL:O    | 1.94                     | 0.50              |
| 1:E:101:PHE:HE2  | 1:E:121:LYS:HB2  | 1.74                     | 0.50              |
| 1:E:160:LYS:N    | 1:E:160:LYS:HD2  | 2.26                     | 0.50              |
| 1:C:49:GLU:CD    | 1:C:95:VAL:HG11  | 2.31                     | 0.50              |
| 1:E:37:LEU:CD2   | 1:E:200:PHE:CE1  | 2.95                     | 0.50              |
| 1:B:146:TRP:HZ2  | 1:C:117:VAL:O    | 1.94                     | 0.50              |
| 1:C:26:ASP:OD1   | 1:D:2:ARG:CZ     | 2.59                     | 0.50              |
| 1:B:37:LEU:CD2   | 1:B:200:PHE:CE1  | 2.95                     | 0.50              |
| 1:D:146:TRP:CH2  | 1:E:102:SER:HB3  | 2.44                     | 0.50              |
| 1:E:77:LEU:CG    | 1:E:78:THR:N     | 2.74                     | 0.50              |
| 1:C:128:LEU:HD23 | 1:C:129:ALA:N    | 2.27                     | 0.50              |
| 1:A:26:ASP:OD1   | 1:B:2:ARG:CZ     | 2.59                     | 0.50              |
| 1:B:77:LEU:CG    | 1:B:78:THR:N     | 2.74                     | 0.50              |
| 1:D:11:ASP:CG    | 1:D:68:PHE:HE2   | 2.15                     | 0.50              |
| 1:C:160:LYS:HD2  | 1:C:160:LYS:N    | 2.26                     | 0.50              |
| 1:A:47:ASN:HB3   | 1:B:41:PHE:HZ    | 0.70                     | 0.50              |
| 1:E:9:LEU:N      | 1:E:9:LEU:HD12   | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:77:LEU:CG    | 1:D:78:THR:N     | 2.74                     | 0.50              |
| 1:A:11:ASP:CG    | 1:A:68:PHE:HE2   | 2.15                     | 0.50              |
| 1:E:163:LEU:HD22 | 1:E:174:LEU:HD13 | 1.93                     | 0.50              |
| 1:E:174:LEU:CG   | 1:E:200:PHE:CZ   | 2.94                     | 0.50              |
| 1:B:49:GLU:CD    | 1:B:95:VAL:HG11  | 2.32                     | 0.50              |
| 1:C:47:ASN:ND2   | 1:D:42:ARG:CD    | 2.66                     | 0.50              |
| 1:A:105:LEU:CD2  | 1:E:147:THR:CG2  | 2.90                     | 0.50              |
| 1:B:128:LEU:HD23 | 1:B:129:ALA:N    | 2.27                     | 0.49              |
| 1:C:49:GLU:CG    | 1:D:41:PHE:CE1   | 2.82                     | 0.49              |
| 1:A:175:LEU:HD22 | 1:A:175:LEU:N    | 2.27                     | 0.49              |
| 1:A:37:LEU:CD2   | 1:A:200:PHE:CE1  | 2.95                     | 0.49              |
| 1:E:49:GLU:CD    | 1:E:95:VAL:HG11  | 2.31                     | 0.49              |
| 1:C:175:LEU:HD22 | 1:C:175:LEU:N    | 2.27                     | 0.49              |
| 1:C:96:GLY:N     | 1:D:99:GLU:OE2   | 2.45                     | 0.49              |
| 1:C:37:LEU:CD2   | 1:C:200:PHE:CE1  | 2.95                     | 0.49              |
| 1:D:175:LEU:N    | 1:D:175:LEU:HD22 | 2.28                     | 0.49              |
| 1:A:41:PHE:CE1   | 1:E:49:GLU:CG    | 2.82                     | 0.49              |
| 1:D:147:THR:CG2  | 1:E:105:LEU:CD2  | 2.90                     | 0.49              |
| 1:C:141:LEU:HD23 | 1:C:198:LEU:O    | 2.13                     | 0.49              |
| 1:C:91:ILE:CD1   | 1:C:122:VAL:HG11 | 2.40                     | 0.49              |
| 1:D:37:LEU:CD2   | 1:D:200:PHE:CE1  | 2.95                     | 0.49              |
| 1:B:91:ILE:CD1   | 1:B:122:VAL:HG11 | 2.40                     | 0.49              |
| 1:B:147:THR:CG2  | 1:C:105:LEU:CD2  | 2.90                     | 0.49              |
| 1:C:57:THR:O     | 1:C:58:LEU:HD23  | 2.13                     | 0.49              |
| 1:C:147:THR:CG2  | 1:D:105:LEU:CD2  | 2.90                     | 0.49              |
| 1:A:128:LEU:HD23 | 1:A:129:ALA:N    | 2.27                     | 0.49              |
| 1:A:49:GLU:CD    | 1:A:95:VAL:HG11  | 2.32                     | 0.49              |
| 1:E:128:LEU:HD23 | 1:E:129:ALA:N    | 2.27                     | 0.49              |
| 1:C:174:LEU:CG   | 1:C:200:PHE:CZ   | 2.94                     | 0.49              |
| 1:D:52:ILE:HG21  | 1:D:54:LEU:HG    | 1.94                     | 0.49              |
| 1:A:160:LYS:O    | 1:A:161:VAL:HG23 | 2.13                     | 0.49              |
| 1:C:11:ASP:CG    | 1:C:68:PHE:HE2   | 2.15                     | 0.49              |
| 1:D:21:ILE:HG22  | 1:D:23:ILE:HG12  | 1.95                     | 0.49              |
| 1:E:141:LEU:HD23 | 1:E:198:LEU:O    | 2.12                     | 0.49              |
| 1:C:21:ILE:HG22  | 1:C:23:ILE:HG12  | 1.95                     | 0.49              |
| 1:D:131:LEU:CD2  | 1:D:172:PHE:CE1  | 2.93                     | 0.49              |
| 1:A:145:SER:OG   | 1:A:148:HIS:HB2  | 2.13                     | 0.49              |
| 1:A:146:TRP:HZ2  | 1:B:117:VAL:O    | 1.94                     | 0.49              |
| 1:D:145:SER:OG   | 1:D:148:HIS:HB2  | 2.13                     | 0.49              |
| 1:E:174:LEU:CG   | 1:E:200:PHE:CE1  | 2.95                     | 0.49              |
| 1:B:145:SER:OG   | 1:B:148:HIS:HB2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:THR:CG2  | 1:B:105:LEU:CD2  | 2.90                     | 0.49              |
| 1:B:141:LEU:N    | 1:B:141:LEU:HD23 | 2.24                     | 0.49              |
| 1:E:52:ILE:HG21  | 1:E:54:LEU:HG    | 1.94                     | 0.49              |
| 1:E:57:THR:O     | 1:E:58:LEU:HD23  | 2.13                     | 0.49              |
| 1:D:141:LEU:HD23 | 1:D:198:LEU:O    | 2.13                     | 0.49              |
| 1:A:90:PHE:CE2   | 1:B:103:ASP:CA   | 2.91                     | 0.49              |
| 1:E:175:LEU:HD22 | 1:E:175:LEU:N    | 2.27                     | 0.49              |
| 1:B:21:ILE:HG22  | 1:B:23:ILE:HG12  | 1.95                     | 0.49              |
| 1:D:57:THR:O     | 1:D:58:LEU:HD23  | 2.13                     | 0.49              |
| 1:B:160:LYS:O    | 1:B:161:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:131:LEU:CD2  | 1:B:172:PHE:CE1  | 2.93                     | 0.49              |
| 1:A:101:PHE:CZ   | 1:A:121:LYS:HB2  | 2.48                     | 0.49              |
| 1:A:175:LEU:CD2  | 1:A:202:PHE:HA   | 2.36                     | 0.49              |
| 1:B:11:ASP:CG    | 1:B:68:PHE:HE2   | 2.15                     | 0.49              |
| 1:E:167:ALA:HB3  | 1:E:170:THR:OG1  | 2.13                     | 0.48              |
| 1:D:160:LYS:O    | 1:D:161:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:57:THR:O     | 1:B:58:LEU:HD23  | 2.13                     | 0.48              |
| 1:A:200:PHE:HD2  | 1:A:202:PHE:CD1  | 2.31                     | 0.48              |
| 1:E:11:ASP:CG    | 1:E:68:PHE:HE2   | 2.15                     | 0.48              |
| 1:E:160:LYS:O    | 1:E:161:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:175:LEU:N    | 1:B:175:LEU:HD22 | 2.28                     | 0.48              |
| 1:A:175:LEU:HD21 | 1:A:203:ARG:HG2  | 1.95                     | 0.48              |
| 1:D:47:ASN:ND2   | 1:E:42:ARG:CD    | 2.66                     | 0.48              |
| 1:E:101:PHE:CZ   | 1:E:121:LYS:HB2  | 2.48                     | 0.48              |
| 1:C:160:LYS:O    | 1:C:161:VAL:HG23 | 2.13                     | 0.48              |
| 1:D:174:LEU:CG   | 1:D:200:PHE:CE1  | 2.95                     | 0.48              |
| 1:B:101:PHE:CZ   | 1:B:121:LYS:HB2  | 2.48                     | 0.48              |
| 1:A:161:VAL:HG12 | 1:A:162:ASP:N    | 2.29                     | 0.48              |
| 1:A:81:ILE:CD1   | 1:A:116:TYR:CE2  | 2.95                     | 0.48              |
| 1:E:79:VAL:CG2   | 1:E:83:GLU:HG3   | 2.43                     | 0.48              |
| 1:C:52:ILE:HG21  | 1:C:54:LEU:HG    | 1.94                     | 0.48              |
| 1:C:146:TRP:HZ2  | 1:D:117:VAL:O    | 1.94                     | 0.48              |
| 1:D:175:LEU:HD21 | 1:D:203:ARG:HG2  | 1.96                     | 0.48              |
| 1:B:141:LEU:HD23 | 1:B:198:LEU:O    | 2.13                     | 0.48              |
| 1:A:141:LEU:HD23 | 1:A:198:LEU:O    | 2.13                     | 0.48              |
| 1:E:145:SER:OG   | 1:E:148:HIS:HB2  | 2.13                     | 0.48              |
| 1:B:79:VAL:CG2   | 1:B:83:GLU:HG3   | 2.43                     | 0.48              |
| 1:E:33:PHE:CE2   | 1:E:89:ILE:HG21  | 2.49                     | 0.48              |
| 1:A:25:ASP:O     | 1:B:1:SER:C      | 2.49                     | 0.48              |
| 1:B:167:ALA:HB3  | 1:B:170:THR:OG1  | 2.13                     | 0.48              |
| 1:B:175:LEU:HD21 | 1:B:203:ARG:HG2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1:SER:CB     | 1:A:5:ARG:HH21   | 2.27                     | 0.48              |
| 1:C:101:PHE:CZ   | 1:C:121:LYS:HB2  | 2.48                     | 0.48              |
| 1:B:1:SER:CB     | 1:B:5:ARG:HH21   | 2.27                     | 0.48              |
| 1:A:79:VAL:CG2   | 1:A:83:GLU:HG3   | 2.43                     | 0.48              |
| 1:C:79:VAL:CG2   | 1:C:83:GLU:HG3   | 2.43                     | 0.48              |
| 1:D:25:ASP:O     | 1:E:1:SER:C      | 2.49                     | 0.48              |
| 1:C:167:ALA:HB3  | 1:C:170:THR:OG1  | 2.13                     | 0.48              |
| 1:D:200:PHE:HD2  | 1:D:202:PHE:CD1  | 2.31                     | 0.48              |
| 1:D:87:PRO:HB2   | 1:D:89:ILE:CD1   | 2.44                     | 0.48              |
| 1:A:167:ALA:HB3  | 1:A:170:THR:OG1  | 2.13                     | 0.48              |
| 1:A:57:THR:O     | 1:A:58:LEU:HD23  | 2.13                     | 0.48              |
| 1:A:33:PHE:CE2   | 1:A:89:ILE:HG21  | 2.49                     | 0.48              |
| 1:D:91:ILE:CD1   | 1:D:122:VAL:HG11 | 2.40                     | 0.48              |
| 1:E:87:PRO:HB2   | 1:E:89:ILE:CD1   | 2.44                     | 0.48              |
| 1:C:163:LEU:HD22 | 1:C:174:LEU:HD13 | 1.93                     | 0.48              |
| 1:C:52:ILE:HG22  | 1:C:54:LEU:HG    | 1.96                     | 0.48              |
| 1:C:1:SER:CB     | 1:C:5:ARG:HH21   | 2.27                     | 0.48              |
| 1:D:35:TYR:OH    | 1:D:143:SER:OG   | 2.32                     | 0.48              |
| 1:D:86:THR:HG22  | 1:D:87:PRO:N     | 2.29                     | 0.48              |
| 1:B:174:LEU:CG   | 1:B:200:PHE:CE1  | 2.95                     | 0.48              |
| 1:B:52:ILE:HG22  | 1:B:54:LEU:HG    | 1.96                     | 0.48              |
| 1:A:52:ILE:HG21  | 1:A:54:LEU:HG    | 1.94                     | 0.48              |
| 1:D:79:VAL:CG2   | 1:D:83:GLU:HG3   | 2.43                     | 0.48              |
| 1:C:86:THR:HG22  | 1:C:87:PRO:N     | 2.29                     | 0.48              |
| 1:D:161:VAL:HG12 | 1:D:162:ASP:N    | 2.28                     | 0.48              |
| 1:D:167:ALA:HB3  | 1:D:170:THR:OG1  | 2.13                     | 0.48              |
| 1:B:25:ASP:O     | 1:C:2:ARG:CA     | 2.54                     | 0.48              |
| 1:C:77:LEU:O     | 1:C:108:VAL:HG22 | 2.14                     | 0.48              |
| 1:C:161:VAL:HG12 | 1:C:162:ASP:N    | 2.29                     | 0.48              |
| 1:B:47:ASN:HB3   | 1:C:41:PHE:HZ    | 0.70                     | 0.48              |
| 1:C:145:SER:OG   | 1:C:148:HIS:HB2  | 2.13                     | 0.48              |
| 1:D:1:SER:CB     | 1:D:5:ARG:HH21   | 2.27                     | 0.48              |
| 1:B:52:ILE:HG21  | 1:B:54:LEU:HG    | 1.94                     | 0.48              |
| 1:B:87:PRO:HB2   | 1:B:89:ILE:CD1   | 2.44                     | 0.48              |
| 1:E:21:ILE:HG22  | 1:E:23:ILE:HG12  | 1.95                     | 0.48              |
| 1:E:161:VAL:HG12 | 1:E:162:ASP:N    | 2.28                     | 0.47              |
| 1:C:21:ILE:CG2   | 1:D:1:SER:OG     | 2.49                     | 0.47              |
| 1:A:174:LEU:CG   | 1:A:200:PHE:CE1  | 2.95                     | 0.47              |
| 1:A:1:SER:OG     | 1:E:21:ILE:CG2   | 2.49                     | 0.47              |
| 1:E:38:GLN:O     | 1:E:39:LYS:HG3   | 2.14                     | 0.47              |
| 1:D:101:PHE:CZ   | 1:D:121:LYS:HB2  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:35:TYR:OH    | 1:D:143:SER:HB3  | 2.15                     | 0.47              |
| 1:D:163:LEU:HD22 | 1:D:174:LEU:HD13 | 1.93                     | 0.47              |
| 1:D:33:PHE:CE2   | 1:D:89:ILE:HG21  | 2.49                     | 0.47              |
| 1:D:77:LEU:O     | 1:D:108:VAL:HG22 | 2.14                     | 0.47              |
| 1:A:147:THR:N    | 1:B:105:LEU:HD13 | 2.06                     | 0.47              |
| 1:B:33:PHE:CE2   | 1:B:89:ILE:HG21  | 2.49                     | 0.47              |
| 1:A:86:THR:HG22  | 1:A:87:PRO:N     | 2.29                     | 0.47              |
| 1:A:38:GLN:O     | 1:A:39:LYS:HG3   | 2.14                     | 0.47              |
| 1:E:35:TYR:OH    | 1:E:143:SER:CB   | 2.63                     | 0.47              |
| 1:E:35:TYR:OH    | 1:E:143:SER:HB3  | 2.14                     | 0.47              |
| 1:E:175:LEU:HD21 | 1:E:203:ARG:HG2  | 1.95                     | 0.47              |
| 1:E:35:TYR:OH    | 1:E:143:SER:OG   | 2.32                     | 0.47              |
| 1:E:1:SER:CB     | 1:E:5:ARG:HH21   | 2.27                     | 0.47              |
| 1:C:175:LEU:HD21 | 1:C:203:ARG:HG2  | 1.95                     | 0.47              |
| 1:B:96:GLY:N     | 1:C:99:GLU:OE2   | 2.45                     | 0.47              |
| 1:D:101:PHE:HE2  | 1:D:121:LYS:HB2  | 1.74                     | 0.47              |
| 1:A:21:ILE:HG22  | 1:A:23:ILE:HG12  | 1.95                     | 0.47              |
| 1:A:101:PHE:HE2  | 1:A:121:LYS:HB2  | 1.74                     | 0.47              |
| 1:A:1:SER:C      | 1:E:25:ASP:O     | 2.49                     | 0.47              |
| 1:C:181:VAL:HG13 | 1:C:181:VAL:O    | 2.14                     | 0.47              |
| 1:D:181:VAL:O    | 1:D:181:VAL:HG13 | 2.14                     | 0.47              |
| 1:B:86:THR:HG22  | 1:B:87:PRO:N     | 2.29                     | 0.47              |
| 1:A:174:LEU:CG   | 1:A:200:PHE:CZ   | 2.94                     | 0.47              |
| 1:C:38:GLN:O     | 1:C:39:LYS:HG3   | 2.14                     | 0.47              |
| 1:D:25:ASP:O     | 1:E:2:ARG:CA     | 2.54                     | 0.47              |
| 1:E:77:LEU:O     | 1:E:108:VAL:HG22 | 2.14                     | 0.47              |
| 1:E:86:THR:HG22  | 1:E:87:PRO:N     | 2.29                     | 0.47              |
| 1:A:46:GLU:CD    | 1:B:42:ARG:CZ    | 2.82                     | 0.47              |
| 1:B:161:VAL:HG12 | 1:B:162:ASP:N    | 2.28                     | 0.47              |
| 1:B:163:LEU:HD22 | 1:B:174:LEU:HD13 | 1.93                     | 0.47              |
| 1:B:35:TYR:OH    | 1:B:143:SER:CB   | 2.63                     | 0.47              |
| 1:B:77:LEU:O     | 1:B:108:VAL:HG22 | 2.14                     | 0.47              |
| 1:D:38:GLN:O     | 1:D:39:LYS:HG3   | 2.14                     | 0.47              |
| 1:A:155:LEU:N    | 1:A:155:LEU:HD22 | 2.30                     | 0.47              |
| 1:D:35:TYR:OH    | 1:D:143:SER:CB   | 2.63                     | 0.47              |
| 1:A:77:LEU:O     | 1:A:108:VAL:HG22 | 2.14                     | 0.47              |
| 1:B:155:LEU:HD22 | 1:B:155:LEU:N    | 2.30                     | 0.47              |
| 1:D:21:ILE:CG2   | 1:E:1:SER:OG     | 2.49                     | 0.47              |
| 1:D:49:GLU:CG    | 1:E:41:PHE:CE1   | 2.81                     | 0.47              |
| 1:C:35:TYR:OH    | 1:C:143:SER:HB3  | 2.15                     | 0.47              |
| 1:C:200:PHE:HD2  | 1:C:202:PHE:CD1  | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:33:PHE:CE2   | 1:C:89:ILE:HG21  | 2.49                     | 0.47              |
| 1:C:87:PRO:HB2   | 1:C:89:ILE:CD1   | 2.44                     | 0.47              |
| 1:E:155:LEU:N    | 1:E:155:LEU:HD22 | 2.30                     | 0.47              |
| 1:E:181:VAL:O    | 1:E:181:VAL:HG13 | 2.14                     | 0.47              |
| 1:B:49:GLU:CG    | 1:B:95:VAL:HG21  | 2.40                     | 0.47              |
| 1:C:35:TYR:OH    | 1:C:143:SER:CB   | 2.63                     | 0.47              |
| 1:D:52:ILE:HG22  | 1:D:54:LEU:HG    | 1.96                     | 0.47              |
| 1:A:87:PRO:HB2   | 1:A:89:ILE:CD1   | 2.44                     | 0.47              |
| 1:B:38:GLN:O     | 1:B:39:LYS:HG3   | 2.14                     | 0.47              |
| 1:A:47:ASN:HD21  | 1:B:42:ARG:CD    | 2.27                     | 0.47              |
| 1:A:101:PHE:HE1  | 1:E:95:VAL:C     | 1.88                     | 0.47              |
| 1:A:2:ARG:CA     | 1:E:25:ASP:O     | 2.54                     | 0.47              |
| 1:B:181:VAL:HG13 | 1:B:181:VAL:O    | 2.15                     | 0.47              |
| 1:E:141:LEU:HD23 | 1:E:141:LEU:N    | 2.25                     | 0.47              |
| 1:B:101:PHE:HE2  | 1:B:121:LYS:HB2  | 1.74                     | 0.47              |
| 1:B:35:TYR:OH    | 1:B:143:SER:HB3  | 2.15                     | 0.47              |
| 1:A:35:TYR:OH    | 1:A:143:SER:HB3  | 2.14                     | 0.47              |
| 1:E:81:ILE:CD1   | 1:E:116:TYR:CE2  | 2.95                     | 0.47              |
| 1:C:155:LEU:N    | 1:C:155:LEU:HD22 | 2.30                     | 0.47              |
| 1:D:160:LYS:HD2  | 1:D:160:LYS:H    | 1.80                     | 0.46              |
| 1:D:81:ILE:CD1   | 1:D:116:TYR:CE2  | 2.95                     | 0.46              |
| 1:E:160:LYS:HD2  | 1:E:160:LYS:H    | 1.81                     | 0.46              |
| 1:D:47:ASN:HD21  | 1:E:42:ARG:CD    | 2.27                     | 0.46              |
| 1:A:42:ARG:CZ    | 1:E:46:GLU:CD    | 2.81                     | 0.46              |
| 1:E:188:CYS:SG   | 1:E:189:CYS:N    | 2.88                     | 0.46              |
| 1:C:35:TYR:OH    | 1:C:143:SER:OG   | 2.32                     | 0.46              |
| 1:A:99:GLU:OE2   | 1:E:96:GLY:N     | 2.45                     | 0.46              |
| 1:B:81:ILE:CD1   | 1:B:116:TYR:CE2  | 2.95                     | 0.46              |
| 1:E:174:LEU:HD23 | 1:E:176:ASN:N    | 2.30                     | 0.46              |
| 1:C:131:LEU:CD2  | 1:C:172:PHE:CE1  | 2.93                     | 0.46              |
| 1:A:35:TYR:OH    | 1:A:143:SER:CB   | 2.63                     | 0.46              |
| 1:B:188:CYS:SG   | 1:B:189:CYS:N    | 2.88                     | 0.46              |
| 1:A:52:ILE:HG22  | 1:A:54:LEU:HG    | 1.96                     | 0.46              |
| 1:D:188:CYS:SG   | 1:D:189:CYS:N    | 2.89                     | 0.46              |
| 1:B:174:LEU:HD23 | 1:B:176:ASN:N    | 2.30                     | 0.46              |
| 1:C:188:CYS:SG   | 1:C:189:CYS:N    | 2.88                     | 0.46              |
| 1:A:181:VAL:HG13 | 1:A:181:VAL:O    | 2.14                     | 0.46              |
| 1:E:52:ILE:HG22  | 1:E:54:LEU:HG    | 1.96                     | 0.46              |
| 1:C:47:ASN:HD21  | 1:D:42:ARG:CD    | 2.27                     | 0.46              |
| 1:D:174:LEU:CG   | 1:D:200:PHE:CZ   | 2.94                     | 0.46              |
| 1:D:155:LEU:N    | 1:D:155:LEU:HD22 | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:LEU:CG   | 1:C:200:PHE:CE1  | 2.95                     | 0.46              |
| 1:C:174:LEU:HD23 | 1:C:176:ASN:N    | 2.31                     | 0.46              |
| 1:D:174:LEU:HD23 | 1:D:176:ASN:N    | 2.31                     | 0.46              |
| 1:C:46:GLU:CD    | 1:D:42:ARG:CZ    | 2.81                     | 0.46              |
| 1:B:200:PHE:HD2  | 1:B:202:PHE:CD1  | 2.31                     | 0.46              |
| 1:E:152:GLU:N    | 1:E:152:GLU:OE1  | 2.48                     | 0.46              |
| 1:C:49:GLU:CG    | 1:C:95:VAL:HG21  | 2.40                     | 0.46              |
| 1:A:49:GLU:CG    | 1:A:95:VAL:HG21  | 2.40                     | 0.46              |
| 1:A:79:VAL:CG2   | 1:A:80:PRO:HD2   | 2.45                     | 0.46              |
| 1:D:46:GLU:CD    | 1:E:42:ARG:CZ    | 2.81                     | 0.46              |
| 1:A:81:ILE:HB    | 1:A:104:LYS:HG2  | 1.37                     | 0.46              |
| 1:B:79:VAL:CG2   | 1:B:80:PRO:HD2   | 2.45                     | 0.46              |
| 1:C:79:VAL:CG2   | 1:C:80:PRO:HD2   | 2.45                     | 0.46              |
| 1:A:188:CYS:SG   | 1:A:189:CYS:N    | 2.88                     | 0.46              |
| 1:D:94:SER:OG    | 1:E:101:PHE:CD1  | 2.55                     | 0.45              |
| 1:E:200:PHE:HD2  | 1:E:202:PHE:CD1  | 2.31                     | 0.45              |
| 1:A:152:GLU:N    | 1:A:152:GLU:OE1  | 2.48                     | 0.45              |
| 1:B:178:THR:HG22 | 1:B:179:GLN:N    | 2.31                     | 0.45              |
| 1:D:79:VAL:CG2   | 1:D:80:PRO:HD2   | 2.45                     | 0.45              |
| 1:B:25:ASP:O     | 1:C:1:SER:C      | 2.49                     | 0.45              |
| 1:C:40:ILE:HD11  | 1:C:200:PHE:CD2  | 2.51                     | 0.45              |
| 1:C:26:ASP:OD1   | 1:D:2:ARG:NH2    | 2.50                     | 0.45              |
| 1:B:35:TYR:OH    | 1:B:143:SER:OG   | 2.32                     | 0.45              |
| 1:B:37:LEU:CD1   | 1:B:52:ILE:CG2   | 2.95                     | 0.45              |
| 1:A:2:ARG:NH2    | 1:E:26:ASP:OD1   | 2.50                     | 0.45              |
| 1:C:81:ILE:HD12  | 1:C:116:TYR:CE1  | 2.51                     | 0.45              |
| 1:D:147:THR:N    | 1:E:105:LEU:HD13 | 2.06                     | 0.45              |
| 1:E:178:THR:HG22 | 1:E:179:GLN:N    | 2.31                     | 0.45              |
| 1:B:152:GLU:OE1  | 1:B:152:GLU:N    | 2.48                     | 0.45              |
| 1:B:147:THR:N    | 1:C:105:LEU:CB   | 2.80                     | 0.45              |
| 1:E:79:VAL:CG2   | 1:E:80:PRO:HD2   | 2.45                     | 0.45              |
| 1:A:147:THR:N    | 1:B:105:LEU:CB   | 2.80                     | 0.45              |
| 1:C:25:ASP:O     | 1:D:2:ARG:CA     | 2.54                     | 0.45              |
| 1:D:26:ASP:OD1   | 1:E:2:ARG:NH2    | 2.50                     | 0.45              |
| 1:D:33:PHE:CD1   | 1:D:35:TYR:CE2   | 3.05                     | 0.45              |
| 1:A:96:GLY:N     | 1:B:99:GLU:OE2   | 2.45                     | 0.45              |
| 1:A:124:LEU:HD12 | 1:A:124:LEU:O    | 2.17                     | 0.45              |
| 1:A:103:ASP:CA   | 1:E:90:PHE:CE2   | 2.91                     | 0.45              |
| 1:D:23:ILE:HD11  | 1:D:29:VAL:CG1   | 2.46                     | 0.45              |
| 1:C:47:ASN:HB3   | 1:D:41:PHE:HZ    | 0.70                     | 0.45              |
| 1:A:160:LYS:H    | 1:A:160:LYS:HD2  | 1.80                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:LEU:CD2  | 1:A:172:PHE:CE1  | 2.93                     | 0.45              |
| 1:C:125:SER:HB3  | 1:D:39:LYS:HZ3   | 1.65                     | 0.45              |
| 1:D:147:THR:N    | 1:E:105:LEU:CB   | 2.80                     | 0.45              |
| 1:C:160:LYS:HD2  | 1:C:160:LYS:H    | 1.80                     | 0.45              |
| 1:D:40:ILE:HD11  | 1:D:200:PHE:CD2  | 2.51                     | 0.45              |
| 1:A:26:ASP:OD1   | 1:B:2:ARG:NH2    | 2.50                     | 0.45              |
| 1:A:174:LEU:HD23 | 1:A:176:ASN:N    | 2.31                     | 0.45              |
| 1:A:178:THR:HG22 | 1:A:179:GLN:N    | 2.31                     | 0.45              |
| 1:E:81:ILE:HD12  | 1:E:116:TYR:CE1  | 2.51                     | 0.45              |
| 1:E:33:PHE:CD1   | 1:E:35:TYR:CE2   | 3.05                     | 0.45              |
| 1:C:25:ASP:O     | 1:D:1:SER:C      | 2.49                     | 0.45              |
| 1:A:105:LEU:CB   | 1:E:147:THR:N    | 2.80                     | 0.45              |
| 1:D:81:ILE:HD12  | 1:D:116:TYR:CE1  | 2.51                     | 0.45              |
| 1:E:79:VAL:HG23  | 1:E:80:PRO:HD2   | 1.99                     | 0.45              |
| 1:E:34:GLU:HA    | 1:E:179:GLN:HE22 | 1.82                     | 0.45              |
| 1:C:81:ILE:CD1   | 1:C:116:TYR:CE2  | 2.95                     | 0.45              |
| 1:D:152:GLU:N    | 1:D:152:GLU:OE1  | 2.48                     | 0.44              |
| 1:C:33:PHE:CD1   | 1:C:35:TYR:CE2   | 3.05                     | 0.44              |
| 1:A:163:LEU:HD22 | 1:A:174:LEU:HD13 | 1.93                     | 0.44              |
| 1:E:124:LEU:HD12 | 1:E:124:LEU:O    | 2.17                     | 0.44              |
| 1:C:152:GLU:OE1  | 1:C:152:GLU:N    | 2.48                     | 0.44              |
| 1:D:174:LEU:CD1  | 1:D:200:PHE:CE1  | 3.00                     | 0.44              |
| 1:B:23:ILE:HD11  | 1:B:29:VAL:CG1   | 2.46                     | 0.44              |
| 1:B:26:ASP:OD1   | 1:C:2:ARG:NH2    | 2.50                     | 0.44              |
| 1:C:34:GLU:HA    | 1:C:179:GLN:HE22 | 1.82                     | 0.44              |
| 1:C:174:LEU:CD1  | 1:C:200:PHE:CE1  | 3.00                     | 0.44              |
| 1:A:23:ILE:HD11  | 1:A:29:VAL:CG1   | 2.46                     | 0.44              |
| 1:B:124:LEU:O    | 1:B:124:LEU:HD12 | 2.17                     | 0.44              |
| 1:B:33:PHE:CD1   | 1:B:35:TYR:CE2   | 3.05                     | 0.44              |
| 1:A:40:ILE:HD11  | 1:A:200:PHE:CD2  | 2.51                     | 0.44              |
| 1:A:79:VAL:HG23  | 1:A:80:PRO:HD2   | 1.99                     | 0.44              |
| 1:B:147:THR:N    | 1:C:105:LEU:HB2  | 2.33                     | 0.44              |
| 1:D:34:GLU:HA    | 1:D:179:GLN:HE22 | 1.82                     | 0.44              |
| 1:B:160:LYS:HD2  | 1:B:160:LYS:H    | 1.80                     | 0.44              |
| 1:E:142:LYS:CD   | 1:E:184:LYS:HZ1  | 2.30                     | 0.44              |
| 1:E:37:LEU:CD1   | 1:E:52:ILE:CG2   | 2.94                     | 0.44              |
| 1:B:46:GLU:CD    | 1:C:42:ARG:CZ    | 2.82                     | 0.44              |
| 1:C:147:THR:N    | 1:D:105:LEU:HB2  | 2.33                     | 0.44              |
| 1:D:124:LEU:O    | 1:D:124:LEU:HD12 | 2.17                     | 0.44              |
| 1:A:34:GLU:HA    | 1:A:179:GLN:HE22 | 1.82                     | 0.44              |
| 1:A:5:ARG:NH2    | 1:E:21:ILE:HD13  | 2.30                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:38:GLN:C     | 1:C:39:LYS:HG3   | 2.38                     | 0.44              |
| 1:D:79:VAL:HG23  | 1:D:80:PRO:HD2   | 1.99                     | 0.44              |
| 1:E:173:GLN:HG2  | 1:E:174:LEU:N    | 2.33                     | 0.44              |
| 1:B:147:THR:N    | 1:C:105:LEU:HD13 | 2.06                     | 0.44              |
| 1:B:47:ASN:HD21  | 1:C:42:ARG:CD    | 2.27                     | 0.44              |
| 1:C:147:THR:N    | 1:D:105:LEU:CB   | 2.79                     | 0.44              |
| 1:A:105:LEU:HB2  | 1:E:147:THR:N    | 2.33                     | 0.44              |
| 1:A:33:PHE:CD1   | 1:A:35:TYR:CE2   | 3.05                     | 0.44              |
| 1:A:37:LEU:CD1   | 1:A:52:ILE:CG2   | 2.95                     | 0.44              |
| 1:E:161:VAL:CG1  | 1:E:177:ALA:CB   | 2.96                     | 0.44              |
| 1:C:178:THR:HG22 | 1:C:179:GLN:N    | 2.31                     | 0.44              |
| 1:C:23:ILE:HD11  | 1:C:29:VAL:CG1   | 2.46                     | 0.44              |
| 1:A:147:THR:N    | 1:B:105:LEU:HB2  | 2.33                     | 0.44              |
| 1:A:141:LEU:HD23 | 1:A:198:LEU:HB3  | 1.97                     | 0.44              |
| 1:A:38:GLN:C     | 1:A:39:LYS:HG3   | 2.38                     | 0.44              |
| 1:C:189:CYS:HB3  | 1:C:191:GLU:OE1  | 2.18                     | 0.44              |
| 1:D:96:GLY:O     | 1:D:98:PRO:HD3   | 2.18                     | 0.44              |
| 1:C:173:GLN:HG2  | 1:C:174:LEU:N    | 2.33                     | 0.44              |
| 1:D:49:GLU:CG    | 1:D:95:VAL:HG21  | 2.40                     | 0.44              |
| 1:D:96:GLY:N     | 1:E:99:GLU:OE2   | 2.45                     | 0.44              |
| 1:C:124:LEU:O    | 1:C:124:LEU:HD12 | 2.17                     | 0.44              |
| 1:D:173:GLN:HG2  | 1:D:174:LEU:N    | 2.33                     | 0.44              |
| 1:B:173:GLN:HG2  | 1:B:174:LEU:N    | 2.33                     | 0.44              |
| 1:A:189:CYS:HB3  | 1:A:191:GLU:OE1  | 2.18                     | 0.44              |
| 1:E:40:ILE:HD11  | 1:E:200:PHE:CD2  | 2.51                     | 0.43              |
| 1:A:173:GLN:HG2  | 1:A:174:LEU:N    | 2.33                     | 0.43              |
| 1:B:96:GLY:O     | 1:B:98:PRO:HD3   | 2.18                     | 0.43              |
| 1:B:174:LEU:CD1  | 1:B:200:PHE:CE1  | 3.00                     | 0.43              |
| 1:A:35:TYR:OH    | 1:A:143:SER:OG   | 2.32                     | 0.43              |
| 1:D:189:CYS:HB3  | 1:D:191:GLU:OE1  | 2.18                     | 0.43              |
| 1:D:161:VAL:CG1  | 1:D:177:ALA:HB1  | 2.45                     | 0.43              |
| 1:A:23:ILE:O     | 1:B:1:SER:CA     | 2.66                     | 0.43              |
| 1:D:19:LEU:N     | 1:D:19:LEU:HD22  | 2.33                     | 0.43              |
| 1:E:19:LEU:N     | 1:E:19:LEU:HD22  | 2.33                     | 0.43              |
| 1:E:131:LEU:CD2  | 1:E:172:PHE:CE1  | 2.93                     | 0.43              |
| 1:B:119:GLN:CA   | 1:B:120:LEU:HD12 | 2.49                     | 0.43              |
| 1:B:76:GLU:HB3   | 1:B:107:ARG:CG   | 2.49                     | 0.43              |
| 1:A:9:LEU:O      | 1:A:13:LEU:HG    | 2.19                     | 0.43              |
| 1:A:19:LEU:HD22  | 1:A:19:LEU:N     | 2.33                     | 0.43              |
| 1:B:150:THR:HG23 | 1:B:151:GLN:N    | 2.33                     | 0.43              |
| 1:E:174:LEU:CD1  | 1:E:200:PHE:CE1  | 3.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:5:ARG:HG3    | 1:E:74:PHE:CD2   | 2.54                     | 0.43              |
| 1:A:174:LEU:CD1  | 1:A:200:PHE:CE1  | 3.00                     | 0.43              |
| 1:E:96:GLY:O     | 1:E:98:PRO:HD3   | 2.18                     | 0.43              |
| 1:C:81:ILE:HB    | 1:C:104:LYS:HG2  | 1.37                     | 0.43              |
| 1:D:23:ILE:O     | 1:E:1:SER:CA     | 2.66                     | 0.43              |
| 1:C:5:ARG:HG3    | 1:C:74:PHE:CD2   | 2.54                     | 0.43              |
| 1:A:25:ASP:O     | 1:B:2:ARG:CA     | 2.54                     | 0.43              |
| 1:B:34:GLU:HA    | 1:B:179:GLN:HE22 | 1.83                     | 0.43              |
| 1:B:79:VAL:HG23  | 1:B:80:PRO:HD2   | 1.99                     | 0.43              |
| 1:C:79:VAL:HG23  | 1:C:80:PRO:HD2   | 1.99                     | 0.43              |
| 1:E:189:CYS:HB3  | 1:E:191:GLU:OE1  | 2.18                     | 0.43              |
| 1:D:147:THR:N    | 1:E:105:LEU:HB2  | 2.33                     | 0.43              |
| 1:E:198:LEU:C    | 1:E:198:LEU:HD13 | 2.39                     | 0.43              |
| 1:C:119:GLN:CA   | 1:C:120:LEU:HD12 | 2.49                     | 0.43              |
| 1:C:96:GLY:O     | 1:C:98:PRO:HD3   | 2.18                     | 0.43              |
| 1:D:161:VAL:CG1  | 1:D:177:ALA:CB   | 2.96                     | 0.43              |
| 1:E:49:GLU:CG    | 1:E:95:VAL:HG21  | 2.40                     | 0.43              |
| 1:D:178:THR:HG22 | 1:D:179:GLN:N    | 2.31                     | 0.43              |
| 1:D:198:LEU:HD13 | 1:D:198:LEU:C    | 2.39                     | 0.43              |
| 1:A:45:VAL:CG2   | 1:A:128:LEU:HD21 | 2.43                     | 0.43              |
| 1:A:101:PHE:HB2  | 1:A:119:GLN:CB   | 2.49                     | 0.43              |
| 1:A:161:VAL:CG1  | 1:A:177:ALA:CB   | 2.96                     | 0.43              |
| 1:D:38:GLN:C     | 1:D:39:LYS:HG3   | 2.38                     | 0.43              |
| 1:B:9:LEU:O      | 1:B:13:LEU:HG    | 2.19                     | 0.43              |
| 1:B:189:CYS:HB3  | 1:B:191:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:150:THR:HG23 | 1:A:151:GLN:N    | 2.33                     | 0.43              |
| 1:C:150:THR:HG23 | 1:C:151:GLN:N    | 2.33                     | 0.43              |
| 1:C:21:ILE:HD13  | 1:D:5:ARG:NH2    | 2.30                     | 0.43              |
| 1:B:5:ARG:HG3    | 1:B:74:PHE:CD2   | 2.54                     | 0.43              |
| 1:C:70:GLU:H     | 1:C:70:GLU:CD    | 2.22                     | 0.43              |
| 1:D:9:LEU:O      | 1:D:13:LEU:HG    | 2.19                     | 0.43              |
| 1:B:19:LEU:N     | 1:B:19:LEU:HD22  | 2.33                     | 0.43              |
| 1:C:198:LEU:C    | 1:C:198:LEU:HD13 | 2.39                     | 0.43              |
| 1:D:170:THR:CG2  | 1:D:171:ARG:N    | 2.82                     | 0.43              |
| 1:D:5:ARG:HG3    | 1:D:74:PHE:CD2   | 2.54                     | 0.43              |
| 1:A:119:GLN:CA   | 1:A:120:LEU:HD12 | 2.49                     | 0.43              |
| 1:B:38:GLN:C     | 1:B:39:LYS:HG3   | 2.38                     | 0.43              |
| 1:E:38:GLN:C     | 1:E:39:LYS:HG3   | 2.38                     | 0.43              |
| 1:C:9:LEU:O      | 1:C:13:LEU:HG    | 2.19                     | 0.43              |
| 1:D:101:PHE:HB2  | 1:D:119:GLN:CB   | 2.49                     | 0.42              |
| 1:A:161:VAL:HB   | 1:A:177:ALA:CB   | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:170:THR:CG2  | 1:A:171:ARG:N    | 2.82                     | 0.42              |
| 1:E:23:ILE:HD11  | 1:E:29:VAL:CG1   | 2.46                     | 0.42              |
| 1:E:36:SER:HB2   | 1:E:55:TRP:CD2   | 2.55                     | 0.42              |
| 1:D:36:SER:HB2   | 1:D:55:TRP:CD2   | 2.55                     | 0.42              |
| 1:A:198:LEU:HD13 | 1:A:198:LEU:C    | 2.39                     | 0.42              |
| 1:A:1:SER:CA     | 1:E:23:ILE:O     | 2.66                     | 0.42              |
| 1:A:76:GLU:HB3   | 1:A:107:ARG:CG   | 2.49                     | 0.42              |
| 1:A:42:ARG:CD    | 1:E:47:ASN:HD21  | 2.27                     | 0.42              |
| 1:E:9:LEU:O      | 1:E:13:LEU:HG    | 2.19                     | 0.42              |
| 1:E:170:THR:CG2  | 1:E:171:ARG:N    | 2.82                     | 0.42              |
| 1:D:37:LEU:CD1   | 1:D:52:ILE:CG2   | 2.95                     | 0.42              |
| 1:E:101:PHE:HB2  | 1:E:119:GLN:CB   | 2.49                     | 0.42              |
| 1:E:161:VAL:HB   | 1:E:177:ALA:CB   | 2.49                     | 0.42              |
| 1:B:147:THR:CA   | 1:C:105:LEU:HB2  | 2.50                     | 0.42              |
| 1:C:141:LEU:CD2  | 1:C:141:LEU:N    | 2.83                     | 0.42              |
| 1:A:96:GLY:O     | 1:A:98:PRO:HD3   | 2.18                     | 0.42              |
| 1:B:101:PHE:HB2  | 1:B:119:GLN:CB   | 2.49                     | 0.42              |
| 1:B:161:VAL:CG1  | 1:B:177:ALA:CB   | 2.96                     | 0.42              |
| 1:D:70:GLU:CD    | 1:D:70:GLU:H     | 2.22                     | 0.42              |
| 1:C:19:LEU:N     | 1:C:19:LEU:HD22  | 2.33                     | 0.42              |
| 1:B:23:ILE:O     | 1:C:1:SER:CA     | 2.66                     | 0.42              |
| 1:B:161:VAL:HB   | 1:B:177:ALA:CB   | 2.49                     | 0.42              |
| 1:B:170:THR:CG2  | 1:B:171:ARG:N    | 2.82                     | 0.42              |
| 1:A:161:VAL:CG1  | 1:A:177:ALA:HB1  | 2.45                     | 0.42              |
| 1:E:150:THR:HG23 | 1:E:151:GLN:N    | 2.33                     | 0.42              |
| 1:E:161:VAL:HG21 | 1:E:177:ALA:HB1  | 2.01                     | 0.42              |
| 1:B:94:SER:OG    | 1:C:101:PHE:CD1  | 2.55                     | 0.42              |
| 1:B:23:ILE:HD11  | 1:C:1:SER:OG     | 2.20                     | 0.42              |
| 1:C:147:THR:CA   | 1:D:105:LEU:HB2  | 2.50                     | 0.42              |
| 1:D:119:GLN:CA   | 1:D:120:LEU:HD12 | 2.49                     | 0.42              |
| 1:D:161:VAL:HG21 | 1:D:177:ALA:HB1  | 2.02                     | 0.42              |
| 1:D:36:SER:HA    | 1:D:162:ASP:HB3  | 2.02                     | 0.42              |
| 1:A:23:ILE:HD11  | 1:B:1:SER:OG     | 2.20                     | 0.42              |
| 1:A:101:PHE:CD1  | 1:E:94:SER:OG    | 2.55                     | 0.42              |
| 1:C:12:VAL:CG2   | 1:C:13:LEU:N     | 2.83                     | 0.42              |
| 1:D:150:THR:HG23 | 1:D:151:GLN:N    | 2.33                     | 0.42              |
| 1:E:119:GLN:CA   | 1:E:120:LEU:HD12 | 2.49                     | 0.42              |
| 1:C:36:SER:HB2   | 1:C:55:TRP:CD2   | 2.55                     | 0.42              |
| 1:C:76:GLU:HB3   | 1:C:107:ARG:CG   | 2.49                     | 0.42              |
| 1:D:141:LEU:N    | 1:D:141:LEU:CD2  | 2.83                     | 0.42              |
| 1:B:198:LEU:C    | 1:B:198:LEU:HD13 | 2.40                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:40:ILE:HD11  | 1:B:200:PHE:CD2  | 2.51                     | 0.42              |
| 1:A:5:ARG:HG3    | 1:A:74:PHE:CD2   | 2.54                     | 0.42              |
| 1:A:70:GLU:CD    | 1:A:70:GLU:H     | 2.22                     | 0.42              |
| 1:E:70:GLU:CD    | 1:E:70:GLU:H     | 2.22                     | 0.42              |
| 1:A:185:GLN:CG   | 1:A:186:TYR:N    | 2.83                     | 0.42              |
| 1:B:48:ASP:OD1   | 1:C:171:ARG:CZ   | 2.68                     | 0.42              |
| 1:C:23:ILE:O     | 1:D:1:SER:CA     | 2.66                     | 0.42              |
| 1:C:48:ASP:OD1   | 1:D:171:ARG:CZ   | 2.68                     | 0.42              |
| 1:A:47:ASN:ND2   | 1:B:42:ARG:CD    | 2.66                     | 0.42              |
| 1:B:36:SER:HA    | 1:B:162:ASP:HB3  | 2.02                     | 0.42              |
| 1:A:36:SER:HB2   | 1:A:55:TRP:CD2   | 2.55                     | 0.42              |
| 1:A:171:ARG:CZ   | 1:E:48:ASP:OD1   | 2.68                     | 0.42              |
| 1:B:70:GLU:H     | 1:B:70:GLU:CD    | 2.22                     | 0.42              |
| 1:B:185:GLN:CG   | 1:B:186:TYR:N    | 2.83                     | 0.42              |
| 1:C:37:LEU:CD1   | 1:C:52:ILE:CG2   | 2.94                     | 0.42              |
| 1:A:48:ASP:OD1   | 1:B:171:ARG:CZ   | 2.68                     | 0.42              |
| 1:A:95:VAL:CG1   | 1:B:121:LYS:NZ   | 2.83                     | 0.42              |
| 1:C:16:CYS:SG    | 1:C:64:CYS:SG    | 3.12                     | 0.42              |
| 1:A:12:VAL:CG2   | 1:A:13:LEU:N     | 2.83                     | 0.42              |
| 1:C:36:SER:HA    | 1:C:162:ASP:HB3  | 2.02                     | 0.42              |
| 1:B:141:LEU:N    | 1:B:141:LEU:CD2  | 2.83                     | 0.42              |
| 1:C:161:VAL:CG1  | 1:C:177:ALA:HB1  | 2.45                     | 0.41              |
| 1:C:141:LEU:HD23 | 1:C:198:LEU:HB3  | 1.97                     | 0.41              |
| 1:C:45:VAL:CG2   | 1:C:128:LEU:HD21 | 2.43                     | 0.41              |
| 1:A:147:THR:CG2  | 1:A:148:HIS:N    | 2.83                     | 0.41              |
| 1:E:141:LEU:N    | 1:E:141:LEU:CD2  | 2.83                     | 0.41              |
| 1:E:42:ARG:HG2   | 1:E:43:ALA:N     | 2.36                     | 0.41              |
| 1:C:198:LEU:HD13 | 1:C:199:SER:N    | 2.35                     | 0.41              |
| 1:C:23:ILE:HD11  | 1:D:1:SER:OG     | 2.19                     | 0.41              |
| 1:B:36:SER:HB2   | 1:B:55:TRP:CD2   | 2.55                     | 0.41              |
| 1:A:36:SER:HA    | 1:A:162:ASP:HB3  | 2.02                     | 0.41              |
| 1:E:45:VAL:CG2   | 1:E:128:LEU:HD21 | 2.43                     | 0.41              |
| 1:D:21:ILE:CG2   | 1:D:23:ILE:HG12  | 2.51                     | 0.41              |
| 1:D:48:ASP:OD1   | 1:E:171:ARG:CZ   | 2.68                     | 0.41              |
| 1:E:36:SER:HA    | 1:E:162:ASP:HB3  | 2.02                     | 0.41              |
| 1:B:198:LEU:HD13 | 1:B:199:SER:N    | 2.36                     | 0.41              |
| 1:E:185:GLN:CG   | 1:E:186:TYR:N    | 2.83                     | 0.41              |
| 1:C:185:GLN:CG   | 1:C:186:TYR:N    | 2.83                     | 0.41              |
| 1:B:147:THR:CG2  | 1:B:148:HIS:N    | 2.83                     | 0.41              |
| 1:A:141:LEU:N    | 1:A:141:LEU:CD2  | 2.83                     | 0.41              |
| 1:A:198:LEU:HD13 | 1:A:199:SER:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:81:ILE:HB    | 1:D:104:LYS:HG2  | 1.37                     | 0.41              |
| 1:D:185:GLN:CG   | 1:D:186:TYR:N    | 2.83                     | 0.41              |
| 1:D:45:VAL:CG2   | 1:D:128:LEU:HD21 | 2.43                     | 0.41              |
| 1:B:21:ILE:CG2   | 1:B:23:ILE:HG12  | 2.51                     | 0.41              |
| 1:B:95:VAL:CG1   | 1:C:121:LYS:NZ   | 2.83                     | 0.41              |
| 1:A:121:LYS:NZ   | 1:E:95:VAL:CG1   | 2.83                     | 0.41              |
| 1:A:1:SER:OG     | 1:E:23:ILE:HD11  | 2.20                     | 0.41              |
| 1:C:161:VAL:CG1  | 1:C:177:ALA:CB   | 2.96                     | 0.41              |
| 1:C:147:THR:CG2  | 1:C:148:HIS:N    | 2.83                     | 0.41              |
| 1:D:42:ARG:HG2   | 1:D:43:ALA:N     | 2.35                     | 0.41              |
| 1:A:21:ILE:CG2   | 1:A:23:ILE:HG12  | 2.51                     | 0.41              |
| 1:D:79:VAL:CG2   | 1:D:80:PRO:N     | 2.83                     | 0.41              |
| 1:D:147:THR:CG2  | 1:E:105:LEU:HB3  | 2.30                     | 0.41              |
| 1:C:161:VAL:HG21 | 1:C:177:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:161:VAL:CB   | 1:A:177:ALA:CB   | 2.99                     | 0.41              |
| 1:A:161:VAL:HG21 | 1:A:177:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:1:SER:OG     | 1:E:23:ILE:CG1   | 2.69                     | 0.41              |
| 1:B:12:VAL:CG2   | 1:B:13:LEU:N     | 2.82                     | 0.41              |
| 1:D:149:SER:HA   | 1:D:193:TYR:CE2  | 2.56                     | 0.41              |
| 1:D:23:ILE:HD11  | 1:E:1:SER:OG     | 2.19                     | 0.41              |
| 1:D:47:ASN:HB3   | 1:E:41:PHE:HZ    | 0.70                     | 0.41              |
| 1:B:23:ILE:CG1   | 1:C:1:SER:OG     | 2.69                     | 0.41              |
| 1:C:170:THR:CG2  | 1:C:171:ARG:N    | 2.82                     | 0.41              |
| 1:C:21:ILE:CG2   | 1:C:23:ILE:HG12  | 2.51                     | 0.41              |
| 1:C:95:VAL:CG1   | 1:D:121:LYS:NZ   | 2.83                     | 0.41              |
| 1:D:89:ILE:N     | 1:D:89:ILE:HD12  | 2.36                     | 0.41              |
| 1:B:161:VAL:HG21 | 1:B:177:ALA:HB1  | 2.02                     | 0.41              |
| 1:B:89:ILE:N     | 1:B:89:ILE:HD12  | 2.36                     | 0.41              |
| 1:B:35:TYR:HH    | 1:B:143:SER:HG   | 1.64                     | 0.41              |
| 1:B:81:ILE:HD12  | 1:B:116:TYR:CE1  | 2.51                     | 0.41              |
| 1:E:81:ILE:HB    | 1:E:104:LYS:HG2  | 1.37                     | 0.41              |
| 1:E:12:VAL:CG2   | 1:E:13:LEU:N     | 2.83                     | 0.41              |
| 1:A:28:PRO:HB3   | 1:A:151:GLN:O    | 2.21                     | 0.41              |
| 1:D:95:VAL:CG1   | 1:E:121:LYS:NZ   | 2.83                     | 0.41              |
| 1:E:141:LEU:HD23 | 1:E:198:LEU:HB3  | 1.97                     | 0.41              |
| 1:A:15:ARG:NH1   | 1:A:68:PHE:CZ    | 2.89                     | 0.41              |
| 1:E:19:LEU:CD2   | 1:E:19:LEU:H     | 2.34                     | 0.41              |
| 1:E:161:VAL:CB   | 1:E:177:ALA:CB   | 2.99                     | 0.40              |
| 1:E:89:ILE:HD12  | 1:E:89:ILE:N     | 2.36                     | 0.40              |
| 1:B:149:SER:HA   | 1:B:193:TYR:CE2  | 2.56                     | 0.40              |
| 1:C:89:ILE:HD12  | 1:C:89:ILE:N     | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:17:SER:HA    | 1:C:18:PRO:HD2   | 1.96                     | 0.40              |
| 1:A:79:VAL:CG2   | 1:A:80:PRO:N     | 2.83                     | 0.40              |
| 1:E:79:VAL:CG2   | 1:E:80:PRO:N     | 2.83                     | 0.40              |
| 1:D:12:VAL:CG2   | 1:D:13:LEU:N     | 2.83                     | 0.40              |
| 1:C:42:ARG:HG2   | 1:C:43:ALA:N     | 2.35                     | 0.40              |
| 1:B:77:LEU:HD12  | 1:B:78:THR:N     | 2.27                     | 0.40              |
| 1:A:163:LEU:HD21 | 1:A:177:ALA:CB   | 2.50                     | 0.40              |
| 1:A:81:ILE:HG23  | 1:A:82:ALA:N     | 2.36                     | 0.40              |
| 1:A:16:CYS:SG    | 1:A:64:CYS:SG    | 3.12                     | 0.40              |
| 1:D:147:THR:CG2  | 1:D:148:HIS:N    | 2.83                     | 0.40              |
| 1:C:161:VAL:HB   | 1:C:177:ALA:CB   | 2.49                     | 0.40              |
| 1:B:21:ILE:HD13  | 1:C:5:ARG:NH2    | 2.30                     | 0.40              |
| 1:D:76:GLU:HB3   | 1:D:107:ARG:CG   | 2.49                     | 0.40              |
| 1:A:89:ILE:N     | 1:A:89:ILE:HD12  | 2.36                     | 0.40              |
| 1:A:1:SER:HB2    | 1:E:23:ILE:O     | 2.22                     | 0.40              |
| 1:A:81:ILE:HD12  | 1:A:116:TYR:CE1  | 2.51                     | 0.40              |
| 1:C:81:ILE:HG23  | 1:C:82:ALA:N     | 2.36                     | 0.40              |
| 1:D:11:ASP:OD1   | 1:D:68:PHE:CE2   | 2.75                     | 0.40              |
| 1:E:11:ASP:OD1   | 1:E:68:PHE:CE2   | 2.75                     | 0.40              |
| 1:B:28:PRO:HB3   | 1:B:151:GLN:O    | 2.21                     | 0.40              |
| 1:C:161:VAL:CB   | 1:C:177:ALA:CB   | 2.99                     | 0.40              |
| 1:C:147:THR:N    | 1:D:105:LEU:HD13 | 2.06                     | 0.40              |
| 1:C:149:SER:HA   | 1:C:193:TYR:CE2  | 2.56                     | 0.40              |
| 1:B:42:ARG:HG2   | 1:B:43:ALA:N     | 2.35                     | 0.40              |
| 1:A:105:LEU:HB2  | 1:E:147:THR:CA   | 2.50                     | 0.40              |
| 1:C:15:ARG:NH1   | 1:C:68:PHE:CZ    | 2.89                     | 0.40              |
| 1:E:198:LEU:HD13 | 1:E:199:SER:N    | 2.35                     | 0.40              |
| 1:B:23:ILE:O     | 1:C:1:SER:HB2    | 2.22                     | 0.40              |
| 1:D:161:VAL:CB   | 1:D:177:ALA:CB   | 2.99                     | 0.40              |
| 1:A:148:HIS:HD2  | 1:B:78:THR:HG22  | 1.74                     | 0.40              |
| 1:B:172:PHE:HA   | 1:B:205:PRO:CD   | 2.49                     | 0.40              |
| 1:E:21:ILE:CG2   | 1:E:23:ILE:HG12  | 2.51                     | 0.40              |
| 1:C:81:ILE:CD1   | 1:C:116:TYR:CZ   | 2.94                     | 0.40              |
| 1:A:11:ASP:OD1   | 1:A:68:PHE:CE2   | 2.75                     | 0.40              |
| 1:B:79:VAL:CG2   | 1:B:80:PRO:N     | 2.83                     | 0.40              |
| 1:C:19:LEU:H     | 1:C:19:LEU:CD2   | 2.34                     | 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     | 201/205 (98%)   | 189 (94%) | 12 (6%) | 0        | 100         | 100 |
| 1   | B     | 201/205 (98%)   | 189 (94%) | 12 (6%) | 0        | 100         | 100 |
| 1   | C     | 201/205 (98%)   | 189 (94%) | 12 (6%) | 0        | 100         | 100 |
| 1   | D     | 201/205 (98%)   | 189 (94%) | 12 (6%) | 0        | 100         | 100 |
| 1   | E     | 201/205 (98%)   | 189 (94%) | 12 (6%) | 0        | 100         | 100 |
| All | All   | 1005/1025 (98%) | 945 (94%) | 60 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 1   | B     | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 1   | C     | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 1   | D     | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 1   | E     | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| All | All   | 955/955 (100%) | 955 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | GLN  |
| 1   | A     | 66  | ASN  |
| 1   | A     | 148 | HIS  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 182 | ASN  |
| 1   | A     | 185 | GLN  |
| 1   | B     | 27  | GLN  |
| 1   | B     | 66  | ASN  |
| 1   | B     | 148 | HIS  |
| 1   | B     | 173 | GLN  |
| 1   | B     | 182 | ASN  |
| 1   | B     | 185 | GLN  |
| 1   | C     | 27  | GLN  |
| 1   | C     | 66  | ASN  |
| 1   | C     | 148 | HIS  |
| 1   | C     | 173 | GLN  |
| 1   | C     | 182 | ASN  |
| 1   | C     | 185 | GLN  |
| 1   | D     | 27  | GLN  |
| 1   | D     | 66  | ASN  |
| 1   | D     | 148 | HIS  |
| 1   | D     | 173 | GLN  |
| 1   | D     | 182 | ASN  |
| 1   | D     | 185 | GLN  |
| 1   | E     | 27  | GLN  |
| 1   | E     | 66  | ASN  |
| 1   | E     | 148 | HIS  |
| 1   | E     | 173 | GLN  |
| 1   | E     | 182 | ASN  |
| 1   | E     | 185 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates 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.