



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:58 pm BST

PDB ID : 4QSL  
Title : Crystal Structure of Listeria Monocytogenes Pyruvate Carboxylase  
Authors : Choi, P.H.; Tong, L.  
Deposited on : 2014-07-04  
Resolution : 3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

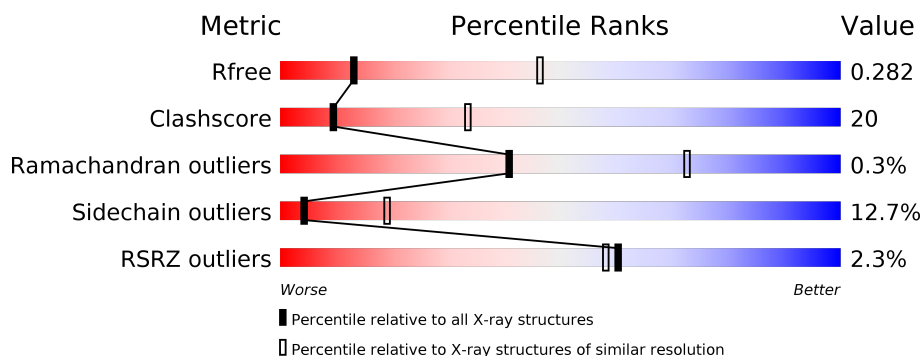
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1177 (3.32-3.24)                                      |
| Clashscore            | 141614                      | 1044 (3.30-3.26)                                      |
| Ramachandran outliers | 138981                      | 1026 (3.30-3.26)                                      |
| Sidechain outliers    | 138945                      | 1025 (3.30-3.26)                                      |
| RSRZ outliers         | 127900                      | 1141 (3.32-3.24)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 1146   | <div> <div>%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>8%</div> </div> </div>   |
| 1   | B     | 1146   | <div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div> |
| 1   | C     | 1146   | <div> <div>4%</div> <div> <div></div> <div>53%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div> |
| 1   | D     | 1146   | <div> <div>%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>5%</div> <div>10%</div> </div> </div> |
| 1   | E     | 1146   | <div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div> |
| 1   | F     | 1146   | <div> <div>%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>8%</div> </div> </div>   |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | G     | 1146   | <div><div><div></div><div></div><div></div><div></div></div><div>3%53%25%18%</div></div>  |
| 1   | H     | 1146   | <div><div><div></div><div></div><div></div><div></div></div><div>%57%28%5%10%</div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60495 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

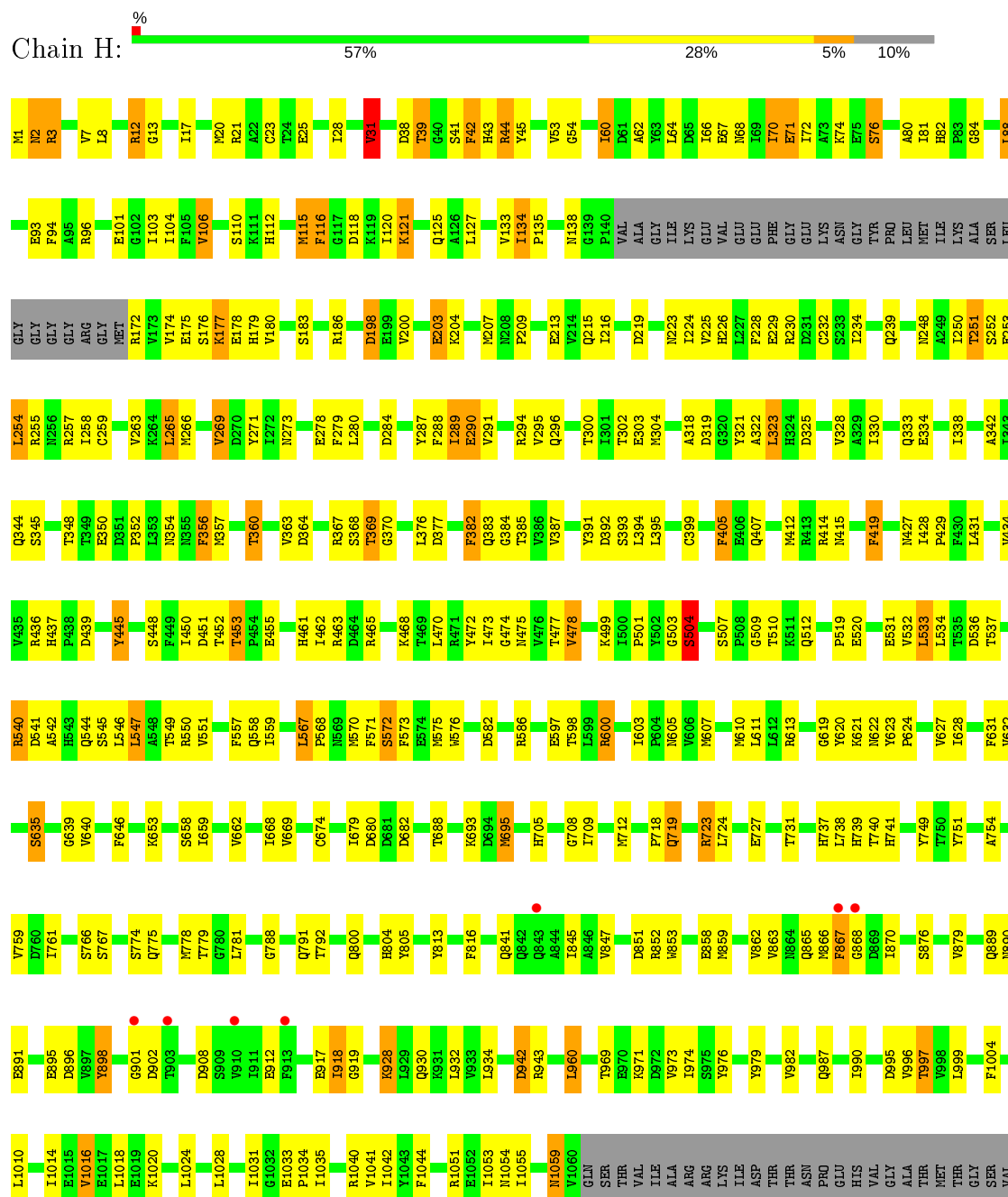
- Molecule 1 is a protein called Pyruvate carboxylase.

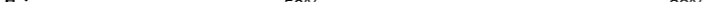
| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | H     | 1029     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7881  | 4992 | 1351 | 1504 | 34 |         |         |       |
| 1   | F     | 1052     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7969  | 5063 | 1353 | 1518 | 35 |         |         |       |
| 1   | E     | 1031     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7492  | 4716 | 1292 | 1459 | 25 |         |         |       |
| 1   | G     | 942      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6909  | 4338 | 1202 | 1341 | 28 |         |         |       |
| 1   | D     | 1029     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7881  | 4992 | 1351 | 1504 | 34 |         |         |       |
| 1   | A     | 1052     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7969  | 5063 | 1353 | 1518 | 35 |         |         |       |
| 1   | B     | 1031     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7492  | 4716 | 1292 | 1459 | 25 |         |         |       |
| 1   | C     | 941      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6902  | 4333 | 1201 | 1340 | 28 |         |         |       |

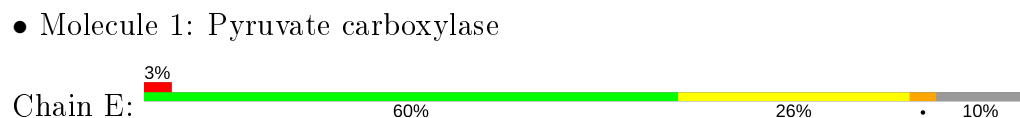
### 3 Residue-property plots

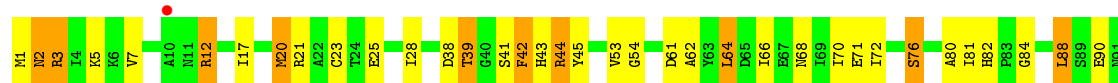
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

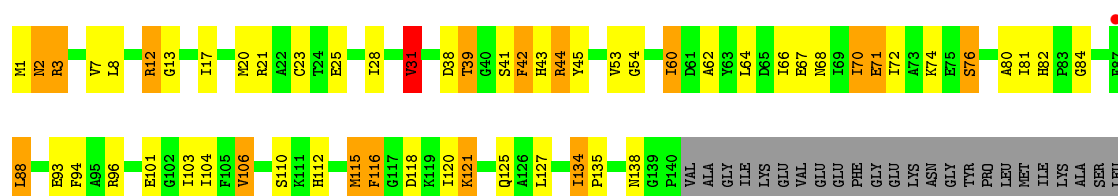
- Molecule 1: Pyruvate carboxylase



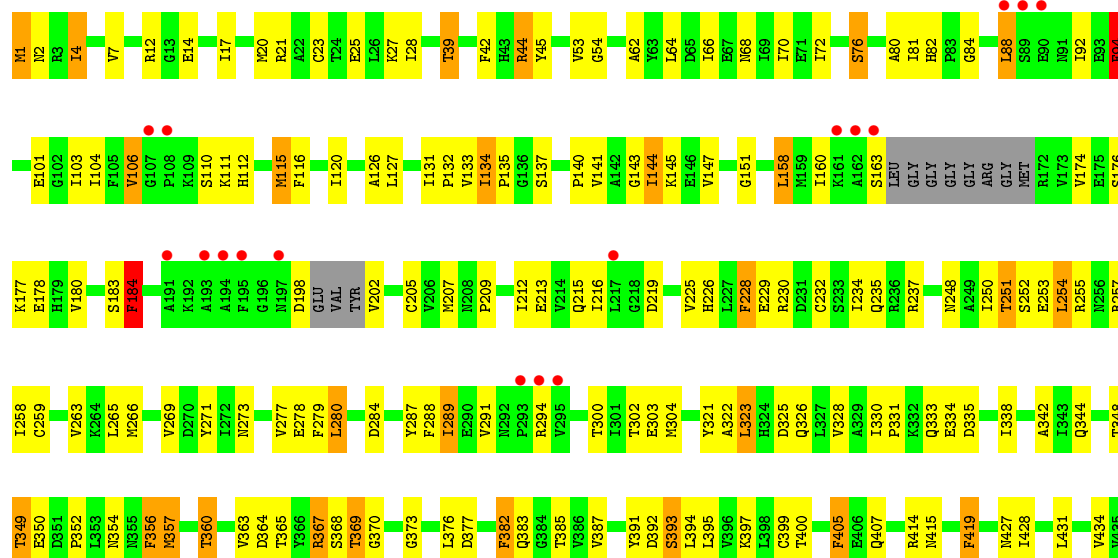
Chain F:  59% 28% 8%

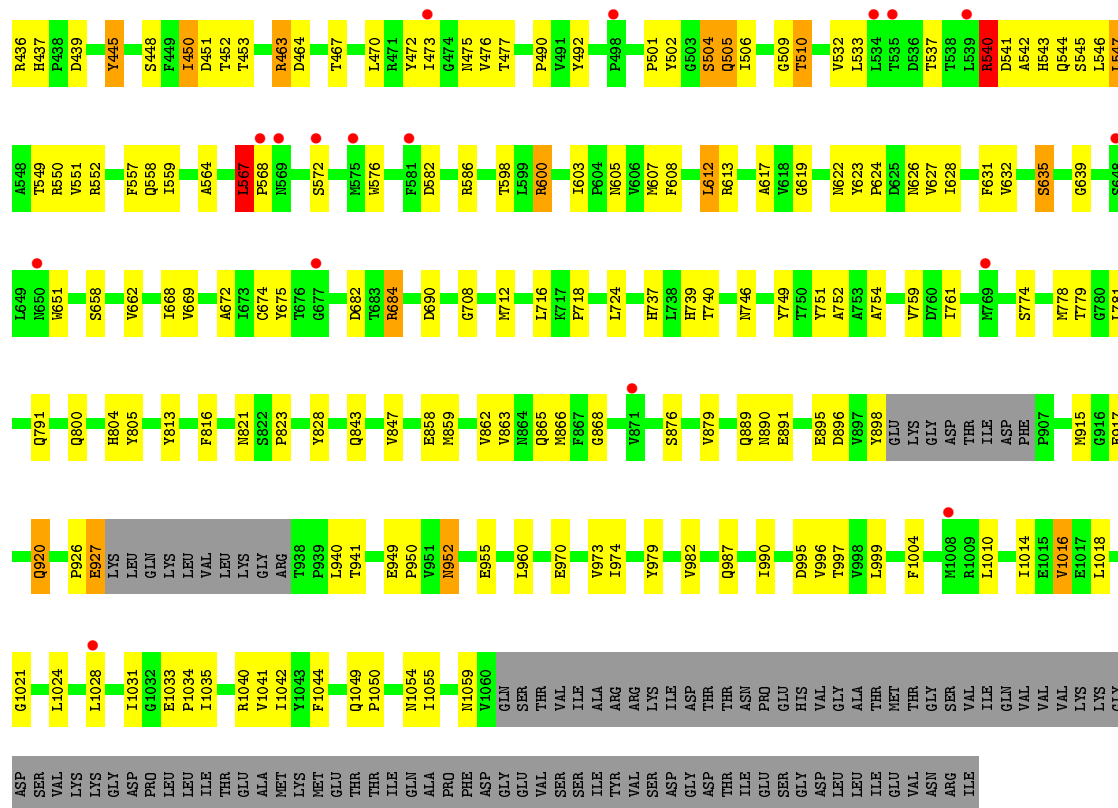




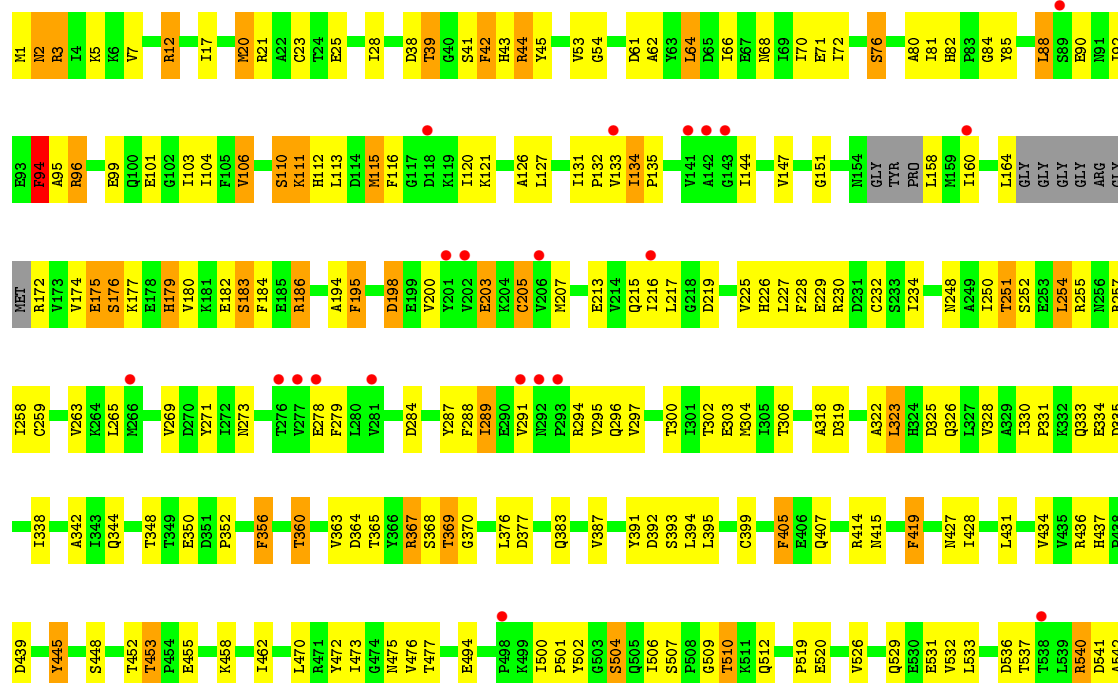


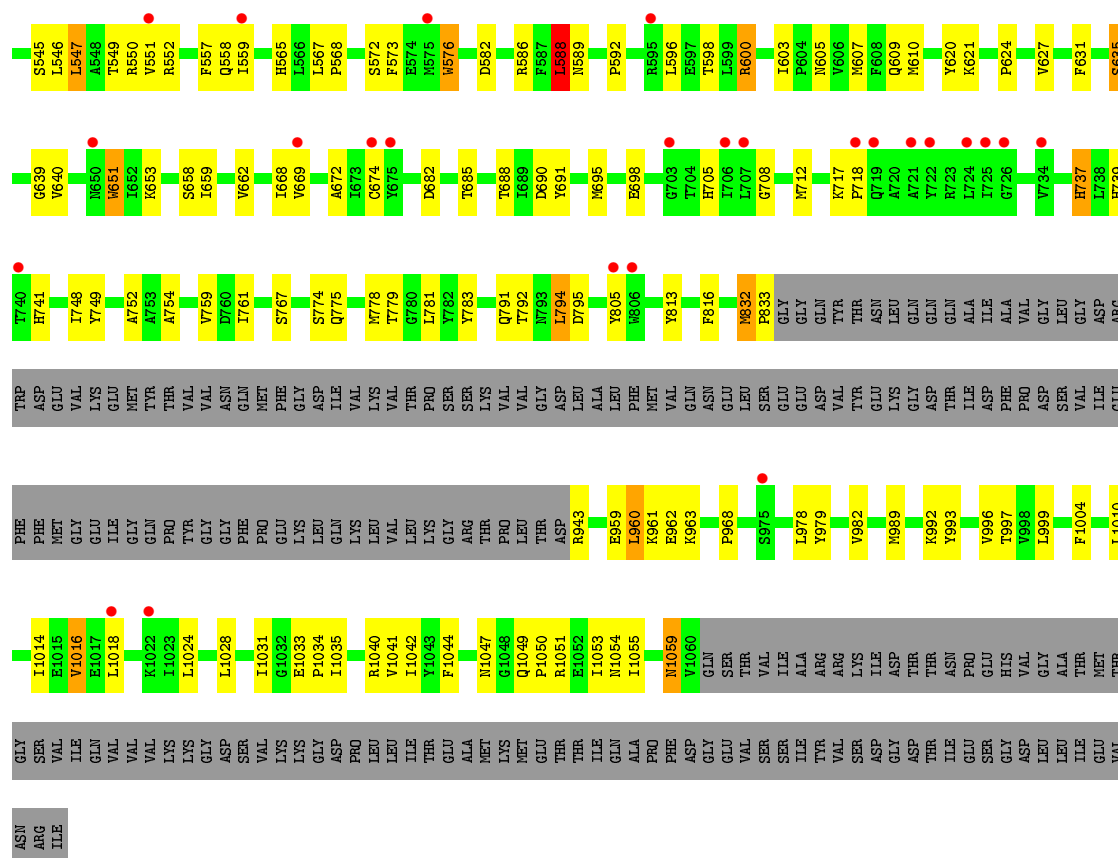






• Molecule 1: Pyruvate carboxylase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 91.36Å 132.62Å 257.54Å<br>86.65° 79.84° 70.07°                      | Depositor        |
| Resolution (Å)  | 47.16 – 3.28<br>47.11 – 3.28  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.9 (47.16-3.28)<br>88.4 (47.11-3.28)                              | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 3.25Å)   | Xtriage          |
| Refinement program  | REFMAC 5.7.0029   | Depositor        |
| R, $R_{free}$   | 0.238 , 0.284<br>0.235 , 0.282                                      | Depositor<br>DCC |
| $R_{free}$ test set   | 7628 reflections (5.02%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 116.2   | Xtriage          |
| Anisotropy  | 0.062   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 86.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$         | Xtriage          |
| Estimated twinning fraction   | 0.398 for h,h-k,h-l<br>0.007 for -h,-h+k,-l<br>0.007 for -h,-k,-h+l | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 60495   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 134.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.46         | 0/8136      | 0.74        | 5/11083 (0.0%)  |
| 1   | B     | 0.45         | 0/7639      | 0.72        | 7/10443 (0.1%)  |
| 1   | C     | 0.46         | 0/7031      | 0.73        | 6/9586 (0.1%)   |
| 1   | D     | 0.47         | 0/8042      | 0.74        | 9/10933 (0.1%)  |
| 1   | E     | 0.45         | 0/7639      | 0.72        | 9/10443 (0.1%)  |
| 1   | F     | 0.46         | 0/8136      | 0.74        | 6/11083 (0.1%)  |
| 1   | G     | 0.47         | 0/7039      | 0.73        | 6/9597 (0.1%)   |
| 1   | H     | 0.48         | 0/8042      | 0.74        | 9/10933 (0.1%)  |
| All | All   | 0.46         | 0/61704     | 0.73        | 57/84101 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | D     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | H     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

All (57) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 115 | MET  | CA-CB-CG  | 8.11  | 127.09      | 113.30   |
| 1   | H     | 115 | MET  | CA-CB-CG  | 8.08  | 127.04      | 113.30   |
| 1   | G     | 690 | ASP  | CB-CG-OD1 | 7.87  | 125.38      | 118.30   |
| 1   | C     | 690 | ASP  | CB-CG-OD1 | 7.80  | 125.32      | 118.30   |
| 1   | H     | 478 | VAL  | CB-CA-C   | -7.79 | 96.61       | 111.40   |
| 1   | D     | 478 | VAL  | CB-CA-C   | -7.27 | 97.59       | 111.40   |
| 1   | A     | 943 | ARG  | NE-CZ-NH2 | -7.19 | 116.70      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | F     | 943  | ARG  | NE-CZ-NH2  | -7.08 | 116.76      | 120.30   |
| 1   | B     | 184  | PHE  | N-CA-CB    | 6.50  | 122.31      | 110.60   |
| 1   | E     | 184  | PHE  | N-CA-CB    | 6.50  | 122.29      | 110.60   |
| 1   | E     | 4    | ILE  | CG1-CB-CG2 | -6.41 | 97.30       | 111.40   |
| 1   | F     | 943  | ARG  | NE-CZ-NH1  | 6.39  | 123.50      | 120.30   |
| 1   | H     | 478  | VAL  | CA-CB-CG2  | 6.38  | 120.46      | 110.90   |
| 1   | A     | 628  | ILE  | CG1-CB-CG2 | -6.34 | 97.45       | 111.40   |
| 1   | B     | 4    | ILE  | CG1-CB-CG2 | -6.32 | 97.49       | 111.40   |
| 1   | F     | 628  | ILE  | CG1-CB-CG2 | -6.32 | 97.50       | 111.40   |
| 1   | D     | 478  | VAL  | CA-CB-CG2  | 6.24  | 120.26      | 110.90   |
| 1   | A     | 943  | ARG  | NE-CZ-NH1  | 6.23  | 123.41      | 120.30   |
| 1   | H     | 367  | ARG  | NE-CZ-NH1  | 6.22  | 123.41      | 120.30   |
| 1   | D     | 367  | ARG  | NE-CZ-NH1  | 6.19  | 123.40      | 120.30   |
| 1   | C     | 96   | ARG  | NE-CZ-NH1  | 6.15  | 123.37      | 120.30   |
| 1   | G     | 94   | PHE  | CB-CG-CD1  | 6.13  | 125.09      | 120.80   |
| 1   | H     | 31   | VAL  | CB-CA-C    | -6.11 | 99.79       | 111.40   |
| 1   | C     | 94   | PHE  | CB-CG-CD1  | 6.04  | 125.03      | 120.80   |
| 1   | D     | 31   | VAL  | CB-CA-C    | -5.95 | 100.09      | 111.40   |
| 1   | E     | 94   | PHE  | CB-CG-CD1  | 5.91  | 124.94      | 120.80   |
| 1   | B     | 450  | ILE  | CA-CB-CG1  | 5.89  | 122.19      | 111.00   |
| 1   | A     | 1029 | ASN  | N-CA-CB    | 5.87  | 121.16      | 110.60   |
| 1   | E     | 540  | ARG  | CG-CD-NE   | 5.86  | 124.10      | 111.80   |
| 1   | B     | 94   | PHE  | CB-CG-CD1  | 5.85  | 124.90      | 120.80   |
| 1   | F     | 1029 | ASN  | N-CA-CB    | 5.85  | 121.13      | 110.60   |
| 1   | C     | 588  | LEU  | CB-CG-CD1  | -5.85 | 101.06      | 111.00   |
| 1   | D     | 695  | MET  | CG-SD-CE   | 5.74  | 109.38      | 100.20   |
| 1   | G     | 588  | LEU  | CB-CG-CD1  | -5.72 | 101.28      | 111.00   |
| 1   | G     | 96   | ARG  | NE-CZ-NH1  | 5.72  | 123.16      | 120.30   |
| 1   | H     | 695  | MET  | CG-SD-CE   | 5.67  | 109.27      | 100.20   |
| 1   | H     | 115  | MET  | N-CA-CB    | -5.55 | 100.61      | 110.60   |
| 1   | H     | 960  | LEU  | CB-CG-CD2  | 5.53  | 120.40      | 111.00   |
| 1   | D     | 115  | MET  | N-CA-CB    | -5.51 | 100.68      | 110.60   |
| 1   | B     | 463  | ARG  | NE-CZ-NH1  | 5.42  | 123.01      | 120.30   |
| 1   | D     | 960  | LEU  | CB-CG-CD2  | 5.36  | 120.11      | 111.00   |
| 1   | C     | 690  | ASP  | CB-CG-OD2  | -5.36 | 113.48      | 118.30   |
| 1   | H     | 567  | LEU  | CB-CG-CD2  | 5.35  | 120.09      | 111.00   |
| 1   | E     | 144  | ILE  | CB-CA-C    | -5.33 | 100.95      | 111.60   |
| 1   | G     | 690  | ASP  | CB-CG-OD2  | -5.32 | 113.51      | 118.30   |
| 1   | B     | 540  | ARG  | CG-CD-NE   | 5.29  | 122.91      | 111.80   |
| 1   | D     | 567  | LEU  | CB-CG-CD2  | 5.27  | 119.95      | 111.00   |
| 1   | F     | 1056 | GLN  | N-CA-CB    | 5.21  | 119.97      | 110.60   |
| 1   | A     | 1056 | GLN  | N-CA-CB    | 5.19  | 119.94      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 94  | PHE  | CB-CG-CD2 | -5.12 | 117.22      | 120.80   |
| 1   | E     | 463 | ARG  | NE-CZ-NH1 | 5.10  | 122.85      | 120.30   |
| 1   | G     | 94  | PHE  | CB-CG-CD2 | -5.09 | 117.24      | 120.80   |
| 1   | E     | 567 | LEU  | CA-CB-CG  | 5.08  | 126.99      | 115.30   |
| 1   | B     | 567 | LEU  | CA-CB-CG  | 5.07  | 126.96      | 115.30   |
| 1   | E     | 143 | GLY  | N-CA-C    | 5.07  | 125.77      | 113.10   |
| 1   | F     | 159 | MET  | CG-SD-CE  | 5.05  | 108.28      | 100.20   |
| 1   | C     | 832 | MET  | CG-SD-CE  | 5.01  | 108.22      | 100.20   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | D     | 504 | SER  | Peptide |
| 1   | F     | 504 | SER  | Peptide |
| 1   | H     | 504 | SER  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 7969  | 0        | 7573     | 289     | 0            |
| 1   | B     | 7492  | 0        | 6807     | 324     | 0            |
| 1   | C     | 6902  | 0        | 6371     | 288     | 0            |
| 1   | D     | 7881  | 0        | 7579     | 288     | 0            |
| 1   | E     | 7492  | 0        | 6807     | 311     | 0            |
| 1   | F     | 7969  | 0        | 7573     | 299     | 0            |
| 1   | G     | 6909  | 0        | 6379     | 282     | 0            |
| 1   | H     | 7881  | 0        | 7579     | 298     | 0            |
| All | All   | 60495 | 0        | 56668    | 2299    | 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 20.

All (2299) 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:345:SER:OG   | 1:D:412:MET:CE   | 1.67                     | 1.40              |
| 1:H:345:SER:OG   | 1:H:412:MET:CE   | 1.68                     | 1.39              |
| 1:E:280:LEU:HD12 | 1:E:289:ILE:CG2  | 1.54                     | 1.37              |
| 1:B:280:LEU:HD12 | 1:B:289:ILE:CG2  | 1.55                     | 1.37              |
| 1:B:279:PHE:N    | 1:B:289:ILE:HD11 | 1.37                     | 1.36              |
| 1:E:279:PHE:N    | 1:E:289:ILE:HD11 | 1.39                     | 1.35              |
| 1:H:345:SER:OG   | 1:H:412:MET:HE1  | 1.21                     | 1.25              |
| 1:D:345:SER:OG   | 1:D:412:MET:HE1  | 1.21                     | 1.24              |
| 1:E:180:VAL:HG12 | 1:E:184:PHE:CZ   | 1.72                     | 1.23              |
| 1:E:144:ILE:HG22 | 1:E:184:PHE:CE2  | 1.78                     | 1.19              |
| 1:B:279:PHE:CA   | 1:B:289:ILE:HD11 | 1.71                     | 1.18              |
| 1:E:14:GLU:OE2   | 1:E:397:LYS:CE   | 1.91                     | 1.17              |
| 1:B:180:VAL:HG12 | 1:B:184:PHE:CZ   | 1.78                     | 1.17              |
| 1:E:279:PHE:CA   | 1:E:289:ILE:HD11 | 1.72                     | 1.17              |
| 1:B:14:GLU:OE2   | 1:B:397:LYS:CE   | 1.91                     | 1.17              |
| 1:B:279:PHE:CA   | 1:B:289:ILE:CD1  | 2.22                     | 1.15              |
| 1:B:612:LEU:HD11 | 1:B:617:ALA:HA   | 1.20                     | 1.15              |
| 1:E:612:LEU:HD11 | 1:E:617:ALA:HA   | 1.20                     | 1.15              |
| 1:E:279:PHE:CA   | 1:E:289:ILE:CD1  | 2.23                     | 1.14              |
| 1:G:960:LEU:HD12 | 1:G:968:PRO:HG3  | 1.25                     | 1.13              |
| 1:C:960:LEU:HD12 | 1:C:968:PRO:HG3  | 1.25                     | 1.13              |
| 1:D:254:LEU:HD22 | 1:D:258:ILE:HD11 | 1.32                     | 1.11              |
| 1:H:254:LEU:HD22 | 1:H:258:ILE:HD11 | 1.32                     | 1.11              |
| 1:E:280:LEU:HD12 | 1:E:289:ILE:HG21 | 1.13                     | 1.10              |
| 1:B:280:LEU:HD12 | 1:B:289:ILE:HG21 | 1.13                     | 1.10              |
| 1:G:61:ASP:HA    | 1:G:64:LEU:HD12  | 1.29                     | 1.09              |
| 1:C:61:ASP:HA    | 1:C:64:LEU:HD12  | 1.29                     | 1.09              |
| 1:D:8:LEU:HA     | 1:D:31:VAL:HG23  | 1.24                     | 1.09              |
| 1:H:8:LEU:HA     | 1:H:31:VAL:HG23  | 1.23                     | 1.09              |
| 1:B:144:ILE:HG22 | 1:B:184:PHE:CE2  | 1.87                     | 1.08              |
| 1:B:158:LEU:HD13 | 1:B:174:VAL:HB   | 1.30                     | 1.07              |
| 1:B:612:LEU:CD1  | 1:B:617:ALA:HA   | 1.86                     | 1.03              |
| 1:E:612:LEU:CD1  | 1:E:617:ALA:HA   | 1.87                     | 1.03              |
| 1:D:345:SER:OG   | 1:D:412:MET:HE3  | 1.53                     | 1.02              |
| 1:C:164:LEU:HA   | 1:C:195:PHE:HE1  | 1.22                     | 1.02              |
| 1:H:345:SER:OG   | 1:H:412:MET:HE3  | 1.54                     | 1.01              |
| 1:E:279:PHE:C    | 1:E:289:ILE:CD1  | 2.29                     | 1.01              |
| 1:B:279:PHE:C    | 1:B:289:ILE:CD1  | 2.29                     | 1.01              |
| 1:A:219:ASP:HB3  | 1:A:323:LEU:HD23 | 1.42                     | 1.01              |
| 1:E:219:ASP:HB3  | 1:E:323:LEU:HD23 | 1.43                     | 1.01              |
| 1:B:219:ASP:HB3  | 1:B:323:LEU:HD23 | 1.43                     | 1.01              |
| 1:E:144:ILE:HG22 | 1:E:184:PHE:CZ   | 1.96                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:THR:OG1  | 1:A:415:ASN:ND2  | 1.94                     | 1.00              |
| 1:F:369:THR:OG1  | 1:F:415:ASN:ND2  | 1.94                     | 1.00              |
| 1:F:219:ASP:HB3  | 1:F:323:LEU:HD23 | 1.44                     | 1.00              |
| 1:G:219:ASP:HB3  | 1:G:323:LEU:HD23 | 1.42                     | 0.99              |
| 1:G:576:TRP:HE1  | 1:G:596:LEU:HB2  | 1.27                     | 0.99              |
| 1:A:156:TYR:O    | 1:A:176:SER:HB2  | 1.61                     | 0.99              |
| 1:E:144:ILE:CG2  | 1:E:184:PHE:CE2  | 2.44                     | 0.99              |
| 1:F:126:ALA:O    | 1:F:131:ILE:CD1  | 2.10                     | 0.99              |
| 1:C:219:ASP:HB3  | 1:C:323:LEU:HD23 | 1.43                     | 0.99              |
| 1:C:576:TRP:HE1  | 1:C:596:LEU:HB2  | 1.28                     | 0.99              |
| 1:G:960:LEU:CD1  | 1:G:968:PRO:HG3  | 1.91                     | 0.98              |
| 1:C:960:LEU:CD1  | 1:C:968:PRO:HG3  | 1.91                     | 0.98              |
| 1:E:915:MET:O    | 1:E:940:LEU:CB   | 2.11                     | 0.98              |
| 1:H:503:GLY:O    | 1:C:5:LYS:NZ     | 1.96                     | 0.98              |
| 1:A:126:ALA:O    | 1:A:131:ILE:CD1  | 2.10                     | 0.98              |
| 1:E:280:LEU:CD1  | 1:E:289:ILE:CG2  | 2.41                     | 0.98              |
| 1:B:280:LEU:CD1  | 1:B:289:ILE:CG2  | 2.41                     | 0.98              |
| 1:G:367:ARG:HH12 | 1:G:1049:GLN:CB  | 1.77                     | 0.97              |
| 1:H:219:ASP:HB3  | 1:H:323:LEU:HD23 | 1.43                     | 0.97              |
| 1:C:369:THR:OG1  | 1:C:415:ASN:ND2  | 1.98                     | 0.97              |
| 1:D:369:THR:OG1  | 1:D:415:ASN:ND2  | 1.96                     | 0.97              |
| 1:G:369:THR:OG1  | 1:G:415:ASN:ND2  | 1.98                     | 0.97              |
| 1:B:158:LEU:HD12 | 1:B:174:VAL:O    | 1.64                     | 0.97              |
| 1:D:219:ASP:HB3  | 1:D:323:LEU:HD23 | 1.44                     | 0.96              |
| 1:B:369:THR:OG1  | 1:B:415:ASN:ND2  | 1.99                     | 0.96              |
| 1:E:369:THR:OG1  | 1:E:415:ASN:ND2  | 1.99                     | 0.96              |
| 1:F:126:ALA:O    | 1:F:131:ILE:HD13 | 1.65                     | 0.96              |
| 1:H:369:THR:OG1  | 1:H:415:ASN:ND2  | 1.98                     | 0.96              |
| 1:A:126:ALA:O    | 1:A:131:ILE:HD13 | 1.66                     | 0.96              |
| 1:C:367:ARG:HH12 | 1:C:1049:GLN:CB  | 1.80                     | 0.95              |
| 1:B:14:GLU:OE2   | 1:B:397:LYS:HE3  | 1.66                     | 0.95              |
| 1:C:164:LEU:HA   | 1:C:195:PHE:CE1  | 2.02                     | 0.95              |
| 1:C:960:LEU:HD11 | 1:C:968:PRO:HB3  | 1.48                     | 0.95              |
| 1:G:960:LEU:HD11 | 1:G:968:PRO:HB3  | 1.48                     | 0.94              |
| 1:E:14:GLU:OE2   | 1:E:397:LYS:HE3  | 1.66                     | 0.94              |
| 1:E:280:LEU:CD1  | 1:E:289:ILE:HG21 | 1.97                     | 0.93              |
| 1:E:14:GLU:OE2   | 1:E:397:LYS:NZ   | 2.02                     | 0.93              |
| 1:E:564:ALA:HB2  | 1:E:603:ILE:HG22 | 1.49                     | 0.93              |
| 1:B:280:LEU:CD1  | 1:B:289:ILE:HG21 | 1.98                     | 0.93              |
| 1:B:564:ALA:HB2  | 1:B:603:ILE:HG22 | 1.49                     | 0.93              |
| 1:B:14:GLU:OE2   | 1:B:397:LYS:NZ   | 2.02                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:3:ARG:HD2    | 1:C:104:ILE:HD11 | 1.51                     | 0.92              |
| 1:G:3:ARG:HD2    | 1:G:104:ILE:HD11 | 1.53                     | 0.90              |
| 1:D:3:ARG:HD2    | 1:D:104:ILE:HD11 | 1.52                     | 0.90              |
| 1:B:279:PHE:HA   | 1:B:289:ILE:HD13 | 1.50                     | 0.90              |
| 1:H:3:ARG:HD2    | 1:H:104:ILE:HD11 | 1.52                     | 0.90              |
| 1:G:576:TRP:NE1  | 1:G:596:LEU:HB2  | 1.86                     | 0.89              |
| 1:F:943:ARG:HD3  | 1:F:946:ALA:HB2  | 1.55                     | 0.89              |
| 1:A:943:ARG:HD3  | 1:A:946:ALA:HB2  | 1.55                     | 0.89              |
| 1:E:279:PHE:HA   | 1:E:289:ILE:HD13 | 1.51                     | 0.89              |
| 1:B:279:PHE:CA   | 1:B:289:ILE:HD13 | 2.00                     | 0.89              |
| 1:B:970:GLU:O    | 1:B:973:VAL:HG22 | 1.72                     | 0.89              |
| 1:C:576:TRP:NE1  | 1:C:596:LEU:HB2  | 1.86                     | 0.89              |
| 1:B:279:PHE:HA   | 1:B:289:ILE:CD1  | 2.01                     | 0.88              |
| 1:E:970:GLU:O    | 1:E:973:VAL:HG22 | 1.73                     | 0.88              |
| 1:B:278:GLU:C    | 1:B:289:ILE:HD11 | 1.92                     | 0.88              |
| 1:E:279:PHE:CA   | 1:E:289:ILE:HD13 | 2.01                     | 0.88              |
| 1:E:279:PHE:HA   | 1:E:289:ILE:CD1  | 2.01                     | 0.88              |
| 1:C:227:LEU:HD23 | 1:C:306:THR:HG21 | 1.55                     | 0.88              |
| 1:E:278:GLU:C    | 1:E:289:ILE:HD11 | 1.94                     | 0.87              |
| 1:A:347:ILE:O    | 1:A:395:LEU:HD12 | 1.74                     | 0.86              |
| 1:F:347:ILE:O    | 1:F:395:LEU:HD12 | 1.74                     | 0.86              |
| 1:D:45:TYR:CE1   | 1:C:1047:ASN:HB3 | 2.09                     | 0.86              |
| 1:C:61:ASP:HA    | 1:C:64:LEU:CD1   | 2.06                     | 0.85              |
| 1:G:61:ASP:HA    | 1:G:64:LEU:CD1   | 2.05                     | 0.85              |
| 1:B:279:PHE:N    | 1:B:289:ILE:CD1  | 2.32                     | 0.85              |
| 1:H:45:TYR:CE1   | 1:G:1047:ASN:HB3 | 2.11                     | 0.84              |
| 1:E:147:VAL:O    | 1:E:151:GLY:N    | 2.09                     | 0.84              |
| 1:E:180:VAL:HG12 | 1:E:184:PHE:HZ   | 1.35                     | 0.83              |
| 1:E:279:PHE:N    | 1:E:289:ILE:CD1  | 2.33                     | 0.83              |
| 1:B:915:MET:O    | 1:B:940:LEU:CB   | 2.26                     | 0.83              |
| 1:D:172:ARG:HH12 | 1:D:186:ARG:CB   | 1.92                     | 0.83              |
| 1:B:101:GLU:HB2  | 1:B:103:ILE:HD13 | 1.60                     | 0.82              |
| 1:E:101:GLU:HB2  | 1:E:103:ILE:HD13 | 1.60                     | 0.82              |
| 1:B:180:VAL:HG12 | 1:B:184:PHE:HZ   | 1.37                     | 0.82              |
| 1:B:144:ILE:HG22 | 1:B:184:PHE:CZ   | 2.14                     | 0.82              |
| 1:C:227:LEU:CD2  | 1:C:306:THR:HG21 | 2.10                     | 0.82              |
| 1:E:349:THR:HG22 | 1:E:393:SER:O    | 1.80                     | 0.82              |
| 1:C:147:VAL:O    | 1:C:151:GLY:N    | 2.11                     | 0.81              |
| 1:F:51:TYR:CE1   | 1:E:1021:GLY:HA3 | 2.15                     | 0.81              |
| 1:G:250:ILE:HD11 | 1:G:255:ARG:HB3  | 1.62                     | 0.81              |
| 1:G:147:VAL:O    | 1:G:151:GLY:N    | 2.11                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:5:LYS:NZ     | 1:D:503:GLY:O    | 2.12                     | 0.81              |
| 1:H:172:ARG:HH12 | 1:H:186:ARG:CB   | 1.94                     | 0.81              |
| 1:B:349:THR:HG22 | 1:B:393:SER:O    | 1.81                     | 0.81              |
| 1:H:8:LEU:HA     | 1:H:31:VAL:CG2   | 2.08                     | 0.81              |
| 1:F:673:ILE:HG22 | 1:F:695:MET:CE   | 2.11                     | 0.81              |
| 1:F:147:VAL:O    | 1:F:151:GLY:N    | 2.12                     | 0.80              |
| 1:A:147:VAL:O    | 1:A:151:GLY:N    | 2.12                     | 0.80              |
| 1:C:250:ILE:HD11 | 1:C:255:ARG:HB3  | 1.63                     | 0.80              |
| 1:A:673:ILE:HG22 | 1:A:695:MET:CE   | 2.12                     | 0.80              |
| 1:D:8:LEU:HA     | 1:D:31:VAL:CG2   | 2.09                     | 0.80              |
| 1:D:254:LEU:CD2  | 1:D:258:ILE:HD11 | 2.11                     | 0.80              |
| 1:G:61:ASP:CA    | 1:G:64:LEU:HD12  | 2.12                     | 0.80              |
| 1:H:254:LEU:CD2  | 1:H:258:ILE:HD11 | 2.11                     | 0.80              |
| 1:A:344:GLN:HG3  | 1:A:399:CYS:SG   | 2.22                     | 0.80              |
| 1:B:144:ILE:CG2  | 1:B:184:PHE:CE2  | 2.64                     | 0.80              |
| 1:G:3:ARG:HG3    | 1:G:319:ASP:OD1  | 1.82                     | 0.80              |
| 1:C:61:ASP:CA    | 1:C:64:LEU:HD12  | 2.12                     | 0.80              |
| 1:G:219:ASP:HB3  | 1:G:323:LEU:CD2  | 2.12                     | 0.80              |
| 1:C:3:ARG:HG3    | 1:C:319:ASP:OD1  | 1.82                     | 0.80              |
| 1:E:843:GLN:O    | 1:E:847:VAL:HG23 | 1.81                     | 0.80              |
| 1:C:344:GLN:HG3  | 1:C:399:CYS:SG   | 2.23                     | 0.79              |
| 1:E:979:TYR:HB3  | 1:E:982:VAL:HG22 | 1.63                     | 0.79              |
| 1:B:843:GLN:O    | 1:B:847:VAL:HG23 | 1.81                     | 0.79              |
| 1:B:876:SER:O    | 1:B:879:VAL:HG12 | 1.81                     | 0.79              |
| 1:H:3:ARG:HG3    | 1:H:319:ASP:OD1  | 1.82                     | 0.79              |
| 1:A:979:TYR:HB3  | 1:A:982:VAL:HG22 | 1.65                     | 0.79              |
| 1:C:66:ILE:O     | 1:C:70:ILE:HD12  | 1.83                     | 0.79              |
| 1:D:3:ARG:HG3    | 1:D:319:ASP:OD1  | 1.82                     | 0.79              |
| 1:E:876:SER:O    | 1:E:879:VAL:HG12 | 1.82                     | 0.79              |
| 1:G:66:ILE:O     | 1:G:70:ILE:HD12  | 1.83                     | 0.79              |
| 1:B:979:TYR:HB3  | 1:B:982:VAL:HG22 | 1.64                     | 0.79              |
| 1:C:219:ASP:HB3  | 1:C:323:LEU:CD2  | 2.13                     | 0.79              |
| 1:D:344:GLN:HG3  | 1:D:399:CYS:SG   | 2.23                     | 0.79              |
| 1:F:943:ARG:O    | 1:F:943:ARG:HG2  | 1.81                     | 0.79              |
| 1:A:943:ARG:O    | 1:A:943:ARG:HG2  | 1.81                     | 0.78              |
| 1:B:72:ILE:O     | 1:B:76:SER:OG    | 2.01                     | 0.78              |
| 1:C:501:PRO:O    | 1:C:504:SER:OG   | 2.01                     | 0.78              |
| 1:E:72:ILE:O     | 1:E:76:SER:OG    | 2.01                     | 0.78              |
| 1:G:344:GLN:HG3  | 1:G:399:CYS:SG   | 2.23                     | 0.78              |
| 1:F:979:TYR:HB3  | 1:F:982:VAL:HG22 | 1.65                     | 0.78              |
| 1:A:219:ASP:HB3  | 1:A:323:LEU:CD2  | 2.13                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:344:GLN:HG3  | 1:E:399:CYS:SG   | 2.24                     | 0.78              |
| 1:F:344:GLN:HG3  | 1:F:399:CYS:SG   | 2.24                     | 0.78              |
| 1:H:344:GLN:HG3  | 1:H:399:CYS:SG   | 2.23                     | 0.78              |
| 1:H:876:SER:O    | 1:H:879:VAL:HG12 | 1.83                     | 0.78              |
| 1:B:66:ILE:O     | 1:B:70:ILE:HD12  | 1.82                     | 0.78              |
| 1:E:66:ILE:O     | 1:E:70:ILE:HD12  | 1.82                     | 0.78              |
| 1:H:510:THR:HG22 | 1:H:607:MET:SD   | 2.22                     | 0.78              |
| 1:A:66:ILE:O     | 1:A:70:ILE:HD12  | 1.82                     | 0.78              |
| 1:A:72:ILE:O     | 1:A:76:SER:OG    | 2.02                     | 0.78              |
| 1:B:219:ASP:HB3  | 1:B:323:LEU:CD2  | 2.13                     | 0.78              |
| 1:B:344:GLN:HG3  | 1:B:399:CYS:SG   | 2.24                     | 0.78              |
| 1:F:72:ILE:O     | 1:F:76:SER:OG    | 2.02                     | 0.78              |
| 1:F:986:TYR:CE1  | 1:F:990:ILE:HD12 | 2.19                     | 0.78              |
| 1:D:876:SER:O    | 1:D:879:VAL:HG12 | 1.83                     | 0.78              |
| 1:E:219:ASP:HB3  | 1:E:323:LEU:CD2  | 2.13                     | 0.78              |
| 1:F:66:ILE:O     | 1:F:70:ILE:HD12  | 1.82                     | 0.78              |
| 1:F:504:SER:HB2  | 1:F:505:GLN:CG   | 2.13                     | 0.78              |
| 1:H:72:ILE:O     | 1:H:76:SER:OG    | 2.01                     | 0.78              |
| 1:D:72:ILE:O     | 1:D:76:SER:OG    | 2.01                     | 0.77              |
| 1:G:501:PRO:O    | 1:G:504:SER:OG   | 2.02                     | 0.77              |
| 1:A:986:TYR:CE1  | 1:A:990:ILE:HD12 | 2.20                     | 0.77              |
| 1:C:540:ARG:NH2  | 1:C:541:ASP:OD1  | 2.18                     | 0.77              |
| 1:D:219:ASP:HB3  | 1:D:323:LEU:CD2  | 2.14                     | 0.77              |
| 1:B:160:ILE:HD11 | 1:B:174:VAL:CG2  | 2.14                     | 0.77              |
| 1:D:510:THR:HG22 | 1:D:607:MET:SD   | 2.23                     | 0.77              |
| 1:G:72:ILE:O     | 1:G:76:SER:OG    | 2.01                     | 0.77              |
| 1:H:219:ASP:HB3  | 1:H:323:LEU:CD2  | 2.15                     | 0.77              |
| 1:E:280:LEU:HD12 | 1:E:289:ILE:HG23 | 1.64                     | 0.77              |
| 1:F:219:ASP:HB3  | 1:F:323:LEU:CD2  | 2.14                     | 0.77              |
| 1:B:280:LEU:HD12 | 1:B:289:ILE:HG23 | 1.65                     | 0.77              |
| 1:C:72:ILE:O     | 1:C:76:SER:OG    | 2.02                     | 0.77              |
| 1:G:540:ARG:NH2  | 1:G:541:ASP:OD1  | 2.18                     | 0.77              |
| 1:C:88:LEU:HB3   | 1:C:94:PHE:HD2   | 1.50                     | 0.77              |
| 1:E:501:PRO:O    | 1:E:504:SER:OG   | 2.03                     | 0.77              |
| 1:B:160:ILE:HD11 | 1:B:174:VAL:HG21 | 1.67                     | 0.76              |
| 1:C:526:VAL:O    | 1:C:529:GLN:N    | 2.18                     | 0.76              |
| 1:D:979:TYR:HB3  | 1:D:982:VAL:HG22 | 1.64                     | 0.76              |
| 1:G:526:VAL:O    | 1:G:529:GLN:N    | 2.18                     | 0.76              |
| 1:G:519:PRO:HB2  | 1:G:705:HIS:NE2  | 2.00                     | 0.76              |
| 1:B:144:ILE:HG22 | 1:B:184:PHE:CD2  | 2.21                     | 0.76              |
| 1:C:691:TYR:O    | 1:C:695:MET:HG2  | 1.85                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:960:LEU:HD11 | 1:C:968:PRO:CB   | 2.15                     | 0.76              |
| 1:G:960:LEU:HD11 | 1:G:968:PRO:CB   | 2.15                     | 0.76              |
| 1:B:228:PHE:HD2  | 1:B:338:ILE:HD11 | 1.50                     | 0.76              |
| 1:C:519:PRO:HB2  | 1:C:705:HIS:NE2  | 2.00                     | 0.76              |
| 1:G:691:TYR:O    | 1:G:695:MET:HG2  | 1.85                     | 0.76              |
| 1:B:88:LEU:HB3   | 1:B:94:PHE:HD2   | 1.50                     | 0.76              |
| 1:F:51:TYR:CE1   | 1:E:1021:GLY:CA  | 2.69                     | 0.76              |
| 1:B:82:HIS:HD2   | 1:B:84:GLY:H     | 1.33                     | 0.76              |
| 1:E:228:PHE:HD2  | 1:E:338:ILE:HD11 | 1.50                     | 0.75              |
| 1:G:88:LEU:HB3   | 1:G:94:PHE:HD2   | 1.52                     | 0.75              |
| 1:A:501:PRO:O    | 1:A:504:SER:OG   | 2.04                     | 0.75              |
| 1:F:124:GLU:O    | 1:F:127:LEU:HG   | 1.86                     | 0.75              |
| 1:B:501:PRO:O    | 1:B:504:SER:OG   | 2.04                     | 0.75              |
| 1:E:88:LEU:HB3   | 1:E:94:PHE:HD2   | 1.51                     | 0.75              |
| 1:H:979:TYR:HB3  | 1:H:982:VAL:HG22 | 1.65                     | 0.75              |
| 1:A:51:TYR:CE1   | 1:B:1021:GLY:HA3 | 2.21                     | 0.75              |
| 1:E:82:HIS:HD2   | 1:E:84:GLY:H     | 1.34                     | 0.75              |
| 1:F:501:PRO:O    | 1:F:504:SER:OG   | 2.05                     | 0.75              |
| 1:G:685:THR:O    | 1:G:688:THR:HG23 | 1.87                     | 0.75              |
| 1:H:82:HIS:HD2   | 1:H:84:GLY:H     | 1.34                     | 0.75              |
| 1:A:124:GLU:O    | 1:A:127:LEU:HG   | 1.86                     | 0.74              |
| 1:C:685:THR:O    | 1:C:688:THR:HG23 | 1.87                     | 0.74              |
| 1:D:82:HIS:HD2   | 1:D:84:GLY:H     | 1.35                     | 0.74              |
| 1:E:88:LEU:HD12  | 1:E:94:PHE:CD2   | 2.23                     | 0.74              |
| 1:H:960:LEU:CD1  | 1:H:976:TYR:CG   | 2.71                     | 0.74              |
| 1:D:45:TYR:CD1   | 1:C:1047:ASN:HB3 | 2.22                     | 0.74              |
| 1:D:501:PRO:O    | 1:D:504:SER:OG   | 2.05                     | 0.74              |
| 1:B:800:GLN:O    | 1:B:804:HIS:ND1  | 2.20                     | 0.74              |
| 1:E:800:GLN:O    | 1:E:804:HIS:ND1  | 2.20                     | 0.74              |
| 1:B:88:LEU:HD12  | 1:B:94:PHE:CD2   | 2.23                     | 0.73              |
| 1:D:960:LEU:CD1  | 1:D:976:TYR:CG   | 2.71                     | 0.73              |
| 1:D:384:GLY:HA3  | 1:C:1050:PRO:HD3 | 1.69                     | 0.73              |
| 1:D:13:GLY:O     | 1:D:17:ILE:HD12  | 1.87                     | 0.73              |
| 1:H:13:GLY:O     | 1:H:17:ILE:HD12  | 1.87                     | 0.73              |
| 1:D:800:GLN:O    | 1:D:804:HIS:ND1  | 2.20                     | 0.73              |
| 1:H:501:PRO:O    | 1:H:504:SER:OG   | 2.05                     | 0.73              |
| 1:D:45:TYR:CE1   | 1:C:1047:ASN:CB  | 2.71                     | 0.73              |
| 1:C:960:LEU:CD1  | 1:C:968:PRO:CG   | 2.65                     | 0.73              |
| 1:F:82:HIS:HD2   | 1:F:84:GLY:H     | 1.36                     | 0.73              |
| 1:G:960:LEU:CD1  | 1:G:968:PRO:CG   | 2.65                     | 0.73              |
| 1:B:141:VAL:HG11 | 1:B:147:VAL:HG22 | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:HIS:HD2   | 1:A:84:GLY:H     | 1.36                     | 0.72              |
| 1:D:960:LEU:HD13 | 1:D:976:TYR:CG   | 2.24                     | 0.72              |
| 1:F:126:ALA:O    | 1:F:131:ILE:HD11 | 1.87                     | 0.72              |
| 1:G:227:LEU:HD22 | 1:G:306:THR:HG21 | 1.71                     | 0.72              |
| 1:H:960:LEU:HD13 | 1:H:976:TYR:CG   | 2.23                     | 0.72              |
| 1:F:627:VAL:HG23 | 1:F:628:ILE:HD12 | 1.68                     | 0.72              |
| 1:A:627:VAL:HG23 | 1:A:628:ILE:HD12 | 1.68                     | 0.72              |
| 1:B:81:ILE:O     | 1:B:106:VAL:HG23 | 1.90                     | 0.72              |
| 1:B:160:ILE:CD1  | 1:B:174:VAL:CG2  | 2.67                     | 0.72              |
| 1:G:175:GLU:HG2  | 1:G:179:HIS:CD2  | 2.24                     | 0.72              |
| 1:A:156:TYR:O    | 1:A:176:SER:CB   | 2.36                     | 0.72              |
| 1:H:45:TYR:CD1   | 1:G:1047:ASN:HB3 | 2.24                     | 0.72              |
| 1:A:126:ALA:O    | 1:A:131:ILE:HD11 | 1.88                     | 0.72              |
| 1:E:234:ILE:HD11 | 1:E:445:TYR:CZ   | 2.25                     | 0.72              |
| 1:A:519:PRO:HB2  | 1:A:705:HIS:NE2  | 2.05                     | 0.72              |
| 1:C:500:ILE:HG21 | 1:C:565:HIS:CD2  | 2.24                     | 0.72              |
| 1:C:510:THR:OG1  | 1:C:607:MET:HG3  | 1.90                     | 0.72              |
| 1:C:228:PHE:CE2  | 1:C:338:ILE:HG13 | 2.24                     | 0.72              |
| 1:E:81:ILE:O     | 1:E:106:VAL:HG23 | 1.90                     | 0.72              |
| 1:A:234:ILE:HD11 | 1:A:445:TYR:CZ   | 2.25                     | 0.71              |
| 1:B:990:ILE:HD11 | 1:B:995:ASP:HA   | 1.72                     | 0.71              |
| 1:F:519:PRO:HB2  | 1:F:705:HIS:NE2  | 2.06                     | 0.71              |
| 1:G:82:HIS:HD2   | 1:G:84:GLY:H     | 1.35                     | 0.71              |
| 1:H:519:PRO:HB2  | 1:H:705:HIS:NE2  | 2.05                     | 0.71              |
| 1:C:82:HIS:HD2   | 1:C:84:GLY:H     | 1.35                     | 0.71              |
| 1:E:990:ILE:HD11 | 1:E:995:ASP:HA   | 1.72                     | 0.71              |
| 1:G:127:LEU:HD22 | 1:G:133:VAL:HG21 | 1.71                     | 0.71              |
| 1:B:158:LEU:CD1  | 1:B:174:VAL:O    | 2.38                     | 0.71              |
| 1:B:234:ILE:HD11 | 1:B:445:TYR:CZ   | 2.25                     | 0.71              |
| 1:D:279:PHE:CA   | 1:D:289:ILE:HD11 | 2.20                     | 0.71              |
| 1:E:279:PHE:C    | 1:E:289:ILE:HD13 | 2.08                     | 0.71              |
| 1:F:234:ILE:HD11 | 1:F:445:TYR:CZ   | 2.26                     | 0.71              |
| 1:A:51:TYR:CE1   | 1:B:1021:GLY:CA  | 2.74                     | 0.71              |
| 1:G:510:THR:OG1  | 1:G:607:MET:HG3  | 1.91                     | 0.71              |
| 1:G:88:LEU:HD12  | 1:G:94:PHE:CD2   | 2.25                     | 0.71              |
| 1:H:279:PHE:CA   | 1:H:289:ILE:HD11 | 2.21                     | 0.71              |
| 1:B:279:PHE:C    | 1:B:289:ILE:HD13 | 2.09                     | 0.71              |
| 1:H:45:TYR:CE1   | 1:G:1047:ASN:CB  | 2.73                     | 0.71              |
| 1:B:437:HIS:CD2  | 1:B:439:ASP:H    | 2.08                     | 0.71              |
| 1:F:504:SER:HB2  | 1:F:505:GLN:HG3  | 1.73                     | 0.71              |
| 1:H:21:ARG:NH2   | 1:G:418:GLU:OE2  | 2.23                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:226:HIS:ND1   | 1:C:259:CYS:HB3   | 2.06                     | 0.71              |
| 1:D:175:GLU:OE2   | 1:D:175:GLU:N     | 2.23                     | 0.71              |
| 1:F:414:ARG:HD3   | 1:E:25:GLU:HG3    | 1.72                     | 0.71              |
| 1:F:511:LYS:HZ3   | 1:F:641:ASP:CG    | 1.94                     | 0.71              |
| 1:C:88:LEU:HD12   | 1:C:94:PHE:CD2    | 2.26                     | 0.70              |
| 1:H:234:ILE:HD11  | 1:H:445:TYR:CZ    | 2.25                     | 0.70              |
| 1:C:127:LEU:HD22  | 1:C:133:VAL:HG21  | 1.72                     | 0.70              |
| 1:D:60:ILE:HD13   | 1:D:60:ILE:H      | 1.53                     | 0.70              |
| 1:E:437:HIS:CD2   | 1:E:439:ASP:H     | 2.08                     | 0.70              |
| 1:E:64:LEU:HD23   | 1:E:88:LEU:HD23   | 1.73                     | 0.70              |
| 1:H:134:ILE:HD12  | 1:H:287:TYR:HB3   | 1.74                     | 0.70              |
| 1:H:60:ILE:H      | 1:H:60:ILE:HD13   | 1.54                     | 0.70              |
| 1:E:14:GLU:OE2    | 1:E:397:LYS:HE2   | 1.90                     | 0.70              |
| 1:B:510:THR:OG1   | 1:B:607:MET:HG3   | 1.90                     | 0.70              |
| 1:E:157:PRO:O     | 1:E:158:LEU:HD23  | 1.92                     | 0.70              |
| 1:B:64:LEU:HD23   | 1:B:88:LEU:HD23   | 1.74                     | 0.70              |
| 1:F:1010:LEU:HD21 | 1:F:1031:ILE:HD11 | 1.74                     | 0.70              |
| 1:A:363:VAL:O     | 1:A:383:GLN:O     | 2.10                     | 0.70              |
| 1:B:14:GLU:OE2    | 1:B:397:LYS:HE2   | 1.90                     | 0.70              |
| 1:D:519:PRO:HB2   | 1:D:705:HIS:NE2   | 2.07                     | 0.70              |
| 1:F:657:VAL:HG22  | 1:F:943:ARG:NH2   | 2.06                     | 0.70              |
| 1:D:370:GLY:O     | 1:C:21:ARG:NH1    | 2.25                     | 0.70              |
| 1:D:234:ILE:HD11  | 1:D:445:TYR:CZ    | 2.26                     | 0.70              |
| 1:H:64:LEU:HD23   | 1:H:88:LEU:HD23   | 1.74                     | 0.70              |
| 1:F:363:VAL:O     | 1:F:383:GLN:O     | 2.10                     | 0.69              |
| 1:A:657:VAL:HG22  | 1:A:943:ARG:NH2   | 2.07                     | 0.69              |
| 1:E:82:HIS:HA     | 1:E:106:VAL:HG23  | 1.74                     | 0.69              |
| 1:B:82:HIS:HA     | 1:B:106:VAL:HG23  | 1.74                     | 0.69              |
| 1:C:234:ILE:HD11  | 1:C:445:TYR:CZ    | 2.28                     | 0.69              |
| 1:C:363:VAL:O     | 1:C:383:GLN:O     | 2.09                     | 0.69              |
| 1:D:64:LEU:HD23   | 1:D:88:LEU:HD23   | 1.75                     | 0.69              |
| 1:F:134:ILE:HD12  | 1:F:287:TYR:HB3   | 1.74                     | 0.69              |
| 1:F:657:VAL:HG22  | 1:F:943:ARG:HH22  | 1.58                     | 0.69              |
| 1:D:363:VAL:O     | 1:D:383:GLN:O     | 2.10                     | 0.69              |
| 1:A:657:VAL:HG22  | 1:A:943:ARG:HH22  | 1.58                     | 0.69              |
| 1:A:370:GLY:O     | 1:B:21:ARG:NH1    | 2.26                     | 0.69              |
| 1:G:363:VAL:O     | 1:G:383:GLN:O     | 2.10                     | 0.69              |
| 1:A:863:VAL:HA    | 1:A:866:MET:HG3   | 1.74                     | 0.68              |
| 1:D:134:ILE:HD12  | 1:D:287:TYR:HB3   | 1.75                     | 0.68              |
| 1:E:180:VAL:HG12  | 1:E:184:PHE:CE1   | 2.28                     | 0.68              |
| 1:H:800:GLN:O     | 1:H:804:HIS:ND1   | 2.20                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:279:PHE:N     | 1:C:289:ILE:HD11  | 2.09                     | 0.68              |
| 1:F:157:PRO:O     | 1:F:158:LEU:HD23  | 1.93                     | 0.68              |
| 1:G:234:ILE:HD11  | 1:G:445:TYR:CZ    | 2.28                     | 0.68              |
| 1:H:363:VAL:O     | 1:H:383:GLN:O     | 2.10                     | 0.68              |
| 1:D:21:ARG:NH1    | 1:C:370:GLY:O     | 2.27                     | 0.68              |
| 1:D:70:ILE:O      | 1:D:74:LYS:HG2    | 1.94                     | 0.68              |
| 1:H:279:PHE:N     | 1:H:289:ILE:HD11  | 2.09                     | 0.68              |
| 1:E:363:VAL:O     | 1:E:383:GLN:O     | 2.10                     | 0.68              |
| 1:F:673:ILE:CG2   | 1:F:695:MET:CE    | 2.71                     | 0.68              |
| 1:G:582:ASP:OD2   | 1:G:586:ARG:NH1   | 2.26                     | 0.68              |
| 1:H:863:VAL:HA    | 1:H:866:MET:HG3   | 1.74                     | 0.68              |
| 1:A:1010:LEU:HD21 | 1:A:1031:ILE:HD11 | 1.75                     | 0.68              |
| 1:D:279:PHE:N     | 1:D:289:ILE:HD11  | 2.09                     | 0.68              |
| 1:A:134:ILE:HD12  | 1:A:287:TYR:HB3   | 1.75                     | 0.68              |
| 1:A:157:PRO:O     | 1:A:158:LEU:HD23  | 1.94                     | 0.68              |
| 1:B:363:VAL:O     | 1:B:383:GLN:O     | 2.10                     | 0.68              |
| 1:C:582:ASP:OD2   | 1:C:586:ARG:NH1   | 2.26                     | 0.68              |
| 1:F:679:ILE:HD13  | 1:F:724:LEU:HD13  | 1.74                     | 0.68              |
| 1:G:279:PHE:N     | 1:G:289:ILE:HD11  | 2.09                     | 0.68              |
| 1:A:673:ILE:CG2   | 1:A:695:MET:CE    | 2.71                     | 0.68              |
| 1:F:863:VAL:HA    | 1:F:866:MET:HG3   | 1.75                     | 0.68              |
| 1:H:70:ILE:O      | 1:H:74:LYS:HG2    | 1.94                     | 0.68              |
| 1:B:143:GLY:O     | 1:B:147:VAL:HG23  | 1.94                     | 0.68              |
| 1:H:582:ASP:OD2   | 1:H:586:ARG:NH1   | 2.27                     | 0.68              |
| 1:D:990:ILE:HD11  | 1:D:995:ASP:HA    | 1.76                     | 0.67              |
| 1:D:582:ASP:OD2   | 1:D:586:ARG:NH1   | 2.28                     | 0.67              |
| 1:B:158:LEU:N     | 1:B:158:LEU:HD12  | 2.09                     | 0.67              |
| 1:D:863:VAL:HA    | 1:D:866:MET:HG3   | 1.75                     | 0.67              |
| 1:E:160:ILE:HD11  | 1:E:174:VAL:HG21  | 1.75                     | 0.67              |
| 1:H:384:GLY:HA3   | 1:G:1050:PRO:HD3  | 1.75                     | 0.67              |
| 1:B:582:ASP:OD2   | 1:B:586:ARG:NH1   | 2.27                     | 0.67              |
| 1:A:679:ILE:HD13  | 1:A:724:LEU:HD13  | 1.75                     | 0.67              |
| 1:D:21:ARG:NH1    | 1:C:370:GLY:C     | 2.47                     | 0.67              |
| 1:B:603:ILE:HG13  | 1:B:608:PHE:CZ    | 2.30                     | 0.67              |
| 1:E:603:ILE:HG13  | 1:E:608:PHE:CZ    | 2.30                     | 0.67              |
| 1:C:198:ASP:O     | 1:C:200:VAL:HG23  | 1.95                     | 0.67              |
| 1:C:66:ILE:HG13   | 1:C:88:LEU:HD11   | 1.77                     | 0.67              |
| 1:H:990:ILE:HD11  | 1:H:995:ASP:HA    | 1.77                     | 0.67              |
| 1:B:603:ILE:HG13  | 1:B:608:PHE:HZ    | 1.60                     | 0.67              |
| 1:H:8:LEU:CA      | 1:H:31:VAL:HG23   | 2.16                     | 0.67              |
| 1:F:198:ASP:O     | 1:F:200:VAL:HG23  | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:582:ASP:OD2  | 1:A:586:ARG:NH1  | 2.28                     | 0.66              |
| 1:B:437:HIS:HD2  | 1:B:439:ASP:N    | 1.91                     | 0.66              |
| 1:F:550:ARG:HG3  | 1:F:816:PHE:CD1  | 2.30                     | 0.66              |
| 1:F:673:ILE:CG2  | 1:F:695:MET:HE3  | 2.25                     | 0.66              |
| 1:E:437:HIS:HD2  | 1:E:439:ASP:N    | 1.92                     | 0.66              |
| 1:E:582:ASP:OD2  | 1:E:586:ARG:NH1  | 2.27                     | 0.66              |
| 1:G:198:ASP:O    | 1:G:200:VAL:HG23 | 1.96                     | 0.66              |
| 1:G:365:THR:HG21 | 1:G:1051:ARG:HD3 | 1.77                     | 0.66              |
| 1:A:550:ARG:HG3  | 1:A:816:PHE:CD1  | 2.31                     | 0.66              |
| 1:A:21:ARG:NH1   | 1:B:370:GLY:O    | 2.28                     | 0.66              |
| 1:C:365:THR:HG21 | 1:C:1051:ARG:HD3 | 1.78                     | 0.66              |
| 1:E:603:ILE:HG13 | 1:E:608:PHE:HZ   | 1.60                     | 0.66              |
| 1:D:1:MET:HE1    | 1:D:319:ASP:HB2  | 1.78                     | 0.66              |
| 1:A:414:ARG:HD3  | 1:B:25:GLU:HG3   | 1.77                     | 0.66              |
| 1:A:673:ILE:CG2  | 1:A:695:MET:HE3  | 2.26                     | 0.66              |
| 1:D:679:ILE:HD13 | 1:D:724:LEU:HD13 | 1.76                     | 0.66              |
| 1:G:250:ILE:HD11 | 1:G:255:ARG:CB   | 2.25                     | 0.66              |
| 1:G:66:ILE:HG13  | 1:G:88:LEU:HD11  | 1.78                     | 0.66              |
| 1:A:198:ASP:O    | 1:A:200:VAL:HG23 | 1.95                     | 0.66              |
| 1:C:1:MET:HE1    | 1:C:319:ASP:HB2  | 1.78                     | 0.66              |
| 1:E:250:ILE:HD11 | 1:E:255:ARG:HB2  | 1.76                     | 0.66              |
| 1:F:250:ILE:HD11 | 1:F:255:ARG:HB2  | 1.77                     | 0.66              |
| 1:F:582:ASP:OD2  | 1:F:586:ARG:NH1  | 2.29                     | 0.66              |
| 1:G:227:LEU:CD2  | 1:G:306:THR:HG21 | 2.26                     | 0.66              |
| 1:B:147:VAL:O    | 1:B:151:GLY:N    | 2.28                     | 0.66              |
| 1:F:120:ILE:HD12 | 1:F:121:LYS:N    | 2.11                     | 0.66              |
| 1:F:504:SER:HB2  | 1:F:505:GLN:HG2  | 1.76                     | 0.66              |
| 1:G:278:GLU:C    | 1:G:289:ILE:HD11 | 2.16                     | 0.66              |
| 1:H:250:ILE:HD11 | 1:H:255:ARG:HB2  | 1.78                     | 0.66              |
| 1:B:250:ILE:HD11 | 1:B:255:ARG:HB2  | 1.77                     | 0.66              |
| 1:A:250:ILE:HD11 | 1:A:255:ARG:HB2  | 1.78                     | 0.65              |
| 1:D:120:ILE:HD12 | 1:D:121:LYS:N    | 2.11                     | 0.65              |
| 1:D:250:ILE:HD11 | 1:D:255:ARG:HB2  | 1.78                     | 0.65              |
| 1:D:370:GLY:C    | 1:C:21:ARG:NH1   | 2.50                     | 0.65              |
| 1:H:176:SER:O    | 1:H:179:HIS:ND1  | 2.26                     | 0.65              |
| 1:B:158:LEU:HD13 | 1:B:174:VAL:CB   | 2.18                     | 0.65              |
| 1:C:278:GLU:C    | 1:C:289:ILE:HD11 | 2.17                     | 0.65              |
| 1:G:1:MET:HE1    | 1:G:319:ASP:HB2  | 1.78                     | 0.65              |
| 1:H:120:ILE:HD12 | 1:H:121:LYS:N    | 2.11                     | 0.65              |
| 1:H:1:MET:HE1    | 1:H:319:ASP:HB2  | 1.78                     | 0.65              |
| 1:H:659:ILE:HG23 | 1:H:669:VAL:HG11 | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:679:ILE:HD13 | 1:H:724:LEU:HD13 | 1.77                     | 0.65              |
| 1:A:151:GLY:HA2  | 1:A:158:LEU:HD11 | 1.78                     | 0.65              |
| 1:C:120:ILE:HD12 | 1:C:121:LYS:N    | 2.11                     | 0.65              |
| 1:C:250:ILE:HD11 | 1:C:255:ARG:CB   | 2.26                     | 0.65              |
| 1:F:370:GLY:O    | 1:E:21:ARG:NH1   | 2.30                     | 0.65              |
| 1:F:21:ARG:NH1   | 1:E:370:GLY:O    | 2.29                     | 0.65              |
| 1:G:127:LEU:CD2  | 1:G:133:VAL:HG21 | 2.26                     | 0.65              |
| 1:H:66:ILE:HG13  | 1:H:88:LEU:HD11  | 1.79                     | 0.65              |
| 1:A:120:ILE:HD12 | 1:A:121:LYS:N    | 2.12                     | 0.65              |
| 1:D:66:ILE:HG13  | 1:D:88:LEU:HD11  | 1.79                     | 0.65              |
| 1:H:352:PRO:HA   | 1:H:356:PHE:CD1  | 2.32                     | 0.65              |
| 1:B:141:VAL:CG1  | 1:B:147:VAL:HG22 | 2.27                     | 0.65              |
| 1:B:603:ILE:HD12 | 1:B:608:PHE:CE1  | 2.32                     | 0.65              |
| 1:D:659:ILE:HG23 | 1:D:669:VAL:HG11 | 1.79                     | 0.65              |
| 1:A:1:MET:HE1    | 1:A:319:ASP:HB2  | 1.77                     | 0.64              |
| 1:A:470:LEU:HD22 | 1:A:1044:PHE:CD2 | 2.32                     | 0.64              |
| 1:B:464:ASP:OD2  | 1:B:467:THR:OG1  | 2.15                     | 0.64              |
| 1:C:127:LEU:CD2  | 1:C:133:VAL:HG21 | 2.27                     | 0.64              |
| 1:D:550:ARG:HG3  | 1:D:816:PHE:CD1  | 2.33                     | 0.64              |
| 1:G:960:LEU:HD13 | 1:G:961:LYS:N    | 2.12                     | 0.64              |
| 1:E:464:ASP:OD2  | 1:E:467:THR:OG1  | 2.15                     | 0.64              |
| 1:E:603:ILE:HD12 | 1:E:608:PHE:CE1  | 2.33                     | 0.64              |
| 1:E:952:ASN:OD1  | 1:E:955:GLU:N    | 2.19                     | 0.64              |
| 1:F:1:MET:HE1    | 1:F:319:ASP:HB2  | 1.78                     | 0.64              |
| 1:F:943:ARG:HD3  | 1:F:946:ALA:CB   | 2.27                     | 0.64              |
| 1:H:901:GLY:HA3  | 1:H:932:LEU:HD22 | 1.79                     | 0.64              |
| 1:A:25:GLU:HG3   | 1:B:414:ARG:HD3  | 1.80                     | 0.64              |
| 1:B:952:ASN:OD1  | 1:B:955:GLU:N    | 2.19                     | 0.64              |
| 1:C:960:LEU:HD13 | 1:C:961:LYS:N    | 2.12                     | 0.64              |
| 1:E:66:ILE:HG13  | 1:E:88:LEU:HD11  | 1.78                     | 0.64              |
| 1:B:66:ILE:HG13  | 1:B:88:LEU:HD11  | 1.78                     | 0.64              |
| 1:H:550:ARG:HG3  | 1:H:816:PHE:CD1  | 2.33                     | 0.64              |
| 1:A:943:ARG:HD3  | 1:A:946:ALA:CB   | 2.27                     | 0.64              |
| 1:B:144:ILE:CG2  | 1:B:184:PHE:CD2  | 2.81                     | 0.64              |
| 1:D:901:GLY:HA3  | 1:D:932:LEU:HD22 | 1.79                     | 0.64              |
| 1:F:504:SER:CB   | 1:F:505:GLN:HG2  | 2.28                     | 0.64              |
| 1:D:328:VAL:HG12 | 1:D:330:ILE:HG13 | 1.80                     | 0.64              |
| 1:H:328:VAL:HG12 | 1:H:330:ILE:HG13 | 1.80                     | 0.64              |
| 1:H:546:LEU:HB3  | 1:H:547:LEU:HD13 | 1.80                     | 0.64              |
| 1:D:198:ASP:O    | 1:D:200:VAL:HG23 | 1.98                     | 0.64              |
| 1:G:174:VAL:HG12 | 1:G:176:SER:H    | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:500:ILE:HG21 | 1:G:565:HIS:CD2  | 2.33                     | 0.64              |
| 1:H:198:ASP:O    | 1:H:200:VAL:HG23 | 1.97                     | 0.64              |
| 1:C:540:ARG:HH21 | 1:C:541:ASP:CG   | 2.01                     | 0.64              |
| 1:A:659:ILE:HG23 | 1:A:669:VAL:HG11 | 1.80                     | 0.63              |
| 1:B:228:PHE:CE2  | 1:B:338:ILE:HG13 | 2.33                     | 0.63              |
| 1:B:740:THR:HG22 | 1:B:751:TYR:CE1  | 2.33                     | 0.63              |
| 1:E:550:ARG:HG3  | 1:E:816:PHE:CD1  | 2.34                     | 0.63              |
| 1:G:120:ILE:HD12 | 1:G:121:LYS:N    | 2.12                     | 0.63              |
| 1:D:546:LEU:HB3  | 1:D:547:LEU:HD13 | 1.81                     | 0.63              |
| 1:B:254:LEU:HD22 | 1:B:258:ILE:HD11 | 1.80                     | 0.63              |
| 1:E:740:THR:HG22 | 1:E:751:TYR:CE1  | 2.33                     | 0.63              |
| 1:F:659:ILE:HG23 | 1:F:669:VAL:HG11 | 1.80                     | 0.63              |
| 1:A:370:GLY:C    | 1:B:21:ARG:NH1   | 2.51                     | 0.63              |
| 1:B:550:ARG:HG3  | 1:B:816:PHE:CD1  | 2.34                     | 0.63              |
| 1:C:227:LEU:HD23 | 1:C:306:THR:CG2  | 2.29                     | 0.63              |
| 1:E:228:PHE:CE2  | 1:E:338:ILE:HG13 | 2.34                     | 0.63              |
| 1:H:541:ASP:OD2  | 1:H:739:HIS:CE1  | 2.52                     | 0.63              |
| 1:C:254:LEU:HD22 | 1:C:258:ILE:HD11 | 1.81                     | 0.63              |
| 1:E:254:LEU:HD22 | 1:E:258:ILE:HD11 | 1.81                     | 0.63              |
| 1:G:659:ILE:HG23 | 1:G:669:VAL:HG11 | 1.79                     | 0.63              |
| 1:B:328:VAL:HG12 | 1:B:330:ILE:HG13 | 1.81                     | 0.63              |
| 1:D:680:ASP:OD1  | 1:D:723:ARG:NH1  | 2.31                     | 0.63              |
| 1:F:328:VAL:HG12 | 1:F:330:ILE:HG13 | 1.81                     | 0.63              |
| 1:G:550:ARG:HG3  | 1:G:816:PHE:CD1  | 2.33                     | 0.63              |
| 1:A:597:GLU:OE1  | 1:A:971:LYS:NZ   | 2.26                     | 0.63              |
| 1:C:174:VAL:HG12 | 1:C:176:SER:H    | 1.64                     | 0.63              |
| 1:C:328:VAL:HG12 | 1:C:330:ILE:HG13 | 1.81                     | 0.63              |
| 1:E:352:PRO:HA   | 1:E:356:PHE:CD1  | 2.33                     | 0.63              |
| 1:F:470:LEU:HD22 | 1:F:1044:PHE:CD2 | 2.34                     | 0.63              |
| 1:H:290:GLU:OE2  | 1:H:291:VAL:N    | 2.31                     | 0.63              |
| 1:A:740:THR:HG22 | 1:A:751:TYR:CE1  | 2.35                     | 0.62              |
| 1:D:740:THR:HG22 | 1:D:751:TYR:CE1  | 2.34                     | 0.62              |
| 1:E:328:VAL:HG12 | 1:E:330:ILE:HG13 | 1.81                     | 0.62              |
| 1:G:254:LEU:HD22 | 1:G:258:ILE:HD11 | 1.81                     | 0.62              |
| 1:H:942:ASP:OD1  | 1:H:942:ASP:N    | 2.32                     | 0.62              |
| 1:B:141:VAL:HG21 | 1:B:202:VAL:CB   | 2.28                     | 0.62              |
| 1:D:352:PRO:HA   | 1:D:356:PHE:CD1  | 2.34                     | 0.62              |
| 1:H:740:THR:HG22 | 1:H:751:TYR:CE1  | 2.34                     | 0.62              |
| 1:C:659:ILE:HG23 | 1:C:669:VAL:HG11 | 1.80                     | 0.62              |
| 1:D:541:ASP:OD2  | 1:D:739:HIS:CE1  | 2.52                     | 0.62              |
| 1:H:680:ASP:OD1  | 1:H:723:ARG:NH1  | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:254:LEU:HD22 | 1:A:258:ILE:HD11 | 1.80                     | 0.62              |
| 1:B:437:HIS:HD2  | 1:B:439:ASP:H    | 1.46                     | 0.62              |
| 1:B:940:LEU:O    | 1:B:941:THR:HG22 | 1.99                     | 0.62              |
| 1:C:526:VAL:O    | 1:C:529:GLN:CB   | 2.47                     | 0.62              |
| 1:G:540:ARG:HH21 | 1:G:541:ASP:CG   | 2.03                     | 0.62              |
| 1:G:546:LEU:HB3  | 1:G:547:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:832:MET:HG3  | 1:C:833:PRO:CD   | 2.30                     | 0.62              |
| 1:D:624:PRO:O    | 1:D:627:VAL:HG22 | 1.99                     | 0.62              |
| 1:F:740:THR:HG22 | 1:F:751:TYR:CE1  | 2.35                     | 0.62              |
| 1:D:942:ASP:N    | 1:D:942:ASP:OD1  | 2.33                     | 0.62              |
| 1:F:624:PRO:O    | 1:F:627:VAL:HG22 | 2.00                     | 0.62              |
| 1:A:541:ASP:OD2  | 1:A:739:HIS:CE1  | 2.52                     | 0.62              |
| 1:C:624:PRO:O    | 1:C:627:VAL:HG22 | 2.00                     | 0.62              |
| 1:G:624:PRO:O    | 1:G:627:VAL:HG22 | 2.00                     | 0.62              |
| 1:A:624:PRO:O    | 1:A:627:VAL:HG22 | 2.00                     | 0.62              |
| 1:B:352:PRO:HA   | 1:B:356:PHE:CD1  | 2.34                     | 0.62              |
| 1:C:546:LEU:HB3  | 1:C:547:LEU:HD13 | 1.82                     | 0.62              |
| 1:G:328:VAL:HG12 | 1:G:330:ILE:HG13 | 1.82                     | 0.62              |
| 1:A:219:ASP:CB   | 1:A:323:LEU:HD23 | 2.27                     | 0.61              |
| 1:F:254:LEU:HD22 | 1:F:258:ILE:HD11 | 1.81                     | 0.61              |
| 1:F:370:GLY:C    | 1:E:21:ARG:NH1   | 2.53                     | 0.61              |
| 1:H:17:ILE:HD11  | 1:H:43:HIS:HB3   | 1.82                     | 0.61              |
| 1:C:550:ARG:HG3  | 1:C:816:PHE:CD1  | 2.35                     | 0.61              |
| 1:G:526:VAL:O    | 1:G:529:GLN:CB   | 2.48                     | 0.61              |
| 1:F:25:GLU:HG3   | 1:E:414:ARG:HD3  | 1.83                     | 0.61              |
| 1:F:546:LEU:HB3  | 1:F:547:LEU:HD13 | 1.82                     | 0.61              |
| 1:H:624:PRO:O    | 1:H:627:VAL:HG22 | 2.00                     | 0.61              |
| 1:D:177:LYS:HG3  | 1:D:178:GLU:H    | 1.64                     | 0.61              |
| 1:G:352:PRO:HA   | 1:G:356:PHE:CD1  | 2.35                     | 0.61              |
| 1:B:624:PRO:O    | 1:B:627:VAL:HG22 | 2.00                     | 0.61              |
| 1:C:537:THR:O    | 1:C:540:ARG:O    | 2.18                     | 0.61              |
| 1:E:180:VAL:CG1  | 1:E:184:PHE:CZ   | 2.66                     | 0.61              |
| 1:G:832:MET:HG3  | 1:G:833:PRO:CD   | 2.31                     | 0.61              |
| 1:H:537:THR:O    | 1:H:540:ARG:O    | 2.19                     | 0.61              |
| 1:A:328:VAL:HG12 | 1:A:330:ILE:HG13 | 1.82                     | 0.61              |
| 1:B:546:LEU:HB3  | 1:B:547:LEU:HD13 | 1.83                     | 0.61              |
| 1:C:352:PRO:HA   | 1:C:356:PHE:CD1  | 2.35                     | 0.61              |
| 1:E:624:PRO:O    | 1:E:627:VAL:HG22 | 2.00                     | 0.61              |
| 1:F:151:GLY:HA2  | 1:F:158:LEU:HD11 | 1.81                     | 0.61              |
| 1:F:174:VAL:HG12 | 1:F:176:SER:H    | 1.64                     | 0.61              |
| 1:F:541:ASP:OD2  | 1:F:739:HIS:CE1  | 2.53                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:537:THR:O     | 1:G:540:ARG:O     | 2.18                     | 0.61              |
| 1:H:360:THR:HA    | 1:H:387:VAL:CG2   | 2.31                     | 0.61              |
| 1:D:537:THR:O     | 1:D:540:ARG:O     | 2.19                     | 0.61              |
| 1:E:749:TYR:CZ    | 1:G:752:ALA:HB1   | 2.36                     | 0.61              |
| 1:A:832:MET:HG2   | 1:A:836:GLN:HG2   | 1.81                     | 0.61              |
| 1:E:219:ASP:CB    | 1:E:323:LEU:HD23  | 2.27                     | 0.61              |
| 1:E:234:ILE:HD11  | 1:E:445:TYR:CE1   | 2.36                     | 0.61              |
| 1:F:175:GLU:OE2   | 1:F:175:GLU:N     | 2.33                     | 0.61              |
| 1:G:360:THR:HA    | 1:G:387:VAL:CG2   | 2.31                     | 0.61              |
| 1:C:360:THR:HA    | 1:C:387:VAL:CG2   | 2.31                     | 0.61              |
| 1:A:942:ASP:N     | 1:A:942:ASP:OD1   | 2.33                     | 0.61              |
| 1:H:360:THR:HA    | 1:H:387:VAL:HG23  | 1.83                     | 0.61              |
| 1:A:21:ARG:NH1    | 1:B:370:GLY:C     | 2.53                     | 0.60              |
| 1:B:219:ASP:CB    | 1:B:323:LEU:HD23  | 2.27                     | 0.60              |
| 1:H:254:LEU:O     | 1:H:258:ILE:HD12  | 2.01                     | 0.60              |
| 1:A:175:GLU:OE2   | 1:A:175:GLU:N     | 2.34                     | 0.60              |
| 1:B:234:ILE:HD11  | 1:B:445:TYR:CE1   | 2.36                     | 0.60              |
| 1:E:213:GLU:OE2   | 1:E:232:CYS:SG    | 2.54                     | 0.60              |
| 1:F:942:ASP:OD1   | 1:F:942:ASP:N     | 2.33                     | 0.60              |
| 1:A:546:LEU:HB3   | 1:A:547:LEU:HD13  | 1.83                     | 0.60              |
| 1:B:537:THR:O     | 1:B:540:ARG:O     | 2.19                     | 0.60              |
| 1:D:254:LEU:O     | 1:D:258:ILE:HD12  | 2.01                     | 0.60              |
| 1:G:110:SER:HA    | 1:G:113:LEU:HD12  | 1.82                     | 0.60              |
| 1:E:537:THR:O     | 1:E:540:ARG:O     | 2.19                     | 0.60              |
| 1:F:126:ALA:C     | 1:F:131:ILE:HD11  | 2.21                     | 0.60              |
| 1:G:576:TRP:CD1   | 1:G:596:LEU:HB2   | 2.37                     | 0.60              |
| 1:C:110:SER:HA    | 1:C:113:LEU:HD12  | 1.82                     | 0.60              |
| 1:C:576:TRP:CD1   | 1:C:596:LEU:HB2   | 2.37                     | 0.60              |
| 1:D:360:THR:HA    | 1:D:387:VAL:CG2   | 2.31                     | 0.60              |
| 1:D:17:ILE:HD11   | 1:D:43:HIS:HB3    | 1.84                     | 0.60              |
| 1:F:1031:ILE:HG22 | 1:F:1042:ILE:HG13 | 1.84                     | 0.60              |
| 1:A:174:VAL:HG12  | 1:A:176:SER:H     | 1.66                     | 0.60              |
| 1:A:537:THR:O     | 1:A:540:ARG:O     | 2.19                     | 0.60              |
| 1:C:541:ASP:OD2   | 1:C:739:HIS:CE1   | 2.55                     | 0.60              |
| 1:E:546:LEU:HB3   | 1:E:547:LEU:HD13  | 1.84                     | 0.60              |
| 1:F:537:THR:O     | 1:F:540:ARG:O     | 2.19                     | 0.60              |
| 1:F:680:ASP:OD1   | 1:F:723:ARG:NH1   | 2.33                     | 0.60              |
| 1:A:1031:ILE:HG22 | 1:A:1042:ILE:HG13 | 1.84                     | 0.60              |
| 1:B:213:GLU:OE2   | 1:B:232:CYS:SG    | 2.55                     | 0.60              |
| 1:D:25:GLU:HG3    | 1:C:414:ARG:HD3   | 1.83                     | 0.60              |
| 1:E:979:TYR:HB3   | 1:E:982:VAL:CG2   | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:611:LEU:HD11 | 1:F:646:PHE:CE1  | 2.37                     | 0.60              |
| 1:F:832:MET:HG2  | 1:F:836:GLN:HG2  | 1.81                     | 0.60              |
| 1:H:611:LEU:HD11 | 1:H:646:PHE:CE1  | 2.37                     | 0.60              |
| 1:B:160:ILE:HD12 | 1:B:174:VAL:HG23 | 1.84                     | 0.60              |
| 1:E:382:PHE:CE1  | 1:E:385:THR:HB   | 2.36                     | 0.60              |
| 1:G:552:ARG:HA   | 1:G:588:LEU:HD11 | 1.83                     | 0.60              |
| 1:H:219:ASP:CB   | 1:H:323:LEU:HD23 | 2.27                     | 0.60              |
| 1:H:12:ARG:NH2   | 1:H:38:ASP:OD1   | 2.34                     | 0.60              |
| 1:C:589:ASN:OD1  | 1:C:989:MET:HE1  | 2.02                     | 0.60              |
| 1:D:12:ARG:NH2   | 1:D:38:ASP:OD1   | 2.34                     | 0.60              |
| 1:F:126:ALA:CA   | 1:F:131:ILE:HD11 | 2.31                     | 0.60              |
| 1:G:541:ASP:OD2  | 1:G:739:HIS:CE1  | 2.55                     | 0.60              |
| 1:A:234:ILE:HD11 | 1:A:445:TYR:CE1  | 2.36                     | 0.60              |
| 1:A:680:ASP:OD1  | 1:A:723:ARG:NH1  | 2.33                     | 0.60              |
| 1:A:979:TYR:HB3  | 1:A:982:VAL:CG2  | 2.32                     | 0.60              |
| 1:D:360:THR:HA   | 1:D:387:VAL:HG23 | 1.84                     | 0.60              |
| 1:E:360:THR:HA   | 1:E:387:VAL:CG2  | 2.31                     | 0.60              |
| 1:E:940:LEU:O    | 1:E:941:THR:HG22 | 2.02                     | 0.60              |
| 1:H:134:ILE:HD12 | 1:H:287:TYR:CB   | 2.32                     | 0.60              |
| 1:A:563:MET:HE1  | 1:A:573:PHE:CD2  | 2.36                     | 0.59              |
| 1:B:360:THR:HA   | 1:B:387:VAL:CG2  | 2.32                     | 0.59              |
| 1:C:470:LEU:HD22 | 1:C:1044:PHE:CD2 | 2.37                     | 0.59              |
| 1:D:290:GLU:OE2  | 1:D:291:VAL:N    | 2.32                     | 0.59              |
| 1:D:219:ASP:CB   | 1:D:323:LEU:HD23 | 2.28                     | 0.59              |
| 1:E:437:HIS:HD2  | 1:E:439:ASP:H    | 1.47                     | 0.59              |
| 1:G:589:ASN:OD1  | 1:G:989:MET:HE1  | 2.02                     | 0.59              |
| 1:E:541:ASP:OD2  | 1:E:739:HIS:CE1  | 2.55                     | 0.59              |
| 1:F:979:TYR:HB3  | 1:F:982:VAL:CG2  | 2.32                     | 0.59              |
| 1:H:370:GLY:O    | 1:G:21:ARG:NH1   | 2.36                     | 0.59              |
| 1:H:414:ARG:HD3  | 1:G:25:GLU:HG3   | 1.82                     | 0.59              |
| 1:F:21:ARG:NH1   | 1:E:370:GLY:C    | 2.55                     | 0.59              |
| 1:A:110:SER:HA   | 1:A:113:LEU:HD12 | 1.83                     | 0.59              |
| 1:D:45:TYR:CE2   | 1:C:1047:ASN:O   | 2.55                     | 0.59              |
| 1:D:611:LEU:HD11 | 1:D:646:PHE:CE1  | 2.37                     | 0.59              |
| 1:D:979:TYR:HB3  | 1:D:982:VAL:CG2  | 2.33                     | 0.59              |
| 1:E:280:LEU:N    | 1:E:289:ILE:HD13 | 2.18                     | 0.59              |
| 1:F:234:ILE:HD11 | 1:F:445:TYR:CE1  | 2.37                     | 0.59              |
| 1:G:470:LEU:HD22 | 1:G:1044:PHE:CD2 | 2.38                     | 0.59              |
| 1:C:552:ARG:HA   | 1:C:588:LEU:HD11 | 1.84                     | 0.59              |
| 1:E:470:LEU:HD22 | 1:E:1044:PHE:CD2 | 2.38                     | 0.59              |
| 1:F:110:SER:HA   | 1:F:113:LEU:HD12 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:134:ILE:HD12 | 1:F:287:TYR:CB   | 2.32                     | 0.59              |
| 1:B:541:ASP:OD2  | 1:B:739:HIS:CE1  | 2.56                     | 0.59              |
| 1:B:979:TYR:HB3  | 1:B:982:VAL:CG2  | 2.32                     | 0.59              |
| 1:E:266:MET:HE2  | 1:E:277:VAL:HG22 | 1.84                     | 0.59              |
| 1:G:360:THR:HA   | 1:G:387:VAL:HG23 | 1.83                     | 0.59              |
| 1:A:126:ALA:C    | 1:A:131:ILE:HD11 | 2.22                     | 0.59              |
| 1:H:234:ILE:HD11 | 1:H:445:TYR:CE1  | 2.37                     | 0.59              |
| 1:A:134:ILE:HD12 | 1:A:287:TYR:CB   | 2.32                     | 0.59              |
| 1:A:865:GLN:HA   | 1:A:868:GLY:O    | 2.03                     | 0.59              |
| 1:C:360:THR:HA   | 1:C:387:VAL:HG23 | 1.83                     | 0.59              |
| 1:E:14:GLU:CD    | 1:E:397:LYS:HE3  | 2.22                     | 0.59              |
| 1:A:126:ALA:CA   | 1:A:131:ILE:HD11 | 2.32                     | 0.59              |
| 1:D:45:TYR:CZ    | 1:C:1047:ASN:HB3 | 2.38                     | 0.59              |
| 1:A:611:LEU:HD11 | 1:A:646:PHE:CE1  | 2.38                     | 0.59              |
| 1:B:382:PHE:CE1  | 1:B:385:THR:HB   | 2.38                     | 0.59              |
| 1:F:511:LYS:NZ   | 1:F:641:ASP:OD1  | 2.35                     | 0.59              |
| 1:H:134:ILE:CD1  | 1:H:287:TYR:CB   | 2.81                     | 0.59              |
| 1:H:64:LEU:CD2   | 1:H:88:LEU:HD23  | 2.33                     | 0.59              |
| 1:A:511:LYS:NZ   | 1:A:641:ASP:OD1  | 2.35                     | 0.58              |
| 1:B:280:LEU:N    | 1:B:289:ILE:HD13 | 2.18                     | 0.58              |
| 1:D:322:ALA:N    | 1:D:325:ASP:OD2  | 2.36                     | 0.58              |
| 1:B:64:LEU:CD2   | 1:B:88:LEU:HD23  | 2.32                     | 0.58              |
| 1:D:134:ILE:HD12 | 1:D:287:TYR:CB   | 2.33                     | 0.58              |
| 1:E:141:VAL:HG21 | 1:E:202:VAL:CB   | 2.33                     | 0.58              |
| 1:H:470:LEU:HD22 | 1:H:1044:PHE:CD2 | 2.38                     | 0.58              |
| 1:H:979:TYR:HB3  | 1:H:982:VAL:CG2  | 2.34                     | 0.58              |
| 1:E:360:THR:HA   | 1:E:387:VAL:HG23 | 1.84                     | 0.58              |
| 1:E:64:LEU:CD2   | 1:E:88:LEU:HD23  | 2.32                     | 0.58              |
| 1:F:134:ILE:CD1  | 1:F:287:TYR:CB   | 2.81                     | 0.58              |
| 1:F:563:MET:HE1  | 1:F:573:PHE:CD2  | 2.37                     | 0.58              |
| 1:B:360:THR:HA   | 1:B:387:VAL:HG23 | 1.84                     | 0.58              |
| 1:B:14:GLU:CD    | 1:B:397:LYS:HE3  | 2.23                     | 0.58              |
| 1:C:653:LYS:O    | 1:C:943:ARG:HD3  | 2.03                     | 0.58              |
| 1:D:470:LEU:HD22 | 1:D:1044:PHE:CD2 | 2.38                     | 0.58              |
| 1:D:64:LEU:CD2   | 1:D:88:LEU:HD23  | 2.34                     | 0.58              |
| 1:E:228:PHE:CD2  | 1:E:338:ILE:HD11 | 2.37                     | 0.58              |
| 1:G:653:LYS:O    | 1:G:943:ARG:HD3  | 2.03                     | 0.58              |
| 1:B:348:THR:OG1  | 1:B:350:GLU:HG3  | 2.04                     | 0.58              |
| 1:D:234:ILE:HD11 | 1:D:445:TYR:CE1  | 2.38                     | 0.58              |
| 1:H:322:ALA:N    | 1:H:325:ASP:OD2  | 2.36                     | 0.58              |
| 1:H:45:TYR:CE2   | 1:G:1047:ASN:O   | 2.57                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:470:LEU:HD22 | 1:B:1044:PHE:CD2 | 2.39                     | 0.58              |
| 1:D:898:TYR:HD1  | 1:D:928:LYS:CE   | 2.16                     | 0.58              |
| 1:A:134:ILE:CD1  | 1:A:287:TYR:CB   | 2.81                     | 0.58              |
| 1:E:823:PRO:O    | 1:G:767:SER:HB3  | 2.04                     | 0.58              |
| 1:F:92:ILE:HD13  | 1:F:113:LEU:HB2  | 1.86                     | 0.58              |
| 1:H:550:ARG:HG3  | 1:H:816:PHE:CE1  | 2.39                     | 0.58              |
| 1:E:322:ALA:N    | 1:E:325:ASP:OD2  | 2.36                     | 0.58              |
| 1:F:322:ALA:N    | 1:F:325:ASP:OD2  | 2.36                     | 0.58              |
| 1:A:360:THR:HA   | 1:A:387:VAL:CG2  | 2.33                     | 0.58              |
| 1:A:511:LYS:HZ3  | 1:A:641:ASP:CG   | 2.07                     | 0.58              |
| 1:B:266:MET:HE2  | 1:B:277:VAL:HG22 | 1.85                     | 0.58              |
| 1:B:603:ILE:CD1  | 1:B:608:PHE:CE1  | 2.86                     | 0.58              |
| 1:D:134:ILE:CD1  | 1:D:287:TYR:CB   | 2.82                     | 0.58              |
| 1:E:278:GLU:HB2  | 1:E:289:ILE:HG13 | 1.84                     | 0.58              |
| 1:H:898:TYR:HD1  | 1:H:928:LYS:CE   | 2.16                     | 0.58              |
| 1:A:322:ALA:N    | 1:A:325:ASP:OD2  | 2.37                     | 0.58              |
| 1:B:101:GLU:CB   | 1:B:103:ILE:HD13 | 2.32                     | 0.58              |
| 1:E:603:ILE:CD1  | 1:E:608:PHE:CE1  | 2.86                     | 0.58              |
| 1:F:382:PHE:CE1  | 1:F:385:THR:HB   | 2.38                     | 0.58              |
| 1:G:53:VAL:HG13  | 1:G:54:GLY:N     | 2.18                     | 0.58              |
| 1:H:177:LYS:HG3  | 1:H:178:GLU:H    | 1.68                     | 0.58              |
| 1:B:749:TYR:CZ   | 1:C:752:ALA:HB1  | 2.39                     | 0.57              |
| 1:B:952:ASN:C    | 1:B:952:ASN:OD1  | 2.42                     | 0.57              |
| 1:C:234:ILE:HD11 | 1:C:445:TYR:CE1  | 2.38                     | 0.57              |
| 1:B:823:PRO:O    | 1:C:767:SER:HB3  | 2.04                     | 0.57              |
| 1:D:174:VAL:C    | 1:D:175:GLU:OE2  | 2.42                     | 0.57              |
| 1:F:213:GLU:OE2  | 1:F:232:CYS:SG   | 2.54                     | 0.57              |
| 1:F:360:THR:HA   | 1:F:387:VAL:CG2  | 2.34                     | 0.57              |
| 1:F:865:GLN:HA   | 1:F:868:GLY:O    | 2.04                     | 0.57              |
| 1:H:175:GLU:HB2  | 1:H:179:HIS:CG   | 2.39                     | 0.57              |
| 1:A:213:GLU:OE2  | 1:A:232:CYS:SG   | 2.54                     | 0.57              |
| 1:B:278:GLU:C    | 1:B:289:ILE:CD1  | 2.69                     | 0.57              |
| 1:B:278:GLU:HB2  | 1:B:289:ILE:HG13 | 1.85                     | 0.57              |
| 1:C:228:PHE:HE2  | 1:C:338:ILE:HG13 | 1.70                     | 0.57              |
| 1:C:53:VAL:HG13  | 1:C:54:GLY:H     | 1.70                     | 0.57              |
| 1:E:101:GLU:CB   | 1:E:103:ILE:HD13 | 2.32                     | 0.57              |
| 1:E:952:ASN:OD1  | 1:E:952:ASN:C    | 2.42                     | 0.57              |
| 1:G:164:LEU:HA   | 1:G:195:PHE:HE1  | 1.68                     | 0.57              |
| 1:C:53:VAL:HG13  | 1:C:54:GLY:N     | 2.18                     | 0.57              |
| 1:G:367:ARG:NH1  | 1:G:1049:GLN:CB  | 2.60                     | 0.57              |
| 1:G:53:VAL:HG13  | 1:G:54:GLY:H     | 1.70                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:520:GLU:OE1  | 1:G:705:HIS:CD2  | 2.57                     | 0.57              |
| 1:A:92:ILE:HD13  | 1:A:113:LEU:HB2  | 1.87                     | 0.57              |
| 1:B:322:ALA:N    | 1:B:325:ASP:OD2  | 2.37                     | 0.57              |
| 1:F:360:THR:HA   | 1:F:387:VAL:HG23 | 1.86                     | 0.57              |
| 1:A:360:THR:HA   | 1:A:387:VAL:HG23 | 1.86                     | 0.57              |
| 1:D:550:ARG:HG3  | 1:D:816:PHE:CE1  | 2.40                     | 0.57              |
| 1:D:551:VAL:HA   | 1:D:813:TYR:CE2  | 2.40                     | 0.57              |
| 1:D:865:GLN:HA   | 1:D:868:GLY:O    | 2.04                     | 0.57              |
| 1:F:80:ALA:HB2   | 1:F:104:ILE:HB   | 1.87                     | 0.57              |
| 1:C:160:ILE:HG22 | 1:C:200:VAL:CG1  | 2.34                     | 0.57              |
| 1:C:520:GLU:OE1  | 1:C:705:HIS:CD2  | 2.57                     | 0.57              |
| 1:E:348:THR:OG1  | 1:E:350:GLU:HG3  | 2.05                     | 0.57              |
| 1:E:926:PRO:O    | 1:E:927:GLU:HB2  | 2.03                     | 0.57              |
| 1:A:550:ARG:HG3  | 1:A:816:PHE:CE1  | 2.40                     | 0.57              |
| 1:B:603:ILE:HD12 | 1:B:608:PHE:HE1  | 1.69                     | 0.57              |
| 1:F:986:TYR:CZ   | 1:F:990:ILE:HD12 | 2.38                     | 0.57              |
| 1:G:160:ILE:HG22 | 1:G:200:VAL:CG1  | 2.34                     | 0.57              |
| 1:E:349:THR:HG23 | 1:E:393:SER:CB   | 2.35                     | 0.57              |
| 1:E:651:TRP:CZ2  | 1:E:920:GLN:HG3  | 2.40                     | 0.57              |
| 1:G:234:ILE:HD11 | 1:G:445:TYR:CE1  | 2.39                     | 0.57              |
| 1:A:382:PHE:CE1  | 1:A:385:THR:HB   | 2.39                     | 0.57              |
| 1:A:557:PHE:CE1  | 1:A:598:THR:HB   | 2.40                     | 0.57              |
| 1:A:673:ILE:HG22 | 1:A:695:MET:HE1  | 1.87                     | 0.57              |
| 1:A:986:TYR:CZ   | 1:A:990:ILE:HD12 | 2.39                     | 0.57              |
| 1:B:394:LEU:HD12 | 1:B:395:LEU:N    | 2.20                     | 0.57              |
| 1:B:504:SER:O    | 1:B:506:ILE:HG12 | 2.05                     | 0.57              |
| 1:C:540:ARG:HH21 | 1:C:541:ASP:CB   | 2.18                     | 0.57              |
| 1:G:550:ARG:HG3  | 1:G:816:PHE:CE1  | 2.40                     | 0.57              |
| 1:B:651:TRP:CZ2  | 1:B:920:GLN:HG3  | 2.40                     | 0.57              |
| 1:B:926:PRO:O    | 1:B:927:GLU:HB2  | 2.04                     | 0.57              |
| 1:F:304:MET:HE3  | 1:F:342:ALA:HB1  | 1.87                     | 0.57              |
| 1:F:713:ALA:HB3  | 1:F:715:LEU:CD1  | 2.34                     | 0.57              |
| 1:G:126:ALA:HB1  | 1:G:131:ILE:HD11 | 1.87                     | 0.57              |
| 1:H:557:PHE:CE1  | 1:H:598:THR:HB   | 2.40                     | 0.57              |
| 1:H:623:TYR:HB3  | 1:H:627:VAL:HG21 | 1.87                     | 0.57              |
| 1:B:859:MET:O    | 1:B:863:VAL:HG23 | 2.05                     | 0.56              |
| 1:F:673:ILE:HG22 | 1:F:695:MET:HE1  | 1.87                     | 0.56              |
| 1:F:859:MET:O    | 1:F:863:VAL:HG23 | 2.05                     | 0.56              |
| 1:G:322:ALA:N    | 1:G:325:ASP:OD2  | 2.38                     | 0.56              |
| 1:G:540:ARG:HH21 | 1:G:541:ASP:HA   | 1.69                     | 0.56              |
| 1:A:304:MET:HE3  | 1:A:342:ALA:HB1  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:53:VAL:HG13   | 1:B:54:GLY:N      | 2.20                     | 0.56              |
| 1:B:865:GLN:HA    | 1:B:868:GLY:O     | 2.05                     | 0.56              |
| 1:D:623:TYR:HB3   | 1:D:627:VAL:HG21  | 1.88                     | 0.56              |
| 1:E:394:LEU:HD12  | 1:E:395:LEU:N     | 2.20                     | 0.56              |
| 1:E:859:MET:O     | 1:E:863:VAL:HG23  | 2.05                     | 0.56              |
| 1:E:865:GLN:HA    | 1:E:868:GLY:O     | 2.05                     | 0.56              |
| 1:H:382:PHE:CE1   | 1:H:385:THR:HB    | 2.40                     | 0.56              |
| 1:A:348:THR:OG1   | 1:A:350:GLU:HG3   | 2.05                     | 0.56              |
| 1:B:304:MET:HE3   | 1:B:342:ALA:HB1   | 1.87                     | 0.56              |
| 1:C:92:ILE:HD13   | 1:C:113:LEU:HB2   | 1.87                     | 0.56              |
| 1:E:603:ILE:HD12  | 1:E:608:PHE:HE1   | 1.70                     | 0.56              |
| 1:F:348:THR:OG1   | 1:F:350:GLU:HG3   | 2.05                     | 0.56              |
| 1:F:673:ILE:HG22  | 1:F:695:MET:HE3   | 1.85                     | 0.56              |
| 1:G:92:ILE:HD13   | 1:G:113:LEU:HB2   | 1.87                     | 0.56              |
| 1:H:45:TYR:CZ     | 1:G:1047:ASN:HB3  | 2.41                     | 0.56              |
| 1:H:551:VAL:HA    | 1:H:813:TYR:CE2   | 2.40                     | 0.56              |
| 1:C:126:ALA:HB1   | 1:C:131:ILE:HD11  | 1.88                     | 0.56              |
| 1:D:8:LEU:CA      | 1:D:31:VAL:HG23   | 2.16                     | 0.56              |
| 1:D:382:PHE:CE1   | 1:D:385:THR:HB    | 2.40                     | 0.56              |
| 1:E:14:GLU:CD     | 1:E:397:LYS:CE    | 2.70                     | 0.56              |
| 1:G:540:ARG:HH21  | 1:G:541:ASP:CB    | 2.19                     | 0.56              |
| 1:G:576:TRP:CZ2   | 1:G:592:PRO:HB2   | 2.40                     | 0.56              |
| 1:H:859:MET:O     | 1:H:863:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:859:MET:O     | 1:A:863:VAL:HG23  | 2.06                     | 0.56              |
| 1:C:322:ALA:N     | 1:C:325:ASP:OD2   | 2.38                     | 0.56              |
| 1:C:576:TRP:CZ2   | 1:C:592:PRO:HB2   | 2.40                     | 0.56              |
| 1:D:859:MET:O     | 1:D:863:VAL:HG23  | 2.05                     | 0.56              |
| 1:E:550:ARG:HG3   | 1:E:816:PHE:CE1   | 2.41                     | 0.56              |
| 1:A:80:ALA:HB2    | 1:A:104:ILE:HB    | 1.88                     | 0.56              |
| 1:A:321:TYR:HB3   | 1:A:325:ASP:OD2   | 2.05                     | 0.56              |
| 1:B:158:LEU:H     | 1:B:158:LEU:HD12  | 1.67                     | 0.56              |
| 1:E:80:ALA:HB2    | 1:E:104:ILE:HB    | 1.88                     | 0.56              |
| 1:E:278:GLU:C     | 1:E:289:ILE:CD1   | 2.70                     | 0.56              |
| 1:F:321:TYR:HB3   | 1:F:325:ASP:OD2   | 2.05                     | 0.56              |
| 1:B:450:ILE:HG22  | 1:B:451:ASP:N     | 2.21                     | 0.56              |
| 1:B:88:LEU:HB3    | 1:B:94:PHE:CD2    | 2.37                     | 0.56              |
| 1:B:987:GLN:O     | 1:B:990:ILE:HG22  | 2.05                     | 0.56              |
| 1:D:1031:ILE:HG23 | 1:D:1042:ILE:HG13 | 1.88                     | 0.56              |
| 1:E:209:PRO:HB2   | 1:E:280:LEU:HD23  | 1.87                     | 0.56              |
| 1:E:987:GLN:O     | 1:E:990:ILE:HG22  | 2.05                     | 0.56              |
| 1:F:1041:VAL:HG12 | 1:F:1043:TYR:CE1  | 2.40                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:1031:ILE:HG23 | 1:H:1042:ILE:HG13 | 1.88                     | 0.56              |
| 1:A:506:ILE:HD11  | 1:A:565:HIS:CE1   | 2.41                     | 0.56              |
| 1:B:209:PRO:HB2   | 1:B:280:LEU:HD23  | 1.87                     | 0.56              |
| 1:B:367:ARG:HH12  | 1:B:1049:GLN:HB2  | 1.70                     | 0.56              |
| 1:C:278:GLU:C     | 1:C:289:ILE:CD1   | 2.74                     | 0.56              |
| 1:D:134:ILE:HD11  | 1:D:287:TYR:HB2   | 1.87                     | 0.56              |
| 1:D:321:TYR:HB3   | 1:D:325:ASP:OD2   | 2.06                     | 0.56              |
| 1:F:160:ILE:HG22  | 1:F:200:VAL:CG1   | 2.35                     | 0.56              |
| 1:G:164:LEU:HA    | 1:G:195:PHE:CE1   | 2.40                     | 0.56              |
| 1:G:278:GLU:C     | 1:G:289:ILE:CD1   | 2.74                     | 0.56              |
| 1:H:134:ILE:HD11  | 1:H:287:TYR:HB2   | 1.87                     | 0.56              |
| 1:B:14:GLU:CD     | 1:B:397:LYS:CE    | 2.71                     | 0.56              |
| 1:D:557:PHE:CE1   | 1:D:598:THR:HB    | 2.41                     | 0.56              |
| 1:D:898:TYR:CD1   | 1:D:928:LYS:HE2   | 2.40                     | 0.56              |
| 1:G:304:MET:HE3   | 1:G:342:ALA:HB1   | 1.87                     | 0.56              |
| 1:A:630:GLU:HG2   | 1:A:953:PHE:HE1   | 1.70                     | 0.56              |
| 1:D:908:ASP:O     | 1:D:912:GLU:HG3   | 2.06                     | 0.56              |
| 1:E:53:VAL:HG13   | 1:E:54:GLY:N      | 2.20                     | 0.56              |
| 1:F:557:PHE:CE1   | 1:F:598:THR:HB    | 2.41                     | 0.56              |
| 1:F:550:ARG:HG3   | 1:F:816:PHE:CE1   | 2.41                     | 0.56              |
| 1:H:321:TYR:HB3   | 1:H:325:ASP:OD2   | 2.06                     | 0.56              |
| 1:H:908:ASP:O     | 1:H:912:GLU:HG3   | 2.06                     | 0.56              |
| 1:E:505:GLN:HA    | 1:E:505:GLN:OE1   | 2.05                     | 0.56              |
| 1:H:600:ARG:NH1   | 1:H:603:ILE:O     | 2.39                     | 0.56              |
| 1:H:865:GLN:HA    | 1:H:868:GLY:O     | 2.06                     | 0.56              |
| 1:H:898:TYR:CD1   | 1:H:928:LYS:HE2   | 2.40                     | 0.56              |
| 1:A:160:ILE:HG22  | 1:A:200:VAL:CG1   | 2.36                     | 0.55              |
| 1:B:349:THR:HG23  | 1:B:393:SER:CB    | 2.36                     | 0.55              |
| 1:G:348:THR:OG1   | 1:G:350:GLU:HG3   | 2.05                     | 0.55              |
| 1:H:175:GLU:N     | 1:H:175:GLU:OE2   | 2.39                     | 0.55              |
| 1:H:541:ASP:OD2   | 1:H:741:HIS:HE1   | 1.89                     | 0.55              |
| 1:A:673:ILE:HG22  | 1:A:695:MET:HE3   | 1.86                     | 0.55              |
| 1:D:80:ALA:HB2    | 1:D:104:ILE:HB    | 1.88                     | 0.55              |
| 1:E:147:VAL:HG21  | 1:E:184:PHE:CE1   | 2.40                     | 0.55              |
| 1:H:80:ALA:HB2    | 1:H:104:ILE:HB    | 1.88                     | 0.55              |
| 1:B:80:ALA:HB2    | 1:B:104:ILE:HB    | 1.88                     | 0.55              |
| 1:C:348:THR:OG1   | 1:C:350:GLU:HG3   | 2.05                     | 0.55              |
| 1:C:832:MET:HG3   | 1:C:833:PRO:HD2   | 1.88                     | 0.55              |
| 1:E:367:ARG:HH12  | 1:E:1049:GLN:HB2  | 1.71                     | 0.55              |
| 1:F:1031:ILE:CG2  | 1:F:1042:ILE:HG13 | 2.36                     | 0.55              |
| 1:F:986:TYR:CE1   | 1:F:990:ILE:CD1   | 2.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:557:PHE:CE1   | 1:G:598:THR:HB    | 2.41                     | 0.55              |
| 1:H:510:THR:CG2   | 1:H:607:MET:SD    | 2.92                     | 0.55              |
| 1:B:126:ALA:HB1   | 1:B:131:ILE:HD11  | 1.88                     | 0.55              |
| 1:E:88:LEU:HB3    | 1:E:94:PHE:CD2    | 2.38                     | 0.55              |
| 1:F:53:VAL:HG13   | 1:F:54:GLY:N      | 2.21                     | 0.55              |
| 1:H:348:THR:OG1   | 1:H:350:GLU:HG3   | 2.06                     | 0.55              |
| 1:H:394:LEU:HD12  | 1:H:395:LEU:N     | 2.21                     | 0.55              |
| 1:A:713:ALA:HB3   | 1:A:715:LEU:CD1   | 2.35                     | 0.55              |
| 1:B:82:HIS:HA     | 1:B:106:VAL:CG2   | 2.37                     | 0.55              |
| 1:B:623:TYR:HB3   | 1:B:627:VAL:HG21  | 1.89                     | 0.55              |
| 1:C:557:PHE:CE1   | 1:C:598:THR:HB    | 2.42                     | 0.55              |
| 1:D:960:LEU:CD1   | 1:D:976:TYR:CD1   | 2.89                     | 0.55              |
| 1:E:82:HIS:HA     | 1:E:106:VAL:CG2   | 2.37                     | 0.55              |
| 1:G:620:TYR:CD2   | 1:G:621:LYS:N     | 2.74                     | 0.55              |
| 1:H:960:LEU:CD1   | 1:H:976:TYR:CD1   | 2.89                     | 0.55              |
| 1:A:1031:ILE:CG2  | 1:A:1042:ILE:HG13 | 2.37                     | 0.55              |
| 1:A:1041:VAL:HG12 | 1:A:1043:TYR:CE1  | 2.41                     | 0.55              |
| 1:A:394:LEU:HD12  | 1:A:395:LEU:N     | 2.22                     | 0.55              |
| 1:A:986:TYR:CE1   | 1:A:990:ILE:CD1   | 2.90                     | 0.55              |
| 1:C:550:ARG:HG3   | 1:C:816:PHE:CE1   | 2.42                     | 0.55              |
| 1:D:345:SER:CB    | 1:D:412:MET:CE    | 2.81                     | 0.55              |
| 1:F:134:ILE:HD11  | 1:F:287:TYR:HB2   | 1.87                     | 0.55              |
| 1:H:53:VAL:HG13   | 1:H:54:GLY:N      | 2.20                     | 0.55              |
| 1:H:987:GLN:O     | 1:H:990:ILE:HG22  | 2.07                     | 0.55              |
| 1:A:134:ILE:HD11  | 1:A:287:TYR:HB2   | 1.87                     | 0.55              |
| 1:A:740:THR:HG22  | 1:A:751:TYR:CZ    | 2.42                     | 0.55              |
| 1:C:1031:ILE:HG23 | 1:C:1042:ILE:HG13 | 1.89                     | 0.55              |
| 1:D:348:THR:OG1   | 1:D:350:GLU:HG3   | 2.06                     | 0.55              |
| 1:F:630:GLU:HG2   | 1:F:953:PHE:HE1   | 1.71                     | 0.55              |
| 1:G:1031:ILE:HG23 | 1:G:1042:ILE:HG13 | 1.89                     | 0.55              |
| 1:A:53:VAL:HG13   | 1:A:54:GLY:N      | 2.21                     | 0.55              |
| 1:D:177:LYS:O     | 1:D:180:VAL:HG23  | 2.07                     | 0.55              |
| 1:D:465:ARG:HG2   | 1:D:465:ARG:O     | 2.07                     | 0.55              |
| 1:B:550:ARG:HG3   | 1:B:816:PHE:CE1   | 2.42                     | 0.55              |
| 1:D:987:GLN:O     | 1:D:990:ILE:HG22  | 2.07                     | 0.55              |
| 1:E:160:ILE:CD1   | 1:E:174:VAL:CG2   | 2.85                     | 0.55              |
| 1:H:465:ARG:O     | 1:H:465:ARG:HG2   | 2.07                     | 0.55              |
| 1:A:63:TYR:HB2    | 1:A:87:PHE:CD2    | 2.42                     | 0.55              |
| 1:B:551:VAL:HA    | 1:B:813:TYR:CE2   | 2.42                     | 0.55              |
| 1:C:394:LEU:HD12  | 1:C:395:LEU:N     | 2.21                     | 0.55              |
| 1:C:540:ARG:HH21  | 1:C:541:ASP:HA    | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:928:LYS:O     | 1:D:932:LEU:HD12  | 2.07                     | 0.55              |
| 1:E:1031:ILE:HG23 | 1:E:1042:ILE:HG13 | 1.89                     | 0.55              |
| 1:E:126:ALA:HB1   | 1:E:131:ILE:HD11  | 1.89                     | 0.55              |
| 1:H:259:CYS:O     | 1:H:263:VAL:HG23  | 2.07                     | 0.55              |
| 1:H:622:ASN:ND2   | 1:H:917:GLU:O     | 2.40                     | 0.55              |
| 1:B:1031:ILE:HG23 | 1:B:1042:ILE:HG13 | 1.89                     | 0.54              |
| 1:B:235:GLN:O     | 1:B:450:ILE:HG13  | 2.07                     | 0.54              |
| 1:D:259:CYS:O     | 1:D:263:VAL:HG23  | 2.08                     | 0.54              |
| 1:D:44:ARG:HD3    | 1:D:45:TYR:CD1    | 2.42                     | 0.54              |
| 1:H:228:PHE:CE2   | 1:H:338:ILE:HG13  | 2.42                     | 0.54              |
| 1:H:345:SER:CB    | 1:H:412:MET:CE    | 2.81                     | 0.54              |
| 1:B:472:TYR:OH    | 1:B:1004:PHE:CD2  | 2.59                     | 0.54              |
| 1:D:394:LEU:HD12  | 1:D:395:LEU:N     | 2.22                     | 0.54              |
| 1:D:53:VAL:HG13   | 1:D:54:GLY:N      | 2.21                     | 0.54              |
| 1:D:510:THR:CG2   | 1:D:607:MET:SD    | 2.93                     | 0.54              |
| 1:E:259:CYS:O     | 1:E:263:VAL:HG23  | 2.07                     | 0.54              |
| 1:F:394:LEU:HD12  | 1:F:395:LEU:N     | 2.23                     | 0.54              |
| 1:G:80:ALA:HB2    | 1:G:104:ILE:HB    | 1.88                     | 0.54              |
| 1:H:928:LYS:O     | 1:H:932:LEU:HD12  | 2.07                     | 0.54              |
| 1:A:600:ARG:NH1   | 1:A:603:ILE:O     | 2.40                     | 0.54              |
| 1:A:908:ASP:O     | 1:A:912:GLU:HG3   | 2.06                     | 0.54              |
| 1:B:740:THR:HG22  | 1:B:751:TYR:CZ    | 2.41                     | 0.54              |
| 1:C:620:TYR:CD2   | 1:C:621:LYS:N     | 2.75                     | 0.54              |
| 1:E:304:MET:HE3   | 1:E:342:ALA:HB1   | 1.88                     | 0.54              |
| 1:F:600:ARG:NH1   | 1:F:603:ILE:O     | 2.40                     | 0.54              |
| 1:F:160:ILE:CG2   | 1:F:200:VAL:HG11  | 2.37                     | 0.54              |
| 1:F:134:ILE:CD1   | 1:F:287:TYR:HB3   | 2.36                     | 0.54              |
| 1:G:160:ILE:CG2   | 1:G:200:VAL:HG11  | 2.37                     | 0.54              |
| 1:G:20:MET:CE     | 1:G:43:HIS:O      | 2.55                     | 0.54              |
| 1:G:394:LEU:HD12  | 1:G:395:LEU:N     | 2.22                     | 0.54              |
| 1:G:620:TYR:HD2   | 1:G:621:LYS:N     | 2.05                     | 0.54              |
| 1:G:832:MET:HG3   | 1:G:833:PRO:HD2   | 1.89                     | 0.54              |
| 1:H:44:ARG:HD3    | 1:H:45:TYR:CD1    | 2.42                     | 0.54              |
| 1:B:120:ILE:HD12  | 1:B:140:PRO:HG3   | 1.88                     | 0.54              |
| 1:C:177:LYS:O     | 1:C:180:VAL:HG23  | 2.08                     | 0.54              |
| 1:C:195:PHE:N     | 1:C:195:PHE:CD2   | 2.75                     | 0.54              |
| 1:D:600:ARG:NH1   | 1:D:603:ILE:O     | 2.41                     | 0.54              |
| 1:F:623:TYR:HB3   | 1:F:627:VAL:HG21  | 1.88                     | 0.54              |
| 1:B:259:CYS:O     | 1:B:263:VAL:HG23  | 2.07                     | 0.54              |
| 1:C:259:CYS:O     | 1:C:263:VAL:HG23  | 2.07                     | 0.54              |
| 1:D:21:ARG:HH12   | 1:C:370:GLY:C     | 2.11                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:209:PRO:CB   | 1:E:280:LEU:HD23 | 2.38                     | 0.54              |
| 1:E:551:VAL:HA   | 1:E:813:TYR:CE2  | 2.43                     | 0.54              |
| 1:F:567:LEU:N    | 1:F:568:PRO:CD   | 2.70                     | 0.54              |
| 1:F:740:THR:HG22 | 1:F:751:TYR:CZ   | 2.43                     | 0.54              |
| 1:B:228:PHE:HD2  | 1:B:338:ILE:CD1  | 2.21                     | 0.54              |
| 1:C:80:ALA:HB2   | 1:C:104:ILE:HB   | 1.88                     | 0.54              |
| 1:C:600:ARG:NH1  | 1:C:603:ILE:O    | 2.41                     | 0.54              |
| 1:D:541:ASP:OD2  | 1:D:741:HIS:HE1  | 1.91                     | 0.54              |
| 1:E:740:THR:HG22 | 1:E:751:TYR:CZ   | 2.42                     | 0.54              |
| 1:F:259:CYS:O    | 1:F:263:VAL:HG23 | 2.07                     | 0.54              |
| 1:F:395:LEU:HD12 | 1:F:395:LEU:H    | 1.71                     | 0.54              |
| 1:A:160:ILE:CG2  | 1:A:200:VAL:HG11 | 2.38                     | 0.54              |
| 1:C:20:MET:CE    | 1:C:43:HIS:O     | 2.56                     | 0.54              |
| 1:D:597:GLU:OE1  | 1:D:971:LYS:NZ   | 2.26                     | 0.54              |
| 1:E:623:TYR:HB3  | 1:E:627:VAL:HG21 | 1.90                     | 0.54              |
| 1:F:120:ILE:HD12 | 1:F:121:LYS:HG2  | 1.90                     | 0.54              |
| 1:G:177:LYS:O    | 1:G:180:VAL:HG23 | 2.08                     | 0.54              |
| 1:H:25:GLU:HG3   | 1:G:414:ARG:HD3  | 1.89                     | 0.54              |
| 1:A:126:ALA:HB1  | 1:A:131:ILE:HD11 | 1.90                     | 0.54              |
| 1:B:600:ARG:NH1  | 1:B:603:ILE:O    | 2.41                     | 0.54              |
| 1:C:160:ILE:CG2  | 1:C:200:VAL:HG11 | 2.38                     | 0.54              |
| 1:E:472:TYR:OH   | 1:E:1004:PHE:CD2 | 2.60                     | 0.54              |
| 1:F:502:TYR:CD1  | 1:F:503:GLY:N    | 2.76                     | 0.54              |
| 1:F:870:ILE:O    | 1:F:872:LYS:NZ   | 2.39                     | 0.54              |
| 1:G:259:CYS:O    | 1:G:263:VAL:HG23 | 2.08                     | 0.54              |
| 1:H:509:GLY:N    | 1:H:512:GLN:OE1  | 2.39                     | 0.54              |
| 1:H:597:GLU:OE1  | 1:H:971:LYS:NZ   | 2.26                     | 0.54              |
| 1:H:862:VAL:O    | 1:H:866:MET:HG2  | 2.08                     | 0.54              |
| 1:A:571:PHE:CD2  | 1:A:572:SER:HB3  | 2.44                     | 0.54              |
| 1:B:209:PRO:CB   | 1:B:280:LEU:HD23 | 2.38                     | 0.54              |
| 1:E:278:GLU:CB   | 1:E:289:ILE:HG13 | 2.38                     | 0.54              |
| 1:F:63:TYR:HB2   | 1:F:87:PHE:CD2   | 2.43                     | 0.54              |
| 1:A:259:CYS:O    | 1:A:263:VAL:HG23 | 2.08                     | 0.53              |
| 1:B:278:GLU:CB   | 1:B:289:ILE:HG13 | 2.38                     | 0.53              |
| 1:D:862:VAL:O    | 1:D:866:MET:HG2  | 2.08                     | 0.53              |
| 1:E:160:ILE:HD11 | 1:E:174:VAL:CG2  | 2.38                     | 0.53              |
| 1:E:147:VAL:HG11 | 1:E:180:VAL:CG1  | 2.38                     | 0.53              |
| 1:E:228:PHE:HD2  | 1:E:338:ILE:CD1  | 2.21                     | 0.53              |
| 1:E:321:TYR:HB3  | 1:E:325:ASP:OD2  | 2.08                     | 0.53              |
| 1:A:134:ILE:CD1  | 1:A:287:TYR:HB3  | 2.37                     | 0.53              |
| 1:A:623:TYR:HB3  | 1:A:627:VAL:HG21 | 1.88                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:160:ILE:HD12 | 1:B:174:VAL:CG2  | 2.37                     | 0.53              |
| 1:B:53:VAL:HG13  | 1:B:54:GLY:H     | 1.72                     | 0.53              |
| 1:F:908:ASP:O    | 1:F:912:GLU:HG3  | 2.07                     | 0.53              |
| 1:F:66:ILE:HG23  | 1:F:94:PHE:CD1   | 2.43                     | 0.53              |
| 1:G:609:GLN:HE22 | 1:G:737:HIS:HE1  | 1.54                     | 0.53              |
| 1:A:849:LEU:HD12 | 1:A:849:LEU:N    | 2.22                     | 0.53              |
| 1:A:870:ILE:O    | 1:A:872:LYS:NZ   | 2.40                     | 0.53              |
| 1:B:321:TYR:HB3  | 1:B:325:ASP:OD2  | 2.09                     | 0.53              |
| 1:E:120:ILE:HD12 | 1:E:140:PRO:HG3  | 1.89                     | 0.53              |
| 1:E:266:MET:HE2  | 1:E:277:VAL:CG2  | 2.37                     | 0.53              |
| 1:E:600:ARG:NH1  | 1:E:603:ILE:O    | 2.41                     | 0.53              |
| 1:F:849:LEU:N    | 1:F:849:LEU:HD12 | 2.22                     | 0.53              |
| 1:G:600:ARG:NH1  | 1:G:603:ILE:O    | 2.41                     | 0.53              |
| 1:H:53:VAL:HG13  | 1:H:54:GLY:H     | 1.73                     | 0.53              |
| 1:A:225:VAL:HG13 | 1:A:333:GLN:NE2  | 2.23                     | 0.53              |
| 1:B:81:ILE:O     | 1:B:106:VAL:CG2  | 2.57                     | 0.53              |
| 1:D:414:ARG:HD3  | 1:C:25:GLU:HG3   | 1.89                     | 0.53              |
| 1:D:622:ASN:ND2  | 1:D:917:GLU:O    | 2.41                     | 0.53              |
| 1:F:571:PHE:CD2  | 1:F:572:SER:HB3  | 2.44                     | 0.53              |
| 1:A:120:ILE:HD12 | 1:A:121:LYS:HG2  | 1.91                     | 0.53              |
| 1:A:134:ILE:HG22 | 1:A:203:GLU:HB3  | 1.89                     | 0.53              |
| 1:C:228:PHE:CD2  | 1:C:338:ILE:CG1  | 2.92                     | 0.53              |
| 1:C:620:TYR:HD2  | 1:C:621:LYS:N    | 2.06                     | 0.53              |
| 1:D:225:VAL:HG13 | 1:D:333:GLN:NE2  | 2.23                     | 0.53              |
| 1:D:304:MET:HE3  | 1:D:342:ALA:HB1  | 1.90                     | 0.53              |
| 1:D:509:GLY:N    | 1:D:512:GLN:OE1  | 2.40                     | 0.53              |
| 1:D:571:PHE:CD2  | 1:D:572:SER:HB3  | 2.44                     | 0.53              |
| 1:F:597:GLU:OE1  | 1:F:971:LYS:NZ   | 2.26                     | 0.53              |
| 1:G:195:PHE:CD2  | 1:G:195:PHE:N    | 2.76                     | 0.53              |
| 1:F:126:ALA:HB1  | 1:F:131:ILE:HD11 | 1.90                     | 0.53              |
| 1:F:54:GLY:HA3   | 1:F:62:ALA:HB1   | 1.91                     | 0.53              |
| 1:G:219:ASP:CB   | 1:G:323:LEU:HD23 | 2.26                     | 0.53              |
| 1:A:134:ILE:CD1  | 1:A:287:TYR:HB2  | 2.38                     | 0.53              |
| 1:D:788:GLY:N    | 1:A:719:GLN:HG2  | 2.24                     | 0.53              |
| 1:D:53:VAL:HG13  | 1:D:54:GLY:H     | 1.73                     | 0.53              |
| 1:E:81:ILE:O     | 1:E:106:VAL:CG2  | 2.57                     | 0.53              |
| 1:F:134:ILE:CD1  | 1:F:287:TYR:HB2  | 2.39                     | 0.53              |
| 1:F:177:LYS:O    | 1:F:180:VAL:HG23 | 2.09                     | 0.53              |
| 1:G:1059:ASN:OD1 | 1:G:1059:ASN:N   | 2.41                     | 0.53              |
| 1:A:395:LEU:HD12 | 1:A:395:LEU:H    | 1.73                     | 0.53              |
| 1:A:567:LEU:N    | 1:A:568:PRO:CD   | 2.71                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:740:THR:HG22 | 1:D:751:TYR:CZ    | 2.44                     | 0.53              |
| 1:H:304:MET:HE3  | 1:H:342:ALA:HB1   | 1.90                     | 0.53              |
| 1:D:1059:ASN:OD1 | 1:D:1059:ASN:N    | 2.42                     | 0.53              |
| 1:D:213:GLU:OE2  | 1:D:232:CYS:SG    | 2.55                     | 0.53              |
| 1:D:251:THR:HG23 | 1:D:254:LEU:HB2   | 1.91                     | 0.53              |
| 1:F:134:ILE:HG22 | 1:F:203:GLU:HB3   | 1.90                     | 0.53              |
| 1:F:225:VAL:HG13 | 1:F:333:GLN:NE2   | 2.24                     | 0.53              |
| 1:F:541:ASP:OD2  | 1:F:741:HIS:HE1   | 1.92                     | 0.53              |
| 1:E:752:ALA:HB1  | 1:G:749:TYR:CZ    | 2.43                     | 0.53              |
| 1:H:1059:ASN:N   | 1:H:1059:ASN:OD1  | 2.42                     | 0.53              |
| 1:H:120:ILE:HD12 | 1:H:121:LYS:HG2   | 1.90                     | 0.53              |
| 1:H:740:THR:HG22 | 1:H:751:TYR:CZ    | 2.44                     | 0.53              |
| 1:E:280:LEU:CD1  | 1:E:289:ILE:HG22  | 2.37                     | 0.53              |
| 1:F:251:THR:HG23 | 1:F:254:LEU:HB2   | 1.90                     | 0.53              |
| 1:G:509:GLY:N    | 1:G:512:GLN:OE1   | 2.39                     | 0.53              |
| 1:H:251:THR:HG23 | 1:H:254:LEU:HB2   | 1.91                     | 0.53              |
| 1:A:66:ILE:HG23  | 1:A:94:PHE:CD1    | 2.44                     | 0.52              |
| 1:D:228:PHE:CE2  | 1:D:338:ILE:HG13  | 2.44                     | 0.52              |
| 1:E:53:VAL:HG13  | 1:E:54:GLY:H      | 1.73                     | 0.52              |
| 1:F:195:PHE:N    | 1:F:195:PHE:CD2   | 2.77                     | 0.52              |
| 1:G:540:ARG:NH2  | 1:G:541:ASP:HA    | 2.25                     | 0.52              |
| 1:A:1010:LEU:HA  | 1:A:1028:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:609:GLN:HE22 | 1:C:737:HIS:HE1   | 1.55                     | 0.52              |
| 1:F:475:ASN:HA   | 1:F:1055:ILE:HG21 | 1.92                     | 0.52              |
| 1:F:551:VAL:HA   | 1:F:813:TYR:CE2   | 2.44                     | 0.52              |
| 1:G:227:LEU:HD21 | 1:G:308:ILE:HD12  | 1.91                     | 0.52              |
| 1:A:251:THR:HG23 | 1:A:254:LEU:HB2   | 1.90                     | 0.52              |
| 1:A:54:GLY:HA3   | 1:A:62:ALA:HB1    | 1.91                     | 0.52              |
| 1:A:551:VAL:HA   | 1:A:813:TYR:CE2   | 2.44                     | 0.52              |
| 1:D:1010:LEU:HA  | 1:D:1028:LEU:HD23 | 1.91                     | 0.52              |
| 1:F:2:ASN:HB2    | 1:F:321:TYR:OH    | 2.10                     | 0.52              |
| 1:A:53:VAL:HG13  | 1:A:54:GLY:H      | 1.74                     | 0.52              |
| 1:A:541:ASP:OD2  | 1:A:741:HIS:HE1   | 1.92                     | 0.52              |
| 1:B:266:MET:HE2  | 1:B:277:VAL:CG2   | 2.38                     | 0.52              |
| 1:E:251:THR:HG23 | 1:E:254:LEU:HB2   | 1.90                     | 0.52              |
| 1:F:509:GLY:N    | 1:F:512:GLN:OE1   | 2.40                     | 0.52              |
| 1:A:195:PHE:N    | 1:A:195:PHE:CD2   | 2.78                     | 0.52              |
| 1:B:226:HIS:ND1  | 1:B:259:CYS:HB3   | 2.24                     | 0.52              |
| 1:B:280:LEU:CD1  | 1:B:289:ILE:HG22  | 2.38                     | 0.52              |
| 1:D:996:VAL:O    | 1:D:999:LEU:HD12  | 2.09                     | 0.52              |
| 1:E:143:GLY:O    | 1:E:147:VAL:HG23  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:472:TYR:OH   | 1:E:1004:PHE:O    | 2.27                     | 0.52              |
| 1:F:230:ARG:NH2  | 1:F:296:GLN:OE1   | 2.43                     | 0.52              |
| 1:G:160:ILE:CG2  | 1:G:200:VAL:CG1   | 2.87                     | 0.52              |
| 1:H:134:ILE:CD1  | 1:H:287:TYR:HB2   | 2.39                     | 0.52              |
| 1:H:134:ILE:CD1  | 1:H:287:TYR:HB3   | 2.36                     | 0.52              |
| 1:A:177:LYS:O    | 1:A:180:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:230:ARG:NH2  | 1:A:296:GLN:OE1   | 2.43                     | 0.52              |
| 1:C:1059:ASN:OD1 | 1:C:1059:ASN:N    | 2.42                     | 0.52              |
| 1:C:304:MET:HE3  | 1:C:342:ALA:HB1   | 1.91                     | 0.52              |
| 1:D:230:ARG:NH2  | 1:D:296:GLN:OE1   | 2.42                     | 0.52              |
| 1:F:53:VAL:HG13  | 1:F:54:GLY:H      | 1.74                     | 0.52              |
| 1:C:213:GLU:OE2  | 1:C:232:CYS:SG    | 2.54                     | 0.52              |
| 1:C:251:THR:HG23 | 1:C:254:LEU:HB2   | 1.90                     | 0.52              |
| 1:C:219:ASP:CB   | 1:C:323:LEU:HD23  | 2.28                     | 0.52              |
| 1:D:120:ILE:HD12 | 1:D:121:LYS:HG2   | 1.91                     | 0.52              |
| 1:D:134:ILE:CD1  | 1:D:287:TYR:HB2   | 2.39                     | 0.52              |
| 1:D:54:GLY:HA3   | 1:D:62:ALA:HB1    | 1.91                     | 0.52              |
| 1:E:54:GLY:HA3   | 1:E:62:ALA:HB1    | 1.90                     | 0.52              |
| 1:F:1041:VAL:CG1 | 1:F:1043:TYR:CE1  | 2.92                     | 0.52              |
| 1:B:160:ILE:CD1  | 1:B:174:VAL:HG23  | 2.39                     | 0.52              |
| 1:C:996:VAL:O    | 1:C:999:LEU:HD12  | 2.09                     | 0.52              |
| 1:G:251:THR:HG23 | 1:G:254:LEU:HB2   | 1.90                     | 0.52              |
| 1:H:996:VAL:O    | 1:H:999:LEU:HD12  | 2.10                     | 0.52              |
| 1:A:2:ASN:HB2    | 1:A:321:TYR:OH    | 2.10                     | 0.52              |
| 1:A:996:VAL:O    | 1:A:999:LEU:HD12  | 2.09                     | 0.52              |
| 1:B:472:TYR:OH   | 1:B:1004:PHE:O    | 2.28                     | 0.52              |
| 1:C:160:ILE:CG2  | 1:C:200:VAL:CG1   | 2.88                     | 0.52              |
| 1:G:164:LEU:HD22 | 1:G:195:PHE:CZ    | 2.44                     | 0.52              |
| 1:H:225:VAL:HG13 | 1:H:333:GLN:NE2   | 2.25                     | 0.52              |
| 1:A:475:ASN:HA   | 1:A:1055:ILE:HG21 | 1.92                     | 0.52              |
| 1:C:23:CYS:HB3   | 1:C:28:ILE:HB     | 1.92                     | 0.52              |
| 1:C:54:GLY:HA3   | 1:C:62:ALA:HB1    | 1.92                     | 0.52              |
| 1:D:2:ASN:HB2    | 1:D:321:TYR:OH    | 2.10                     | 0.52              |
| 1:D:226:HIS:H    | 1:D:333:GLN:HE22  | 1.58                     | 0.52              |
| 1:E:180:VAL:CG1  | 1:E:184:PHE:HZ    | 2.14                     | 0.52              |
| 1:E:557:PHE:CE1  | 1:E:598:THR:HB    | 2.45                     | 0.52              |
| 1:G:250:ILE:CD1  | 1:G:255:ARG:HB3   | 2.37                     | 0.52              |
| 1:H:177:LYS:O    | 1:H:180:VAL:HG23  | 2.10                     | 0.52              |
| 1:B:54:GLY:HA3   | 1:B:62:ALA:HB1    | 1.91                     | 0.51              |
| 1:C:367:ARG:NH1  | 1:C:1049:GLN:CB   | 2.63                     | 0.51              |
| 1:C:509:GLY:N    | 1:C:512:GLN:OE1   | 2.40                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:177:LYS:CG   | 1:D:178:GLU:H     | 2.22                     | 0.51              |
| 1:D:465:ARG:CG   | 1:D:465:ARG:O     | 2.58                     | 0.51              |
| 1:D:475:ASN:HA   | 1:D:1055:ILE:HG21 | 1.92                     | 0.51              |
| 1:E:266:MET:CE   | 1:E:277:VAL:HG22  | 2.39                     | 0.51              |
| 1:F:996:VAL:O    | 1:F:999:LEU:HD12  | 2.09                     | 0.51              |
| 1:G:54:GLY:HA3   | 1:G:62:ALA:HB1    | 1.93                     | 0.51              |
| 1:H:115:MET:HG2  | 1:H:125:GLN:HG3   | 1.92                     | 0.51              |
| 1:H:541:ASP:OD2  | 1:H:741:HIS:CE1   | 2.63                     | 0.51              |
| 1:A:734:VAL:HG12 | 1:A:735:PRO:HD2   | 1.92                     | 0.51              |
| 1:B:557:PHE:CE1  | 1:B:598:THR:HB    | 2.45                     | 0.51              |
| 1:E:147:VAL:HG21 | 1:E:184:PHE:HE1   | 1.74                     | 0.51              |
| 1:F:1010:LEU:HA  | 1:F:1028:LEU:HD23 | 1.92                     | 0.51              |
| 1:G:17:ILE:HA    | 1:G:20:MET:HG3    | 1.91                     | 0.51              |
| 1:G:23:CYS:HB3   | 1:G:28:ILE:HB     | 1.92                     | 0.51              |
| 1:H:226:HIS:H    | 1:H:333:GLN:HE22  | 1.58                     | 0.51              |
| 1:H:54:GLY:HA3   | 1:H:62:ALA:HB1    | 1.92                     | 0.51              |
| 1:B:356:PHE:CD1  | 1:B:356:PHE:N     | 2.79                     | 0.51              |
| 1:B:996:VAL:O    | 1:B:999:LEU:HD12  | 2.10                     | 0.51              |
| 1:C:88:LEU:HB3   | 1:C:94:PHE:CD2    | 2.38                     | 0.51              |
| 1:D:120:ILE:HD12 | 1:D:121:LYS:H     | 1.76                     | 0.51              |
| 1:E:540:ARG:NH2  | 1:E:541:ASP:OD1   | 2.44                     | 0.51              |
| 1:E:996:VAL:O    | 1:E:999:LEU:HD12  | 2.10                     | 0.51              |
| 1:G:225:VAL:HG13 | 1:G:333:GLN:NE2   | 2.26                     | 0.51              |
| 1:G:228:PHE:CE2  | 1:G:338:ILE:HG13  | 2.45                     | 0.51              |
| 1:G:996:VAL:O    | 1:G:999:LEU:HD12  | 2.09                     | 0.51              |
| 1:H:475:ASN:HA   | 1:H:1055:ILE:HG21 | 1.93                     | 0.51              |
| 1:H:66:ILE:HG23  | 1:H:94:PHE:HD1    | 1.75                     | 0.51              |
| 1:B:131:ILE:HD12 | 1:B:132:PRO:O     | 2.10                     | 0.51              |
| 1:B:158:LEU:CD1  | 1:B:174:VAL:HB    | 2.22                     | 0.51              |
| 1:E:131:ILE:HD12 | 1:E:132:PRO:O     | 2.10                     | 0.51              |
| 1:F:2:ASN:HB3    | 1:F:319:ASP:OD2   | 2.11                     | 0.51              |
| 1:F:734:VAL:HG12 | 1:F:735:PRO:HD2   | 1.93                     | 0.51              |
| 1:G:540:ARG:HH21 | 1:G:541:ASP:CA    | 2.23                     | 0.51              |
| 1:H:1010:LEU:HA  | 1:H:1028:LEU:HD23 | 1.92                     | 0.51              |
| 1:H:465:ARG:O    | 1:H:465:ARG:CG    | 2.58                     | 0.51              |
| 1:H:571:PHE:CD2  | 1:H:572:SER:HB3   | 2.45                     | 0.51              |
| 1:H:93:GLU:O     | 1:H:96:ARG:HG2    | 2.11                     | 0.51              |
| 1:B:251:THR:HG23 | 1:B:254:LEU:HB2   | 1.91                     | 0.51              |
| 1:B:266:MET:CE   | 1:B:277:VAL:HG22  | 2.40                     | 0.51              |
| 1:B:288:PHE:CD1  | 1:B:288:PHE:C     | 2.84                     | 0.51              |
| 1:B:475:ASN:HA   | 1:B:1055:ILE:HG21 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:194:ALA:C    | 1:C:195:PHE:HD2   | 2.14                     | 0.51              |
| 1:C:225:VAL:HG13 | 1:C:333:GLN:NE2   | 2.26                     | 0.51              |
| 1:F:160:ILE:CG2  | 1:F:200:VAL:CG1   | 2.88                     | 0.51              |
| 1:F:862:VAL:O    | 1:F:866:MET:HG2   | 2.09                     | 0.51              |
| 1:H:2:ASN:HB2    | 1:H:321:TYR:OH    | 2.10                     | 0.51              |
| 1:A:1041:VAL:CG1 | 1:A:1043:TYR:CE1  | 2.93                     | 0.51              |
| 1:A:2:ASN:HB3    | 1:A:319:ASP:OD2   | 2.11                     | 0.51              |
| 1:C:183:SER:HA   | 1:C:186:ARG:HD2   | 1.92                     | 0.51              |
| 1:C:228:PHE:CD2  | 1:C:338:ILE:HG13  | 2.46                     | 0.51              |
| 1:D:754:ALA:HB1  | 1:D:759:VAL:HG11  | 1.92                     | 0.51              |
| 1:E:475:ASN:HA   | 1:E:1055:ILE:HG21 | 1.92                     | 0.51              |
| 1:E:749:TYR:CZ   | 1:G:752:ALA:CB    | 2.94                     | 0.51              |
| 1:G:183:SER:HA   | 1:G:186:ARG:HD2   | 1.92                     | 0.51              |
| 1:H:278:GLU:C    | 1:H:289:ILE:CD1   | 2.79                     | 0.51              |
| 1:A:506:ILE:CD1  | 1:A:565:HIS:CE1   | 2.93                     | 0.51              |
| 1:A:509:GLY:N    | 1:A:512:GLN:OE1   | 2.41                     | 0.51              |
| 1:D:93:GLU:O     | 1:D:96:ARG:HG2    | 2.11                     | 0.51              |
| 1:E:279:PHE:C    | 1:E:289:ILE:HD12  | 2.26                     | 0.51              |
| 1:E:675:TYR:CE2  | 1:E:716:LEU:CD1   | 2.93                     | 0.51              |
| 1:H:120:ILE:HD12 | 1:H:121:LYS:H     | 1.76                     | 0.51              |
| 1:B:552:ARG:HD2  | 1:B:1004:PHE:CD1  | 2.46                     | 0.51              |
| 1:B:279:PHE:C    | 1:B:289:ILE:HD12  | 2.26                     | 0.51              |
| 1:B:626:ASN:CG   | 1:B:950:PRO:HB3   | 2.31                     | 0.51              |
| 1:C:250:ILE:CD1  | 1:C:255:ARG:HB3   | 2.37                     | 0.51              |
| 1:D:112:HIS:CE1  | 1:D:271:TYR:HA    | 2.46                     | 0.51              |
| 1:E:12:ARG:CZ    | 1:E:391:TYR:CD1   | 2.94                     | 0.51              |
| 1:E:180:VAL:O    | 1:E:184:PHE:CE2   | 2.64                     | 0.51              |
| 1:E:626:ASN:CG   | 1:E:950:PRO:HB3   | 2.31                     | 0.51              |
| 1:F:44:ARG:HD3   | 1:F:45:TYR:CD1    | 2.46                     | 0.51              |
| 1:H:230:ARG:NH2  | 1:H:296:GLN:OE1   | 2.43                     | 0.51              |
| 1:A:754:ALA:HB1  | 1:A:759:VAL:HG11  | 1.93                     | 0.51              |
| 1:C:131:ILE:HD12 | 1:C:132:PRO:O     | 2.11                     | 0.51              |
| 1:C:2:ASN:HB3    | 1:C:319:ASP:OD2   | 2.11                     | 0.51              |
| 1:D:134:ILE:CD1  | 1:D:287:TYR:HB3   | 2.38                     | 0.51              |
| 1:G:131:ILE:HD12 | 1:G:132:PRO:O     | 2.11                     | 0.51              |
| 1:G:134:ILE:HG22 | 1:G:203:GLU:HB3   | 1.93                     | 0.51              |
| 1:H:354:ASN:HD22 | 1:H:357:MET:CB    | 2.23                     | 0.51              |
| 1:H:754:ALA:HB1  | 1:H:759:VAL:HG11  | 1.93                     | 0.51              |
| 1:A:1059:ASN:N   | 1:A:1059:ASN:OD1  | 2.42                     | 0.51              |
| 1:A:44:ARG:HD3   | 1:A:45:TYR:CD1    | 2.46                     | 0.51              |
| 1:A:511:LYS:NZ   | 1:A:641:ASP:CG    | 2.64                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:862:VAL:O    | 1:A:866:MET:HG2   | 2.10                     | 0.51              |
| 1:B:12:ARG:CZ    | 1:B:391:TYR:CD1   | 2.94                     | 0.51              |
| 1:C:832:MET:HG3  | 1:C:833:PRO:HD3   | 1.93                     | 0.51              |
| 1:E:226:HIS:H    | 1:E:333:GLN:HE22  | 1.58                     | 0.51              |
| 1:H:788:GLY:N    | 1:F:719:GLN:HG2   | 2.25                     | 0.51              |
| 1:G:2:ASN:HB3    | 1:G:319:ASP:OD2   | 2.12                     | 0.51              |
| 1:H:737:HIS:HA   | 1:H:761:ILE:O     | 2.11                     | 0.51              |
| 1:A:160:ILE:CG2  | 1:A:200:VAL:CG1   | 2.89                     | 0.50              |
| 1:A:1:MET:HE1    | 1:A:319:ASP:CB    | 2.40                     | 0.50              |
| 1:C:475:ASN:HA   | 1:C:1055:ILE:HG21 | 1.92                     | 0.50              |
| 1:D:115:MET:HG2  | 1:D:125:GLN:HG3   | 1.93                     | 0.50              |
| 1:D:662:VAL:HB   | 1:D:669:VAL:HG22  | 1.93                     | 0.50              |
| 1:D:719:GLN:HG2  | 1:A:788:GLY:N     | 2.26                     | 0.50              |
| 1:D:541:ASP:OD2  | 1:D:741:HIS:CE1   | 2.64                     | 0.50              |
| 1:E:502:TYR:HD1  | 1:E:503:GLY:N     | 2.08                     | 0.50              |
| 1:E:752:ALA:CB   | 1:G:749:TYR:CZ    | 2.94                     | 0.50              |
| 1:F:1:MET:HE1    | 1:F:319:ASP:CB    | 2.41                     | 0.50              |
| 1:F:737:HIS:HA   | 1:F:761:ILE:O     | 2.12                     | 0.50              |
| 1:H:112:HIS:CE1  | 1:H:271:TYR:HA    | 2.46                     | 0.50              |
| 1:H:960:LEU:HD13 | 1:H:976:TYR:CD2   | 2.46                     | 0.50              |
| 1:A:215:GLN:C    | 1:A:216:ILE:HD12  | 2.32                     | 0.50              |
| 1:B:226:HIS:H    | 1:B:333:GLN:HE22  | 1.58                     | 0.50              |
| 1:B:228:PHE:CD2  | 1:B:338:ILE:HD11  | 2.37                     | 0.50              |
| 1:B:675:TYR:CE2  | 1:B:716:LEU:CD1   | 2.94                     | 0.50              |
| 1:C:44:ARG:HD3   | 1:C:45:TYR:CD1    | 2.46                     | 0.50              |
| 1:C:510:THR:OG1  | 1:C:607:MET:CG    | 2.58                     | 0.50              |
| 1:C:651:TRP:NE1  | 1:C:653:LYS:CB    | 2.75                     | 0.50              |
| 1:D:278:GLU:C    | 1:D:289:ILE:CD1   | 2.79                     | 0.50              |
| 1:G:475:ASN:HA   | 1:G:1055:ILE:HG21 | 1.92                     | 0.50              |
| 1:H:453:THR:HG22 | 1:H:455:GLU:OE1   | 2.11                     | 0.50              |
| 1:A:737:HIS:HA   | 1:A:761:ILE:O     | 2.12                     | 0.50              |
| 1:C:120:ILE:HD12 | 1:C:121:LYS:H     | 1.76                     | 0.50              |
| 1:D:44:ARG:HD3   | 1:D:45:TYR:CE1    | 2.46                     | 0.50              |
| 1:D:453:THR:HG22 | 1:D:455:GLU:OE1   | 2.12                     | 0.50              |
| 1:E:23:CYS:HB3   | 1:E:28:ILE:HB     | 1.92                     | 0.50              |
| 1:E:540:ARG:HH21 | 1:E:541:ASP:CG    | 2.15                     | 0.50              |
| 1:E:541:ASP:HA   | 1:E:544:GLN:HB3   | 1.94                     | 0.50              |
| 1:F:1059:ASN:OD1 | 1:F:1059:ASN:N    | 2.43                     | 0.50              |
| 1:G:1010:LEU:HA  | 1:G:1028:LEU:HD23 | 1.93                     | 0.50              |
| 1:G:127:LEU:HD22 | 1:G:133:VAL:CG2   | 2.41                     | 0.50              |
| 1:H:116:PHE:N    | 1:H:116:PHE:CD1   | 2.77                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:356:PHE:N    | 1:H:356:PHE:HD1   | 2.10                     | 0.50              |
| 1:B:180:VAL:CG1  | 1:B:184:PHE:CZ    | 2.72                     | 0.50              |
| 1:F:570:MET:HG3  | 1:F:573:PHE:HE1   | 1.76                     | 0.50              |
| 1:H:428:ILE:HA   | 1:H:431:LEU:HD12  | 1.93                     | 0.50              |
| 1:H:42:PHE:HA    | 1:H:45:TYR:CD2    | 2.46                     | 0.50              |
| 1:H:662:VAL:HB   | 1:H:669:VAL:HG22  | 1.94                     | 0.50              |
| 1:C:453:THR:HG22 | 1:C:455:GLU:OE1   | 2.12                     | 0.50              |
| 1:C:610:MET:HG2  | 1:C:640:VAL:HG11  | 1.94                     | 0.50              |
| 1:D:7:VAL:HG11   | 1:D:23:CYS:SG     | 2.52                     | 0.50              |
| 1:G:112:HIS:O    | 1:G:116:PHE:HD2   | 1.95                     | 0.50              |
| 1:G:194:ALA:C    | 1:G:195:PHE:HD2   | 2.15                     | 0.50              |
| 1:G:662:VAL:HB   | 1:G:669:VAL:HG22  | 1.93                     | 0.50              |
| 1:G:737:HIS:HA   | 1:G:761:ILE:O     | 2.11                     | 0.50              |
| 1:C:134:ILE:HG22 | 1:C:203:GLU:HB3   | 1.94                     | 0.50              |
| 1:C:540:ARG:HH21 | 1:C:541:ASP:CA    | 2.24                     | 0.50              |
| 1:D:66:ILE:HG23  | 1:D:94:PHE:HD1    | 1.76                     | 0.50              |
| 1:E:112:HIS:CE1  | 1:E:271:TYR:HA    | 2.47                     | 0.50              |
| 1:E:552:ARG:HD2  | 1:E:1004:PHE:CD1  | 2.46                     | 0.50              |
| 1:F:219:ASP:CB   | 1:F:323:LEU:HD23  | 2.28                     | 0.50              |
| 1:F:754:ALA:HB1  | 1:F:759:VAL:HG11  | 1.94                     | 0.50              |
| 1:G:610:MET:HG2  | 1:G:640:VAL:HG11  | 1.94                     | 0.50              |
| 1:H:2:ASN:HB3    | 1:H:319:ASP:OD2   | 2.11                     | 0.50              |
| 1:B:23:CYS:HB3   | 1:B:28:ILE:HB     | 1.93                     | 0.50              |
| 1:C:1010:LEU:HA  | 1:C:1028:LEU:HD23 | 1.93                     | 0.50              |
| 1:C:215:GLN:C    | 1:C:216:ILE:HD12  | 2.32                     | 0.50              |
| 1:C:304:MET:HE2  | 1:C:399:CYS:CB    | 2.41                     | 0.50              |
| 1:C:551:VAL:HA   | 1:C:813:TYR:CE2   | 2.46                     | 0.50              |
| 1:C:589:ASN:OD1  | 1:C:989:MET:CE    | 2.60                     | 0.50              |
| 1:F:112:HIS:CE1  | 1:F:271:TYR:HA    | 2.47                     | 0.50              |
| 1:G:7:VAL:HG11   | 1:G:23:CYS:SG     | 2.52                     | 0.50              |
| 1:G:453:THR:HG22 | 1:G:455:GLU:OE1   | 2.12                     | 0.50              |
| 1:G:832:MET:HG3  | 1:G:833:PRO:HD3   | 1.94                     | 0.50              |
| 1:H:356:PHE:CD1  | 1:H:356:PHE:N     | 2.79                     | 0.50              |
| 1:H:44:ARG:HD3   | 1:H:45:TYR:CE1    | 2.47                     | 0.50              |
| 1:H:567:LEU:N    | 1:H:568:PRO:CD    | 2.73                     | 0.50              |
| 1:C:230:ARG:NH2  | 1:C:296:GLN:OE1   | 2.45                     | 0.50              |
| 1:D:12:ARG:NH1   | 1:D:391:TYR:CB    | 2.74                     | 0.50              |
| 1:D:42:PHE:HA    | 1:D:45:TYR:CD2    | 2.46                     | 0.50              |
| 1:D:532:VAL:HG12 | 1:D:791:GLN:O     | 2.12                     | 0.50              |
| 1:G:589:ASN:OD1  | 1:G:989:MET:CE    | 2.60                     | 0.50              |
| 1:A:134:ILE:CG2  | 1:A:203:GLU:HB3   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:112:HIS:CE1  | 1:A:271:TYR:HA    | 2.47                     | 0.50              |
| 1:B:180:VAL:HG12 | 1:B:184:PHE:CE1   | 2.38                     | 0.50              |
| 1:B:228:PHE:CD2  | 1:B:338:ILE:CG1   | 2.95                     | 0.50              |
| 1:C:737:HIS:HA   | 1:C:761:ILE:O     | 2.12                     | 0.50              |
| 1:D:176:SER:OG   | 1:D:177:LYS:HE2   | 2.12                     | 0.50              |
| 1:D:2:ASN:HB3    | 1:D:319:ASP:OD2   | 2.11                     | 0.50              |
| 1:D:737:HIS:HA   | 1:D:761:ILE:O     | 2.12                     | 0.50              |
| 1:E:228:PHE:CD2  | 1:E:338:ILE:CG1   | 2.95                     | 0.50              |
| 1:F:622:ASN:ND2  | 1:F:917:GLU:O     | 2.45                     | 0.50              |
| 1:H:21:ARG:NH1   | 1:G:370:GLY:O     | 2.44                     | 0.50              |
| 1:G:44:ARG:HD3   | 1:G:45:TYR:CD1    | 2.47                     | 0.50              |
| 1:G:510:THR:OG1  | 1:G:607:MET:CG    | 2.58                     | 0.50              |
| 1:H:17:ILE:HA    | 1:H:20:MET:HG3    | 1.93                     | 0.50              |
| 1:H:719:GLN:HG2  | 1:F:788:GLY:N     | 2.27                     | 0.50              |
| 1:H:532:VAL:HG12 | 1:H:791:GLN:O     | 2.12                     | 0.50              |
| 1:A:226:HIS:H    | 1:A:333:GLN:HE22  | 1.58                     | 0.49              |
| 1:B:134:ILE:HD12 | 1:B:287:TYR:CB    | 2.42                     | 0.49              |
| 1:C:7:VAL:HG11   | 1:C:23:CYS:SG     | 2.52                     | 0.49              |
| 1:D:116:PHE:CD1  | 1:D:116:PHE:N     | 2.77                     | 0.49              |
| 1:E:428:ILE:HA   | 1:E:431:LEU:HD12  | 1.94                     | 0.49              |
| 1:F:541:ASP:OD2  | 1:F:741:HIS:CE1   | 2.65                     | 0.49              |
| 1:A:570:MET:HG3  | 1:A:573:PHE:HE1   | 1.77                     | 0.49              |
| 1:B:177:LYS:O    | 1:B:178:GLU:CB    | 2.60                     | 0.49              |
| 1:B:540:ARG:HA   | 1:B:543:HIS:HE2   | 1.77                     | 0.49              |
| 1:D:546:LEU:CD1  | 1:D:774:SER:HB2   | 2.42                     | 0.49              |
| 1:E:356:PHE:N    | 1:E:356:PHE:CD1   | 2.81                     | 0.49              |
| 1:F:532:VAL:HG12 | 1:F:791:GLN:O     | 2.12                     | 0.49              |
| 1:G:111:LYS:O    | 1:G:115:MET:HG2   | 2.12                     | 0.49              |
| 1:G:213:GLU:O    | 1:G:229:GLU:HA    | 2.12                     | 0.49              |
| 1:G:428:ILE:HA   | 1:G:431:LEU:HD12  | 1.93                     | 0.49              |
| 1:H:265:LEU:HG   | 1:H:266:MET:HE2   | 1.94                     | 0.49              |
| 1:B:754:ALA:HB1  | 1:B:759:VAL:HG11  | 1.94                     | 0.49              |
| 1:C:356:PHE:CD1  | 1:C:356:PHE:N     | 2.81                     | 0.49              |
| 1:C:662:VAL:HB   | 1:C:669:VAL:HG22  | 1.94                     | 0.49              |
| 1:C:546:LEU:CD1  | 1:C:774:SER:HB2   | 2.43                     | 0.49              |
| 1:D:356:PHE:CD1  | 1:D:356:PHE:N     | 2.80                     | 0.49              |
| 1:E:1010:LEU:HA  | 1:E:1028:LEU:HD23 | 1.94                     | 0.49              |
| 1:E:754:ALA:HB1  | 1:E:759:VAL:HG11  | 1.94                     | 0.49              |
| 1:E:546:LEU:CD1  | 1:E:774:SER:HB2   | 2.43                     | 0.49              |
| 1:F:134:ILE:CG2  | 1:F:203:GLU:HB3   | 2.43                     | 0.49              |
| 1:F:42:PHE:HA    | 1:F:45:TYR:CD2    | 2.47                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:428:ILE:HA   | 1:F:431:LEU:HD12  | 1.94                     | 0.49              |
| 1:F:712:MET:O    | 1:F:741:HIS:HD2   | 1.95                     | 0.49              |
| 1:H:7:VAL:HG11   | 1:H:23:CYS:SG     | 2.52                     | 0.49              |
| 1:B:1010:LEU:HA  | 1:B:1028:LEU:HD23 | 1.94                     | 0.49              |
| 1:B:356:PHE:N    | 1:B:356:PHE:HD1   | 2.09                     | 0.49              |
| 1:C:112:HIS:O    | 1:C:116:PHE:HD2   | 1.96                     | 0.49              |
| 1:C:226:HIS:H    | 1:C:333:GLN:HE22  | 1.58                     | 0.49              |
| 1:D:17:ILE:HA    | 1:D:20:MET:HG3    | 1.94                     | 0.49              |
| 1:D:213:GLU:O    | 1:D:229:GLU:HA    | 2.12                     | 0.49              |
| 1:D:370:GLY:C    | 1:C:21:ARG:HH12   | 2.14                     | 0.49              |
| 1:D:428:ILE:HA   | 1:D:431:LEU:HD12  | 1.94                     | 0.49              |
| 1:F:226:HIS:H    | 1:F:333:GLN:HE22  | 1.59                     | 0.49              |
| 1:G:754:ALA:HB1  | 1:G:759:VAL:HG11  | 1.94                     | 0.49              |
| 1:H:474:GLY:O    | 1:H:478:VAL:HG23  | 2.12                     | 0.49              |
| 1:H:708:GLY:HA2  | 1:H:737:HIS:O     | 2.12                     | 0.49              |
| 1:H:851:ASP:OD2  | 1:H:852:ARG:N     | 2.45                     | 0.49              |
| 1:A:42:PHE:HA    | 1:A:45:TYR:CD2    | 2.47                     | 0.49              |
| 1:A:563:MET:HB3  | 1:A:573:PHE:HE2   | 1.75                     | 0.49              |
| 1:A:541:ASP:OD2  | 1:A:741:HIS:CE1   | 2.66                     | 0.49              |
| 1:A:622:ASN:ND2  | 1:A:917:GLU:O     | 2.46                     | 0.49              |
| 1:B:112:HIS:CE1  | 1:B:271:TYR:HA    | 2.47                     | 0.49              |
| 1:B:567:LEU:N    | 1:B:568:PRO:CD    | 2.75                     | 0.49              |
| 1:C:127:LEU:HD22 | 1:C:133:VAL:CG2   | 2.42                     | 0.49              |
| 1:C:17:ILE:HA    | 1:C:20:MET:HG3    | 1.94                     | 0.49              |
| 1:C:540:ARG:NH2  | 1:C:541:ASP:HA    | 2.26                     | 0.49              |
| 1:F:111:LYS:O    | 1:F:115:MET:HG2   | 2.12                     | 0.49              |
| 1:G:230:ARG:NH2  | 1:G:296:GLN:OE1   | 2.46                     | 0.49              |
| 1:G:520:GLU:OE1  | 1:G:705:HIS:NE2   | 2.45                     | 0.49              |
| 1:G:88:LEU:HB3   | 1:G:94:PHE:CD2    | 2.39                     | 0.49              |
| 1:H:12:ARG:NH1   | 1:H:391:TYR:CB    | 2.75                     | 0.49              |
| 1:H:546:LEU:CD1  | 1:H:774:SER:HB2   | 2.42                     | 0.49              |
| 1:A:453:THR:HG22 | 1:A:455:GLU:OE1   | 2.12                     | 0.49              |
| 1:A:370:GLY:C    | 1:B:21:ARG:HH12   | 2.16                     | 0.49              |
| 1:B:368:SER:HA   | 1:B:419:PHE:CE1   | 2.48                     | 0.49              |
| 1:B:541:ASP:HA   | 1:B:544:GLN:HB3   | 1.95                     | 0.49              |
| 1:B:603:ILE:CD1  | 1:B:608:PHE:CZ    | 2.95                     | 0.49              |
| 1:D:356:PHE:HD1  | 1:D:356:PHE:N     | 2.11                     | 0.49              |
| 1:E:226:HIS:ND1  | 1:E:259:CYS:HB3   | 2.27                     | 0.49              |
| 1:G:176:SER:O    | 1:G:179:HIS:CD2   | 2.65                     | 0.49              |
| 1:G:215:GLN:C    | 1:G:216:ILE:HD12  | 2.33                     | 0.49              |
| 1:G:356:PHE:CD1  | 1:G:356:PHE:N     | 2.81                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:546:LEU:CD1  | 1:G:774:SER:HB2  | 2.43                     | 0.49              |
| 1:G:551:VAL:HA   | 1:G:813:TYR:CE2  | 2.47                     | 0.49              |
| 1:H:176:SER:OG   | 1:H:177:LYS:HE2  | 2.12                     | 0.49              |
| 1:A:226:HIS:ND1  | 1:A:259:CYS:HB3  | 2.28                     | 0.49              |
| 1:B:112:HIS:O    | 1:B:116:PHE:HD2  | 1.95                     | 0.49              |
| 1:B:428:ILE:HA   | 1:B:431:LEU:HD12 | 1.95                     | 0.49              |
| 1:B:546:LEU:CD1  | 1:B:774:SER:HB2  | 2.43                     | 0.49              |
| 1:C:520:GLU:OE1  | 1:C:705:HIS:NE2  | 2.46                     | 0.49              |
| 1:C:754:ALA:HB1  | 1:C:759:VAL:HG11 | 1.94                     | 0.49              |
| 1:D:851:ASP:OD2  | 1:D:852:ARG:N    | 2.45                     | 0.49              |
| 1:E:215:GLN:C    | 1:E:216:ILE:HD12 | 2.33                     | 0.49              |
| 1:E:228:PHE:CD2  | 1:E:338:ILE:HG13 | 2.48                     | 0.49              |
| 1:E:567:LEU:N    | 1:E:568:PRO:CD   | 2.75                     | 0.49              |
| 1:F:708:GLY:HA2  | 1:F:737:HIS:O    | 2.13                     | 0.49              |
| 1:G:182:GLU:O    | 1:G:186:ARG:HD2  | 2.13                     | 0.49              |
| 1:G:437:HIS:CE1  | 1:G:439:ASP:HB2  | 2.48                     | 0.49              |
| 1:G:519:PRO:HB2  | 1:G:705:HIS:HE2  | 1.76                     | 0.49              |
| 1:G:532:VAL:HG12 | 1:G:791:GLN:O    | 2.13                     | 0.49              |
| 1:H:23:CYS:HB3   | 1:H:28:ILE:HB    | 1.95                     | 0.49              |
| 1:H:540:ARG:O    | 1:H:542:ALA:N    | 2.43                     | 0.49              |
| 1:A:111:LYS:O    | 1:A:115:MET:HG2  | 2.13                     | 0.49              |
| 1:A:511:LYS:NZ   | 1:A:641:ASP:OD2  | 2.46                     | 0.49              |
| 1:A:532:VAL:HG12 | 1:A:791:GLN:O    | 2.12                     | 0.49              |
| 1:B:510:THR:OG1  | 1:B:607:MET:CG   | 2.59                     | 0.49              |
| 1:D:567:LEU:N    | 1:D:568:PRO:CD   | 2.74                     | 0.49              |
| 1:E:112:HIS:O    | 1:E:116:PHE:HD2  | 1.95                     | 0.49              |
| 1:E:7:VAL:HG11   | 1:E:23:CYS:SG    | 2.53                     | 0.49              |
| 1:F:453:THR:HG22 | 1:F:455:GLU:OE1  | 2.12                     | 0.49              |
| 1:G:112:HIS:CE1  | 1:G:271:TYR:HA   | 2.47                     | 0.49              |
| 1:A:708:GLY:HA2  | 1:A:737:HIS:O    | 2.13                     | 0.49              |
| 1:C:519:PRO:HB2  | 1:C:705:HIS:HE2  | 1.75                     | 0.49              |
| 1:C:532:VAL:HG12 | 1:C:791:GLN:O    | 2.13                     | 0.49              |
| 1:D:23:CYS:HB3   | 1:D:28:ILE:HB    | 1.95                     | 0.49              |
| 1:D:540:ARG:O    | 1:D:542:ALA:N    | 2.43                     | 0.49              |
| 1:D:960:LEU:HD13 | 1:D:976:TYR:CD2  | 2.47                     | 0.49              |
| 1:E:225:VAL:HG13 | 1:E:333:GLN:NE2  | 2.28                     | 0.49              |
| 1:E:708:GLY:HA2  | 1:E:737:HIS:O    | 2.13                     | 0.49              |
| 1:A:7:VAL:HG11   | 1:A:23:CYS:SG    | 2.53                     | 0.49              |
| 1:A:712:MET:O    | 1:A:741:HIS:HD2  | 1.96                     | 0.49              |
| 1:B:708:GLY:HA2  | 1:B:737:HIS:O    | 2.13                     | 0.49              |
| 1:C:111:LYS:O    | 1:C:115:MET:HG2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:182:GLU:O    | 1:C:186:ARG:HD2  | 2.13                     | 0.49              |
| 1:C:112:HIS:CE1  | 1:C:271:TYR:HA   | 2.47                     | 0.49              |
| 1:D:708:GLY:HA2  | 1:D:737:HIS:O    | 2.13                     | 0.49              |
| 1:E:64:LEU:CD2   | 1:E:88:LEU:CD2   | 2.91                     | 0.49              |
| 1:F:213:GLU:O    | 1:F:229:GLU:HA   | 2.12                     | 0.49              |
| 1:F:23:CYS:HB3   | 1:F:28:ILE:HB    | 1.94                     | 0.49              |
| 1:F:534:LEU:O    | 1:F:570:MET:HE3  | 2.12                     | 0.49              |
| 1:F:918:ILE:HD12 | 1:F:919:GLY:H    | 1.78                     | 0.49              |
| 1:G:226:HIS:H    | 1:G:333:GLN:HE22 | 1.58                     | 0.49              |
| 1:H:918:ILE:HD12 | 1:H:919:GLY:H    | 1.77                     | 0.49              |
| 1:A:709:ILE:HB   | 1:A:738:LEU:CD1  | 2.43                     | 0.48              |
| 1:B:44:ARG:HD3   | 1:B:45:TYR:CD1   | 2.47                     | 0.48              |
| 1:C:213:GLU:O    | 1:C:229:GLU:HA   | 2.13                     | 0.48              |
| 1:D:620:TYR:CE2  | 1:D:621:LYS:HE3  | 2.47                     | 0.48              |
| 1:F:215:GLN:C    | 1:F:216:ILE:HD12 | 2.34                     | 0.48              |
| 1:F:563:MET:HB3  | 1:F:573:PHE:HE2  | 1.76                     | 0.48              |
| 1:H:42:PHE:HA    | 1:H:45:TYR:HD2   | 1.78                     | 0.48              |
| 1:A:546:LEU:CD1  | 1:A:774:SER:HB2  | 2.42                     | 0.48              |
| 1:A:918:ILE:HD12 | 1:A:919:GLY:H    | 1.78                     | 0.48              |
| 1:B:7:VAL:HG11   | 1:B:23:CYS:SG    | 2.53                     | 0.48              |
| 1:C:356:PHE:HD1  | 1:C:356:PHE:N    | 2.12                     | 0.48              |
| 1:C:12:ARG:NH1   | 1:C:38:ASP:OD2   | 2.46                     | 0.48              |
| 1:D:42:PHE:HA    | 1:D:45:TYR:HD2   | 1.78                     | 0.48              |
| 1:D:541:ASP:HA   | 1:D:544:GLN:HB3  | 1.94                     | 0.48              |
| 1:E:288:PHE:C    | 1:E:288:PHE:CD1  | 2.87                     | 0.48              |
| 1:F:226:HIS:ND1  | 1:F:259:CYS:HB3  | 2.28                     | 0.48              |
| 1:F:662:VAL:HB   | 1:F:669:VAL:HG22 | 1.95                     | 0.48              |
| 1:F:709:ILE:HB   | 1:F:738:LEU:CD1  | 2.43                     | 0.48              |
| 1:H:226:HIS:ND1  | 1:H:259:CYS:HB3  | 2.28                     | 0.48              |
| 1:A:213:GLU:O    | 1:A:229:GLU:HA   | 2.12                     | 0.48              |
| 1:A:228:PHE:CE2  | 1:A:338:ILE:HG13 | 2.48                     | 0.48              |
| 1:B:12:ARG:CZ    | 1:B:391:TYR:HD1  | 2.25                     | 0.48              |
| 1:B:532:VAL:HG12 | 1:B:791:GLN:O    | 2.12                     | 0.48              |
| 1:C:960:LEU:HD11 | 1:C:968:PRO:CG   | 2.36                     | 0.48              |
| 1:D:215:GLN:C    | 1:D:216:ILE:HD12 | 2.34                     | 0.48              |
| 1:D:534:LEU:O    | 1:D:570:MET:HE3  | 2.12                     | 0.48              |
| 1:E:532:VAL:HG12 | 1:E:791:GLN:O    | 2.12                     | 0.48              |
| 1:G:42:PHE:HA    | 1:G:45:TYR:CD2   | 2.47                     | 0.48              |
| 1:H:611:LEU:HD11 | 1:H:646:PHE:CD1  | 2.48                     | 0.48              |
| 1:H:712:MET:O    | 1:H:741:HIS:HD2  | 1.96                     | 0.48              |
| 1:A:156:TYR:CB   | 1:A:157:PRO:HD3  | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:ARG:HH12  | 1:B:370:GLY:C    | 2.17                     | 0.48              |
| 1:A:23:CYS:HB3   | 1:A:28:ILE:HB    | 1.95                     | 0.48              |
| 1:D:611:LEU:HD11 | 1:D:646:PHE:CD1  | 2.48                     | 0.48              |
| 1:E:44:ARG:HD3   | 1:E:45:TYR:CD1   | 2.48                     | 0.48              |
| 1:F:228:PHE:CE2  | 1:F:338:ILE:HG13 | 2.48                     | 0.48              |
| 1:F:546:LEU:CD1  | 1:F:774:SER:HB2  | 2.42                     | 0.48              |
| 1:G:356:PHE:HD1  | 1:G:356:PHE:N    | 2.12                     | 0.48              |
| 1:G:960:LEU:HD11 | 1:G:968:PRO:CG   | 2.36                     | 0.48              |
| 1:A:533:LEU:O    | 1:A:761:ILE:HA   | 2.14                     | 0.48              |
| 1:A:534:LEU:O    | 1:A:570:MET:HE3  | 2.13                     | 0.48              |
| 1:B:662:VAL:HB   | 1:B:669:VAL:HG22 | 1.94                     | 0.48              |
| 1:D:474:GLY:O    | 1:D:478:VAL:HG23 | 2.13                     | 0.48              |
| 1:E:12:ARG:CZ    | 1:E:391:TYR:HD1  | 2.25                     | 0.48              |
| 1:F:611:LEU:HD11 | 1:F:646:PHE:CD1  | 2.48                     | 0.48              |
| 1:G:182:GLU:O    | 1:G:186:ARG:NE   | 2.45                     | 0.48              |
| 1:G:12:ARG:NH1   | 1:G:38:ASP:OD2   | 2.47                     | 0.48              |
| 1:G:473:ILE:O    | 1:G:477:THR:OG1  | 2.26                     | 0.48              |
| 1:G:567:LEU:N    | 1:G:568:PRO:CD   | 2.76                     | 0.48              |
| 1:G:992:LYS:HE3  | 1:G:993:TYR:CZ   | 2.47                     | 0.48              |
| 1:H:213:GLU:OE2  | 1:H:232:CYS:SG   | 2.55                     | 0.48              |
| 1:A:611:LEU:HD11 | 1:A:646:PHE:CD1  | 2.48                     | 0.48              |
| 1:B:228:PHE:CD2  | 1:B:338:ILE:HG13 | 2.48                     | 0.48              |
| 1:B:64:LEU:CD2   | 1:B:88:LEU:CD2   | 2.91                     | 0.48              |
| 1:B:82:HIS:CD2   | 1:B:84:GLY:H     | 2.23                     | 0.48              |
| 1:B:626:ASN:ND2  | 1:B:950:PRO:HB3  | 2.28                     | 0.48              |
| 1:C:1:MET:HE1    | 1:C:319:ASP:CB   | 2.42                     | 0.48              |
| 1:C:473:ILE:O    | 1:C:477:THR:OG1  | 2.26                     | 0.48              |
| 1:C:960:LEU:C    | 1:C:960:LEU:HD13 | 2.33                     | 0.48              |
| 1:C:992:LYS:HE3  | 1:C:993:TYR:CZ   | 2.48                     | 0.48              |
| 1:E:603:ILE:CD1  | 1:E:608:PHE:CZ   | 2.96                     | 0.48              |
| 1:F:473:ILE:O    | 1:F:477:THR:OG1  | 2.26                     | 0.48              |
| 1:F:7:VAL:HG11   | 1:F:23:CYS:SG    | 2.54                     | 0.48              |
| 1:G:960:LEU:HD13 | 1:G:960:LEU:C    | 2.33                     | 0.48              |
| 1:H:213:GLU:O    | 1:H:229:GLU:HA   | 2.14                     | 0.48              |
| 1:H:534:LEU:O    | 1:H:570:MET:HE3  | 2.13                     | 0.48              |
| 1:B:180:VAL:O    | 1:B:184:PHE:CE2  | 2.67                     | 0.48              |
| 1:B:737:HIS:HA   | 1:B:761:ILE:O    | 2.13                     | 0.48              |
| 1:D:437:HIS:CE1  | 1:D:439:ASP:HB2  | 2.49                     | 0.48              |
| 1:D:712:MET:O    | 1:D:741:HIS:HD2  | 1.96                     | 0.48              |
| 1:E:737:HIS:HA   | 1:E:761:ILE:O    | 2.13                     | 0.48              |
| 1:E:626:ASN:ND2  | 1:E:950:PRO:HB3  | 2.28                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:144:ILE:HG23  | 1:G:184:PHE:CD2  | 2.49                     | 0.48              |
| 1:C:176:SER:O     | 1:C:179:HIS:CD2  | 2.66                     | 0.48              |
| 1:C:963:LYS:HA    | 1:C:963:LYS:HE3  | 1.96                     | 0.48              |
| 1:D:265:LEU:HG    | 1:D:266:MET:HE2  | 1.95                     | 0.48              |
| 1:D:918:ILE:HD12  | 1:D:919:GLY:H    | 1.78                     | 0.48              |
| 1:F:42:PHE:HA     | 1:F:45:TYR:HD2   | 1.78                     | 0.48              |
| 1:F:533:LEU:O     | 1:F:761:ILE:HA   | 2.14                     | 0.48              |
| 1:G:1:MET:HE1     | 1:G:319:ASP:CB   | 2.43                     | 0.48              |
| 1:B:144:ILE:HD12  | 1:B:145:LYS:H    | 1.79                     | 0.48              |
| 1:C:175:GLU:HG3   | 1:C:179:HIS:CD2  | 2.48                     | 0.48              |
| 1:C:428:ILE:HA    | 1:C:431:LEU:HD12 | 1.94                     | 0.48              |
| 1:C:437:HIS:CE1   | 1:C:439:ASP:HB2  | 2.49                     | 0.48              |
| 1:B:749:TYR:CZ    | 1:C:752:ALA:CB   | 2.97                     | 0.48              |
| 1:D:354:ASN:HD22  | 1:D:357:MET:CB   | 2.26                     | 0.48              |
| 1:E:662:VAL:HB    | 1:E:669:VAL:HG22 | 1.94                     | 0.48              |
| 1:F:120:ILE:HD12  | 1:F:121:LYS:H    | 1.76                     | 0.48              |
| 1:F:541:ASP:HA    | 1:F:544:GLN:HB3  | 1.95                     | 0.48              |
| 1:A:112:HIS:O     | 1:A:116:PHE:HD2  | 1.95                     | 0.48              |
| 1:A:428:ILE:HA    | 1:A:431:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:541:ASP:HA    | 1:A:544:GLN:HB3  | 1.95                     | 0.48              |
| 1:C:42:PHE:HA     | 1:C:45:TYR:CD2   | 2.48                     | 0.48              |
| 1:E:280:LEU:N     | 1:E:289:ILE:CD1  | 2.74                     | 0.48              |
| 1:F:1041:VAL:HG11 | 1:F:1043:TYR:HE1 | 1.77                     | 0.48              |
| 1:H:370:GLY:C     | 1:G:21:ARG:NH1   | 2.68                     | 0.48              |
| 1:H:437:HIS:CE1   | 1:H:439:ASP:HB2  | 2.49                     | 0.48              |
| 1:H:709:ILE:HB    | 1:H:738:LEU:CD1  | 2.44                     | 0.48              |
| 1:C:510:THR:OG1   | 1:C:607:MET:SD   | 2.71                     | 0.47              |
| 1:D:226:HIS:ND1   | 1:D:259:CYS:HB3  | 2.29                     | 0.47              |
| 1:F:347:ILE:O     | 1:F:395:LEU:CD1  | 2.55                     | 0.47              |
| 1:F:370:GLY:C     | 1:E:21:ARG:HH12  | 2.18                     | 0.47              |
| 1:F:511:LYS:NZ    | 1:F:641:ASP:CG   | 2.64                     | 0.47              |
| 1:G:120:ILE:HD12  | 1:G:121:LYS:H    | 1.79                     | 0.47              |
| 1:G:651:TRP:NE1   | 1:G:653:LYS:CB   | 2.77                     | 0.47              |
| 1:G:533:LEU:O     | 1:G:761:ILE:HA   | 2.14                     | 0.47              |
| 1:H:1:MET:HE1     | 1:H:319:ASP:CB   | 2.43                     | 0.47              |
| 1:H:559:ILE:HD13  | 1:H:805:TYR:CG   | 2.49                     | 0.47              |
| 1:A:662:VAL:HB    | 1:A:669:VAL:HG22 | 1.95                     | 0.47              |
| 1:B:180:VAL:CG1   | 1:B:184:PHE:HZ   | 2.17                     | 0.47              |
| 1:C:533:LEU:O     | 1:C:761:ILE:HA   | 2.15                     | 0.47              |
| 1:E:675:TYR:CE2   | 1:E:716:LEU:HD12 | 2.49                     | 0.47              |
| 1:G:42:PHE:HA     | 1:G:45:TYR:HD2   | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:194:ALA:HB1  | 1:A:195:PHE:CE2  | 2.49                     | 0.47              |
| 1:C:182:GLU:O    | 1:C:186:ARG:NE   | 2.46                     | 0.47              |
| 1:B:752:ALA:HB1  | 1:C:749:TYR:CZ   | 2.48                     | 0.47              |
| 1:D:1:MET:HE1    | 1:D:319:ASP:CB   | 2.43                     | 0.47              |
| 1:E:368:SER:HA   | 1:E:419:PHE:CE1  | 2.49                     | 0.47              |
| 1:E:509:GLY:HA3  | 1:E:605:ASN:O    | 2.14                     | 0.47              |
| 1:E:64:LEU:HD23  | 1:E:88:LEU:CD2   | 2.44                     | 0.47              |
| 1:G:144:ILE:HA   | 1:G:184:PHE:CE2  | 2.50                     | 0.47              |
| 1:H:610:MET:HG2  | 1:H:640:VAL:HG11 | 1.95                     | 0.47              |
| 1:H:82:HIS:CD2   | 1:H:84:GLY:H     | 2.24                     | 0.47              |
| 1:B:1:MET:HE2    | 1:B:4:ILE:O      | 2.13                     | 0.47              |
| 1:B:280:LEU:N    | 1:B:289:ILE:CD1  | 2.75                     | 0.47              |
| 1:D:176:SER:O    | 1:D:179:HIS:ND1  | 2.26                     | 0.47              |
| 1:F:112:HIS:O    | 1:F:116:PHE:HD2  | 1.96                     | 0.47              |
| 1:F:437:HIS:CE1  | 1:F:439:ASP:HB2  | 2.49                     | 0.47              |
| 1:G:510:THR:OG1  | 1:G:607:MET:SD   | 2.71                     | 0.47              |
| 1:H:64:LEU:CD2   | 1:H:88:LEU:CD2   | 2.92                     | 0.47              |
| 1:H:898:TYR:HD1  | 1:H:928:LYS:HE2  | 1.77                     | 0.47              |
| 1:B:215:GLN:C    | 1:B:216:ILE:HD12 | 2.35                     | 0.47              |
| 1:C:509:GLY:HA3  | 1:C:605:ASN:O    | 2.14                     | 0.47              |
| 1:C:567:LEU:N    | 1:C:568:PRO:CD   | 2.77                     | 0.47              |
| 1:D:709:ILE:HB   | 1:D:738:LEU:CD1  | 2.45                     | 0.47              |
| 1:E:134:ILE:HD12 | 1:E:287:TYR:CB   | 2.44                     | 0.47              |
| 1:E:356:PHE:N    | 1:E:356:PHE:HD1  | 2.11                     | 0.47              |
| 1:E:354:ASN:ND2  | 1:E:357:MET:HB3  | 2.29                     | 0.47              |
| 1:E:1:MET:HE2    | 1:E:4:ILE:O      | 2.14                     | 0.47              |
| 1:F:509:GLY:HA3  | 1:F:605:ASN:O    | 2.14                     | 0.47              |
| 1:A:42:PHE:HA    | 1:A:45:TYR:HD2   | 1.79                     | 0.47              |
| 1:A:509:GLY:HA3  | 1:A:605:ASN:O    | 2.14                     | 0.47              |
| 1:B:225:VAL:HG13 | 1:B:333:GLN:NE2  | 2.30                     | 0.47              |
| 1:B:540:ARG:O    | 1:B:542:ALA:N    | 2.46                     | 0.47              |
| 1:D:405:PHE:CD2  | 1:D:405:PHE:C    | 2.88                     | 0.47              |
| 1:E:540:ARG:O    | 1:E:542:ALA:N    | 2.45                     | 0.47              |
| 1:F:996:VAL:O    | 1:F:997:THR:C    | 2.53                     | 0.47              |
| 1:H:304:MET:HE2  | 1:H:399:CYS:CB   | 2.44                     | 0.47              |
| 1:H:352:PRO:HA   | 1:H:356:PHE:CE1  | 2.49                     | 0.47              |
| 1:H:620:TYR:CE2  | 1:H:621:LYS:HE3  | 2.48                     | 0.47              |
| 1:H:631:PHE:CD2  | 1:H:631:PHE:C    | 2.88                     | 0.47              |
| 1:A:437:HIS:CE1  | 1:A:439:ASP:HB2  | 2.50                     | 0.47              |
| 1:A:559:ILE:HD13 | 1:A:805:TYR:CG   | 2.50                     | 0.47              |
| 1:B:559:ILE:HD13 | 1:B:805:TYR:CG   | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:778:MET:HG3   | 1:C:779:THR:N     | 2.29                     | 0.47              |
| 1:D:369:THR:O     | 1:D:376:LEU:HD11  | 2.15                     | 0.47              |
| 1:E:1018:LEU:HD11 | 1:E:1024:LEU:HD11 | 1.95                     | 0.47              |
| 1:E:450:ILE:HG22  | 1:E:451:ASP:N     | 2.29                     | 0.47              |
| 1:E:533:LEU:O     | 1:E:761:ILE:HA    | 2.15                     | 0.47              |
| 1:G:963:LYS:HA    | 1:G:963:LYS:HE3   | 1.96                     | 0.47              |
| 1:H:450:ILE:HG22  | 1:H:451:ASP:N     | 2.29                     | 0.47              |
| 1:H:546:LEU:HD11  | 1:H:774:SER:HB2   | 1.97                     | 0.47              |
| 1:A:120:ILE:HD12  | 1:A:121:LYS:H     | 1.78                     | 0.47              |
| 1:A:347:ILE:O     | 1:A:395:LEU:CD1   | 2.55                     | 0.47              |
| 1:B:64:LEU:HD23   | 1:B:88:LEU:CD2    | 2.44                     | 0.47              |
| 1:B:675:TYR:CE2   | 1:B:716:LEU:HD12  | 2.50                     | 0.47              |
| 1:B:533:LEU:O     | 1:B:761:ILE:HA    | 2.15                     | 0.47              |
| 1:C:3:ARG:CD      | 1:C:104:ILE:HD11  | 2.35                     | 0.47              |
| 1:C:90:GLU:HA     | 1:C:113:LEU:HD22  | 1.97                     | 0.47              |
| 1:C:226:HIS:CE1   | 1:C:259:CYS:HB3   | 2.49                     | 0.47              |
| 1:C:227:LEU:HD22  | 1:C:306:THR:HG21  | 1.93                     | 0.47              |
| 1:C:708:GLY:HA2   | 1:C:737:HIS:O     | 2.14                     | 0.47              |
| 1:D:559:ILE:HD13  | 1:D:805:TYR:CG    | 2.49                     | 0.47              |
| 1:E:111:LYS:O     | 1:E:115:MET:HG2   | 2.14                     | 0.47              |
| 1:G:157:PRO:O     | 1:G:205:CYS:HB2   | 2.15                     | 0.47              |
| 1:G:509:GLY:HA3   | 1:G:605:ASN:O     | 2.14                     | 0.47              |
| 1:B:111:LYS:O     | 1:B:115:MET:HG2   | 2.14                     | 0.47              |
| 1:B:17:ILE:HA     | 1:B:20:MET:HG3    | 1.96                     | 0.47              |
| 1:B:651:TRP:CE2   | 1:B:920:GLN:HG3   | 2.50                     | 0.47              |
| 1:D:64:LEU:CD2    | 1:D:88:LEU:CD2    | 2.93                     | 0.47              |
| 1:E:213:GLU:O     | 1:E:229:GLU:HA    | 2.14                     | 0.47              |
| 1:F:540:ARG:O     | 1:F:542:ALA:N     | 2.45                     | 0.47              |
| 1:H:541:ASP:HA    | 1:H:544:GLN:HB3   | 1.96                     | 0.47              |
| 1:A:1041:VAL:HG11 | 1:A:1043:TYR:HE1  | 1.78                     | 0.47              |
| 1:D:70:ILE:HG21   | 1:D:101:GLU:HG3   | 1.96                     | 0.47              |
| 1:D:610:MET:HG2   | 1:D:640:VAL:HG11  | 1.96                     | 0.47              |
| 1:E:17:ILE:HA     | 1:E:20:MET:HG3    | 1.97                     | 0.47              |
| 1:E:4:ILE:HD12    | 1:E:319:ASP:OD1   | 2.14                     | 0.47              |
| 1:E:559:ILE:HD13  | 1:E:805:TYR:CG    | 2.50                     | 0.47              |
| 1:F:194:ALA:HB1   | 1:F:195:PHE:CE2   | 2.50                     | 0.47              |
| 1:G:300:THR:O     | 1:G:303:GLU:HB2   | 2.14                     | 0.47              |
| 1:G:708:GLY:HA2   | 1:G:737:HIS:O     | 2.14                     | 0.47              |
| 1:G:778:MET:HG3   | 1:G:779:THR:N     | 2.29                     | 0.47              |
| 1:H:473:ILE:O     | 1:H:477:THR:OG1   | 2.26                     | 0.47              |
| 1:H:619:GLY:HA3   | 1:H:623:TYR:HE2   | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1018:LEU:HD11 | 1:B:1024:LEU:HD11 | 1.96                     | 0.47              |
| 1:B:1041:VAL:HG22 | 1:B:1054:ASN:OD1  | 2.15                     | 0.47              |
| 1:B:622:ASN:ND2   | 1:B:917:GLU:O     | 2.47                     | 0.47              |
| 1:D:116:PHE:N     | 1:D:116:PHE:HD1   | 2.13                     | 0.47              |
| 1:D:546:LEU:HD11  | 1:D:774:SER:HB2   | 1.97                     | 0.47              |
| 1:E:1041:VAL:HG22 | 1:E:1054:ASN:OD1  | 2.15                     | 0.47              |
| 1:B:213:GLU:O     | 1:B:229:GLU:HA    | 2.14                     | 0.46              |
| 1:B:718:PRO:HG2   | 1:B:749:TYR:CD2   | 2.50                     | 0.46              |
| 1:E:651:TRP:CE2   | 1:E:920:GLN:HG3   | 2.50                     | 0.46              |
| 1:F:106:VAL:HG13  | 1:F:318:ALA:HB2   | 1.97                     | 0.46              |
| 1:G:1041:VAL:HG22 | 1:G:1054:ASN:OD1  | 2.15                     | 0.46              |
| 1:G:81:ILE:HG13   | 1:G:103:ILE:HG21  | 1.97                     | 0.46              |
| 1:G:90:GLU:HA     | 1:G:113:LEU:HD22  | 1.97                     | 0.46              |
| 1:H:116:PHE:N     | 1:H:116:PHE:HD1   | 2.13                     | 0.46              |
| 1:H:369:THR:O     | 1:H:376:LEU:HD11  | 2.15                     | 0.46              |
| 1:A:148:GLU:O     | 1:A:152:GLU:N     | 2.46                     | 0.46              |
| 1:C:106:VAL:HG13  | 1:C:318:ALA:HB2   | 1.97                     | 0.46              |
| 1:C:134:ILE:HD12  | 1:C:287:TYR:CB    | 2.45                     | 0.46              |
| 1:C:300:THR:O     | 1:C:303:GLU:HB2   | 2.14                     | 0.46              |
| 1:C:81:ILE:HG13   | 1:C:103:ILE:HG21  | 1.97                     | 0.46              |
| 1:D:300:THR:O     | 1:D:303:GLU:HB2   | 2.15                     | 0.46              |
| 1:D:369:THR:HG1   | 1:D:415:ASN:ND2   | 2.07                     | 0.46              |
| 1:G:134:ILE:HD12  | 1:G:287:TYR:CB    | 2.45                     | 0.46              |
| 1:A:513:ILE:HD12  | 1:A:513:ILE:N     | 2.30                     | 0.46              |
| 1:A:563:MET:CE    | 1:A:573:PHE:CE2   | 2.98                     | 0.46              |
| 1:A:847:VAL:HG11  | 1:A:889:GLN:OE1   | 2.15                     | 0.46              |
| 1:C:1041:VAL:HG22 | 1:C:1054:ASN:OD1  | 2.15                     | 0.46              |
| 1:C:42:PHE:HA     | 1:C:45:TYR:HD2    | 1.80                     | 0.46              |
| 1:D:82:HIS:CD2    | 1:D:84:GLY:H      | 2.25                     | 0.46              |
| 1:F:369:THR:O     | 1:F:376:LEU:HD11  | 2.14                     | 0.46              |
| 1:G:20:MET:HE3    | 1:G:43:HIS:O      | 2.15                     | 0.46              |
| 1:H:21:ARG:NH1    | 1:G:370:GLY:C     | 2.68                     | 0.46              |
| 1:H:509:GLY:HA3   | 1:H:605:ASN:O     | 2.16                     | 0.46              |
| 1:A:331:PRO:HB2   | 1:A:335:ASP:HB2   | 1.97                     | 0.46              |
| 1:B:70:ILE:HG21   | 1:B:101:GLU:HG3   | 1.98                     | 0.46              |
| 1:B:300:THR:O     | 1:B:303:GLU:HB2   | 2.15                     | 0.46              |
| 1:B:509:GLY:HA3   | 1:B:605:ASN:O     | 2.15                     | 0.46              |
| 1:C:20:MET:HE3    | 1:C:43:HIS:O      | 2.15                     | 0.46              |
| 1:D:631:PHE:C     | 1:D:631:PHE:CD2   | 2.89                     | 0.46              |
| 1:E:70:ILE:HG21   | 1:E:101:GLU:HG3   | 1.98                     | 0.46              |
| 1:F:21:ARG:HH12   | 1:E:370:GLY:C     | 2.19                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1041:VAL:CG1  | 1:F:1043:TYR:HE1  | 2.29                     | 0.46              |
| 1:G:3:ARG:CD      | 1:G:104:ILE:HD11  | 2.35                     | 0.46              |
| 1:G:106:VAL:HG13  | 1:G:318:ALA:HB2   | 1.97                     | 0.46              |
| 1:H:405:PHE:C     | 1:H:405:PHE:CD2   | 2.89                     | 0.46              |
| 1:B:540:ARG:HA    | 1:B:543:HIS:NE2   | 2.31                     | 0.46              |
| 1:F:1010:LEU:HD21 | 1:F:1031:ILE:CD1  | 2.42                     | 0.46              |
| 1:F:513:ILE:N     | 1:F:513:ILE:HD12  | 2.30                     | 0.46              |
| 1:F:559:ILE:HD13  | 1:F:805:TYR:CG    | 2.51                     | 0.46              |
| 1:F:620:TYR:CD2   | 1:F:621:LYS:HB3   | 2.51                     | 0.46              |
| 1:F:847:VAL:HG11  | 1:F:889:GLN:OE1   | 2.16                     | 0.46              |
| 1:H:106:VAL:HG13  | 1:H:318:ALA:HB2   | 1.97                     | 0.46              |
| 1:H:319:ASP:OD2   | 1:H:321:TYR:HE2   | 1.99                     | 0.46              |
| 1:B:81:ILE:HG13   | 1:B:103:ILE:HG21  | 1.96                     | 0.46              |
| 1:D:847:VAL:HG11  | 1:D:889:GLN:OE1   | 2.15                     | 0.46              |
| 1:E:369:THR:O     | 1:E:376:LEU:HD11  | 2.16                     | 0.46              |
| 1:E:718:PRO:HG2   | 1:E:749:TYR:CD2   | 2.50                     | 0.46              |
| 1:H:70:ILE:HG21   | 1:H:101:GLU:HG3   | 1.97                     | 0.46              |
| 1:A:540:ARG:O     | 1:A:542:ALA:N     | 2.45                     | 0.46              |
| 1:B:778:MET:HG3   | 1:B:779:THR:N     | 2.30                     | 0.46              |
| 1:C:546:LEU:HD11  | 1:C:774:SER:HB2   | 1.97                     | 0.46              |
| 1:D:319:ASP:OD2   | 1:D:321:TYR:HE2   | 1.99                     | 0.46              |
| 1:D:509:GLY:HA3   | 1:D:605:ASN:O     | 2.16                     | 0.46              |
| 1:E:177:LYS:O     | 1:E:178:GLU:CB    | 2.62                     | 0.46              |
| 1:E:300:THR:O     | 1:E:303:GLU:HB2   | 2.15                     | 0.46              |
| 1:E:82:HIS:CD2    | 1:E:84:GLY:H      | 2.24                     | 0.46              |
| 1:F:331:PRO:HB2   | 1:F:335:ASP:HB2   | 1.98                     | 0.46              |
| 1:A:106:VAL:HG13  | 1:A:318:ALA:HB2   | 1.98                     | 0.46              |
| 1:A:369:THR:O     | 1:A:376:LEU:HD11  | 2.15                     | 0.46              |
| 1:A:68:ASN:O      | 1:A:72:ILE:HG13   | 2.16                     | 0.46              |
| 1:A:546:LEU:HD11  | 1:A:774:SER:HB2   | 1.98                     | 0.46              |
| 1:D:304:MET:HE2   | 1:D:399:CYS:CB    | 2.46                     | 0.46              |
| 1:D:81:ILE:HG13   | 1:D:103:ILE:HG21  | 1.98                     | 0.46              |
| 1:F:546:LEU:HD11  | 1:F:774:SER:HB2   | 1.98                     | 0.46              |
| 1:F:68:ASN:O      | 1:F:72:ILE:HG13   | 2.16                     | 0.46              |
| 1:H:215:GLN:C     | 1:H:216:ILE:HD12  | 2.36                     | 0.46              |
| 1:A:1018:LEU:HD11 | 1:A:1024:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:794:LEU:HD12  | 1:A:795:ASP:O     | 2.16                     | 0.46              |
| 1:A:893:SER:O     | 1:A:897:VAL:HG13  | 2.16                     | 0.46              |
| 1:A:996:VAL:O     | 1:A:997:THR:C     | 2.54                     | 0.46              |
| 1:B:369:THR:O     | 1:B:376:LEU:HD11  | 2.16                     | 0.46              |
| 1:D:619:GLY:HA3   | 1:D:623:TYR:HE2   | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:266:MET:CE    | 1:E:277:VAL:CG2   | 2.94                     | 0.46              |
| 1:E:546:LEU:HD11  | 1:E:774:SER:HB2   | 1.97                     | 0.46              |
| 1:E:622:ASN:ND2   | 1:E:917:GLU:O     | 2.48                     | 0.46              |
| 1:F:794:LEU:HD12  | 1:F:795:ASP:O     | 2.16                     | 0.46              |
| 1:G:576:TRP:CD1   | 1:G:596:LEU:HD22  | 2.51                     | 0.46              |
| 1:H:81:ILE:HG13   | 1:H:103:ILE:HG21  | 1.98                     | 0.46              |
| 1:H:541:ASP:OD2   | 1:H:739:HIS:HE1   | 1.99                     | 0.46              |
| 1:A:620:TYR:CD2   | 1:A:621:LYS:HB3   | 2.51                     | 0.46              |
| 1:C:304:MET:HE2   | 1:C:399:CYS:HB2   | 1.98                     | 0.46              |
| 1:D:257:ARG:NH2   | 1:D:284:ASP:O     | 2.49                     | 0.46              |
| 1:D:541:ASP:OD2   | 1:D:739:HIS:HE1   | 1.99                     | 0.46              |
| 1:D:533:LEU:O     | 1:D:761:ILE:HA    | 2.15                     | 0.46              |
| 1:D:898:TYR:HD1   | 1:D:928:LYS:HE2   | 1.77                     | 0.46              |
| 1:F:1018:LEU:HD11 | 1:F:1024:LEU:HD11 | 1.97                     | 0.46              |
| 1:H:177:LYS:CG    | 1:H:178:GLU:H     | 2.25                     | 0.46              |
| 1:H:280:LEU:HG    | 1:H:289:ILE:HG12  | 1.98                     | 0.46              |
| 1:A:541:ASP:OD2   | 1:A:739:HIS:HE1   | 1.98                     | 0.45              |
| 1:B:288:PHE:CD1   | 1:B:289:ILE:N     | 2.84                     | 0.45              |
| 1:C:369:THR:O     | 1:C:376:LEU:HD11  | 2.16                     | 0.45              |
| 1:D:12:ARG:HH12   | 1:D:391:TYR:HB2   | 1.81                     | 0.45              |
| 1:D:106:VAL:HG13  | 1:D:318:ALA:HB2   | 1.97                     | 0.45              |
| 1:E:778:MET:HG3   | 1:E:779:THR:N     | 2.31                     | 0.45              |
| 1:F:156:TYR:CB    | 1:F:157:PRO:HD3   | 2.46                     | 0.45              |
| 1:G:226:HIS:ND1   | 1:G:259:CYS:HB3   | 2.31                     | 0.45              |
| 1:G:546:LEU:HD11  | 1:G:774:SER:HB2   | 1.97                     | 0.45              |
| 1:A:610:MET:HG2   | 1:A:640:VAL:HG11  | 1.97                     | 0.45              |
| 1:B:266:MET:CE    | 1:B:277:VAL:CG2   | 2.94                     | 0.45              |
| 1:B:278:GLU:O     | 1:B:289:ILE:HG12  | 2.16                     | 0.45              |
| 1:B:134:ILE:CD1   | 1:B:287:TYR:CB    | 2.95                     | 0.45              |
| 1:B:68:ASN:O      | 1:B:72:ILE:HG13   | 2.16                     | 0.45              |
| 1:C:559:ILE:HD13  | 1:C:805:TYR:CG    | 2.51                     | 0.45              |
| 1:E:155:GLY:O     | 1:E:158:LEU:HD21  | 2.15                     | 0.45              |
| 1:E:209:PRO:CG    | 1:E:280:LEU:HD23  | 2.47                     | 0.45              |
| 1:F:148:GLU:O     | 1:F:152:GLU:N     | 2.47                     | 0.45              |
| 1:G:160:ILE:HG22  | 1:G:200:VAL:HG11  | 1.97                     | 0.45              |
| 1:G:369:THR:O     | 1:G:376:LEU:HD11  | 2.16                     | 0.45              |
| 1:H:3:ARG:CD      | 1:H:104:ILE:HD11  | 2.35                     | 0.45              |
| 1:H:12:ARG:HH12   | 1:H:391:TYR:HB2   | 1.82                     | 0.45              |
| 1:H:847:VAL:HG11  | 1:H:889:GLN:OE1   | 2.15                     | 0.45              |
| 1:A:778:MET:HG3   | 1:A:779:THR:N     | 2.31                     | 0.45              |
| 1:B:448:SER:O     | 1:B:452:THR:HG23  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1018:LEU:HD11 | 1:C:1024:LEU:HD11 | 1.97                     | 0.45              |
| 1:D:450:ILE:HG22  | 1:D:451:ASP:N     | 2.31                     | 0.45              |
| 1:E:257:ARG:NH2   | 1:E:284:ASP:O     | 2.49                     | 0.45              |
| 1:E:437:HIS:CD2   | 1:E:439:ASP:N     | 2.73                     | 0.45              |
| 1:F:17:ILE:HA     | 1:F:20:MET:HG3    | 1.98                     | 0.45              |
| 1:F:610:MET:HG2   | 1:F:640:VAL:HG11  | 1.97                     | 0.45              |
| 1:G:365:THR:HG21  | 1:G:1051:ARG:CD   | 2.43                     | 0.45              |
| 1:G:559:ILE:HD13  | 1:G:805:TYR:CG    | 2.51                     | 0.45              |
| 1:H:64:LEU:HD23   | 1:H:88:LEU:CD2    | 2.45                     | 0.45              |
| 1:H:766:SER:O     | 1:H:767:SER:C     | 2.55                     | 0.45              |
| 1:A:448:SER:O     | 1:A:452:THR:HG23  | 2.16                     | 0.45              |
| 1:A:673:ILE:HG21  | 1:A:695:MET:HE3   | 1.98                     | 0.45              |
| 1:B:354:ASN:ND2   | 1:B:357:MET:HB3   | 2.31                     | 0.45              |
| 1:C:160:ILE:HG22  | 1:C:200:VAL:HG11  | 1.98                     | 0.45              |
| 1:C:331:PRO:HB2   | 1:C:335:ASP:HB2   | 1.98                     | 0.45              |
| 1:E:253:GLU:OE2   | 1:E:257:ARG:NH1   | 2.50                     | 0.45              |
| 1:E:278:GLU:O     | 1:E:289:ILE:HG12  | 2.16                     | 0.45              |
| 1:F:563:MET:CE    | 1:F:573:PHE:CE2   | 2.99                     | 0.45              |
| 1:F:70:ILE:HG21   | 1:F:101:GLU:HG3   | 1.99                     | 0.45              |
| 1:F:893:SER:O     | 1:F:897:VAL:HG13  | 2.17                     | 0.45              |
| 1:G:164:LEU:HD22  | 1:G:195:PHE:CE1   | 2.50                     | 0.45              |
| 1:G:331:PRO:HB2   | 1:G:335:ASP:HB2   | 1.98                     | 0.45              |
| 1:G:68:ASN:O      | 1:G:72:ILE:HG13   | 2.16                     | 0.45              |
| 1:H:257:ARG:NH2   | 1:H:284:ASP:O     | 2.49                     | 0.45              |
| 1:H:847:VAL:HG12  | 1:H:847:VAL:O     | 2.17                     | 0.45              |
| 1:B:257:ARG:NH2   | 1:B:284:ASP:O     | 2.49                     | 0.45              |
| 1:B:752:ALA:CB    | 1:C:749:TYR:CZ    | 3.00                     | 0.45              |
| 1:D:280:LEU:HG    | 1:D:289:ILE:HG12  | 1.99                     | 0.45              |
| 1:D:68:ASN:O      | 1:D:72:ILE:HG13   | 2.16                     | 0.45              |
| 1:D:996:VAL:O     | 1:D:997:THR:C     | 2.54                     | 0.45              |
| 1:E:684:ARG:HH11  | 1:E:684:ARG:HA    | 1.82                     | 0.45              |
| 1:E:68:ASN:O      | 1:E:72:ILE:HG13   | 2.16                     | 0.45              |
| 1:E:81:ILE:HG13   | 1:E:103:ILE:HG21  | 1.97                     | 0.45              |
| 1:H:472:TYR:OH    | 1:H:1004:PHE:O    | 2.27                     | 0.45              |
| 1:H:1018:LEU:HD11 | 1:H:1024:LEU:HD11 | 1.97                     | 0.45              |
| 1:H:778:MET:HG3   | 1:H:779:THR:N     | 2.32                     | 0.45              |
| 1:H:930:GLN:O     | 1:H:934:LEU:HG    | 2.16                     | 0.45              |
| 1:A:1041:VAL:CG1  | 1:A:1043:TYR:HE1  | 2.30                     | 0.45              |
| 1:A:657:VAL:HG22  | 1:A:943:ARG:CZ    | 2.47                     | 0.45              |
| 1:B:228:PHE:CD1   | 1:B:228:PHE:N     | 2.85                     | 0.45              |
| 1:C:448:SER:O     | 1:C:452:THR:HG23  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3:ARG:CD      | 1:D:104:ILE:HD11  | 2.35                     | 0.45              |
| 1:F:288:PHE:C     | 1:F:288:PHE:CD1   | 2.90                     | 0.45              |
| 1:F:405:PHE:C     | 1:F:405:PHE:CD2   | 2.89                     | 0.45              |
| 1:F:541:ASP:OD2   | 1:F:739:HIS:HE1   | 1.99                     | 0.45              |
| 1:G:134:ILE:CG2   | 1:G:203:GLU:HB3   | 2.47                     | 0.45              |
| 1:G:144:ILE:HG23  | 1:G:184:PHE:HD2   | 1.80                     | 0.45              |
| 1:G:996:VAL:O     | 1:G:997:THR:C     | 2.54                     | 0.45              |
| 1:H:17:ILE:O      | 1:H:21:ARG:HG3    | 2.17                     | 0.45              |
| 1:H:68:ASN:O      | 1:H:72:ILE:HG13   | 2.16                     | 0.45              |
| 1:H:533:LEU:O     | 1:H:761:ILE:HA    | 2.15                     | 0.45              |
| 1:H:653:LYS:O     | 1:H:943:ARG:HD3   | 2.15                     | 0.45              |
| 1:A:960:LEU:CD2   | 1:A:964:MET:HB2   | 2.46                     | 0.45              |
| 1:B:253:GLU:OE2   | 1:B:257:ARG:NH1   | 2.50                     | 0.45              |
| 1:B:546:LEU:HD11  | 1:B:774:SER:HB2   | 1.98                     | 0.45              |
| 1:D:1018:LEU:HD11 | 1:D:1024:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:653:LYS:O     | 1:D:943:ARG:HD3   | 2.15                     | 0.45              |
| 1:D:930:GLN:O     | 1:D:934:LEU:HG    | 2.17                     | 0.45              |
| 1:E:448:SER:O     | 1:E:452:THR:HG23  | 2.17                     | 0.45              |
| 1:F:160:ILE:HG22  | 1:F:200:VAL:HG11  | 1.98                     | 0.45              |
| 1:F:450:ILE:HG22  | 1:F:451:ASP:N     | 2.29                     | 0.45              |
| 1:G:1018:LEU:HD11 | 1:G:1024:LEU:HD11 | 1.98                     | 0.45              |
| 1:G:352:PRO:HA    | 1:G:356:PHE:CE1   | 2.52                     | 0.45              |
| 1:A:1010:LEU:HD21 | 1:A:1031:ILE:CD1  | 2.44                     | 0.45              |
| 1:A:300:THR:O     | 1:A:303:GLU:HB2   | 2.16                     | 0.45              |
| 1:A:304:MET:HE2   | 1:A:399:CYS:CB    | 2.47                     | 0.45              |
| 1:B:437:HIS:CD2   | 1:B:439:ASP:N     | 2.73                     | 0.45              |
| 1:B:543:HIS:ND1   | 1:B:551:VAL:HB    | 2.31                     | 0.45              |
| 1:C:368:SER:HA    | 1:C:419:PHE:CE1   | 2.52                     | 0.45              |
| 1:C:794:LEU:HD12  | 1:C:795:ASP:O     | 2.17                     | 0.45              |
| 1:D:847:VAL:HG12  | 1:D:847:VAL:O     | 2.17                     | 0.45              |
| 1:F:44:ARG:HD3    | 1:F:45:TYR:CE1    | 2.51                     | 0.45              |
| 1:F:502:TYR:HD1   | 1:F:503:GLY:N     | 2.14                     | 0.45              |
| 1:F:673:ILE:HG21  | 1:F:695:MET:HE3   | 1.98                     | 0.45              |
| 1:A:257:ARG:NH2   | 1:A:284:ASP:O     | 2.50                     | 0.45              |
| 1:B:619:GLY:HA3   | 1:B:623:TYR:HE2   | 1.80                     | 0.45              |
| 1:C:576:TRP:CD1   | 1:C:596:LEU:HD22  | 2.52                     | 0.45              |
| 1:D:64:LEU:HD23   | 1:D:88:LEU:CD2    | 2.45                     | 0.45              |
| 1:E:352:PRO:HA    | 1:E:356:PHE:CE1   | 2.51                     | 0.45              |
| 1:F:657:VAL:HG22  | 1:F:943:ARG:CZ    | 2.47                     | 0.45              |
| 1:F:960:LEU:CD2   | 1:F:964:MET:HB2   | 2.46                     | 0.45              |
| 1:A:131:ILE:O     | 1:A:131:ILE:HG12  | 2.14                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:44:ARG:HD3    | 1:A:45:TYR:CE1   | 2.52                     | 0.45              |
| 1:A:450:ILE:HG22  | 1:A:451:ASP:N    | 2.30                     | 0.45              |
| 1:B:367:ARG:NH1   | 1:B:1049:GLN:HB2 | 2.31                     | 0.45              |
| 1:B:510:THR:OG1   | 1:B:607:MET:SD   | 2.73                     | 0.45              |
| 1:C:257:ARG:NH2   | 1:C:284:ASP:O    | 2.49                     | 0.45              |
| 1:D:1041:VAL:HG22 | 1:D:1054:ASN:OD1 | 2.17                     | 0.45              |
| 1:D:118:ASP:OD2   | 1:D:120:ILE:HG13 | 2.17                     | 0.45              |
| 1:D:352:PRO:HA    | 1:D:356:PHE:CE1  | 2.51                     | 0.45              |
| 1:E:54:GLY:HA3    | 1:E:62:ALA:CB    | 2.47                     | 0.45              |
| 1:F:131:ILE:O     | 1:F:131:ILE:HG12 | 2.15                     | 0.45              |
| 1:F:253:GLU:OE2   | 1:F:257:ARG:NH1  | 2.50                     | 0.45              |
| 1:F:778:MET:HG3   | 1:F:779:THR:N    | 2.32                     | 0.45              |
| 1:G:368:SER:HA    | 1:G:419:PHE:CE1  | 2.52                     | 0.45              |
| 1:G:20:MET:HE1    | 1:G:43:HIS:O     | 2.15                     | 0.45              |
| 1:H:369:THR:HG1   | 1:H:415:ASN:ND2  | 2.10                     | 0.45              |
| 1:H:234:ILE:CD1   | 1:H:445:TYR:CZ   | 2.98                     | 0.45              |
| 1:H:693:LYS:HG2   | 1:H:731:THR:OG1  | 2.16                     | 0.45              |
| 1:H:996:VAL:O     | 1:H:997:THR:C    | 2.54                     | 0.45              |
| 1:A:70:ILE:HG21   | 1:A:101:GLU:HG3  | 1.99                     | 0.44              |
| 1:A:160:ILE:HG22  | 1:A:200:VAL:HG11 | 1.98                     | 0.44              |
| 1:B:996:VAL:O     | 1:B:997:THR:C    | 2.56                     | 0.44              |
| 1:C:134:ILE:CG2   | 1:C:203:GLU:HB3  | 2.47                     | 0.44              |
| 1:D:448:SER:O     | 1:D:452:THR:HG23 | 2.16                     | 0.44              |
| 1:E:42:PHE:HA     | 1:E:45:TYR:CD2   | 2.52                     | 0.44              |
| 1:F:257:ARG:NH2   | 1:F:284:ASP:O    | 2.50                     | 0.44              |
| 1:G:70:ILE:HG21   | 1:G:101:GLU:HG3  | 1.98                     | 0.44              |
| 1:H:414:ARG:NH1   | 1:G:21:ARG:HD3   | 2.32                     | 0.44              |
| 1:A:17:ILE:HA     | 1:A:20:MET:HG3   | 1.99                     | 0.44              |
| 1:A:253:GLU:OE2   | 1:A:257:ARG:NH1  | 2.50                     | 0.44              |
| 1:B:209:PRO:CG    | 1:B:280:LEU:HD23 | 2.48                     | 0.44              |
| 1:B:54:GLY:HA3    | 1:B:62:ALA:CB    | 2.48                     | 0.44              |
| 1:C:17:ILE:O      | 1:C:21:ARG:HG3   | 2.17                     | 0.44              |
| 1:C:352:PRO:HA    | 1:C:356:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:651:TRP:HE1   | 1:C:653:LYS:CB   | 2.31                     | 0.44              |
| 1:C:70:ILE:HG21   | 1:C:101:GLU:HG3  | 1.98                     | 0.44              |
| 1:E:331:PRO:HB2   | 1:E:335:ASP:HB2  | 1.97                     | 0.44              |
| 1:E:367:ARG:NH1   | 1:E:1049:GLN:HB2 | 2.31                     | 0.44              |
| 1:E:952:ASN:O     | 1:E:952:ASN:OD1  | 2.35                     | 0.44              |
| 1:F:448:SER:O     | 1:F:452:THR:HG23 | 2.17                     | 0.44              |
| 1:F:930:GLN:O     | 1:F:934:LEU:HG   | 2.17                     | 0.44              |
| 1:G:257:ARG:NH2   | 1:G:284:ASP:O    | 2.49                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:118:ASP:OD2   | 1:H:120:ILE:HG13  | 2.17                     | 0.44              |
| 1:H:718:PRO:HG2   | 1:H:749:TYR:CD2   | 2.52                     | 0.44              |
| 1:C:365:THR:HG21  | 1:C:1051:ARG:CD   | 2.45                     | 0.44              |
| 1:D:253:GLU:OE2   | 1:D:257:ARG:NH1   | 2.50                     | 0.44              |
| 1:F:319:ASP:OD2   | 1:F:321:TYR:HE2   | 2.00                     | 0.44              |
| 1:F:368:SER:HA    | 1:F:419:PHE:CE1   | 2.51                     | 0.44              |
| 1:G:741:HIS:CD2   | 1:G:775:GLN:HE21  | 2.36                     | 0.44              |
| 1:G:794:LEU:HD12  | 1:G:795:ASP:O     | 2.17                     | 0.44              |
| 1:H:448:SER:O     | 1:H:452:THR:HG23  | 2.16                     | 0.44              |
| 1:A:90:GLU:HA     | 1:A:113:LEU:HD22  | 2.00                     | 0.44              |
| 1:B:626:ASN:OD1   | 1:B:950:PRO:HB3   | 2.17                     | 0.44              |
| 1:C:68:ASN:O      | 1:C:72:ILE:HG13   | 2.17                     | 0.44              |
| 1:C:996:VAL:O     | 1:C:997:THR:C     | 2.55                     | 0.44              |
| 1:D:712:MET:N     | 1:D:712:MET:SD    | 2.89                     | 0.44              |
| 1:E:234:ILE:CD1   | 1:E:445:TYR:CZ    | 2.98                     | 0.44              |
| 1:E:626:ASN:OD1   | 1:E:950:PRO:HB3   | 2.17                     | 0.44              |
| 1:F:51:TYR:CE1    | 1:E:1021:GLY:HA2  | 2.50                     | 0.44              |
| 1:G:405:PHE:C     | 1:G:405:PHE:CD2   | 2.90                     | 0.44              |
| 1:H:1041:VAL:HG22 | 1:H:1054:ASN:OD1  | 2.17                     | 0.44              |
| 1:H:368:SER:HA    | 1:H:419:PHE:CE1   | 2.53                     | 0.44              |
| 1:H:427:ASN:ND2   | 1:H:431:LEU:HD11  | 2.31                     | 0.44              |
| 1:A:1014:ILE:HD12 | 1:A:1016:VAL:HG12 | 2.00                     | 0.44              |
| 1:A:509:GLY:N     | 1:A:605:ASN:HB2   | 2.33                     | 0.44              |
| 1:A:570:MET:HG3   | 1:A:573:PHE:CE1   | 2.52                     | 0.44              |
| 1:B:44:ARG:HD3    | 1:B:45:TYR:CE1    | 2.52                     | 0.44              |
| 1:B:821:ASN:N     | 1:B:821:ASN:OD1   | 2.49                     | 0.44              |
| 1:B:952:ASN:O     | 1:B:952:ASN:OD1   | 2.35                     | 0.44              |
| 1:C:718:PRO:HG2   | 1:C:749:TYR:CD2   | 2.52                     | 0.44              |
| 1:E:134:ILE:CD1   | 1:E:287:TYR:CB    | 2.96                     | 0.44              |
| 1:E:427:ASN:ND2   | 1:E:431:LEU:HD11  | 2.32                     | 0.44              |
| 1:E:619:GLY:HA3   | 1:E:623:TYR:HE2   | 1.81                     | 0.44              |
| 1:E:746:ASN:HD22  | 1:G:748:ILE:HG21  | 1.82                     | 0.44              |
| 1:H:300:THR:O     | 1:H:303:GLU:HB2   | 2.17                     | 0.44              |
| 1:C:12:ARG:NH2    | 1:C:391:TYR:CD2   | 2.85                     | 0.44              |
| 1:C:20:MET:HE1    | 1:C:43:HIS:O      | 2.16                     | 0.44              |
| 1:D:17:ILE:O      | 1:D:21:ARG:HG3    | 2.18                     | 0.44              |
| 1:D:693:LYS:HG2   | 1:D:731:THR:OG1   | 2.17                     | 0.44              |
| 1:F:1014:ILE:HD12 | 1:F:1016:VAL:HG12 | 2.00                     | 0.44              |
| 1:F:709:ILE:HB    | 1:F:738:LEU:HD12  | 1.99                     | 0.44              |
| 1:G:448:SER:O     | 1:G:452:THR:HG23  | 2.18                     | 0.44              |
| 1:G:519:PRO:CB    | 1:G:705:HIS:NE2   | 2.78                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:718:PRO:HG2  | 1:G:749:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:54:GLY:HA3   | 1:A:62:ALA:CB    | 2.48                     | 0.44              |
| 1:A:930:GLN:O    | 1:A:934:LEU:HG   | 2.17                     | 0.44              |
| 1:B:42:PHE:HA    | 1:B:45:TYR:CD2   | 2.53                     | 0.44              |
| 1:B:540:ARG:NH2  | 1:B:541:ASP:OD1  | 2.51                     | 0.44              |
| 1:B:631:PHE:C    | 1:B:631:PHE:CD2  | 2.91                     | 0.44              |
| 1:C:186:ARG:CZ   | 1:C:186:ARG:HB3  | 2.47                     | 0.44              |
| 1:E:156:TYR:N    | 1:E:157:PRO:CD   | 2.80                     | 0.44              |
| 1:E:1:MET:HE1    | 1:E:4:ILE:HB     | 2.00                     | 0.44              |
| 1:F:619:GLY:HA3  | 1:F:623:TYR:HE2  | 1.81                     | 0.44              |
| 1:F:679:ILE:CD1  | 1:F:724:LEU:HD13 | 2.44                     | 0.44              |
| 1:F:90:GLU:HA    | 1:F:113:LEU:HD22 | 2.00                     | 0.44              |
| 1:H:253:GLU:OE2  | 1:H:257:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:319:ASP:OD2  | 1:A:321:TYR:HE2  | 2.01                     | 0.44              |
| 1:A:234:ILE:CD1  | 1:A:445:TYR:CZ   | 2.99                     | 0.44              |
| 1:C:519:PRO:CB   | 1:C:705:HIS:NE2  | 2.78                     | 0.44              |
| 1:C:741:HIS:CD2  | 1:C:775:GLN:HE21 | 2.36                     | 0.44              |
| 1:C:992:LYS:HE3  | 1:C:993:TYR:CE2  | 2.53                     | 0.44              |
| 1:D:81:ILE:O     | 1:D:106:VAL:HG23 | 2.18                     | 0.44              |
| 1:D:234:ILE:CD1  | 1:D:445:TYR:CZ   | 2.99                     | 0.44              |
| 1:E:44:ARG:HD3   | 1:E:45:TYR:CE1   | 2.53                     | 0.44              |
| 1:E:996:VAL:O    | 1:E:997:THR:C    | 2.56                     | 0.44              |
| 1:F:17:ILE:O     | 1:F:21:ARG:HG3   | 2.17                     | 0.44              |
| 1:B:228:PHE:HD1  | 1:B:228:PHE:N    | 2.16                     | 0.44              |
| 1:B:684:ARG:HH11 | 1:B:684:ARG:HA   | 1.83                     | 0.44              |
| 1:D:279:PHE:C    | 1:D:289:ILE:HD11 | 2.38                     | 0.44              |
| 1:D:45:TYR:CD1   | 1:C:1047:ASN:CB  | 2.97                     | 0.44              |
| 1:E:147:VAL:HG11 | 1:E:180:VAL:HG11 | 2.00                     | 0.44              |
| 1:E:160:ILE:HD12 | 1:E:174:VAL:CG2  | 2.47                     | 0.44              |
| 1:E:369:THR:OG1  | 1:E:370:GLY:N    | 2.50                     | 0.44              |
| 1:F:847:VAL:O    | 1:F:847:VAL:HG12 | 2.17                     | 0.44              |
| 1:G:278:GLU:CB   | 1:G:289:ILE:CD1  | 2.96                     | 0.44              |
| 1:H:81:ILE:O     | 1:H:106:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:746:ASN:HD22 | 1:C:748:ILE:HG21 | 1.83                     | 0.43              |
| 1:D:1033:GLU:HG3 | 1:D:1034:PRO:HD2 | 2.00                     | 0.43              |
| 1:D:766:SER:O    | 1:D:767:SER:C    | 2.57                     | 0.43              |
| 1:D:969:THR:O    | 1:D:973:VAL:HG23 | 2.18                     | 0.43              |
| 1:F:570:MET:HG3  | 1:F:573:PHE:CE1  | 2.52                     | 0.43              |
| 1:F:673:ILE:HG21 | 1:F:695:MET:CE   | 2.48                     | 0.43              |
| 1:G:230:ARG:HD3  | 1:G:302:THR:OG1  | 2.18                     | 0.43              |
| 1:G:278:GLU:HB2  | 1:G:289:ILE:CD1  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:754:ALA:HB1  | 1:A:759:VAL:CG1  | 2.49                     | 0.43              |
| 1:A:847:VAL:HG12 | 1:A:847:VAL:O    | 2.17                     | 0.43              |
| 1:B:331:PRO:HB2  | 1:B:335:ASP:HB2  | 1.98                     | 0.43              |
| 1:C:288:PHE:C    | 1:C:288:PHE:CD1  | 2.91                     | 0.43              |
| 1:C:278:GLU:HB2  | 1:C:289:ILE:CD1  | 2.48                     | 0.43              |
| 1:D:898:TYR:HD1  | 1:D:928:LYS:HE3  | 1.81                     | 0.43              |
| 1:E:228:PHE:CD1  | 1:E:228:PHE:N    | 2.87                     | 0.43              |
| 1:F:300:THR:O    | 1:F:303:GLU:HB2  | 2.17                     | 0.43              |
| 1:F:54:GLY:HA3   | 1:F:62:ALA:CB    | 2.48                     | 0.43              |
| 1:G:288:PHE:CD1  | 1:G:288:PHE:C    | 2.91                     | 0.43              |
| 1:B:134:ILE:HG23 | 1:B:135:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:279:PHE:CA   | 1:C:289:ILE:HD11 | 2.48                     | 0.43              |
| 1:C:600:ARG:HG3  | 1:C:639:GLY:HA3  | 1.99                     | 0.43              |
| 1:E:349:THR:HG23 | 1:E:393:SER:HB2  | 2.00                     | 0.43              |
| 1:E:821:ASN:OD1  | 1:E:821:ASN:N    | 2.49                     | 0.43              |
| 1:G:712:MET:SD   | 1:G:712:MET:N    | 2.88                     | 0.43              |
| 1:H:279:PHE:C    | 1:H:289:ILE:HD11 | 2.38                     | 0.43              |
| 1:H:712:MET:SD   | 1:H:712:MET:N    | 2.90                     | 0.43              |
| 1:H:898:TYR:H    | 1:H:898:TYR:HD2  | 1.65                     | 0.43              |
| 1:A:17:ILE:O     | 1:A:21:ARG:HG3   | 2.18                     | 0.43              |
| 1:C:278:GLU:CB   | 1:C:289:ILE:CD1  | 2.96                     | 0.43              |
| 1:D:427:ASN:ND2  | 1:D:431:LEU:HD11 | 2.32                     | 0.43              |
| 1:F:234:ILE:CD1  | 1:F:445:TYR:CZ   | 2.99                     | 0.43              |
| 1:G:81:ILE:O     | 1:G:106:VAL:HG23 | 2.18                     | 0.43              |
| 1:H:741:HIS:CE1  | 1:H:775:GLN:NE2  | 2.86                     | 0.43              |
| 1:H:969:THR:O    | 1:H:973:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:673:ILE:HG21 | 1:A:695:MET:CE   | 2.49                     | 0.43              |
| 1:B:174:VAL:HG12 | 1:B:176:SER:H    | 1.83                     | 0.43              |
| 1:C:158:LEU:C    | 1:C:205:CYS:SG   | 2.97                     | 0.43              |
| 1:D:368:SER:HA   | 1:D:419:PHE:CE1  | 2.54                     | 0.43              |
| 1:D:709:ILE:HB   | 1:D:738:LEU:HD12 | 2.00                     | 0.43              |
| 1:E:847:VAL:HG12 | 1:E:847:VAL:O    | 2.18                     | 0.43              |
| 1:G:12:ARG:NH2   | 1:G:391:TYR:CD2  | 2.85                     | 0.43              |
| 1:G:620:TYR:CE1  | 1:G:978:LEU:O    | 2.72                     | 0.43              |
| 1:H:709:ILE:HB   | 1:H:738:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:1033:GLU:HG3 | 1:A:1034:PRO:HD2 | 2.00                     | 0.43              |
| 1:A:619:GLY:HA3  | 1:A:623:TYR:HE2  | 1.82                     | 0.43              |
| 1:B:352:PRO:HA   | 1:B:356:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:230:ARG:HD3  | 1:C:302:THR:OG1  | 2.19                     | 0.43              |
| 1:C:540:ARG:O    | 1:C:542:ALA:N    | 2.46                     | 0.43              |
| 1:C:54:GLY:HA3   | 1:C:62:ALA:CB    | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:847:VAL:CG1  | 1:E:889:GLN:OE1  | 2.67                     | 0.43              |
| 1:F:173:VAL:HG13 | 1:F:205:CYS:SG   | 2.58                     | 0.43              |
| 1:G:288:PHE:CE2  | 1:G:291:VAL:HG23 | 2.54                     | 0.43              |
| 1:G:600:ARG:HG3  | 1:G:639:GLY:HA3  | 1.99                     | 0.43              |
| 1:H:898:TYR:HD1  | 1:H:928:LYS:HE3  | 1.82                     | 0.43              |
| 1:A:368:SER:HA   | 1:A:419:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:81:ILE:HG13  | 1:A:103:ILE:HG21 | 2.00                     | 0.43              |
| 1:B:427:ASN:ND2  | 1:B:431:LEU:HD11 | 2.33                     | 0.43              |
| 1:B:234:ILE:CD1  | 1:B:445:TYR:CZ   | 2.99                     | 0.43              |
| 1:B:603:ILE:CG1  | 1:B:608:PHE:CZ   | 3.00                     | 0.43              |
| 1:C:288:PHE:CE2  | 1:C:291:VAL:HG23 | 2.54                     | 0.43              |
| 1:C:541:ASP:OD2  | 1:C:739:HIS:HE1  | 2.01                     | 0.43              |
| 1:E:17:ILE:O     | 1:E:21:ARG:HG3   | 2.18                     | 0.43              |
| 1:E:288:PHE:CD1  | 1:E:289:ILE:N    | 2.86                     | 0.43              |
| 1:E:288:PHE:CE2  | 1:E:291:VAL:HG23 | 2.53                     | 0.43              |
| 1:E:631:PHE:CD2  | 1:E:631:PHE:C    | 2.92                     | 0.43              |
| 1:G:279:PHE:CA   | 1:G:289:ILE:HD11 | 2.48                     | 0.43              |
| 1:G:54:GLY:HA3   | 1:G:62:ALA:CB    | 2.49                     | 0.43              |
| 1:H:174:VAL:HG12 | 1:H:176:SER:H    | 1.84                     | 0.43              |
| 1:H:519:PRO:HB2  | 1:H:705:HIS:CD2  | 2.53                     | 0.43              |
| 1:A:126:ALA:CB   | 1:A:131:ILE:HD11 | 2.48                     | 0.43              |
| 1:B:39:THR:HG22  | 1:B:44:ARG:HH21  | 1.82                     | 0.43              |
| 1:B:847:VAL:CG1  | 1:B:889:GLN:OE1  | 2.67                     | 0.43              |
| 1:C:44:ARG:HD3   | 1:C:45:TYR:CE1   | 2.53                     | 0.43              |
| 1:F:51:TYR:CD1   | 1:E:1021:GLY:HA2 | 2.54                     | 0.43              |
| 1:E:134:ILE:HG23 | 1:E:135:PRO:HD2  | 2.00                     | 0.43              |
| 1:E:603:ILE:CG1  | 1:E:608:PHE:CZ   | 3.00                     | 0.43              |
| 1:F:66:ILE:HG23  | 1:F:94:PHE:HD1   | 1.81                     | 0.43              |
| 1:G:540:ARG:O    | 1:G:542:ALA:N    | 2.46                     | 0.43              |
| 1:G:959:GLU:O    | 1:G:963:LYS:HG2  | 2.18                     | 0.43              |
| 1:H:8:LEU:CA     | 1:H:31:VAL:CG2   | 2.89                     | 0.43              |
| 1:H:600:ARG:HG3  | 1:H:639:GLY:HA3  | 2.00                     | 0.43              |
| 1:A:718:PRO:HG2  | 1:A:749:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:448:SER:O    | 1:B:452:THR:CG2  | 2.67                     | 0.43              |
| 1:B:82:HIS:HB2   | 1:B:106:VAL:HG21 | 2.00                     | 0.43              |
| 1:C:674:CYS:HB3  | 1:C:712:MET:HE1  | 2.01                     | 0.43              |
| 1:C:620:TYR:CE1  | 1:C:978:LEU:O    | 2.72                     | 0.43              |
| 1:D:54:GLY:HA3   | 1:D:62:ALA:CB    | 2.48                     | 0.43              |
| 1:D:718:PRO:HG2  | 1:D:749:TYR:CD2  | 2.53                     | 0.43              |
| 1:D:778:MET:HG3  | 1:D:779:THR:N    | 2.34                     | 0.43              |
| 1:D:841:GLN:HG2  | 1:D:853:TRP:CZ2  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:39:THR:HG22  | 1:E:44:ARG:HH21  | 1.82                     | 0.43              |
| 1:E:675:TYR:CE2  | 1:E:716:LEU:HD13 | 2.54                     | 0.43              |
| 1:F:126:ALA:CB   | 1:F:131:ILE:HD11 | 2.48                     | 0.43              |
| 1:F:81:ILE:HG13  | 1:F:103:ILE:HG21 | 2.00                     | 0.43              |
| 1:F:867:PHE:CD1  | 1:F:867:PHE:N    | 2.85                     | 0.43              |
| 1:A:563:MET:HB3  | 1:A:573:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:679:ILE:CD1  | 1:A:724:LEU:HD13 | 2.44                     | 0.43              |
| 1:B:847:VAL:O    | 1:B:847:VAL:HG12 | 2.19                     | 0.43              |
| 1:C:39:THR:HG22  | 1:C:44:ARG:HH21  | 1.83                     | 0.43              |
| 1:D:39:THR:HG22  | 1:D:44:ARG:HH21  | 1.84                     | 0.43              |
| 1:D:898:TYR:H    | 1:D:898:TYR:HD2  | 1.65                     | 0.43              |
| 1:F:50:ALA:O     | 1:E:1021:GLY:O   | 2.37                     | 0.43              |
| 1:F:209:PRO:HB2  | 1:F:280:LEU:HD22 | 2.01                     | 0.43              |
| 1:G:541:ASP:OD2  | 1:G:739:HIS:HE1  | 2.02                     | 0.43              |
| 1:G:992:LYS:HE3  | 1:G:993:TYR:CE2  | 2.54                     | 0.43              |
| 1:H:45:TYR:CD1   | 1:G:1047:ASN:CB  | 2.99                     | 0.43              |
| 1:H:674:CYS:HB3  | 1:H:712:MET:HE1  | 2.01                     | 0.43              |
| 1:A:288:PHE:CD1  | 1:A:288:PHE:C    | 2.92                     | 0.42              |
| 1:A:405:PHE:CD2  | 1:A:405:PHE:C    | 2.91                     | 0.42              |
| 1:A:519:PRO:HB2  | 1:A:705:HIS:CD2  | 2.54                     | 0.42              |
| 1:A:563:MET:HE1  | 1:A:573:PHE:CE2  | 2.52                     | 0.42              |
| 1:A:867:PHE:N    | 1:A:867:PHE:CD1  | 2.86                     | 0.42              |
| 1:B:405:PHE:C    | 1:B:405:PHE:CD2  | 2.92                     | 0.42              |
| 1:B:464:ASP:CG   | 1:B:467:THR:OG1  | 2.58                     | 0.42              |
| 1:B:718:PRO:CG   | 1:B:749:TYR:CD2  | 3.02                     | 0.42              |
| 1:C:348:THR:HG22 | 1:C:394:LEU:HA   | 2.01                     | 0.42              |
| 1:C:427:ASN:ND2  | 1:C:431:LEU:HD11 | 2.34                     | 0.42              |
| 1:C:712:MET:N    | 1:C:712:MET:SD   | 2.89                     | 0.42              |
| 1:C:959:GLU:O    | 1:C:963:LYS:HG2  | 2.19                     | 0.42              |
| 1:E:448:SER:O    | 1:E:452:THR:CG2  | 2.67                     | 0.42              |
| 1:E:82:HIS:HB2   | 1:E:106:VAL:HG21 | 2.00                     | 0.42              |
| 1:F:304:MET:HE2  | 1:F:399:CYS:CB   | 2.49                     | 0.42              |
| 1:F:519:PRO:HB2  | 1:F:705:HIS:CD2  | 2.54                     | 0.42              |
| 1:F:754:ALA:HB1  | 1:F:759:VAL:CG1  | 2.49                     | 0.42              |
| 1:H:1033:GLU:HG3 | 1:H:1034:PRO:HD2 | 2.01                     | 0.42              |
| 1:H:39:THR:HG22  | 1:H:44:ARG:HH21  | 1.84                     | 0.42              |
| 1:H:54:GLY:HA3   | 1:H:62:ALA:CB    | 2.49                     | 0.42              |
| 1:H:631:PHE:O    | 1:H:635:SER:OG   | 2.37                     | 0.42              |
| 1:H:867:PHE:N    | 1:H:867:PHE:CD1  | 2.85                     | 0.42              |
| 1:A:209:PRO:HB2  | 1:A:280:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:620:TYR:HD1  | 1:A:979:TYR:CE1  | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:672:ALA:HA    | 1:A:708:GLY:O     | 2.20                     | 0.42              |
| 1:A:709:ILE:HB    | 1:A:738:LEU:HD12  | 1.99                     | 0.42              |
| 1:A:969:THR:O     | 1:A:973:VAL:HG23  | 2.19                     | 0.42              |
| 1:B:288:PHE:CE2   | 1:B:291:VAL:HG23  | 2.54                     | 0.42              |
| 1:B:349:THR:HG23  | 1:B:393:SER:HB2   | 2.01                     | 0.42              |
| 1:B:540:ARG:HH21  | 1:B:541:ASP:CG    | 2.23                     | 0.42              |
| 1:C:1014:ILE:HD12 | 1:C:1016:VAL:HG12 | 2.01                     | 0.42              |
| 1:C:134:ILE:HG23  | 1:C:135:PRO:HD2   | 1.99                     | 0.42              |
| 1:E:464:ASP:CG    | 1:E:467:THR:OG1   | 2.58                     | 0.42              |
| 1:E:712:MET:SD    | 1:E:712:MET:N     | 2.89                     | 0.42              |
| 1:F:1033:GLU:HG3  | 1:F:1034:PRO:HD2  | 2.01                     | 0.42              |
| 1:F:39:THR:HG22   | 1:F:44:ARG:HH21   | 1.84                     | 0.42              |
| 1:F:500:ILE:HG22  | 1:F:501:PRO:O     | 2.19                     | 0.42              |
| 1:H:278:GLU:C     | 1:H:289:ILE:HD11  | 2.40                     | 0.42              |
| 1:A:81:ILE:O      | 1:A:106:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:39:THR:HG22   | 1:A:44:ARG:HH21   | 1.84                     | 0.42              |
| 1:B:712:MET:SD    | 1:B:712:MET:N     | 2.89                     | 0.42              |
| 1:D:278:GLU:C     | 1:D:289:ILE:HD11  | 2.40                     | 0.42              |
| 1:D:600:ARG:HG3   | 1:D:639:GLY:HA3   | 2.01                     | 0.42              |
| 1:E:600:ARG:HG3   | 1:E:639:GLY:HA3   | 2.01                     | 0.42              |
| 1:F:134:ILE:HG23  | 1:F:135:PRO:HD2   | 2.01                     | 0.42              |
| 1:F:969:THR:O     | 1:F:973:VAL:HG23  | 2.19                     | 0.42              |
| 1:G:1014:ILE:HD12 | 1:G:1016:VAL:HG12 | 2.01                     | 0.42              |
| 1:G:674:CYS:HB3   | 1:G:712:MET:HE1   | 2.01                     | 0.42              |
| 1:H:21:ARG:CZ     | 1:G:418:GLU:OE2   | 2.68                     | 0.42              |
| 1:A:134:ILE:HG23  | 1:A:135:PRO:HD2   | 2.01                     | 0.42              |
| 1:C:144:ILE:HA    | 1:C:184:PHE:CE2   | 2.54                     | 0.42              |
| 1:C:81:ILE:O      | 1:C:106:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:463:ARG:HG3   | 1:D:468:LYS:HE3   | 2.02                     | 0.42              |
| 1:D:519:PRO:HB2   | 1:D:705:HIS:CD2   | 2.54                     | 0.42              |
| 1:E:228:PHE:N     | 1:E:228:PHE:HD1   | 2.18                     | 0.42              |
| 1:E:490:PRO:HD2   | 1:E:492:TYR:CE2   | 2.54                     | 0.42              |
| 1:F:428:ILE:HB    | 1:F:429:PRO:HD3   | 2.01                     | 0.42              |
| 1:F:563:MET:HB3   | 1:F:573:PHE:CE2   | 2.54                     | 0.42              |
| 1:G:304:MET:CE    | 1:G:399:CYS:CB    | 2.98                     | 0.42              |
| 1:G:44:ARG:HD3    | 1:G:45:TYR:CE1    | 2.54                     | 0.42              |
| 1:H:134:ILE:HG21  | 1:H:203:GLU:HB2   | 2.01                     | 0.42              |
| 1:D:680:ASP:HB3   | 1:A:787:ASN:ND2   | 2.35                     | 0.42              |
| 1:B:600:ARG:HG3   | 1:B:639:GLY:HA3   | 2.01                     | 0.42              |
| 1:B:674:CYS:HB3   | 1:B:712:MET:HE1   | 2.00                     | 0.42              |
| 1:B:675:TYR:CE2   | 1:B:716:LEU:HD13  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:754:ALA:HB1  | 1:B:759:VAL:CG1  | 2.49                     | 0.42              |
| 1:C:509:GLY:N    | 1:C:605:ASN:HB2  | 2.34                     | 0.42              |
| 1:D:8:LEU:CA     | 1:D:31:VAL:CG2   | 2.89                     | 0.42              |
| 1:D:741:HIS:CE1  | 1:D:775:GLN:NE2  | 2.87                     | 0.42              |
| 1:E:373:GLY:O    | 1:E:400:THR:HA   | 2.19                     | 0.42              |
| 1:F:81:ILE:O     | 1:F:106:VAL:HG23 | 2.19                     | 0.42              |
| 1:F:620:TYR:HD1  | 1:F:979:TYR:CE1  | 2.38                     | 0.42              |
| 1:F:713:ALA:HB3  | 1:F:715:LEU:HD12 | 1.99                     | 0.42              |
| 1:G:1033:GLU:HG3 | 1:G:1034:PRO:HD2 | 2.00                     | 0.42              |
| 1:G:17:ILE:O     | 1:G:21:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:288:PHE:CE2  | 1:A:291:VAL:HG23 | 2.55                     | 0.42              |
| 1:A:519:PRO:CB   | 1:A:705:HIS:NE2  | 2.80                     | 0.42              |
| 1:B:365:THR:CG2  | 1:B:1050:PRO:O   | 2.67                     | 0.42              |
| 1:B:862:VAL:O    | 1:B:866:MET:N    | 2.52                     | 0.42              |
| 1:D:754:ALA:HB1  | 1:D:759:VAL:CG1  | 2.49                     | 0.42              |
| 1:D:898:TYR:CD1  | 1:D:928:LYS:CE   | 2.99                     | 0.42              |
| 1:E:348:THR:HG22 | 1:E:394:LEU:HA   | 2.01                     | 0.42              |
| 1:E:304:MET:HE2  | 1:E:399:CYS:CB   | 2.49                     | 0.42              |
| 1:E:718:PRO:CG   | 1:E:749:TYR:CD2  | 3.02                     | 0.42              |
| 1:F:718:PRO:HG2  | 1:F:749:TYR:CD2  | 2.54                     | 0.42              |
| 1:H:680:ASP:HB3  | 1:F:787:ASN:ND2  | 2.35                     | 0.42              |
| 1:H:115:MET:CG   | 1:H:125:GLN:HG3  | 2.48                     | 0.42              |
| 1:C:448:SER:O    | 1:C:452:THR:CG2  | 2.67                     | 0.42              |
| 1:C:586:ARG:NH1  | 1:C:586:ARG:HB2  | 2.34                     | 0.42              |
| 1:D:631:PHE:O    | 1:D:635:SER:OG   | 2.38                     | 0.42              |
| 1:D:867:PHE:N    | 1:D:867:PHE:CD1  | 2.86                     | 0.42              |
| 1:E:144:ILE:HD12 | 1:E:145:LYS:H    | 1.83                     | 0.42              |
| 1:E:304:MET:CE   | 1:E:399:CYS:HB2  | 2.49                     | 0.42              |
| 1:E:862:VAL:O    | 1:E:866:MET:N    | 2.52                     | 0.42              |
| 1:F:288:PHE:CE2  | 1:F:291:VAL:HG23 | 2.55                     | 0.42              |
| 1:G:134:ILE:HG23 | 1:G:135:PRO:HD2  | 1.99                     | 0.42              |
| 1:G:348:THR:HG22 | 1:G:394:LEU:HA   | 2.02                     | 0.42              |
| 1:E:828:TYR:CE2  | 1:G:783:TYR:HB3  | 2.54                     | 0.42              |
| 1:H:224:ILE:HG22 | 1:H:263:VAL:HG13 | 2.02                     | 0.42              |
| 1:H:41:SER:OG    | 1:H:43:HIS:HD2   | 2.02                     | 0.42              |
| 1:A:161:LYS:HB2  | 1:A:201:TYR:CE2  | 2.54                     | 0.42              |
| 1:A:427:ASN:ND2  | 1:A:431:LEU:HD11 | 2.35                     | 0.42              |
| 1:C:217:LEU:HD12 | 1:C:227:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:828:TYR:CE2  | 1:C:783:TYR:HB3  | 2.54                     | 0.42              |
| 1:G:304:MET:CE   | 1:G:399:CYS:HB2  | 2.49                     | 0.42              |
| 1:G:39:THR:HG22  | 1:G:44:ARG:HH21  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:1014:ILE:HD12 | 1:H:1016:VAL:HG12 | 2.01                     | 0.42              |
| 1:H:209:PRO:HB2   | 1:H:280:LEU:HD22  | 2.01                     | 0.42              |
| 1:H:519:PRO:CB    | 1:H:705:HIS:NE2   | 2.80                     | 0.42              |
| 1:H:754:ALA:HB1   | 1:H:759:VAL:CG1   | 2.49                     | 0.42              |
| 1:A:157:PRO:C     | 1:A:205:CYS:HB2   | 2.40                     | 0.42              |
| 1:A:428:ILE:HB    | 1:A:429:PRO:HD3   | 2.02                     | 0.42              |
| 1:A:448:SER:O     | 1:A:452:THR:CG2   | 2.68                     | 0.42              |
| 1:B:17:ILE:O      | 1:B:21:ARG:HG3    | 2.19                     | 0.42              |
| 1:B:490:PRO:HD2   | 1:B:492:TYR:CE2   | 2.55                     | 0.42              |
| 1:C:304:MET:CE    | 1:C:399:CYS:HB2   | 2.49                     | 0.42              |
| 1:D:134:ILE:HG21  | 1:D:203:GLU:HB2   | 2.02                     | 0.42              |
| 1:D:209:PRO:HB2   | 1:D:280:LEU:HD22  | 2.01                     | 0.42              |
| 1:E:754:ALA:HB1   | 1:E:759:VAL:CG1   | 2.49                     | 0.42              |
| 1:G:427:ASN:ND2   | 1:G:431:LEU:HD11  | 2.35                     | 0.42              |
| 1:H:898:TYR:CD1   | 1:H:928:LYS:CE    | 2.99                     | 0.42              |
| 1:A:66:ILE:HG23   | 1:A:94:PHE:HD1    | 1.83                     | 0.42              |
| 1:B:278:GLU:C     | 1:B:289:ILE:CG1   | 2.89                     | 0.42              |
| 1:B:348:THR:HG22  | 1:B:394:LEU:HA    | 2.02                     | 0.42              |
| 1:B:473:ILE:O     | 1:B:477:THR:OG1   | 2.26                     | 0.42              |
| 1:D:224:ILE:HG22  | 1:D:263:VAL:HG13  | 2.02                     | 0.42              |
| 1:E:42:PHE:HA     | 1:E:45:TYR:HD2    | 1.83                     | 0.42              |
| 1:F:161:LYS:HB2   | 1:F:201:TYR:CE2   | 2.54                     | 0.42              |
| 1:F:563:MET:HE1   | 1:F:573:PHE:CE2   | 2.53                     | 0.42              |
| 1:F:82:HIS:CD2    | 1:F:84:GLY:H      | 2.26                     | 0.42              |
| 1:H:198:ASP:N     | 1:H:198:ASP:OD1   | 2.53                     | 0.42              |
| 1:A:63:TYR:HB2    | 1:A:87:PHE:CE2    | 2.54                     | 0.41              |
| 1:A:847:VAL:HB    | 1:A:849:LEU:CD1   | 2.50                     | 0.41              |
| 1:B:133:VAL:HG12  | 1:B:134:ILE:N     | 2.35                     | 0.41              |
| 1:B:304:MET:CE    | 1:B:399:CYS:HB2   | 2.50                     | 0.41              |
| 1:B:675:TYR:HE2   | 1:B:716:LEU:HA    | 1.84                     | 0.41              |
| 1:C:198:ASP:N     | 1:C:198:ASP:OD1   | 2.53                     | 0.41              |
| 1:C:519:PRO:HB2   | 1:C:705:HIS:CD2   | 2.54                     | 0.41              |
| 1:D:1014:ILE:HD12 | 1:D:1016:VAL:HG12 | 2.01                     | 0.41              |
| 1:D:174:VAL:CA    | 1:D:175:GLU:OE2   | 2.68                     | 0.41              |
| 1:D:198:ASP:OD1   | 1:D:198:ASP:N     | 2.53                     | 0.41              |
| 1:D:448:SER:O     | 1:D:452:THR:CG2   | 2.67                     | 0.41              |
| 1:E:1014:ILE:HD12 | 1:E:1016:VAL:HG12 | 2.01                     | 0.41              |
| 1:F:509:GLY:N     | 1:F:605:ASN:HB2   | 2.35                     | 0.41              |
| 1:G:586:ARG:HB2   | 1:G:586:ARG:NH1   | 2.35                     | 0.41              |
| 1:G:754:ALA:HB1   | 1:G:759:VAL:CG1   | 2.50                     | 0.41              |
| 1:H:288:PHE:CD1   | 1:H:288:PHE:C     | 2.92                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:448:SER:O     | 1:H:452:THR:CG2   | 2.67                     | 0.41              |
| 1:A:230:ARG:HD3   | 1:A:302:THR:OG1   | 2.20                     | 0.41              |
| 1:A:600:ARG:HG3   | 1:A:639:GLY:HA3   | 2.02                     | 0.41              |
| 1:B:266:MET:HE1   | 1:B:291:VAL:CG1   | 2.50                     | 0.41              |
| 1:E:473:ILE:O     | 1:E:477:THR:OG1   | 2.26                     | 0.41              |
| 1:E:672:ALA:HA    | 1:E:708:GLY:O     | 2.19                     | 0.41              |
| 1:F:194:ALA:C     | 1:F:195:PHE:CD2   | 2.94                     | 0.41              |
| 1:F:230:ARG:HD3   | 1:F:302:THR:OG1   | 2.20                     | 0.41              |
| 1:G:448:SER:O     | 1:G:452:THR:CG2   | 2.68                     | 0.41              |
| 1:G:519:PRO:HB2   | 1:G:705:HIS:CD2   | 2.54                     | 0.41              |
| 1:H:463:ARG:HG3   | 1:H:468:LYS:HE3   | 2.03                     | 0.41              |
| 1:A:194:ALA:C     | 1:A:195:PHE:CD2   | 2.94                     | 0.41              |
| 1:A:685:THR:O     | 1:A:688:THR:HG23  | 2.21                     | 0.41              |
| 1:B:1014:ILE:HD12 | 1:B:1016:VAL:HG12 | 2.02                     | 0.41              |
| 1:B:1033:GLU:HG3  | 1:B:1034:PRO:HD2  | 2.01                     | 0.41              |
| 1:B:158:LEU:HA    | 1:B:205:CYS:H     | 1.85                     | 0.41              |
| 1:C:1033:GLU:HG3  | 1:C:1034:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:45:TYR:CE1    | 1:C:1047:ASN:CG   | 2.94                     | 0.41              |
| 1:C:41:SER:OG     | 1:C:43:HIS:HD2    | 2.03                     | 0.41              |
| 1:C:754:ALA:HB1   | 1:C:759:VAL:CG1   | 2.50                     | 0.41              |
| 1:C:85:TYR:CZ     | 1:C:297:VAL:HG22  | 2.55                     | 0.41              |
| 1:E:212:ILE:HG23  | 1:E:229:GLU:HB2   | 2.02                     | 0.41              |
| 1:F:448:SER:O     | 1:F:452:THR:CG2   | 2.68                     | 0.41              |
| 1:F:672:ALA:HA    | 1:F:708:GLY:O     | 2.21                     | 0.41              |
| 1:G:144:ILE:HA    | 1:G:184:PHE:HE2   | 1.84                     | 0.41              |
| 1:H:134:ILE:HG23  | 1:H:135:PRO:HD2   | 2.02                     | 0.41              |
| 1:H:280:LEU:HD23  | 1:H:280:LEU:HA    | 1.92                     | 0.41              |
| 1:H:304:MET:CE    | 1:H:399:CYS:HB2   | 2.50                     | 0.41              |
| 1:H:718:PRO:CG    | 1:H:749:TYR:CD2   | 3.04                     | 0.41              |
| 1:H:841:GLN:HG2   | 1:H:853:TRP:CZ2   | 2.55                     | 0.41              |
| 1:A:137:SER:CB    | 1:A:141:VAL:HG22  | 2.50                     | 0.41              |
| 1:B:369:THR:OG1   | 1:B:370:GLY:N     | 2.53                     | 0.41              |
| 1:D:428:ILE:HB    | 1:D:429:PRO:HD3   | 2.02                     | 0.41              |
| 1:D:628:ILE:O     | 1:D:632:VAL:HG23  | 2.21                     | 0.41              |
| 1:D:679:ILE:CD1   | 1:D:724:LEU:HD13  | 2.45                     | 0.41              |
| 1:E:7:VAL:HG12    | 1:E:28:ILE:CG2    | 2.50                     | 0.41              |
| 1:F:519:PRO:CB    | 1:F:705:HIS:NE2   | 2.81                     | 0.41              |
| 1:A:82:HIS:CD2    | 1:A:84:GLY:H      | 2.26                     | 0.41              |
| 1:C:405:PHE:CD2   | 1:C:405:PHE:C     | 2.93                     | 0.41              |
| 1:D:280:LEU:HA    | 1:D:280:LEU:HD23  | 1.92                     | 0.41              |
| 1:E:674:CYS:HB3   | 1:E:712:MET:HE1   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:675:TYR:HE2  | 1:E:716:LEU:HA    | 1.84                     | 0.41              |
| 1:F:600:ARG:HG3  | 1:F:639:GLY:HA3   | 2.02                     | 0.41              |
| 1:F:63:TYR:HB2   | 1:F:87:PHE:CE2    | 2.55                     | 0.41              |
| 1:G:41:SER:OG    | 1:G:43:HIS:HD2    | 2.03                     | 0.41              |
| 1:H:17:ILE:HD11  | 1:H:43:HIS:CB     | 2.49                     | 0.41              |
| 1:H:134:ILE:CG2  | 1:H:203:GLU:HB2   | 2.51                     | 0.41              |
| 1:H:628:ILE:O    | 1:H:632:VAL:HG23  | 2.21                     | 0.41              |
| 1:B:672:ALA:HA   | 1:B:708:GLY:O     | 2.20                     | 0.41              |
| 1:B:7:VAL:HG12   | 1:B:28:ILE:CG2    | 2.50                     | 0.41              |
| 1:D:115:MET:CG   | 1:D:125:GLN:HG3   | 2.49                     | 0.41              |
| 1:G:158:LEU:C    | 1:G:205:CYS:SG    | 2.99                     | 0.41              |
| 1:G:672:ALA:HA   | 1:G:708:GLY:O     | 2.20                     | 0.41              |
| 1:G:95:ALA:O     | 1:G:99:GLU:HG3    | 2.21                     | 0.41              |
| 1:A:198:ASP:N    | 1:A:198:ASP:OD1   | 2.54                     | 0.41              |
| 1:A:470:LEU:HB3  | 1:A:1044:PHE:CE2  | 2.55                     | 0.41              |
| 1:B:450:ILE:CG2  | 1:B:451:ASP:N     | 2.84                     | 0.41              |
| 1:B:631:PHE:O    | 1:B:635:SER:OG    | 2.38                     | 0.41              |
| 1:D:138:ASN:N    | 1:D:138:ASN:OD1   | 2.52                     | 0.41              |
| 1:E:1033:GLU:HG3 | 1:E:1034:PRO:HD2  | 2.02                     | 0.41              |
| 1:E:266:MET:HE1  | 1:E:291:VAL:CG1   | 2.51                     | 0.41              |
| 1:E:304:MET:CE   | 1:E:399:CYS:CB    | 2.98                     | 0.41              |
| 1:F:1044:PHE:HE2 | 1:F:1053:ILE:HD11 | 1.86                     | 0.41              |
| 1:F:157:PRO:O    | 1:F:205:CYS:HB2   | 2.20                     | 0.41              |
| 1:F:288:PHE:CD1  | 1:F:289:ILE:N     | 2.89                     | 0.41              |
| 1:F:490:PRO:HD2  | 1:F:492:TYR:CE2   | 2.56                     | 0.41              |
| 1:G:134:ILE:CD1  | 1:G:287:TYR:CB    | 2.98                     | 0.41              |
| 1:H:428:ILE:HB   | 1:H:429:PRO:HD3   | 2.03                     | 0.41              |
| 1:A:224:ILE:HG22 | 1:A:263:VAL:HG13  | 2.03                     | 0.41              |
| 1:B:373:GLY:O    | 1:B:400:THR:HA    | 2.20                     | 0.41              |
| 1:B:42:PHE:HA    | 1:B:45:TYR:HD2    | 1.84                     | 0.41              |
| 1:C:672:ALA:HA   | 1:C:708:GLY:O     | 2.20                     | 0.41              |
| 1:E:631:PHE:O    | 1:E:635:SER:OG    | 2.38                     | 0.41              |
| 1:F:427:ASN:ND2  | 1:F:431:LEU:HD11  | 2.36                     | 0.41              |
| 1:F:67:GLU:O     | 1:F:71:GLU:HG2    | 2.21                     | 0.41              |
| 1:F:847:VAL:HB   | 1:F:849:LEU:CD1   | 2.51                     | 0.41              |
| 1:G:766:SER:O    | 1:G:767:SER:C     | 2.59                     | 0.41              |
| 1:G:589:ASN:CG   | 1:G:989:MET:HE2   | 2.40                     | 0.41              |
| 1:A:304:MET:CE   | 1:A:399:CYS:HB2   | 2.50                     | 0.41              |
| 1:C:589:ASN:CG   | 1:C:989:MET:HE2   | 2.40                     | 0.41              |
| 1:C:95:ALA:O     | 1:C:99:GLU:HG3    | 2.21                     | 0.41              |
| 1:D:1044:PHE:HE2 | 1:D:1053:ILE:HD11 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:41:SER:OG    | 1:D:43:HIS:HD2    | 2.03                     | 0.41              |
| 1:E:133:VAL:HG12 | 1:E:134:ILE:N     | 2.36                     | 0.41              |
| 1:F:224:ILE:HG22 | 1:F:263:VAL:HG13  | 2.03                     | 0.41              |
| 1:G:509:GLY:N    | 1:G:605:ASN:HB2   | 2.35                     | 0.41              |
| 1:H:138:ASN:OD1  | 1:H:138:ASN:N     | 2.53                     | 0.41              |
| 1:H:536:ASP:HB3  | 1:H:573:PHE:HD1   | 1.86                     | 0.41              |
| 1:A:490:PRO:HD2  | 1:A:492:TYR:CE2   | 2.56                     | 0.41              |
| 1:A:67:GLU:O     | 1:A:71:GLU:HG2    | 2.21                     | 0.41              |
| 1:B:212:ILE:HG23 | 1:B:229:GLU:HB2   | 2.03                     | 0.41              |
| 1:B:304:MET:CE   | 1:B:399:CYS:CB    | 2.99                     | 0.41              |
| 1:C:718:PRO:CG   | 1:C:749:TYR:CD2   | 3.04                     | 0.41              |
| 1:D:134:ILE:HG23 | 1:D:135:PRO:HD2   | 2.03                     | 0.41              |
| 1:G:1044:PHE:HE2 | 1:G:1053:ILE:HD11 | 1.85                     | 0.41              |
| 1:A:51:TYR:CE1   | 1:B:1021:GLY:HA2  | 2.54                     | 0.41              |
| 1:B:12:ARG:NE    | 1:B:391:TYR:CD1   | 2.89                     | 0.41              |
| 1:C:304:MET:CE   | 1:C:399:CYS:CB    | 2.99                     | 0.41              |
| 1:D:134:ILE:CG2  | 1:D:203:GLU:HB2   | 2.51                     | 0.41              |
| 1:F:685:THR:O    | 1:F:688:THR:HG23  | 2.21                     | 0.41              |
| 1:F:88:LEU:HB3   | 1:F:94:PHE:CD2    | 2.56                     | 0.41              |
| 1:H:288:PHE:CD1  | 1:H:289:ILE:N     | 2.89                     | 0.41              |
| 1:H:382:PHE:CD1  | 1:H:385:THR:HB    | 2.56                     | 0.41              |
| 1:H:67:GLU:O     | 1:H:71:GLU:HG2    | 2.21                     | 0.41              |
| 1:C:134:ILE:CD1  | 1:C:287:TYR:CB    | 2.98                     | 0.40              |
| 1:C:536:ASP:HB3  | 1:C:573:PHE:HD1   | 1.86                     | 0.40              |
| 1:D:258:ILE:CG2  | 1:D:279:PHE:CD2   | 3.04                     | 0.40              |
| 1:D:862:VAL:O    | 1:D:866:MET:N     | 2.54                     | 0.40              |
| 1:E:365:THR:CG2  | 1:E:1050:PRO:O    | 2.68                     | 0.40              |
| 1:E:12:ARG:NE    | 1:E:391:TYR:CD1   | 2.90                     | 0.40              |
| 1:F:862:VAL:O    | 1:F:866:MET:N     | 2.53                     | 0.40              |
| 1:F:911:ILE:O    | 1:F:915:MET:N     | 2.50                     | 0.40              |
| 1:H:45:TYR:CE1   | 1:G:1047:ASN:CG   | 2.95                     | 0.40              |
| 1:G:198:ASP:O    | 1:G:200:VAL:CG2   | 2.68                     | 0.40              |
| 1:G:373:GLY:O    | 1:G:400:THR:HA    | 2.20                     | 0.40              |
| 1:G:651:TRP:HE1  | 1:G:653:LYS:CB    | 2.35                     | 0.40              |
| 1:H:265:LEU:O    | 1:H:269:VAL:HG22  | 2.20                     | 0.40              |
| 1:H:620:TYR:HD1  | 1:H:979:TYR:CE1   | 2.39                     | 0.40              |
| 1:H:679:ILE:CD1  | 1:H:724:LEU:HD13  | 2.46                     | 0.40              |
| 1:A:1044:PHE:HE2 | 1:A:1053:ILE:HD11 | 1.86                     | 0.40              |
| 1:A:212:ILE:HG23 | 1:A:229:GLU:HB2   | 2.04                     | 0.40              |
| 1:A:713:ALA:HB3  | 1:A:715:LEU:HD12  | 2.01                     | 0.40              |
| 1:A:862:VAL:O    | 1:A:866:MET:N     | 2.53                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:137:SER:CB   | 1:B:141:VAL:HG22  | 2.50                     | 0.40              |
| 1:B:505:GLN:C    | 1:B:506:ILE:HG12  | 2.41                     | 0.40              |
| 1:C:234:ILE:CD1  | 1:C:445:TYR:CZ    | 3.01                     | 0.40              |
| 1:D:13:GLY:C     | 1:D:17:ILE:HD12   | 2.41                     | 0.40              |
| 1:D:620:TYR:HD1  | 1:D:979:TYR:CE1   | 2.39                     | 0.40              |
| 1:E:540:ARG:NH1  | 1:E:578:GLY:HA3   | 2.37                     | 0.40              |
| 1:F:540:ARG:HD2  | 1:F:540:ARG:HH11  | 1.69                     | 0.40              |
| 1:G:198:ASP:N    | 1:G:198:ASP:OD1   | 2.52                     | 0.40              |
| 1:G:718:PRO:CG   | 1:G:749:TYR:CD2   | 3.05                     | 0.40              |
| 1:H:133:VAL:HG12 | 1:H:134:ILE:N     | 2.36                     | 0.40              |
| 1:H:177:LYS:HG2  | 1:H:179:HIS:CE1   | 2.56                     | 0.40              |
| 1:H:258:ILE:CG2  | 1:H:279:PHE:CD2   | 3.04                     | 0.40              |
| 1:A:173:VAL:HG13 | 1:A:205:CYS:SG    | 2.61                     | 0.40              |
| 1:C:1044:PHE:HE2 | 1:C:1053:ILE:HD11 | 1.86                     | 0.40              |
| 1:C:631:PHE:O    | 1:C:635:SER:OG    | 2.37                     | 0.40              |
| 1:C:979:TYR:CB   | 1:C:982:VAL:HG22  | 2.51                     | 0.40              |
| 1:D:67:GLU:O     | 1:D:71:GLU:HG2    | 2.21                     | 0.40              |
| 1:E:278:GLU:C    | 1:E:289:ILE:CG1   | 2.90                     | 0.40              |
| 1:E:541:ASP:OD2  | 1:E:739:HIS:HE1   | 2.01                     | 0.40              |
| 1:F:198:ASP:OD1  | 1:F:198:ASP:N     | 2.55                     | 0.40              |
| 1:F:304:MET:CE   | 1:F:399:CYS:HB2   | 2.50                     | 0.40              |
| 1:B:230:ARG:HD3  | 1:B:302:THR:OG1   | 2.21                     | 0.40              |
| 1:B:541:ASP:OD2  | 1:B:739:HIS:HE1   | 2.02                     | 0.40              |
| 1:C:472:TYR:OH   | 1:C:1004:PHE:O    | 2.28                     | 0.40              |
| 1:D:265:LEU:O    | 1:D:269:VAL:HG22  | 2.20                     | 0.40              |
| 1:F:331:PRO:HG2  | 1:F:336:ILE:HG12  | 2.03                     | 0.40              |
| 1:G:472:TYR:OH   | 1:G:1004:PHE:O    | 2.28                     | 0.40              |
| 1:H:1044:PHE:HE2 | 1:H:1053:ILE:HD11 | 1.86                     | 0.40              |
| 1:H:862:VAL:O    | 1:H:866:MET:N     | 2.54                     | 0.40              |
| 1:A:373:GLY:O    | 1:A:400:THR:HA    | 2.22                     | 0.40              |
| 1:B:628:ILE:O    | 1:B:632:VAL:HG23  | 2.21                     | 0.40              |
| 1:D:45:TYR:CZ    | 1:C:1047:ASN:O    | 2.74                     | 0.40              |
| 1:C:288:PHE:CD1  | 1:C:289:ILE:N     | 2.90                     | 0.40              |
| 1:D:304:MET:CE   | 1:D:399:CYS:HB2   | 2.51                     | 0.40              |
| 1:D:536:ASP:HB3  | 1:D:573:PHE:HD1   | 1.87                     | 0.40              |
| 1:D:674:CYS:HB3  | 1:D:712:MET:HE1   | 2.04                     | 0.40              |
| 1:E:405:PHE:CD2  | 1:E:405:PHE:C     | 2.95                     | 0.40              |
| 1:F:470:LEU:HB3  | 1:F:1044:PHE:CE2  | 2.56                     | 0.40              |
| 1:F:131:ILE:N    | 1:F:131:ILE:HD13  | 2.36                     | 0.40              |
| 1:F:137:SER:CB   | 1:F:141:VAL:HG22  | 2.51                     | 0.40              |
| 1:F:266:MET:HE1  | 1:F:271:TYR:CE1   | 2.56                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:212:ILE:HG23 | 1:G:229:GLU:HB2 | 2.04                     | 0.40              |
| 1:H:230:ARG:HD3  | 1:H:302:THR:OG1 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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     | 1048/1146 (91%) | 988 (94%)  | 57 (5%)  | 3 (0%)   | 41          | 72 |
| 1   | B     | 1021/1146 (89%) | 966 (95%)  | 53 (5%)  | 2 (0%)   | 47          | 77 |
| 1   | C     | 933/1146 (81%)  | 882 (94%)  | 47 (5%)  | 4 (0%)   | 34          | 67 |
| 1   | D     | 1025/1146 (89%) | 967 (94%)  | 55 (5%)  | 3 (0%)   | 41          | 72 |
| 1   | E     | 1021/1146 (89%) | 962 (94%)  | 56 (6%)  | 3 (0%)   | 41          | 72 |
| 1   | F     | 1048/1146 (91%) | 992 (95%)  | 54 (5%)  | 2 (0%)   | 47          | 77 |
| 1   | G     | 934/1146 (82%)  | 881 (94%)  | 49 (5%)  | 4 (0%)   | 34          | 67 |
| 1   | H     | 1025/1146 (89%) | 966 (94%)  | 56 (6%)  | 3 (0%)   | 41          | 72 |
| All | All   | 8055/9168 (88%) | 7604 (94%) | 427 (5%) | 24 (0%)  | 41          | 72 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 273 | ASN  |
| 1   | F     | 273 | ASN  |
| 1   | E     | 273 | ASN  |
| 1   | G     | 176 | SER  |
| 1   | G     | 273 | ASN  |
| 1   | D     | 273 | ASN  |
| 1   | A     | 273 | ASN  |
| 1   | B     | 273 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 176  | SER  |
| 1   | C     | 273  | ASN  |
| 1   | A     | 176  | SER  |
| 1   | F     | 176  | SER  |
| 1   | D     | 176  | SER  |
| 1   | H     | 997  | THR  |
| 1   | E     | 506  | ILE  |
| 1   | G     | 506  | ILE  |
| 1   | C     | 506  | ILE  |
| 1   | H     | 1035 | ILE  |
| 1   | E     | 1035 | ILE  |
| 1   | G     | 1035 | ILE  |
| 1   | D     | 1035 | ILE  |
| 1   | B     | 1035 | ILE  |
| 1   | C     | 1035 | ILE  |
| 1   | A     | 1035 | ILE  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 814/981 (83%)   | 710 (87%)  | 104 (13%) | 4           | 18 |
| 1   | B     | 719/981 (73%)   | 626 (87%)  | 93 (13%)  | 4           | 18 |
| 1   | C     | 676/981 (69%)   | 587 (87%)  | 89 (13%)  | 4           | 17 |
| 1   | D     | 819/981 (84%)   | 719 (88%)  | 100 (12%) | 5           | 20 |
| 1   | E     | 719/981 (73%)   | 625 (87%)  | 94 (13%)  | 4           | 18 |
| 1   | F     | 814/981 (83%)   | 710 (87%)  | 104 (13%) | 4           | 18 |
| 1   | G     | 677/981 (69%)   | 591 (87%)  | 86 (13%)  | 4           | 19 |
| 1   | H     | 819/981 (84%)   | 718 (88%)  | 101 (12%) | 4           | 20 |
| All | All   | 6057/7848 (77%) | 5286 (87%) | 771 (13%) | 4           | 19 |

All (771) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 2   | ASN  |
| 1   | H     | 3   | ARG  |
| 1   | H     | 12  | ARG  |
| 1   | H     | 31  | VAL  |
| 1   | H     | 39  | THR  |
| 1   | H     | 42  | PHE  |
| 1   | H     | 44  | ARG  |
| 1   | H     | 60  | ILE  |
| 1   | H     | 70  | ILE  |
| 1   | H     | 71  | GLU  |
| 1   | H     | 76  | SER  |
| 1   | H     | 88  | LEU  |
| 1   | H     | 106 | VAL  |
| 1   | H     | 110 | SER  |
| 1   | H     | 116 | PHE  |
| 1   | H     | 121 | LYS  |
| 1   | H     | 127 | LEU  |
| 1   | H     | 134 | ILE  |
| 1   | H     | 177 | LYS  |
| 1   | H     | 183 | SER  |
| 1   | H     | 198 | ASP  |
| 1   | H     | 203 | GLU  |
| 1   | H     | 204 | LYS  |
| 1   | H     | 207 | MET  |
| 1   | H     | 223 | ASN  |
| 1   | H     | 239 | GLN  |
| 1   | H     | 248 | ASN  |
| 1   | H     | 251 | THR  |
| 1   | H     | 252 | SER  |
| 1   | H     | 254 | LEU  |
| 1   | H     | 265 | LEU  |
| 1   | H     | 269 | VAL  |
| 1   | H     | 289 | ILE  |
| 1   | H     | 290 | GLU  |
| 1   | H     | 294 | ARG  |
| 1   | H     | 295 | VAL  |
| 1   | H     | 323 | LEU  |
| 1   | H     | 334 | GLU  |
| 1   | H     | 356 | PHE  |
| 1   | H     | 360 | THR  |
| 1   | H     | 364 | ASP  |
| 1   | H     | 369 | THR  |
| 1   | H     | 377 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 382 | PHE  |
| 1   | H     | 392 | ASP  |
| 1   | H     | 393 | SER  |
| 1   | H     | 405 | PHE  |
| 1   | H     | 407 | GLN  |
| 1   | H     | 419 | PHE  |
| 1   | H     | 434 | VAL  |
| 1   | H     | 436 | ARG  |
| 1   | H     | 445 | TYR  |
| 1   | H     | 453 | THR  |
| 1   | H     | 461 | HIS  |
| 1   | H     | 462 | ILE  |
| 1   | H     | 499 | LYS  |
| 1   | H     | 504 | SER  |
| 1   | H     | 507 | SER  |
| 1   | H     | 520 | GLU  |
| 1   | H     | 531 | GLU  |
| 1   | H     | 533 | LEU  |
| 1   | H     | 540 | ARG  |
| 1   | H     | 545 | SER  |
| 1   | H     | 547 | LEU  |
| 1   | H     | 549 | THR  |
| 1   | H     | 558 | GLN  |
| 1   | H     | 572 | SER  |
| 1   | H     | 575 | MET  |
| 1   | H     | 576 | TRP  |
| 1   | H     | 600 | ARG  |
| 1   | H     | 613 | ARG  |
| 1   | H     | 635 | SER  |
| 1   | H     | 658 | SER  |
| 1   | H     | 668 | ILE  |
| 1   | H     | 682 | ASP  |
| 1   | H     | 688 | THR  |
| 1   | H     | 695 | MET  |
| 1   | H     | 719 | GLN  |
| 1   | H     | 723 | ARG  |
| 1   | H     | 727 | GLU  |
| 1   | H     | 781 | LEU  |
| 1   | H     | 792 | THR  |
| 1   | H     | 845 | ILE  |
| 1   | H     | 858 | GLU  |
| 1   | H     | 867 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 870  | ILE  |
| 1   | H     | 890  | ASN  |
| 1   | H     | 891  | GLU  |
| 1   | H     | 895  | GLU  |
| 1   | H     | 896  | ASP  |
| 1   | H     | 898  | TYR  |
| 1   | H     | 902  | ASP  |
| 1   | H     | 918  | ILE  |
| 1   | H     | 928  | LYS  |
| 1   | H     | 942  | ASP  |
| 1   | H     | 974  | ILE  |
| 1   | H     | 1016 | VAL  |
| 1   | H     | 1020 | LYS  |
| 1   | H     | 1040 | ARG  |
| 1   | H     | 1051 | ARG  |
| 1   | H     | 1059 | ASN  |
| 1   | F     | 2    | ASN  |
| 1   | F     | 39   | THR  |
| 1   | F     | 42   | PHE  |
| 1   | F     | 44   | ARG  |
| 1   | F     | 60   | ILE  |
| 1   | F     | 71   | GLU  |
| 1   | F     | 76   | SER  |
| 1   | F     | 106  | VAL  |
| 1   | F     | 110  | SER  |
| 1   | F     | 115  | MET  |
| 1   | F     | 121  | LYS  |
| 1   | F     | 127  | LEU  |
| 1   | F     | 131  | ILE  |
| 1   | F     | 134  | ILE  |
| 1   | F     | 159  | MET  |
| 1   | F     | 163  | SER  |
| 1   | F     | 183  | SER  |
| 1   | F     | 195  | PHE  |
| 1   | F     | 198  | ASP  |
| 1   | F     | 205  | CYS  |
| 1   | F     | 207  | MET  |
| 1   | F     | 239  | GLN  |
| 1   | F     | 251  | THR  |
| 1   | F     | 252  | SER  |
| 1   | F     | 254  | LEU  |
| 1   | F     | 265  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 269 | VAL  |
| 1   | F     | 289 | ILE  |
| 1   | F     | 294 | ARG  |
| 1   | F     | 295 | VAL  |
| 1   | F     | 323 | LEU  |
| 1   | F     | 326 | GLN  |
| 1   | F     | 334 | GLU  |
| 1   | F     | 360 | THR  |
| 1   | F     | 367 | ARG  |
| 1   | F     | 369 | THR  |
| 1   | F     | 382 | PHE  |
| 1   | F     | 392 | ASP  |
| 1   | F     | 393 | SER  |
| 1   | F     | 395 | LEU  |
| 1   | F     | 405 | PHE  |
| 1   | F     | 407 | GLN  |
| 1   | F     | 419 | PHE  |
| 1   | F     | 434 | VAL  |
| 1   | F     | 436 | ARG  |
| 1   | F     | 445 | TYR  |
| 1   | F     | 453 | THR  |
| 1   | F     | 462 | ILE  |
| 1   | F     | 463 | ARG  |
| 1   | F     | 476 | VAL  |
| 1   | F     | 504 | SER  |
| 1   | F     | 505 | GLN  |
| 1   | F     | 507 | SER  |
| 1   | F     | 510 | THR  |
| 1   | F     | 520 | GLU  |
| 1   | F     | 531 | GLU  |
| 1   | F     | 540 | ARG  |
| 1   | F     | 545 | SER  |
| 1   | F     | 547 | LEU  |
| 1   | F     | 549 | THR  |
| 1   | F     | 558 | GLN  |
| 1   | F     | 572 | SER  |
| 1   | F     | 576 | TRP  |
| 1   | F     | 600 | ARG  |
| 1   | F     | 635 | SER  |
| 1   | F     | 652 | ILE  |
| 1   | F     | 658 | SER  |
| 1   | F     | 668 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 682  | ASP  |
| 1   | F     | 695  | MET  |
| 1   | F     | 719  | GLN  |
| 1   | F     | 723  | ARG  |
| 1   | F     | 727  | GLU  |
| 1   | F     | 734  | VAL  |
| 1   | F     | 781  | LEU  |
| 1   | F     | 792  | THR  |
| 1   | F     | 794  | LEU  |
| 1   | F     | 811  | HIS  |
| 1   | F     | 820  | LEU  |
| 1   | F     | 845  | ILE  |
| 1   | F     | 867  | PHE  |
| 1   | F     | 870  | ILE  |
| 1   | F     | 890  | ASN  |
| 1   | F     | 891  | GLU  |
| 1   | F     | 895  | GLU  |
| 1   | F     | 896  | ASP  |
| 1   | F     | 897  | VAL  |
| 1   | F     | 902  | ASP  |
| 1   | F     | 918  | ILE  |
| 1   | F     | 940  | LEU  |
| 1   | F     | 942  | ASP  |
| 1   | F     | 943  | ARG  |
| 1   | F     | 957  | LYS  |
| 1   | F     | 960  | LEU  |
| 1   | F     | 974  | ILE  |
| 1   | F     | 1016 | VAL  |
| 1   | F     | 1030 | SER  |
| 1   | F     | 1031 | ILE  |
| 1   | F     | 1037 | ASP  |
| 1   | F     | 1040 | ARG  |
| 1   | F     | 1049 | GLN  |
| 1   | F     | 1054 | ASN  |
| 1   | F     | 1056 | GLN  |
| 1   | F     | 1059 | ASN  |
| 1   | E     | 1    | MET  |
| 1   | E     | 2    | ASN  |
| 1   | E     | 27   | LYS  |
| 1   | E     | 39   | THR  |
| 1   | E     | 44   | ARG  |
| 1   | E     | 76   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 88  | LEU  |
| 1   | E     | 92  | ILE  |
| 1   | E     | 94  | PHE  |
| 1   | E     | 106 | VAL  |
| 1   | E     | 110 | SER  |
| 1   | E     | 115 | MET  |
| 1   | E     | 127 | LEU  |
| 1   | E     | 134 | ILE  |
| 1   | E     | 144 | ILE  |
| 1   | E     | 163 | SER  |
| 1   | E     | 183 | SER  |
| 1   | E     | 184 | PHE  |
| 1   | E     | 198 | ASP  |
| 1   | E     | 207 | MET  |
| 1   | E     | 228 | PHE  |
| 1   | E     | 237 | ARG  |
| 1   | E     | 248 | ASN  |
| 1   | E     | 251 | THR  |
| 1   | E     | 252 | SER  |
| 1   | E     | 254 | LEU  |
| 1   | E     | 265 | LEU  |
| 1   | E     | 269 | VAL  |
| 1   | E     | 280 | LEU  |
| 1   | E     | 289 | ILE  |
| 1   | E     | 294 | ARG  |
| 1   | E     | 323 | LEU  |
| 1   | E     | 326 | GLN  |
| 1   | E     | 334 | GLU  |
| 1   | E     | 349 | THR  |
| 1   | E     | 356 | PHE  |
| 1   | E     | 357 | MET  |
| 1   | E     | 360 | THR  |
| 1   | E     | 364 | ASP  |
| 1   | E     | 367 | ARG  |
| 1   | E     | 369 | THR  |
| 1   | E     | 377 | ASP  |
| 1   | E     | 382 | PHE  |
| 1   | E     | 392 | ASP  |
| 1   | E     | 393 | SER  |
| 1   | E     | 405 | PHE  |
| 1   | E     | 407 | GLN  |
| 1   | E     | 419 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 434 | VAL  |
| 1   | E     | 436 | ARG  |
| 1   | E     | 445 | TYR  |
| 1   | E     | 453 | THR  |
| 1   | E     | 463 | ARG  |
| 1   | E     | 476 | VAL  |
| 1   | E     | 502 | TYR  |
| 1   | E     | 504 | SER  |
| 1   | E     | 505 | GLN  |
| 1   | E     | 507 | SER  |
| 1   | E     | 510 | THR  |
| 1   | E     | 531 | GLU  |
| 1   | E     | 540 | ARG  |
| 1   | E     | 545 | SER  |
| 1   | E     | 547 | LEU  |
| 1   | E     | 549 | THR  |
| 1   | E     | 558 | GLN  |
| 1   | E     | 567 | LEU  |
| 1   | E     | 572 | SER  |
| 1   | E     | 576 | TRP  |
| 1   | E     | 600 | ARG  |
| 1   | E     | 612 | LEU  |
| 1   | E     | 613 | ARG  |
| 1   | E     | 635 | SER  |
| 1   | E     | 658 | SER  |
| 1   | E     | 668 | ILE  |
| 1   | E     | 682 | ASP  |
| 1   | E     | 684 | ARG  |
| 1   | E     | 690 | ASP  |
| 1   | E     | 724 | LEU  |
| 1   | E     | 781 | LEU  |
| 1   | E     | 858 | GLU  |
| 1   | E     | 890 | ASN  |
| 1   | E     | 891 | GLU  |
| 1   | E     | 895 | GLU  |
| 1   | E     | 896 | ASP  |
| 1   | E     | 898 | TYR  |
| 1   | E     | 920 | GLN  |
| 1   | E     | 927 | GLU  |
| 1   | E     | 949 | GLU  |
| 1   | E     | 952 | ASN  |
| 1   | E     | 960 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 974  | ILE  |
| 1   | E     | 1016 | VAL  |
| 1   | E     | 1040 | ARG  |
| 1   | E     | 1059 | ASN  |
| 1   | G     | 2    | ASN  |
| 1   | G     | 3    | ARG  |
| 1   | G     | 12   | ARG  |
| 1   | G     | 20   | MET  |
| 1   | G     | 39   | THR  |
| 1   | G     | 42   | PHE  |
| 1   | G     | 44   | ARG  |
| 1   | G     | 64   | LEU  |
| 1   | G     | 71   | GLU  |
| 1   | G     | 76   | SER  |
| 1   | G     | 88   | LEU  |
| 1   | G     | 94   | PHE  |
| 1   | G     | 96   | ARG  |
| 1   | G     | 106  | VAL  |
| 1   | G     | 110  | SER  |
| 1   | G     | 111  | LYS  |
| 1   | G     | 115  | MET  |
| 1   | G     | 134  | ILE  |
| 1   | G     | 163  | SER  |
| 1   | G     | 179  | HIS  |
| 1   | G     | 183  | SER  |
| 1   | G     | 186  | ARG  |
| 1   | G     | 195  | PHE  |
| 1   | G     | 198  | ASP  |
| 1   | G     | 205  | CYS  |
| 1   | G     | 207  | MET  |
| 1   | G     | 248  | ASN  |
| 1   | G     | 251  | THR  |
| 1   | G     | 252  | SER  |
| 1   | G     | 254  | LEU  |
| 1   | G     | 265  | LEU  |
| 1   | G     | 269  | VAL  |
| 1   | G     | 289  | ILE  |
| 1   | G     | 294  | ARG  |
| 1   | G     | 295  | VAL  |
| 1   | G     | 323  | LEU  |
| 1   | G     | 326  | GLN  |
| 1   | G     | 334  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 356 | PHE  |
| 1   | G     | 360 | THR  |
| 1   | G     | 364 | ASP  |
| 1   | G     | 367 | ARG  |
| 1   | G     | 369 | THR  |
| 1   | G     | 377 | ASP  |
| 1   | G     | 392 | ASP  |
| 1   | G     | 393 | SER  |
| 1   | G     | 405 | PHE  |
| 1   | G     | 407 | GLN  |
| 1   | G     | 419 | PHE  |
| 1   | G     | 434 | VAL  |
| 1   | G     | 436 | ARG  |
| 1   | G     | 445 | TYR  |
| 1   | G     | 453 | THR  |
| 1   | G     | 458 | LYS  |
| 1   | G     | 462 | ILE  |
| 1   | G     | 476 | VAL  |
| 1   | G     | 494 | GLU  |
| 1   | G     | 502 | TYR  |
| 1   | G     | 504 | SER  |
| 1   | G     | 507 | SER  |
| 1   | G     | 510 | THR  |
| 1   | G     | 540 | ARG  |
| 1   | G     | 545 | SER  |
| 1   | G     | 547 | LEU  |
| 1   | G     | 549 | THR  |
| 1   | G     | 558 | GLN  |
| 1   | G     | 572 | SER  |
| 1   | G     | 576 | TRP  |
| 1   | G     | 588 | LEU  |
| 1   | G     | 600 | ARG  |
| 1   | G     | 635 | SER  |
| 1   | G     | 651 | TRP  |
| 1   | G     | 658 | SER  |
| 1   | G     | 668 | ILE  |
| 1   | G     | 682 | ASP  |
| 1   | G     | 698 | GLU  |
| 1   | G     | 717 | LYS  |
| 1   | G     | 737 | HIS  |
| 1   | G     | 781 | LEU  |
| 1   | G     | 792 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 794  | LEU  |
| 1   | G     | 960  | LEU  |
| 1   | G     | 962  | GLU  |
| 1   | G     | 1016 | VAL  |
| 1   | G     | 1040 | ARG  |
| 1   | G     | 1059 | ASN  |
| 1   | D     | 2    | ASN  |
| 1   | D     | 3    | ARG  |
| 1   | D     | 12   | ARG  |
| 1   | D     | 31   | VAL  |
| 1   | D     | 39   | THR  |
| 1   | D     | 42   | PHE  |
| 1   | D     | 44   | ARG  |
| 1   | D     | 60   | ILE  |
| 1   | D     | 70   | ILE  |
| 1   | D     | 71   | GLU  |
| 1   | D     | 76   | SER  |
| 1   | D     | 88   | LEU  |
| 1   | D     | 106  | VAL  |
| 1   | D     | 110  | SER  |
| 1   | D     | 116  | PHE  |
| 1   | D     | 121  | LYS  |
| 1   | D     | 127  | LEU  |
| 1   | D     | 134  | ILE  |
| 1   | D     | 177  | LYS  |
| 1   | D     | 183  | SER  |
| 1   | D     | 198  | ASP  |
| 1   | D     | 203  | GLU  |
| 1   | D     | 204  | LYS  |
| 1   | D     | 207  | MET  |
| 1   | D     | 223  | ASN  |
| 1   | D     | 248  | ASN  |
| 1   | D     | 251  | THR  |
| 1   | D     | 252  | SER  |
| 1   | D     | 254  | LEU  |
| 1   | D     | 265  | LEU  |
| 1   | D     | 269  | VAL  |
| 1   | D     | 289  | ILE  |
| 1   | D     | 290  | GLU  |
| 1   | D     | 294  | ARG  |
| 1   | D     | 295  | VAL  |
| 1   | D     | 323  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 334 | GLU  |
| 1   | D     | 356 | PHE  |
| 1   | D     | 360 | THR  |
| 1   | D     | 364 | ASP  |
| 1   | D     | 369 | THR  |
| 1   | D     | 377 | ASP  |
| 1   | D     | 382 | PHE  |
| 1   | D     | 392 | ASP  |
| 1   | D     | 393 | SER  |
| 1   | D     | 405 | PHE  |
| 1   | D     | 407 | GLN  |
| 1   | D     | 419 | PHE  |
| 1   | D     | 434 | VAL  |
| 1   | D     | 436 | ARG  |
| 1   | D     | 445 | TYR  |
| 1   | D     | 453 | THR  |
| 1   | D     | 461 | HIS  |
| 1   | D     | 462 | ILE  |
| 1   | D     | 499 | LYS  |
| 1   | D     | 504 | SER  |
| 1   | D     | 507 | SER  |
| 1   | D     | 520 | GLU  |
| 1   | D     | 531 | GLU  |
| 1   | D     | 533 | LEU  |
| 1   | D     | 540 | ARG  |
| 1   | D     | 545 | SER  |
| 1   | D     | 547 | LEU  |
| 1   | D     | 549 | THR  |
| 1   | D     | 558 | GLN  |
| 1   | D     | 572 | SER  |
| 1   | D     | 576 | TRP  |
| 1   | D     | 600 | ARG  |
| 1   | D     | 613 | ARG  |
| 1   | D     | 635 | SER  |
| 1   | D     | 658 | SER  |
| 1   | D     | 668 | ILE  |
| 1   | D     | 682 | ASP  |
| 1   | D     | 688 | THR  |
| 1   | D     | 695 | MET  |
| 1   | D     | 719 | GLN  |
| 1   | D     | 723 | ARG  |
| 1   | D     | 727 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 734  | VAL  |
| 1   | D     | 781  | LEU  |
| 1   | D     | 792  | THR  |
| 1   | D     | 845  | ILE  |
| 1   | D     | 858  | GLU  |
| 1   | D     | 867  | PHE  |
| 1   | D     | 870  | ILE  |
| 1   | D     | 890  | ASN  |
| 1   | D     | 891  | GLU  |
| 1   | D     | 895  | GLU  |
| 1   | D     | 896  | ASP  |
| 1   | D     | 898  | TYR  |
| 1   | D     | 902  | ASP  |
| 1   | D     | 918  | ILE  |
| 1   | D     | 928  | LYS  |
| 1   | D     | 942  | ASP  |
| 1   | D     | 974  | ILE  |
| 1   | D     | 1016 | VAL  |
| 1   | D     | 1020 | LYS  |
| 1   | D     | 1040 | ARG  |
| 1   | D     | 1051 | ARG  |
| 1   | D     | 1059 | ASN  |
| 1   | A     | 2    | ASN  |
| 1   | A     | 39   | THR  |
| 1   | A     | 42   | PHE  |
| 1   | A     | 44   | ARG  |
| 1   | A     | 60   | ILE  |
| 1   | A     | 71   | GLU  |
| 1   | A     | 76   | SER  |
| 1   | A     | 106  | VAL  |
| 1   | A     | 110  | SER  |
| 1   | A     | 115  | MET  |
| 1   | A     | 121  | LYS  |
| 1   | A     | 127  | LEU  |
| 1   | A     | 131  | ILE  |
| 1   | A     | 134  | ILE  |
| 1   | A     | 159  | MET  |
| 1   | A     | 163  | SER  |
| 1   | A     | 176  | SER  |
| 1   | A     | 183  | SER  |
| 1   | A     | 195  | PHE  |
| 1   | A     | 198  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 205 | CYS  |
| 1   | A     | 207 | MET  |
| 1   | A     | 251 | THR  |
| 1   | A     | 252 | SER  |
| 1   | A     | 254 | LEU  |
| 1   | A     | 265 | LEU  |
| 1   | A     | 269 | VAL  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 294 | ARG  |
| 1   | A     | 295 | VAL  |
| 1   | A     | 323 | LEU  |
| 1   | A     | 326 | GLN  |
| 1   | A     | 334 | GLU  |
| 1   | A     | 360 | THR  |
| 1   | A     | 367 | ARG  |
| 1   | A     | 369 | THR  |
| 1   | A     | 382 | PHE  |
| 1   | A     | 392 | ASP  |
| 1   | A     | 393 | SER  |
| 1   | A     | 395 | LEU  |
| 1   | A     | 405 | PHE  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 419 | PHE  |
| 1   | A     | 434 | VAL  |
| 1   | A     | 436 | ARG  |
| 1   | A     | 445 | TYR  |
| 1   | A     | 453 | THR  |
| 1   | A     | 462 | ILE  |
| 1   | A     | 463 | ARG  |
| 1   | A     | 476 | VAL  |
| 1   | A     | 504 | SER  |
| 1   | A     | 507 | SER  |
| 1   | A     | 510 | THR  |
| 1   | A     | 520 | GLU  |
| 1   | A     | 531 | GLU  |
| 1   | A     | 540 | ARG  |
| 1   | A     | 545 | SER  |
| 1   | A     | 547 | LEU  |
| 1   | A     | 549 | THR  |
| 1   | A     | 558 | GLN  |
| 1   | A     | 572 | SER  |
| 1   | A     | 576 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 600  | ARG  |
| 1   | A     | 635  | SER  |
| 1   | A     | 652  | ILE  |
| 1   | A     | 658  | SER  |
| 1   | A     | 668  | ILE  |
| 1   | A     | 682  | ASP  |
| 1   | A     | 688  | THR  |
| 1   | A     | 695  | MET  |
| 1   | A     | 719  | GLN  |
| 1   | A     | 723  | ARG  |
| 1   | A     | 727  | GLU  |
| 1   | A     | 734  | VAL  |
| 1   | A     | 781  | LEU  |
| 1   | A     | 792  | THR  |
| 1   | A     | 794  | LEU  |
| 1   | A     | 811  | HIS  |
| 1   | A     | 820  | LEU  |
| 1   | A     | 845  | ILE  |
| 1   | A     | 867  | PHE  |
| 1   | A     | 870  | ILE  |
| 1   | A     | 890  | ASN  |
| 1   | A     | 891  | GLU  |
| 1   | A     | 895  | GLU  |
| 1   | A     | 896  | ASP  |
| 1   | A     | 897  | VAL  |
| 1   | A     | 902  | ASP  |
| 1   | A     | 918  | ILE  |
| 1   | A     | 940  | LEU  |
| 1   | A     | 942  | ASP  |
| 1   | A     | 943  | ARG  |
| 1   | A     | 957  | LYS  |
| 1   | A     | 960  | LEU  |
| 1   | A     | 974  | ILE  |
| 1   | A     | 1016 | VAL  |
| 1   | A     | 1030 | SER  |
| 1   | A     | 1031 | ILE  |
| 1   | A     | 1037 | ASP  |
| 1   | A     | 1040 | ARG  |
| 1   | A     | 1049 | GLN  |
| 1   | A     | 1054 | ASN  |
| 1   | A     | 1056 | GLN  |
| 1   | A     | 1059 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 1   | MET  |
| 1   | B     | 2   | ASN  |
| 1   | B     | 27  | LYS  |
| 1   | B     | 39  | THR  |
| 1   | B     | 44  | ARG  |
| 1   | B     | 76  | SER  |
| 1   | B     | 88  | LEU  |
| 1   | B     | 92  | ILE  |
| 1   | B     | 94  | PHE  |
| 1   | B     | 106 | VAL  |
| 1   | B     | 110 | SER  |
| 1   | B     | 115 | MET  |
| 1   | B     | 127 | LEU  |
| 1   | B     | 134 | ILE  |
| 1   | B     | 144 | ILE  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 163 | SER  |
| 1   | B     | 183 | SER  |
| 1   | B     | 184 | PHE  |
| 1   | B     | 198 | ASP  |
| 1   | B     | 207 | MET  |
| 1   | B     | 228 | PHE  |
| 1   | B     | 237 | ARG  |
| 1   | B     | 248 | ASN  |
| 1   | B     | 251 | THR  |
| 1   | B     | 252 | SER  |
| 1   | B     | 254 | LEU  |
| 1   | B     | 265 | LEU  |
| 1   | B     | 269 | VAL  |
| 1   | B     | 280 | LEU  |
| 1   | B     | 289 | ILE  |
| 1   | B     | 294 | ARG  |
| 1   | B     | 323 | LEU  |
| 1   | B     | 326 | GLN  |
| 1   | B     | 334 | GLU  |
| 1   | B     | 349 | THR  |
| 1   | B     | 356 | PHE  |
| 1   | B     | 357 | MET  |
| 1   | B     | 360 | THR  |
| 1   | B     | 364 | ASP  |
| 1   | B     | 367 | ARG  |
| 1   | B     | 369 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 377 | ASP  |
| 1   | B     | 382 | PHE  |
| 1   | B     | 392 | ASP  |
| 1   | B     | 393 | SER  |
| 1   | B     | 405 | PHE  |
| 1   | B     | 407 | GLN  |
| 1   | B     | 419 | PHE  |
| 1   | B     | 434 | VAL  |
| 1   | B     | 436 | ARG  |
| 1   | B     | 445 | TYR  |
| 1   | B     | 453 | THR  |
| 1   | B     | 463 | ARG  |
| 1   | B     | 476 | VAL  |
| 1   | B     | 502 | TYR  |
| 1   | B     | 504 | SER  |
| 1   | B     | 505 | GLN  |
| 1   | B     | 510 | THR  |
| 1   | B     | 540 | ARG  |
| 1   | B     | 545 | SER  |
| 1   | B     | 547 | LEU  |
| 1   | B     | 549 | THR  |
| 1   | B     | 558 | GLN  |
| 1   | B     | 567 | LEU  |
| 1   | B     | 572 | SER  |
| 1   | B     | 576 | TRP  |
| 1   | B     | 600 | ARG  |
| 1   | B     | 612 | LEU  |
| 1   | B     | 613 | ARG  |
| 1   | B     | 635 | SER  |
| 1   | B     | 658 | SER  |
| 1   | B     | 668 | ILE  |
| 1   | B     | 682 | ASP  |
| 1   | B     | 684 | ARG  |
| 1   | B     | 690 | ASP  |
| 1   | B     | 724 | LEU  |
| 1   | B     | 781 | LEU  |
| 1   | B     | 858 | GLU  |
| 1   | B     | 890 | ASN  |
| 1   | B     | 891 | GLU  |
| 1   | B     | 895 | GLU  |
| 1   | B     | 896 | ASP  |
| 1   | B     | 898 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 920  | GLN  |
| 1   | B     | 927  | GLU  |
| 1   | B     | 949  | GLU  |
| 1   | B     | 952  | ASN  |
| 1   | B     | 960  | LEU  |
| 1   | B     | 974  | ILE  |
| 1   | B     | 1016 | VAL  |
| 1   | B     | 1040 | ARG  |
| 1   | B     | 1059 | ASN  |
| 1   | C     | 2    | ASN  |
| 1   | C     | 3    | ARG  |
| 1   | C     | 12   | ARG  |
| 1   | C     | 20   | MET  |
| 1   | C     | 39   | THR  |
| 1   | C     | 42   | PHE  |
| 1   | C     | 44   | ARG  |
| 1   | C     | 64   | LEU  |
| 1   | C     | 71   | GLU  |
| 1   | C     | 76   | SER  |
| 1   | C     | 88   | LEU  |
| 1   | C     | 94   | PHE  |
| 1   | C     | 96   | ARG  |
| 1   | C     | 106  | VAL  |
| 1   | C     | 110  | SER  |
| 1   | C     | 111  | LYS  |
| 1   | C     | 115  | MET  |
| 1   | C     | 134  | ILE  |
| 1   | C     | 172  | ARG  |
| 1   | C     | 175  | GLU  |
| 1   | C     | 179  | HIS  |
| 1   | C     | 183  | SER  |
| 1   | C     | 186  | ARG  |
| 1   | C     | 195  | PHE  |
| 1   | C     | 198  | ASP  |
| 1   | C     | 203  | GLU  |
| 1   | C     | 205  | CYS  |
| 1   | C     | 207  | MET  |
| 1   | C     | 248  | ASN  |
| 1   | C     | 251  | THR  |
| 1   | C     | 252  | SER  |
| 1   | C     | 254  | LEU  |
| 1   | C     | 265  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 269 | VAL  |
| 1   | C     | 289 | ILE  |
| 1   | C     | 294 | ARG  |
| 1   | C     | 295 | VAL  |
| 1   | C     | 323 | LEU  |
| 1   | C     | 326 | GLN  |
| 1   | C     | 334 | GLU  |
| 1   | C     | 356 | PHE  |
| 1   | C     | 360 | THR  |
| 1   | C     | 364 | ASP  |
| 1   | C     | 367 | ARG  |
| 1   | C     | 369 | THR  |
| 1   | C     | 377 | ASP  |
| 1   | C     | 392 | ASP  |
| 1   | C     | 393 | SER  |
| 1   | C     | 405 | PHE  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 419 | PHE  |
| 1   | C     | 434 | VAL  |
| 1   | C     | 436 | ARG  |
| 1   | C     | 445 | TYR  |
| 1   | C     | 453 | THR  |
| 1   | C     | 458 | LYS  |
| 1   | C     | 462 | ILE  |
| 1   | C     | 476 | VAL  |
| 1   | C     | 494 | GLU  |
| 1   | C     | 502 | TYR  |
| 1   | C     | 504 | SER  |
| 1   | C     | 507 | SER  |
| 1   | C     | 510 | THR  |
| 1   | C     | 531 | GLU  |
| 1   | C     | 540 | ARG  |
| 1   | C     | 545 | SER  |
| 1   | C     | 547 | LEU  |
| 1   | C     | 549 | THR  |
| 1   | C     | 558 | GLN  |
| 1   | C     | 572 | SER  |
| 1   | C     | 576 | TRP  |
| 1   | C     | 588 | LEU  |
| 1   | C     | 600 | ARG  |
| 1   | C     | 635 | SER  |
| 1   | C     | 651 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 658  | SER  |
| 1   | C     | 668  | ILE  |
| 1   | C     | 682  | ASP  |
| 1   | C     | 698  | GLU  |
| 1   | C     | 717  | LYS  |
| 1   | C     | 737  | HIS  |
| 1   | C     | 781  | LEU  |
| 1   | C     | 792  | THR  |
| 1   | C     | 794  | LEU  |
| 1   | C     | 960  | LEU  |
| 1   | C     | 962  | GLU  |
| 1   | C     | 1016 | VAL  |
| 1   | C     | 1040 | ARG  |
| 1   | C     | 1059 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 2   | ASN  |
| 1   | H     | 43  | HIS  |
| 1   | H     | 82  | HIS  |
| 1   | H     | 112 | HIS  |
| 1   | H     | 221 | HIS  |
| 1   | H     | 226 | HIS  |
| 1   | H     | 333 | GLN  |
| 1   | H     | 337 | HIS  |
| 1   | H     | 354 | ASN  |
| 1   | H     | 415 | ASN  |
| 1   | H     | 479 | ASN  |
| 1   | H     | 558 | GLN  |
| 1   | H     | 741 | HIS  |
| 1   | H     | 787 | ASN  |
| 1   | H     | 842 | GLN  |
| 1   | H     | 890 | ASN  |
| 1   | F     | 2   | ASN  |
| 1   | F     | 43  | HIS  |
| 1   | F     | 82  | HIS  |
| 1   | F     | 112 | HIS  |
| 1   | F     | 179 | HIS  |
| 1   | F     | 221 | HIS  |
| 1   | F     | 226 | HIS  |
| 1   | F     | 333 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 337  | HIS  |
| 1   | F     | 383  | GLN  |
| 1   | F     | 415  | ASN  |
| 1   | F     | 461  | HIS  |
| 1   | F     | 479  | ASN  |
| 1   | F     | 505  | GLN  |
| 1   | F     | 558  | GLN  |
| 1   | F     | 565  | HIS  |
| 1   | F     | 741  | HIS  |
| 1   | F     | 787  | ASN  |
| 1   | F     | 830  | HIS  |
| 1   | F     | 865  | GLN  |
| 1   | F     | 890  | ASN  |
| 1   | F     | 1029 | ASN  |
| 1   | E     | 2    | ASN  |
| 1   | E     | 43   | HIS  |
| 1   | E     | 82   | HIS  |
| 1   | E     | 112  | HIS  |
| 1   | E     | 221  | HIS  |
| 1   | E     | 226  | HIS  |
| 1   | E     | 333  | GLN  |
| 1   | E     | 337  | HIS  |
| 1   | E     | 354  | ASN  |
| 1   | E     | 383  | GLN  |
| 1   | E     | 415  | ASN  |
| 1   | E     | 437  | HIS  |
| 1   | E     | 479  | ASN  |
| 1   | E     | 558  | GLN  |
| 1   | E     | 637  | GLN  |
| 1   | E     | 746  | ASN  |
| 1   | E     | 787  | ASN  |
| 1   | E     | 842  | GLN  |
| 1   | E     | 865  | GLN  |
| 1   | G     | 2    | ASN  |
| 1   | G     | 43   | HIS  |
| 1   | G     | 82   | HIS  |
| 1   | G     | 112  | HIS  |
| 1   | G     | 221  | HIS  |
| 1   | G     | 226  | HIS  |
| 1   | G     | 333  | GLN  |
| 1   | G     | 337  | HIS  |
| 1   | G     | 383  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 415 | ASN  |
| 1   | G     | 461 | HIS  |
| 1   | G     | 479 | ASN  |
| 1   | G     | 558 | GLN  |
| 1   | G     | 737 | HIS  |
| 1   | G     | 746 | ASN  |
| 1   | G     | 787 | ASN  |
| 1   | G     | 830 | HIS  |
| 1   | D     | 2   | ASN  |
| 1   | D     | 43  | HIS  |
| 1   | D     | 82  | HIS  |
| 1   | D     | 112 | HIS  |
| 1   | D     | 221 | HIS  |
| 1   | D     | 226 | HIS  |
| 1   | D     | 333 | GLN  |
| 1   | D     | 337 | HIS  |
| 1   | D     | 354 | ASN  |
| 1   | D     | 383 | GLN  |
| 1   | D     | 415 | ASN  |
| 1   | D     | 479 | ASN  |
| 1   | D     | 486 | HIS  |
| 1   | D     | 558 | GLN  |
| 1   | D     | 741 | HIS  |
| 1   | D     | 787 | ASN  |
| 1   | D     | 842 | GLN  |
| 1   | D     | 890 | ASN  |
| 1   | A     | 2   | ASN  |
| 1   | A     | 43  | HIS  |
| 1   | A     | 82  | HIS  |
| 1   | A     | 112 | HIS  |
| 1   | A     | 179 | HIS  |
| 1   | A     | 221 | HIS  |
| 1   | A     | 226 | HIS  |
| 1   | A     | 333 | GLN  |
| 1   | A     | 337 | HIS  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 461 | HIS  |
| 1   | A     | 479 | ASN  |
| 1   | A     | 558 | GLN  |
| 1   | A     | 565 | HIS  |
| 1   | A     | 741 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 787  | ASN  |
| 1   | A     | 830  | HIS  |
| 1   | A     | 865  | GLN  |
| 1   | A     | 890  | ASN  |
| 1   | A     | 1029 | ASN  |
| 1   | B     | 43   | HIS  |
| 1   | B     | 82   | HIS  |
| 1   | B     | 112  | HIS  |
| 1   | B     | 221  | HIS  |
| 1   | B     | 226  | HIS  |
| 1   | B     | 333  | GLN  |
| 1   | B     | 337  | HIS  |
| 1   | B     | 354  | ASN  |
| 1   | B     | 383  | GLN  |
| 1   | B     | 415  | ASN  |
| 1   | B     | 437  | HIS  |
| 1   | B     | 479  | ASN  |
| 1   | B     | 505  | GLN  |
| 1   | B     | 558  | GLN  |
| 1   | B     | 637  | GLN  |
| 1   | B     | 746  | ASN  |
| 1   | B     | 787  | ASN  |
| 1   | B     | 842  | GLN  |
| 1   | B     | 865  | GLN  |
| 1   | C     | 2    | ASN  |
| 1   | C     | 43   | HIS  |
| 1   | C     | 82   | HIS  |
| 1   | C     | 112  | HIS  |
| 1   | C     | 221  | HIS  |
| 1   | C     | 226  | HIS  |
| 1   | C     | 333  | GLN  |
| 1   | C     | 337  | HIS  |
| 1   | C     | 415  | ASN  |
| 1   | C     | 479  | ASN  |
| 1   | C     | 558  | GLN  |
| 1   | C     | 565  | HIS  |
| 1   | C     | 737  | HIS  |
| 1   | C     | 746  | ASN  |
| 1   | C     | 787  | ASN  |
| 1   | C     | 830  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 1052/1146 (91%) | -0.22  | 11 (1%) 82 82  | 74, 124, 168, 201     | 0     |
| 1   | B     | 1031/1146 (89%) | -0.13  | 34 (3%) 46 44  | 72, 153, 205, 246     | 0     |
| 1   | C     | 941/1146 (82%)  | -0.00  | 46 (4%) 29 28  | 72, 147, 212, 265     | 0     |
| 1   | D     | 1029/1146 (89%) | -0.20  | 12 (1%) 79 78  | 58, 118, 188, 231     | 0     |
| 1   | E     | 1031/1146 (89%) | -0.15  | 35 (3%) 45 43  | 68, 149, 205, 248     | 0     |
| 1   | F     | 1052/1146 (91%) | -0.25  | 8 (0%) 86 86   | 72, 123, 168, 204     | 0     |
| 1   | G     | 942/1146 (82%)  | -0.07  | 32 (3%) 45 43  | 70, 141, 208, 267     | 0     |
| 1   | H     | 1029/1146 (89%) | -0.21  | 7 (0%) 87 88   | 59, 114, 185, 232     | 0     |
| All | All   | 8107/9168 (88%) | -0.16  | 185 (2%) 60 58 | 58, 132, 199, 267     | 0     |

All (185) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 675 | TYR  | 7.6  |
| 1   | C     | 726 | GLY  | 6.5  |
| 1   | C     | 675 | TYR  | 5.9  |
| 1   | E     | 194 | ALA  | 5.7  |
| 1   | B     | 194 | ALA  | 5.6  |
| 1   | B     | 535 | THR  | 5.5  |
| 1   | H     | 901 | GLY  | 5.4  |
| 1   | C     | 718 | PRO  | 5.0  |
| 1   | G     | 719 | GLN  | 5.0  |
| 1   | B     | 572 | SER  | 4.8  |
| 1   | E     | 108 | PRO  | 4.8  |
| 1   | E     | 535 | THR  | 4.8  |
| 1   | E     | 293 | PRO  | 4.7  |
| 1   | E     | 572 | SER  | 4.7  |
| 1   | H     | 903 | THR  | 4.6  |
| 1   | G     | 674 | CYS  | 4.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 718  | PRO  | 4.3  |
| 1   | B     | 581  | PHE  | 4.3  |
| 1   | C     | 719  | GLN  | 4.3  |
| 1   | E     | 575  | MET  | 4.2  |
| 1   | B     | 294  | ARG  | 4.2  |
| 1   | A     | 1018 | LEU  | 4.2  |
| 1   | G     | 734  | VAL  | 4.1  |
| 1   | C     | 206  | VAL  | 4.1  |
| 1   | C     | 721  | ALA  | 4.0  |
| 1   | F     | 692  | TYR  | 4.0  |
| 1   | G     | 650  | ASN  | 3.9  |
| 1   | E     | 193  | ALA  | 3.9  |
| 1   | G     | 730  | ASP  | 3.9  |
| 1   | B     | 293  | PRO  | 3.9  |
| 1   | B     | 108  | PRO  | 3.8  |
| 1   | E     | 294  | ARG  | 3.7  |
| 1   | C     | 734  | VAL  | 3.7  |
| 1   | D     | 909  | SER  | 3.7  |
| 1   | C     | 707  | LEU  | 3.6  |
| 1   | E     | 534  | LEU  | 3.5  |
| 1   | G     | 696  | ALA  | 3.5  |
| 1   | C     | 674  | CYS  | 3.5  |
| 1   | G     | 141  | VAL  | 3.4  |
| 1   | C     | 202  | VAL  | 3.4  |
| 1   | B     | 871  | VAL  | 3.4  |
| 1   | C     | 1022 | LYS  | 3.4  |
| 1   | D     | 843  | GLN  | 3.4  |
| 1   | F     | 1018 | LEU  | 3.4  |
| 1   | H     | 868  | GLY  | 3.4  |
| 1   | E     | 107  | GLY  | 3.3  |
| 1   | B     | 569  | ASN  | 3.3  |
| 1   | H     | 913  | PHE  | 3.3  |
| 1   | G     | 726  | GLY  | 3.2  |
| 1   | B     | 89   | SER  | 3.2  |
| 1   | A     | 692  | TYR  | 3.2  |
| 1   | C     | 291  | VAL  | 3.2  |
| 1   | C     | 292  | ASN  | 3.2  |
| 1   | D     | 903  | THR  | 3.2  |
| 1   | B     | 648  | SER  | 3.1  |
| 1   | C     | 281  | VAL  | 3.1  |
| 1   | C     | 143  | GLY  | 3.1  |
| 1   | B     | 568  | PRO  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 163  | SER  | 3.0  |
| 1   | C     | 216  | ILE  | 3.0  |
| 1   | E     | 568  | PRO  | 3.0  |
| 1   | C     | 201  | TYR  | 3.0  |
| 1   | F     | 1023 | ILE  | 3.0  |
| 1   | C     | 575  | MET  | 3.0  |
| 1   | F     | 1046 | LEU  | 2.9  |
| 1   | C     | 160  | ILE  | 2.9  |
| 1   | B     | 193  | ALA  | 2.9  |
| 1   | A     | 1046 | LEU  | 2.9  |
| 1   | C     | 141  | VAL  | 2.9  |
| 1   | E     | 90   | GLU  | 2.9  |
| 1   | G     | 806  | TRP  | 2.9  |
| 1   | G     | 967  | GLU  | 2.8  |
| 1   | C     | 276  | THR  | 2.8  |
| 1   | G     | 678  | ASP  | 2.8  |
| 1   | C     | 724  | LEU  | 2.8  |
| 1   | G     | 144  | ILE  | 2.8  |
| 1   | C     | 595  | ARG  | 2.8  |
| 1   | G     | 805  | TYR  | 2.8  |
| 1   | H     | 843  | GLN  | 2.8  |
| 1   | D     | 932  | LEU  | 2.8  |
| 1   | C     | 142  | ALA  | 2.8  |
| 1   | E     | 197  | ASN  | 2.7  |
| 1   | E     | 676  | THR  | 2.7  |
| 1   | B     | 534  | LEU  | 2.7  |
| 1   | E     | 709  | ILE  | 2.7  |
| 1   | E     | 998  | VAL  | 2.7  |
| 1   | B     | 575  | MET  | 2.7  |
| 1   | B     | 90   | GLU  | 2.7  |
| 1   | E     | 292  | ASN  | 2.7  |
| 1   | G     | 676  | THR  | 2.7  |
| 1   | C     | 498  | PRO  | 2.7  |
| 1   | A     | 1023 | ILE  | 2.7  |
| 1   | E     | 569  | ASN  | 2.6  |
| 1   | E     | 677  | GLY  | 2.6  |
| 1   | G     | 143  | GLY  | 2.6  |
| 1   | C     | 1018 | LEU  | 2.6  |
| 1   | D     | 868  | GLY  | 2.6  |
| 1   | C     | 133  | VAL  | 2.6  |
| 1   | G     | 207  | MET  | 2.6  |
| 1   | B     | 88   | LEU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 706  | ILE  | 2.6  |
| 1   | G     | 751  | TYR  | 2.6  |
| 1   | B     | 163  | SER  | 2.6  |
| 1   | C     | 293  | PRO  | 2.6  |
| 1   | H     | 910  | VAL  | 2.5  |
| 1   | D     | 870  | ILE  | 2.5  |
| 1   | C     | 551  | VAL  | 2.5  |
| 1   | A     | 689  | ILE  | 2.5  |
| 1   | B     | 107  | GLY  | 2.5  |
| 1   | G     | 142  | ALA  | 2.5  |
| 1   | B     | 162  | ALA  | 2.5  |
| 1   | A     | 677  | GLY  | 2.4  |
| 1   | G     | 813  | TYR  | 2.4  |
| 1   | B     | 1028 | LEU  | 2.4  |
| 1   | F     | 1024 | LEU  | 2.4  |
| 1   | E     | 567  | LEU  | 2.4  |
| 1   | B     | 677  | GLY  | 2.4  |
| 1   | C     | 725  | ILE  | 2.4  |
| 1   | C     | 669  | VAL  | 2.4  |
| 1   | C     | 650  | ASN  | 2.4  |
| 1   | G     | 679  | ILE  | 2.4  |
| 1   | E     | 642  | VAL  | 2.4  |
| 1   | D     | 836  | GLN  | 2.4  |
| 1   | F     | 675  | TYR  | 2.4  |
| 1   | E     | 716  | LEU  | 2.4  |
| 1   | B     | 539  | LEU  | 2.4  |
| 1   | G     | 786  | VAL  | 2.3  |
| 1   | E     | 195  | PHE  | 2.3  |
| 1   | C     | 277  | VAL  | 2.3  |
| 1   | G     | 710  | LYS  | 2.3  |
| 1   | E     | 648  | SER  | 2.3  |
| 1   | D     | 87   | PHE  | 2.3  |
| 1   | C     | 89   | SER  | 2.3  |
| 1   | G     | 740  | THR  | 2.3  |
| 1   | E     | 735  | PRO  | 2.3  |
| 1   | B     | 195  | PHE  | 2.3  |
| 1   | G     | 140  | PRO  | 2.3  |
| 1   | G     | 202  | VAL  | 2.3  |
| 1   | G     | 575  | MET  | 2.2  |
| 1   | C     | 278  | GLU  | 2.2  |
| 1   | F     | 277  | VAL  | 2.2  |
| 1   | G     | 551  | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 538  | THR  | 2.2  |
| 1   | E     | 539  | LEU  | 2.2  |
| 1   | E     | 198  | ASP  | 2.2  |
| 1   | G     | 293  | PRO  | 2.2  |
| 1   | A     | 228  | PHE  | 2.2  |
| 1   | B     | 769  | MET  | 2.2  |
| 1   | E     | 871  | VAL  | 2.2  |
| 1   | C     | 722  | TYR  | 2.2  |
| 1   | D     | 227  | LEU  | 2.2  |
| 1   | E     | 941  | THR  | 2.2  |
| 1   | B     | 650  | ASN  | 2.2  |
| 1   | D     | 901  | GLY  | 2.2  |
| 1   | E     | 749  | TYR  | 2.2  |
| 1   | B     | 295  | VAL  | 2.2  |
| 1   | H     | 867  | PHE  | 2.1  |
| 1   | C     | 559  | ILE  | 2.1  |
| 1   | C     | 118  | ASP  | 2.1  |
| 1   | G     | 10   | ALA  | 2.1  |
| 1   | C     | 805  | TYR  | 2.1  |
| 1   | B     | 197  | ASN  | 2.1  |
| 1   | E     | 581  | PHE  | 2.1  |
| 1   | C     | 975  | SER  | 2.1  |
| 1   | D     | 910  | VAL  | 2.1  |
| 1   | F     | 575  | MET  | 2.1  |
| 1   | A     | 575  | MET  | 2.1  |
| 1   | A     | 913  | PHE  | 2.1  |
| 1   | C     | 740  | THR  | 2.1  |
| 1   | E     | 162  | ALA  | 2.1  |
| 1   | B     | 217  | LEU  | 2.1  |
| 1   | E     | 191  | ALA  | 2.1  |
| 1   | G     | 677  | GLY  | 2.1  |
| 1   | E     | 643  | PHE  | 2.1  |
| 1   | A     | 1049 | GLN  | 2.1  |
| 1   | B     | 161  | LYS  | 2.1  |
| 1   | D     | 216  | ILE  | 2.1  |
| 1   | B     | 498  | PRO  | 2.0  |
| 1   | C     | 703  | GLY  | 2.0  |
| 1   | B     | 191  | ALA  | 2.0  |
| 1   | C     | 266  | MET  | 2.0  |
| 1   | C     | 806  | TRP  | 2.0  |
| 1   | B     | 1008 | MET  | 2.0  |
| 1   | A     | 1024 | LEU  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 473 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.