



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3E8K  
Title : Crystal structure of HK97 Prohead II  
Authors : Gertsman, I.; Speir, J.; Johnson, J.E.  
Deposited on : 2008-08-20  
Resolution : 3.65 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

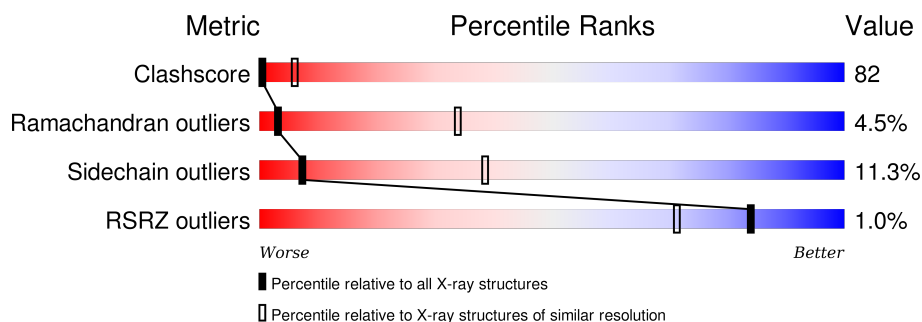
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1125 (3.82-3.50)                                      |
| Ramachandran outliers | 100387                      | 1079 (3.82-3.50)                                      |
| Sidechain outliers    | 100360                      | 1078 (3.82-3.50)                                      |
| RSRZ outliers         | 91569                       | 1017 (3.82-3.50)                                      |

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. 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     | 273    | <div> <div>30%</div> <div>52%</div> <div>11%</div> <div>6%</div> </div>  |
| 1   | B     | 273    | <div> <div>27%</div> <div>49%</div> <div>15%</div> <div>8%</div> </div>  |
| 1   | C     | 273    | <div> <div>31%</div> <div>51%</div> <div>9%</div> <div>9%</div> </div>   |
| 1   | D     | 273    | <div> <div>31%</div> <div>53%</div> <div>8%</div> <div>7%</div> </div>   |
| 1   | E     | 273    | <div> <div>25%</div> <div>56%</div> <div>12%</div> <div>7%</div> </div>  |
| 1   | F     | 273    | <div> <div>23%</div> <div>52%</div> <div>14%</div> <div>9%</div> </div>  |
| 1   | G     | 273    | <div> <div>30%</div> <div>49%</div> <div>10%</div> <div>10%</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13590 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 Major capsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 256      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1978  | 1238 | 346 | 384 | 10 |         |         |       |
| 1   | B     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1934  | 1209 | 339 | 377 | 9  |         |         |       |
| 1   | C     | 248      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1918  | 1198 | 337 | 375 | 8  |         |         |       |
| 1   | D     | 254      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1961  | 1228 | 343 | 381 | 9  |         |         |       |
| 1   | E     | 255      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1970  | 1233 | 345 | 383 | 9  |         |         |       |
| 1   | F     | 248      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1918  | 1198 | 337 | 375 | 8  |         |         |       |
| 1   | G     | 247      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1911  | 1193 | 336 | 374 | 8  |         |         |       |

There are 35 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| A     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| A     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| A     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| A     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| A     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |
| B     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| B     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| B     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| B     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| B     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |
| C     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| C     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| C     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| C     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| C     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |

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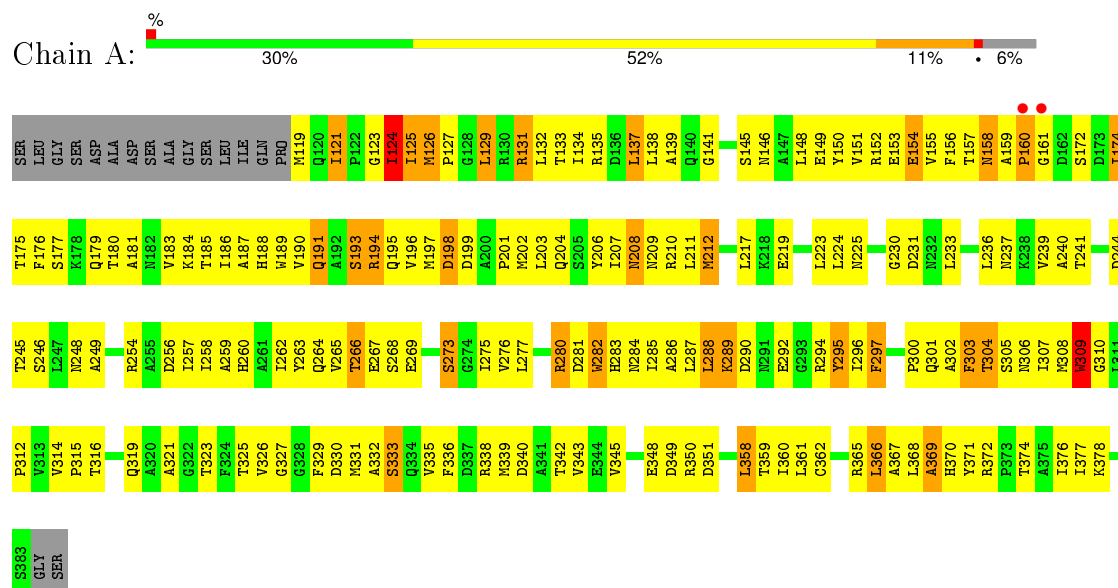
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| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| D     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| D     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| D     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| D     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| D     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |
| E     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| E     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| E     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| E     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| E     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |
| F     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| F     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| F     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| F     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| F     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |
| G     | 159     | ALA      | -      | LINKER     | UNP P49861 |
| G     | 160     | PRO      | -      | LINKER     | UNP P49861 |
| G     | 161     | GLY      | -      | LINKER     | UNP P49861 |
| G     | 162     | ASP      | -      | LINKER     | UNP P49861 |
| G     | 336     | PHE      | TRP    | ENGINEERED | UNP P49861 |

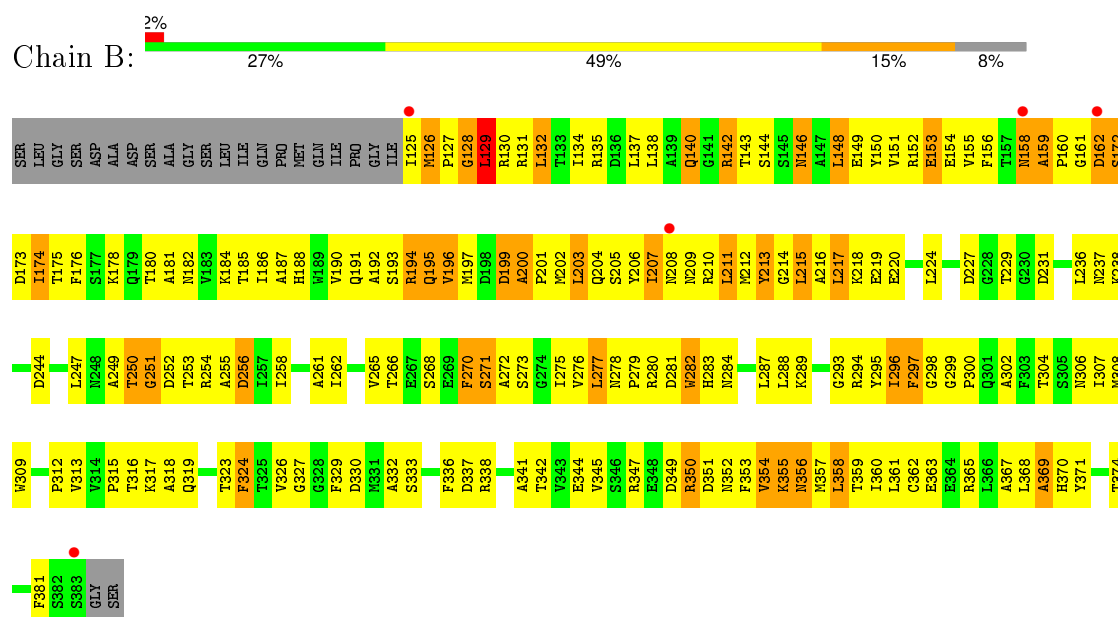
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 ( $\text{RSRZ} > 2$ ). 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.

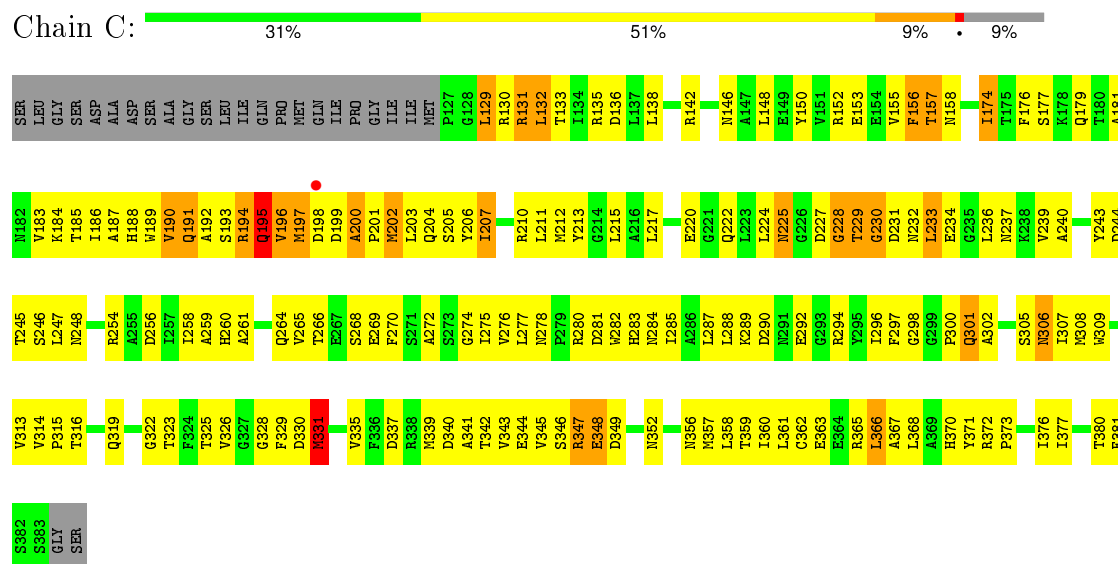
#### • Molecule 1: Major capsid protein



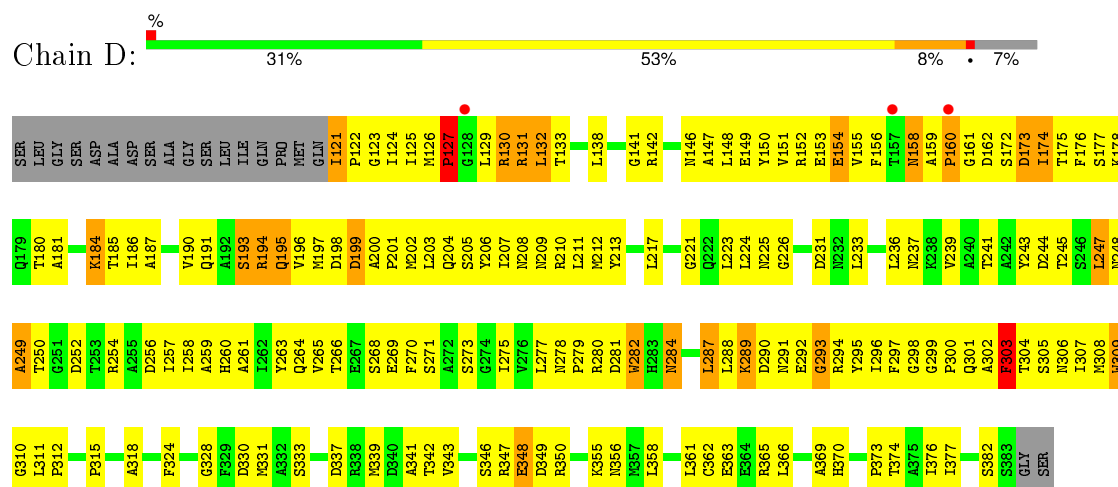
#### • Molecule 1: Major capsid protein



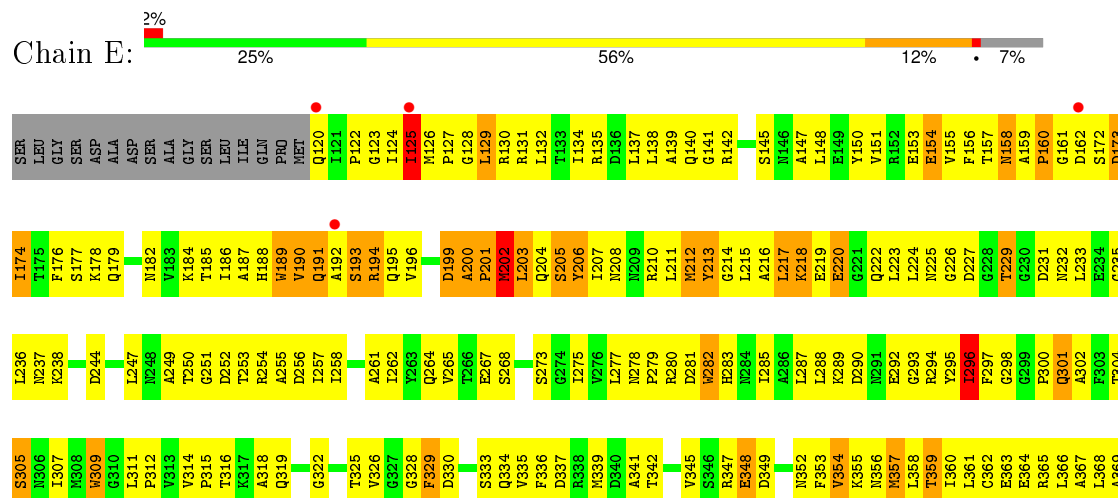
- Molecule 1: Major capsid protein

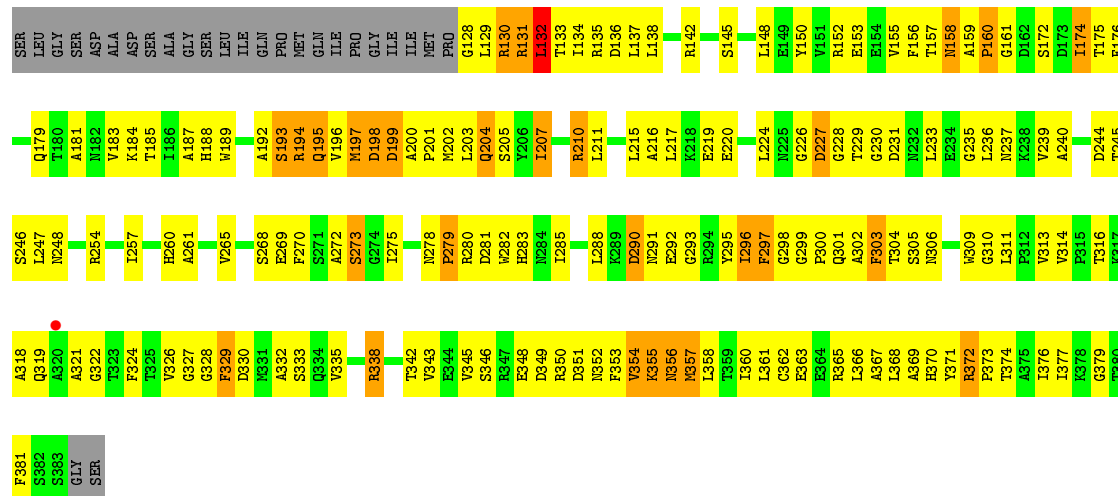


- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | I 2 2 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 553.03Å 574.39Å 587.36Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 35.00 – 3.65<br>34.99 – 3.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 64.8 (35.00-3.65)<br>54.3 (34.99-3.65)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.18  | Depositor        |
| $R_{sym}$   | 0.18  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.97 (at 3.66Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.366 , (Not available)<br>0.311 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.5  | Xtriage          |
| Anisotropy  | 0.013   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.99 , -38.8  | EDS              |
| Estimated twinning fraction   | 0.276 for -h,-l,-k  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.23$ , $\langle L^2 \rangle = 0.09$ | Xtriage          |
| Outliers  | 0 of 656526 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.75  | EDS              |
| Total number of atoms   | 13590   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 32.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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     | 0.41         | 1/2013 (0.0%)  | 0.68        | 2/2730 (0.1%)   |
| 1   | B     | 0.42         | 0/1968         | 0.82        | 11/2669 (0.4%)  |
| 1   | C     | 0.36         | 0/1952         | 0.68        | 2/2647 (0.1%)   |
| 1   | D     | 0.37         | 1/1996 (0.1%)  | 0.68        | 5/2708 (0.2%)   |
| 1   | E     | 0.40         | 1/2005 (0.0%)  | 0.70        | 5/2720 (0.2%)   |
| 1   | F     | 0.42         | 0/1952         | 0.83        | 11/2647 (0.4%)  |
| 1   | G     | 0.40         | 0/1944         | 0.77        | 9/2636 (0.3%)   |
| All | All   | 0.40         | 3/13830 (0.0%) | 0.74        | 45/18757 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 329 | PHE  | C-N   | -5.66 | 1.21        | 1.34     |
| 1   | A     | 212 | MET  | C-N   | -5.28 | 1.21        | 1.34     |
| 1   | D     | 288 | LEU  | C-N   | -5.03 | 1.22        | 1.34     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 200 | ALA  | C-N-CD  | -9.66 | 99.35       | 120.60   |
| 1   | G     | 272 | ALA  | CB-CA-C | -8.25 | 97.73       | 110.10   |
| 1   | G     | 228 | GLY  | N-CA-C  | 8.21  | 133.63      | 113.10   |
| 1   | D     | 193 | SER  | N-CA-CB | -7.66 | 99.01       | 110.50   |
| 1   | G     | 195 | GLN  | N-CA-C  | -7.24 | 91.46       | 111.00   |
| 1   | F     | 194 | ARG  | CB-CA-C | -6.97 | 96.46       | 110.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 196 | VAL  | N-CA-C  | -6.97 | 92.19       | 111.00   |
| 1   | F     | 332 | ALA  | N-CA-CB | -6.81 | 100.56      | 110.10   |
| 1   | B     | 194 | ARG  | CB-CA-C | -6.79 | 96.83       | 110.40   |
| 1   | D     | 226 | GLY  | N-CA-C  | 6.75  | 129.98      | 113.10   |
| 1   | B     | 195 | GLN  | CB-CA-C | -6.71 | 96.97       | 110.40   |
| 1   | F     | 272 | ALA  | CB-CA-C | -6.38 | 100.53      | 110.10   |
| 1   | F     | 204 | GLN  | CB-CA-C | -6.19 | 98.03       | 110.40   |
| 1   | F     | 249 | ALA  | CB-CA-C | 6.18  | 119.37      | 110.10   |
| 1   | B     | 369 | ALA  | O-C-N   | -6.17 | 112.82      | 122.70   |
| 1   | E     | 192 | ALA  | CB-CA-C | -6.17 | 100.85      | 110.10   |
| 1   | A     | 333 | SER  | N-CA-CB | 6.15  | 119.72      | 110.50   |
| 1   | G     | 273 | SER  | N-CA-CB | -5.99 | 101.51      | 110.50   |
| 1   | D     | 250 | THR  | N-CA-C  | 5.96  | 127.09      | 111.00   |
| 1   | G     | 210 | ARG  | N-CA-CB | -5.93 | 99.93       | 110.60   |
| 1   | B     | 251 | GLY  | N-CA-C  | 5.89  | 127.83      | 113.10   |
| 1   | G     | 207 | ILE  | CB-CA-C | -5.89 | 99.82       | 111.60   |
| 1   | F     | 250 | THR  | N-CA-C  | -5.88 | 95.12       | 111.00   |
| 1   | B     | 250 | THR  | CB-CA-C | -5.81 | 95.92       | 111.60   |
| 1   | A     | 249 | ALA  | CB-CA-C | -5.79 | 101.42      | 110.10   |
| 1   | D     | 249 | ALA  | CB-CA-C | -5.73 | 101.51      | 110.10   |
| 1   | B     | 272 | ALA  | N-CA-CB | -5.64 | 102.21      | 110.10   |
| 1   | G     | 227 | ASP  | N-CA-C  | 5.63  | 126.19      | 111.00   |
| 1   | C     | 331 | MET  | N-CA-CB | -5.56 | 100.60      | 110.60   |
| 1   | B     | 203 | LEU  | N-CA-C  | -5.45 | 96.30       | 111.00   |
| 1   | G     | 194 | ARG  | CB-CA-C | -5.42 | 99.57       | 110.40   |
| 1   | B     | 271 | SER  | CB-CA-C | -5.38 | 99.87       | 110.10   |
| 1   | E     | 193 | SER  | N-CA-C  | 5.33  | 125.39      | 111.00   |
| 1   | F     | 212 | MET  | O-C-N   | 5.31  | 131.20      | 122.70   |
| 1   | B     | 128 | GLY  | N-CA-C  | -5.30 | 99.85       | 113.10   |
| 1   | E     | 202 | MET  | N-CA-C  | 5.28  | 125.27      | 111.00   |
| 1   | D     | 123 | GLY  | N-CA-C  | -5.25 | 99.97       | 113.10   |
| 1   | G     | 207 | ILE  | N-CA-C  | 5.25  | 125.16      | 111.00   |
| 1   | B     | 250 | THR  | N-CA-C  | 5.22  | 125.09      | 111.00   |
| 1   | C     | 272 | ALA  | CB-CA-C | -5.21 | 102.29      | 110.10   |
| 1   | F     | 257 | ILE  | CB-CA-C | -5.17 | 101.25      | 111.60   |
| 1   | E     | 203 | LEU  | N-CA-CB | -5.10 | 100.19      | 110.40   |
| 1   | F     | 205 | SER  | N-CA-C  | -5.10 | 97.22       | 111.00   |
| 1   | E     | 218 | LYS  | CB-CA-C | -5.05 | 100.29      | 110.40   |
| 1   | F     | 288 | LEU  | C-N-CA  | -5.01 | 109.18      | 121.70   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 369 | ALA  | Mainchain |

## 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     | 1978  | 0        | 1946     | 311     | 0            |
| 1   | B     | 1934  | 0        | 1896     | 343     | 0            |
| 1   | C     | 1918  | 0        | 1878     | 343     | 0            |
| 1   | D     | 1961  | 0        | 1929     | 330     | 0            |
| 1   | E     | 1970  | 0        | 1937     | 365     | 0            |
| 1   | F     | 1918  | 0        | 1878     | 347     | 0            |
| 1   | G     | 1911  | 0        | 1870     | 285     | 0            |
| All | All   | 13590 | 0        | 13334    | 2213    | 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 82.

All (2213) 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:E:127:PRO:HB2  | 1:E:213:TYR:CD1  | 1.32                     | 1.62              |
| 1:D:125:ILE:HD11 | 1:D:208:ASN:CG   | 1.32                     | 1.49              |
| 1:D:125:ILE:HD11 | 1:D:208:ASN:ND2  | 1.26                     | 1.45              |
| 1:C:196:VAL:HG12 | 1:C:203:LEU:CD1  | 1.44                     | 1.45              |
| 1:B:201:PRO:O    | 1:B:204:GLN:CB   | 1.67                     | 1.41              |
| 1:G:197:MET:CE   | 1:G:358:LEU:HD21 | 1.56                     | 1.36              |
| 1:E:233:LEU:CD1  | 1:E:366:LEU:HD11 | 1.56                     | 1.33              |
| 1:C:213:TYR:CZ   | 1:C:217:LEU:HD11 | 1.64                     | 1.33              |
| 1:D:203:LEU:O    | 1:D:207:ILE:HD13 | 1.24                     | 1.32              |
| 1:E:127:PRO:CB   | 1:E:213:TYR:HD1  | 1.44                     | 1.30              |
| 1:F:199:ASP:O    | 1:F:201:PRO:HD2  | 1.31                     | 1.29              |
| 1:E:206:TYR:O    | 1:E:210:ARG:HB2  | 1.28                     | 1.29              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:HD11 | 1.59                     | 1.29              |
| 1:C:194:ARG:O    | 1:C:196:VAL:N    | 1.66                     | 1.28              |
| 1:F:203:LEU:O    | 1:F:206:TYR:CB   | 1.80                     | 1.27              |
| 1:F:203:LEU:O    | 1:F:206:TYR:HB3  | 1.29                     | 1.26              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:227:ASP:HB3  | 1:E:229:THR:CG2  | 1.65                     | 1.26              |
| 1:B:211:LEU:HD12 | 1:B:211:LEU:O    | 1.28                     | 1.26              |
| 1:E:202:MET:O    | 1:E:205:SER:HB3  | 1.07                     | 1.25              |
| 1:G:197:MET:CE   | 1:G:358:LEU:CD2  | 2.13                     | 1.25              |
| 1:B:193:SER:O    | 1:B:196:VAL:CG2  | 1.87                     | 1.23              |
| 1:C:346:SER:O    | 1:C:359:THR:HG22 | 1.36                     | 1.23              |
| 1:G:278:ASN:OD1  | 1:G:279:PRO:HD2  | 1.38                     | 1.22              |
| 1:A:287:LEU:C    | 1:A:288:LEU:HD23 | 1.58                     | 1.22              |
| 1:A:287:LEU:HD12 | 1:A:287:LEU:O    | 1.39                     | 1.21              |
| 1:D:125:ILE:CD1  | 1:D:208:ASN:OD1  | 1.89                     | 1.20              |
| 1:A:285:ILE:O    | 1:A:288:LEU:CD2  | 1.91                     | 1.19              |
| 1:E:202:MET:HE3  | 1:E:203:LEU:H    | 1.05                     | 1.18              |
| 1:A:285:ILE:O    | 1:A:288:LEU:HD21 | 1.02                     | 1.17              |
| 1:C:210:ARG:NH2  | 1:D:153:GLU:CD   | 1.97                     | 1.17              |
| 1:D:247:LEU:O    | 1:D:247:LEU:HD23 | 1.45                     | 1.17              |
| 1:D:127:PRO:HG3  | 1:D:212:MET:HE3  | 1.23                     | 1.16              |
| 1:A:368:LEU:HD21 | 1:A:370:HIS:NE2  | 1.60                     | 1.16              |
| 1:D:190:VAL:HG12 | 1:D:211:LEU:HD21 | 1.28                     | 1.16              |
| 1:B:215:LEU:CD2  | 1:B:215:LEU:C    | 2.12                     | 1.15              |
| 1:D:127:PRO:HD3  | 1:D:212:MET:HE2  | 1.17                     | 1.15              |
| 1:A:269:GLU:HB3  | 1:F:217:LEU:HD21 | 1.22                     | 1.15              |
| 1:C:129:LEU:HD11 | 1:D:331:MET:CE   | 1.75                     | 1.15              |
| 1:E:127:PRO:CB   | 1:E:213:TYR:CD1  | 2.23                     | 1.14              |
| 1:G:197:MET:HE1  | 1:G:358:LEU:CD2  | 1.74                     | 1.14              |
| 1:D:190:VAL:CG1  | 1:D:211:LEU:HD21 | 1.78                     | 1.14              |
| 1:C:233:LEU:HD23 | 1:C:233:LEU:N    | 1.49                     | 1.14              |
| 1:C:129:LEU:HD11 | 1:D:331:MET:HE1  | 1.21                     | 1.14              |
| 1:C:213:TYR:CE2  | 1:C:217:LEU:HD11 | 1.84                     | 1.13              |
| 1:B:250:THR:HB   | 1:B:251:GLY:CA   | 1.76                     | 1.13              |
| 1:D:125:ILE:CD1  | 1:D:208:ASN:CG   | 2.17                     | 1.13              |
| 1:C:195:GLN:HE22 | 1:C:198:ASP:CB   | 1.60                     | 1.13              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:HD21 | 1.78                     | 1.13              |
| 1:F:194:ARG:O    | 1:F:197:MET:HB3  | 1.48                     | 1.13              |
| 1:D:127:PRO:HD3  | 1:D:212:MET:CE   | 1.76                     | 1.13              |
| 1:F:200:ALA:HB3  | 1:F:201:PRO:HD3  | 1.20                     | 1.13              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:CD1  | 2.22                     | 1.13              |
| 1:B:131:ARG:NH2  | 1:B:220:GLU:OE1  | 1.81                     | 1.12              |
| 1:F:142:ARG:HG3  | 1:F:337:ASP:HB2  | 1.16                     | 1.12              |
| 1:D:125:ILE:CD1  | 1:D:208:ASN:ND2  | 2.12                     | 1.12              |
| 1:G:338:ARG:HH11 | 1:G:338:ARG:CG   | 1.58                     | 1.12              |
| 1:B:201:PRO:C    | 1:B:204:GLN:H    | 1.52                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:215:LEU:HD23 | 1:B:215:LEU:C    | 1.65                     | 1.11              |
| 1:C:225:ASN:HB3  | 1:C:237:ASN:HD22 | 1.08                     | 1.11              |
| 1:E:202:MET:HE3  | 1:E:203:LEU:N    | 1.65                     | 1.11              |
| 1:B:277:LEU:HD23 | 1:B:277:LEU:N    | 1.52                     | 1.11              |
| 1:F:343:VAL:HG12 | 1:F:362:CYS:HB3  | 1.24                     | 1.11              |
| 1:G:198:ASP:O    | 1:G:199:ASP:OD1  | 1.69                     | 1.10              |
| 1:F:203:LEU:C    | 1:F:203:LEU:CD2  | 2.18                     | 1.10              |
| 1:F:142:ARG:CG   | 1:F:337:ASP:HB2  | 1.79                     | 1.10              |
| 1:B:193:SER:O    | 1:B:196:VAL:HG23 | 1.49                     | 1.10              |
| 1:B:212:MET:O    | 1:B:215:LEU:N    | 1.83                     | 1.10              |
| 1:E:215:LEU:O    | 1:E:218:LYS:HB3  | 1.52                     | 1.09              |
| 1:E:227:ASP:HB3  | 1:E:229:THR:HG23 | 1.31                     | 1.09              |
| 1:B:127:PRO:HA   | 1:B:129:LEU:HD13 | 1.18                     | 1.09              |
| 1:B:201:PRO:O    | 1:B:204:GLN:HB3  | 1.44                     | 1.09              |
| 1:E:194:ARG:HA   | 1:E:358:LEU:CD1  | 1.82                     | 1.09              |
| 1:A:125:ILE:CG2  | 1:A:204:GLN:NE2  | 2.15                     | 1.09              |
| 1:F:203:LEU:C    | 1:F:203:LEU:HD23 | 1.68                     | 1.09              |
| 1:C:287:LEU:HD22 | 1:C:300:PRO:HB3  | 1.35                     | 1.09              |
| 1:A:288:LEU:HD23 | 1:A:288:LEU:N    | 1.56                     | 1.09              |
| 1:B:296:ILE:HD13 | 1:B:296:ILE:H    | 1.16                     | 1.08              |
| 1:C:196:VAL:HG13 | 1:C:203:LEU:HD21 | 1.08                     | 1.08              |
| 1:E:202:MET:O    | 1:E:205:SER:CB   | 2.01                     | 1.08              |
| 1:A:285:ILE:C    | 1:A:288:LEU:HD21 | 1.74                     | 1.08              |
| 1:G:129:LEU:CD2  | 1:G:131:ARG:HB2  | 1.84                     | 1.08              |
| 1:F:247:LEU:HD23 | 1:F:247:LEU:N    | 1.48                     | 1.08              |
| 1:D:127:PRO:CD   | 1:D:212:MET:HE2  | 1.82                     | 1.07              |
| 1:G:158:ASN:OD1  | 1:G:172:SER:HA   | 1.53                     | 1.07              |
| 1:C:130:ARG:HG3  | 1:D:271:SER:HB2  | 1.36                     | 1.07              |
| 1:A:197:MET:SD   | 1:A:203:LEU:HD13 | 1.95                     | 1.07              |
| 1:C:194:ARG:NH1  | 1:C:347:ARG:HH22 | 1.51                     | 1.07              |
| 1:A:153:GLU:OE1  | 1:F:210:ARG:NH2  | 1.88                     | 1.07              |
| 1:E:203:LEU:O    | 1:E:206:TYR:N    | 1.85                     | 1.06              |
| 1:D:122:PRO:HG3  | 1:D:343:VAL:O    | 1.54                     | 1.06              |
| 1:D:127:PRO:HG3  | 1:D:212:MET:CE   | 1.83                     | 1.06              |
| 1:G:129:LEU:HD22 | 1:G:131:ARG:HB2  | 1.12                     | 1.06              |
| 1:B:250:THR:CB   | 1:B:251:GLY:HA3  | 1.78                     | 1.06              |
| 1:C:232:ASN:C    | 1:C:233:LEU:HD23 | 1.76                     | 1.05              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:CD2  | 2.35                     | 1.05              |
| 1:D:129:LEU:HD22 | 1:D:130:ARG:H    | 1.16                     | 1.05              |
| 1:A:202:MET:O    | 1:A:206:TYR:N    | 1.88                     | 1.05              |
| 1:C:195:GLN:NE2  | 1:C:198:ASP:HB3  | 1.70                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:329:PHE:HA   | 1:G:332:ALA:HB3  | 1.39                     | 1.04              |
| 1:C:187:ALA:HB2  | 1:C:363:GLU:HA   | 1.39                     | 1.04              |
| 1:F:324:PHE:HD2  | 1:F:381:PHE:CE1  | 1.73                     | 1.04              |
| 1:C:203:LEU:O    | 1:C:206:TYR:N    | 1.88                     | 1.04              |
| 1:D:203:LEU:O    | 1:D:207:ILE:CD1  | 2.04                     | 1.04              |
| 1:F:246:SER:C    | 1:F:247:LEU:HD23 | 1.77                     | 1.04              |
| 1:B:201:PRO:O    | 1:B:204:GLN:CA   | 2.07                     | 1.03              |
| 1:F:194:ARG:NH1  | 1:F:347:ARG:NH1  | 2.06                     | 1.03              |
| 1:D:249:ALA:O    | 1:D:252:ASP:OD2  | 1.75                     | 1.03              |
| 1:C:196:VAL:HG13 | 1:C:203:LEU:CD2  | 1.87                     | 1.03              |
| 1:G:158:ASN:HD22 | 1:G:159:ALA:N    | 1.54                     | 1.03              |
| 1:B:158:ASN:HB2  | 1:B:172:SER:HA   | 1.35                     | 1.03              |
| 1:B:201:PRO:O    | 1:B:204:GLN:N    | 1.91                     | 1.03              |
| 1:C:195:GLN:HE22 | 1:C:198:ASP:HB3  | 0.89                     | 1.03              |
| 1:A:287:LEU:C    | 1:A:288:LEU:CD2  | 2.27                     | 1.03              |
| 1:B:215:LEU:HD23 | 1:B:215:LEU:O    | 1.56                     | 1.02              |
| 1:A:127:PRO:HB3  | 1:A:212:MET:HB3  | 1.39                     | 1.02              |
| 1:E:233:LEU:HD11 | 1:E:366:LEU:HD11 | 1.03                     | 1.02              |
| 1:C:201:PRO:O    | 1:C:204:GLN:HB2  | 1.59                     | 1.02              |
| 1:F:210:ARG:HG2  | 1:F:210:ARG:HH11 | 1.20                     | 1.01              |
| 1:D:125:ILE:HD11 | 1:D:208:ASN:HD21 | 1.26                     | 1.01              |
| 1:F:131:ARG:NH2  | 1:F:220:GLU:OE1  | 1.93                     | 1.01              |
| 1:B:217:LEU:C    | 1:B:217:LEU:CD1  | 2.30                     | 1.00              |
| 1:B:250:THR:HB   | 1:B:251:GLY:HA3  | 1.01                     | 1.00              |
| 1:F:203:LEU:HD22 | 1:F:204:GLN:N    | 1.74                     | 1.00              |
| 1:B:201:PRO:O    | 1:B:204:GLN:HB2  | 1.61                     | 1.00              |
| 1:G:296:ILE:HG22 | 1:G:297:PHE:N    | 1.76                     | 1.00              |
| 1:E:194:ARG:HA   | 1:E:358:LEU:HD13 | 1.39                     | 1.00              |
| 1:A:368:LEU:CD2  | 1:A:370:HIS:NE2  | 2.24                     | 1.00              |
| 1:A:125:ILE:CG2  | 1:A:204:GLN:HE22 | 1.71                     | 1.00              |
| 1:E:227:ASP:HB3  | 1:E:229:THR:HG21 | 1.41                     | 1.00              |
| 1:D:127:PRO:CD   | 1:D:212:MET:CE   | 2.36                     | 1.00              |
| 1:D:247:LEU:HD23 | 1:D:247:LEU:C    | 1.81                     | 1.00              |
| 1:F:324:PHE:CD2  | 1:F:381:PHE:HE1  | 1.78                     | 1.00              |
| 1:G:199:ASP:C    | 1:G:201:PRO:HD2  | 1.82                     | 0.99              |
| 1:G:338:ARG:HH11 | 1:G:338:ARG:HG3  | 0.86                     | 0.99              |
| 1:B:217:LEU:HD13 | 1:B:217:LEU:C    | 1.77                     | 0.99              |
| 1:C:194:ARG:O    | 1:C:196:VAL:HG23 | 1.62                     | 0.99              |
| 1:G:303:PHE:HD2  | 1:G:304:THR:H    | 1.07                     | 0.99              |
| 1:B:195:GLN:C    | 1:B:197:MET:N    | 2.06                     | 0.99              |
| 1:A:125:ILE:HG21 | 1:A:204:GLN:NE2  | 1.74                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:184:LYS:NZ   | 1:G:230:GLY:O    | 1.93                     | 0.99              |
| 1:A:233:LEU:HD11 | 1:A:366:LEU:HD11 | 1.43                     | 0.98              |
| 1:E:125:ILE:CD1  | 1:E:127:PRO:HD3  | 1.92                     | 0.98              |
| 1:F:204:GLN:C    | 1:F:206:TYR:H    | 1.63                     | 0.98              |
| 1:D:127:PRO:CG   | 1:D:212:MET:CE   | 2.42                     | 0.98              |
| 1:F:329:PHE:N    | 1:F:329:PHE:HD1  | 1.62                     | 0.98              |
| 1:C:202:MET:O    | 1:C:205:SER:N    | 1.96                     | 0.98              |
| 1:C:213:TYR:CE2  | 1:C:217:LEU:HD21 | 1.97                     | 0.98              |
| 1:G:202:MET:O    | 1:G:205:SER:OG   | 1.81                     | 0.97              |
| 1:B:249:ALA:HB3  | 1:B:252:ASP:OD2  | 1.64                     | 0.97              |
| 1:G:227:ASP:O    | 1:G:227:ASP:OD1  | 1.82                     | 0.97              |
| 1:F:244:ASP:OD2  | 1:F:247:LEU:HD21 | 1.63                     | 0.97              |
| 1:F:202:MET:O    | 1:F:205:SER:N    | 1.97                     | 0.97              |
| 1:G:301:GLN:HG3  | 1:G:302:ALA:H    | 1.26                     | 0.97              |
| 1:E:157:THR:HG22 | 1:E:267:GLU:HG3  | 1.45                     | 0.97              |
| 1:D:206:TYR:HH   | 1:E:371:TYR:HE2  | 1.13                     | 0.96              |
| 1:D:127:PRO:CG   | 1:D:212:MET:HE3  | 1.95                     | 0.96              |
| 1:C:270:PHE:HE2  | 1:C:331:MET:HG2  | 1.30                     | 0.96              |
| 1:C:201:PRO:O    | 1:C:204:GLN:N    | 1.99                     | 0.95              |
| 1:C:130:ARG:CG   | 1:D:271:SER:HB2  | 1.95                     | 0.95              |
| 1:E:233:LEU:HD11 | 1:E:366:LEU:CD1  | 1.96                     | 0.95              |
| 1:C:287:LEU:HD22 | 1:C:300:PRO:CB   | 1.96                     | 0.95              |
| 1:A:125:ILE:HG23 | 1:A:204:GLN:HE22 | 1.32                     | 0.94              |
| 1:D:282:TRP:HE1  | 1:D:304:THR:HA   | 1.32                     | 0.94              |
| 1:G:129:LEU:HD22 | 1:G:131:ARG:CB   | 1.97                     | 0.94              |
| 1:F:200:ALA:O    | 1:F:202:MET:N    | 2.01                     | 0.94              |
| 1:G:301:GLN:HG3  | 1:G:302:ALA:N    | 1.82                     | 0.94              |
| 1:B:288:LEU:O    | 1:B:296:ILE:HD11 | 1.68                     | 0.94              |
| 1:E:227:ASP:CB   | 1:E:229:THR:HG23 | 1.98                     | 0.94              |
| 1:D:125:ILE:CD1  | 1:D:208:ASN:HD21 | 1.77                     | 0.93              |
| 1:E:157:THR:HG22 | 1:E:267:GLU:CG   | 1.98                     | 0.93              |
| 1:D:125:ILE:HD11 | 1:D:208:ASN:OD1  | 1.57                     | 0.93              |
| 1:F:203:LEU:O    | 1:F:203:LEU:HD23 | 1.66                     | 0.93              |
| 1:C:183:VAL:HA   | 1:C:367:ALA:HB2  | 1.49                     | 0.93              |
| 1:F:345:VAL:HG13 | 1:F:358:LEU:HD21 | 1.50                     | 0.93              |
| 1:E:207:ILE:HG13 | 1:E:208:ASN:H    | 1.32                     | 0.93              |
| 1:A:195:GLN:HG3  | 1:A:196:VAL:HG23 | 1.51                     | 0.93              |
| 1:B:207:ILE:O    | 1:B:211:LEU:HB3  | 1.67                     | 0.93              |
| 1:F:197:MET:SD   | 1:F:197:MET:O    | 2.27                     | 0.93              |
| 1:C:366:LEU:HD22 | 1:C:367:ALA:H    | 1.32                     | 0.93              |
| 1:G:174:ILE:H    | 1:G:174:ILE:HD13 | 1.33                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:329:PHE:HD2  | 1:G:329:PHE:H    | 0.98                     | 0.93              |
| 1:C:213:TYR:HE2  | 1:C:217:LEU:HD21 | 1.34                     | 0.92              |
| 1:B:288:LEU:O    | 1:B:296:ILE:CD1  | 2.16                     | 0.92              |
| 1:A:265:VAL:HG22 | 1:A:377:ILE:HD13 | 1.51                     | 0.92              |
| 1:F:253:THR:HG23 | 1:F:256:ASP:OD1  | 1.68                     | 0.92              |
| 1:B:277:LEU:CD2  | 1:B:277:LEU:N    | 2.29                     | 0.92              |
| 1:G:197:MET:HE2  | 1:G:358:LEU:CD2  | 1.96                     | 0.92              |
| 1:B:195:GLN:C    | 1:B:197:MET:H    | 1.66                     | 0.92              |
| 1:G:197:MET:HE3  | 1:G:358:LEU:HD21 | 1.52                     | 0.92              |
| 1:E:210:ARG:HH22 | 1:F:153:GLU:CD   | 1.73                     | 0.92              |
| 1:F:225:ASN:HB3  | 1:F:237:ASN:HD22 | 1.33                     | 0.92              |
| 1:G:351:ASP:O    | 1:G:355:LYS:HG2  | 1.70                     | 0.91              |
| 1:F:200:ALA:CB   | 1:F:201:PRO:HD3  | 2.00                     | 0.91              |
| 1:G:304:THR:HG22 | 1:G:305:SER:H    | 1.36                     | 0.91              |
| 1:B:211:LEU:HD12 | 1:B:211:LEU:C    | 1.72                     | 0.91              |
| 1:F:194:ARG:NH1  | 1:F:347:ARG:HH12 | 1.64                     | 0.91              |
| 1:G:132:LEU:HB2  | 1:G:136:ASP:HB2  | 1.52                     | 0.91              |
| 1:F:200:ALA:HB3  | 1:F:201:PRO:CD   | 1.99                     | 0.91              |
| 1:A:174:ILE:H    | 1:A:174:ILE:HD13 | 1.33                     | 0.91              |
| 1:G:303:PHE:HD2  | 1:G:304:THR:N    | 1.69                     | 0.91              |
| 1:G:329:PHE:HA   | 1:G:332:ALA:CB   | 1.99                     | 0.91              |
| 1:C:213:TYR:CE1  | 1:C:217:LEU:HD11 | 2.05                     | 0.91              |
| 1:A:263:TYR:OH   | 1:A:267:GLU:OE2  | 1.87                     | 0.91              |
| 1:F:199:ASP:O    | 1:F:201:PRO:CD   | 2.18                     | 0.90              |
| 1:C:233:LEU:HD11 | 1:C:366:LEU:CD1  | 2.01                     | 0.90              |
| 1:E:174:ILE:H    | 1:E:174:ILE:HD13 | 1.36                     | 0.90              |
| 1:D:126:MET:SD   | 1:D:127:PRO:HD2  | 2.11                     | 0.90              |
| 1:F:202:MET:SD   | 1:F:203:LEU:N    | 2.45                     | 0.90              |
| 1:C:347:ARG:O    | 1:C:349:ASP:N    | 2.05                     | 0.90              |
| 1:E:233:LEU:HD13 | 1:E:366:LEU:HD11 | 1.53                     | 0.90              |
| 1:G:197:MET:HE1  | 1:G:358:LEU:HD21 | 1.41                     | 0.90              |
| 1:E:345:VAL:HG22 | 1:E:360:ILE:HA   | 1.54                     | 0.90              |
| 1:G:338:ARG:NH1  | 1:G:338:ARG:HG3  | 1.67                     | 0.89              |
| 1:F:174:ILE:H    | 1:F:174:ILE:HD13 | 1.36                     | 0.89              |
| 1:F:211:LEU:HD21 | 1:F:362:CYS:SG   | 2.13                     | 0.89              |
| 1:F:194:ARG:O    | 1:F:197:MET:CB   | 2.20                     | 0.89              |
| 1:D:194:ARG:HG2  | 1:D:195:GLN:H    | 1.37                     | 0.89              |
| 1:B:195:GLN:O    | 1:B:197:MET:N    | 2.04                     | 0.89              |
| 1:C:206:TYR:OH   | 1:C:210:ARG:NH1  | 2.05                     | 0.89              |
| 1:E:220:GLU:OE2  | 1:E:316:THR:CG2  | 2.21                     | 0.89              |
| 1:C:344:GLU:HB2  | 1:C:361:LEU:HD11 | 1.55                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:206:TYR:O    | 1:E:210:ARG:CB   | 2.19                     | 0.89              |
| 1:G:327:GLY:O    | 1:G:329:PHE:CD2  | 2.25                     | 0.89              |
| 1:B:155:VAL:CG1  | 1:B:374:THR:HB   | 2.03                     | 0.89              |
| 1:F:354:VAL:HG13 | 1:F:355:LYS:HG3  | 1.52                     | 0.89              |
| 1:E:155:VAL:HG23 | 1:E:174:ILE:HG22 | 1.53                     | 0.89              |
| 1:F:247:LEU:N    | 1:F:247:LEU:CD2  | 2.30                     | 0.88              |
| 1:G:200:ALA:O    | 1:G:204:GLN:N    | 2.06                     | 0.88              |
| 1:C:233:LEU:N    | 1:C:233:LEU:CD2  | 2.30                     | 0.88              |
| 1:D:190:VAL:HG12 | 1:D:211:LEU:CD2  | 2.03                     | 0.88              |
| 1:D:247:LEU:HD21 | 1:D:260:HIS:HB3  | 1.56                     | 0.88              |
| 1:F:343:VAL:CG1  | 1:F:362:CYS:HB3  | 2.01                     | 0.88              |
| 1:B:127:PRO:CA   | 1:B:129:LEU:HD13 | 2.02                     | 0.88              |
| 1:A:195:GLN:HG3  | 1:A:196:VAL:H    | 1.37                     | 0.88              |
| 1:G:197:MET:HE2  | 1:G:358:LEU:HD22 | 1.55                     | 0.88              |
| 1:F:155:VAL:HG23 | 1:F:174:ILE:HG22 | 1.56                     | 0.87              |
| 1:C:366:LEU:HD22 | 1:C:367:ALA:N    | 1.89                     | 0.87              |
| 1:E:137:LEU:HD22 | 1:E:329:PHE:HB2  | 1.56                     | 0.87              |
| 1:F:131:ARG:HD2  | 1:F:315:PRO:O    | 1.74                     | 0.87              |
| 1:B:185:THR:HG22 | 1:B:365:ARG:HG2  | 1.54                     | 0.87              |
| 1:B:155:VAL:CG1  | 1:B:374:THR:CB   | 2.52                     | 0.87              |
| 1:B:345:VAL:HG12 | 1:B:360:ILE:HA   | 1.56                     | 0.87              |
| 1:E:295:TYR:OH   | 1:F:256:ASP:OD2  | 1.91                     | 0.87              |
| 1:C:194:ARG:CZ   | 1:C:347:ARG:HH22 | 1.88                     | 0.87              |
| 1:A:155:VAL:HG23 | 1:A:174:ILE:HG22 | 1.54                     | 0.87              |
| 1:B:342:THR:O    | 1:B:362:CYS:HA   | 1.72                     | 0.87              |
| 1:F:361:LEU:O    | 1:F:361:LEU:HD13 | 1.75                     | 0.87              |
| 1:C:130:ARG:HG3  | 1:D:271:SER:CB   | 2.04                     | 0.86              |
| 1:C:287:LEU:CD2  | 1:C:300:PRO:CB   | 2.52                     | 0.86              |
| 1:A:158:ASN:CG   | 1:A:172:SER:HA   | 1.94                     | 0.86              |
| 1:G:200:ALA:N    | 1:G:201:PRO:CD   | 2.38                     | 0.86              |
| 1:A:343:VAL:HG12 | 1:A:362:CYS:HB2  | 1.54                     | 0.86              |
| 1:A:141:GLY:O    | 1:A:336:PHE:HA   | 1.74                     | 0.86              |
| 1:B:159:ALA:O    | 1:B:172:SER:HB3  | 1.73                     | 0.86              |
| 1:E:158:ASN:CG   | 1:E:172:SER:HA   | 1.95                     | 0.86              |
| 1:C:213:TYR:CE2  | 1:C:217:LEU:CD1  | 2.58                     | 0.86              |
| 1:G:316:THR:HG22 | 1:G:318:ALA:H    | 1.37                     | 0.86              |
| 1:E:233:LEU:CD1  | 1:E:366:LEU:CD1  | 2.51                     | 0.86              |
| 1:G:155:VAL:HG11 | 1:G:374:THR:OG1  | 1.75                     | 0.86              |
| 1:D:122:PRO:HG3  | 1:D:343:VAL:HG23 | 1.58                     | 0.86              |
| 1:G:199:ASP:HB3  | 1:G:202:MET:HB3  | 1.56                     | 0.85              |
| 1:C:357:MET:HE1  | 1:D:178:LYS:HG2  | 1.59                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:155:VAL:HG12 | 1:D:374:THR:OG1  | 1.76                     | 0.85              |
| 1:E:207:ILE:HG13 | 1:E:208:ASN:N    | 1.91                     | 0.85              |
| 1:A:300:PRO:HA   | 1:A:303:PHE:HB3  | 1.59                     | 0.85              |
| 1:C:197:MET:SD   | 1:C:358:LEU:CD1  | 2.65                     | 0.85              |
| 1:G:197:MET:CE   | 1:G:358:LEU:HD22 | 2.04                     | 0.85              |
| 1:D:207:ILE:HG13 | 1:D:211:LEU:HD12 | 1.57                     | 0.85              |
| 1:C:203:LEU:O    | 1:C:206:TYR:CB   | 2.25                     | 0.85              |
| 1:C:258:ILE:HD11 | 1:C:275:ILE:HG12 | 1.59                     | 0.85              |
| 1:E:202:MET:CE   | 1:E:203:LEU:N    | 2.39                     | 0.85              |
| 1:G:329:PHE:HD2  | 1:G:329:PHE:N    | 1.75                     | 0.84              |
| 1:B:194:ARG:NH2  | 1:B:347:ARG:NH2  | 2.25                     | 0.84              |
| 1:B:215:LEU:C    | 1:B:215:LEU:HD22 | 1.96                     | 0.84              |
| 1:D:194:ARG:HG2  | 1:D:195:GLN:N    | 1.91                     | 0.84              |
| 1:B:132:LEU:HD23 | 1:B:132:LEU:H    | 1.42                     | 0.84              |
| 1:B:127:PRO:C    | 1:B:129:LEU:H    | 1.81                     | 0.84              |
| 1:B:156:PHE:HB3  | 1:B:158:ASN:OD1  | 1.78                     | 0.84              |
| 1:E:213:TYR:O    | 1:E:217:LEU:HB2  | 1.77                     | 0.84              |
| 1:F:203:LEU:CD2  | 1:F:204:GLN:N    | 2.38                     | 0.84              |
| 1:E:220:GLU:OE2  | 1:E:316:THR:HG21 | 1.77                     | 0.83              |
| 1:E:355:LYS:O    | 1:E:357:MET:HG2  | 1.78                     | 0.83              |
| 1:A:296:ILE:HG23 | 1:A:297:PHE:CD2  | 2.12                     | 0.83              |
| 1:D:158:ASN:CG   | 1:D:172:SER:HA   | 1.97                     | 0.83              |
| 1:B:296:ILE:CD1  | 1:B:296:ILE:H    | 1.91                     | 0.83              |
| 1:F:158:ASN:CG   | 1:F:172:SER:HA   | 1.98                     | 0.83              |
| 1:B:194:ARG:HH22 | 1:B:347:ARG:HH22 | 1.23                     | 0.83              |
| 1:F:142:ARG:HG2  | 1:F:337:ASP:O    | 1.78                     | 0.83              |
| 1:G:132:LEU:HB2  | 1:G:136:ASP:CB   | 2.08                     | 0.83              |
| 1:E:210:ARG:NH2  | 1:F:153:GLU:OE1  | 2.10                     | 0.83              |
| 1:C:196:VAL:HG12 | 1:C:203:LEU:CG   | 2.08                     | 0.83              |
| 1:F:202:MET:HG3  | 1:F:203:LEU:H    | 1.43                     | 0.83              |
| 1:C:233:LEU:CD1  | 1:C:366:LEU:HD11 | 2.09                     | 0.82              |
| 1:D:132:LEU:H    | 1:D:132:LEU:HD23 | 1.41                     | 0.82              |
| 1:B:217:LEU:HD13 | 1:B:217:LEU:O    | 1.78                     | 0.82              |
| 1:A:194:ARG:O    | 1:A:198:ASP:HB2  | 1.79                     | 0.82              |
| 1:A:159:ALA:HB1  | 1:A:160:PRO:HD2  | 1.62                     | 0.82              |
| 1:B:316:THR:HG22 | 1:B:318:ALA:H    | 1.44                     | 0.82              |
| 1:C:210:ARG:NH2  | 1:D:153:GLU:OE1  | 2.03                     | 0.82              |
| 1:A:275:ILE:HD12 | 1:A:308:MET:SD   | 2.20                     | 0.82              |
| 1:F:194:ARG:HH12 | 1:F:347:ARG:HH12 | 1.26                     | 0.82              |
| 1:D:129:LEU:HD22 | 1:D:130:ARG:N    | 1.94                     | 0.82              |
| 1:B:131:ARG:NH2  | 1:B:220:GLU:CD   | 2.32                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:332:ALA:HB1  | 1:G:376:ILE:HD11 | 1.62                     | 0.82              |
| 1:G:198:ASP:O    | 1:G:199:ASP:CG   | 2.16                     | 0.82              |
| 1:E:138:LEU:HD23 | 1:E:329:PHE:HB3  | 1.59                     | 0.82              |
| 1:A:376:ILE:C    | 1:A:377:ILE:HD12 | 1.99                     | 0.81              |
| 1:B:277:LEU:HD23 | 1:B:277:LEU:H    | 1.43                     | 0.81              |
| 1:A:129:LEU:H    | 1:A:129:LEU:HD23 | 1.45                     | 0.81              |
| 1:D:202:MET:HA   | 1:D:205:SER:OG   | 1.80                     | 0.81              |
| 1:C:270:PHE:CE2  | 1:C:331:MET:HG2  | 2.14                     | 0.81              |
| 1:E:132:LEU:H    | 1:E:132:LEU:HD23 | 1.43                     | 0.81              |
| 1:F:203:LEU:O    | 1:F:206:TYR:HB2  | 1.76                     | 0.81              |
| 1:G:138:LEU:HD23 | 1:G:329:PHE:HB3  | 1.61                     | 0.81              |
| 1:F:129:LEU:HD12 | 1:F:129:LEU:H    | 1.45                     | 0.81              |
| 1:G:158:ASN:ND2  | 1:G:159:ALA:N    | 2.29                     | 0.81              |
| 1:B:207:ILE:O    | 1:B:211:LEU:CB   | 2.28                     | 0.81              |
| 1:F:194:ARG:CZ   | 1:F:347:ARG:NH1  | 2.44                     | 0.81              |
| 1:D:190:VAL:CG1  | 1:D:211:LEU:CD2  | 2.59                     | 0.81              |
| 1:G:290:ASP:HB3  | 1:G:292:GLU:HB3  | 1.63                     | 0.81              |
| 1:A:153:GLU:CD   | 1:F:210:ARG:HH21 | 1.84                     | 0.81              |
| 1:F:287:LEU:HD23 | 1:F:287:LEU:H    | 1.46                     | 0.81              |
| 1:D:155:VAL:CG1  | 1:D:374:THR:CB   | 2.60                     | 0.80              |
| 1:D:155:VAL:CG1  | 1:D:374:THR:OG1  | 2.29                     | 0.80              |
| 1:B:336:PHE:HB2  | 1:B:367:ALA:HB3  | 1.63                     | 0.80              |
| 1:D:303:PHE:HA   | 1:D:306:ASN:HB3  | 1.63                     | 0.80              |
| 1:E:211:LEU:HD21 | 1:E:360:ILE:HD13 | 1.63                     | 0.80              |
| 1:E:215:LEU:O    | 1:E:218:LYS:CB   | 2.27                     | 0.80              |
| 1:C:207:ILE:HA   | 1:C:211:LEU:HB3  | 1.63                     | 0.80              |
| 1:F:327:GLY:N    | 1:F:329:PHE:HE1  | 1.79                     | 0.80              |
| 1:E:322:GLY:HA2  | 1:E:381:PHE:HB2  | 1.63                     | 0.80              |
| 1:C:366:LEU:C    | 1:C:366:LEU:HD13 | 2.01                     | 0.80              |
| 1:D:295:TYR:HD1  | 1:D:299:GLY:HA2  | 1.46                     | 0.80              |
| 1:F:202:MET:CG   | 1:F:203:LEU:N    | 2.44                     | 0.80              |
| 1:B:125:ILE:HG12 | 1:B:127:PRO:HD3  | 1.64                     | 0.80              |
| 1:C:184:LYS:HD2  | 1:C:231:ASP:HA   | 1.64                     | 0.80              |
| 1:B:158:ASN:H    | 1:B:158:ASN:ND2  | 1.76                     | 0.80              |
| 1:A:266:THR:HG21 | 1:F:279:PRO:HB3  | 1.64                     | 0.80              |
| 1:G:281:ASP:OD2  | 1:G:322:GLY:N    | 2.12                     | 0.80              |
| 1:C:233:LEU:CD1  | 1:C:366:LEU:CD1  | 2.60                     | 0.80              |
| 1:F:204:GLN:C    | 1:F:206:TYR:N    | 2.32                     | 0.79              |
| 1:G:338:ARG:NH1  | 1:G:338:ARG:CG   | 2.30                     | 0.79              |
| 1:B:127:PRO:O    | 1:B:129:LEU:HD22 | 1.83                     | 0.79              |
| 1:C:131:ARG:NH2  | 1:C:220:GLU:OE1  | 2.14                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:349:ASP:OD1  | 1:D:350:ARG:N    | 2.16                     | 0.79              |
| 1:F:195:GLN:O    | 1:F:198:ASP:N    | 2.12                     | 0.79              |
| 1:A:195:GLN:O    | 1:A:199:ASP:CG   | 2.20                     | 0.79              |
| 1:F:244:ASP:OD2  | 1:F:247:LEU:CD2  | 2.30                     | 0.79              |
| 1:B:159:ALA:HB1  | 1:B:160:PRO:HD2  | 1.62                     | 0.79              |
| 1:C:210:ARG:HH22 | 1:D:153:GLU:CD   | 1.83                     | 0.79              |
| 1:A:123:GLY:O    | 1:A:124:ILE:HG23 | 1.81                     | 0.79              |
| 1:E:215:LEU:O    | 1:E:218:LYS:N    | 2.16                     | 0.79              |
| 1:C:194:ARG:HG2  | 1:C:195:GLN:N    | 1.97                     | 0.79              |
| 1:E:342:THR:O    | 1:E:362:CYS:HA   | 1.81                     | 0.79              |
| 1:D:159:ALA:HB1  | 1:D:160:PRO:HD2  | 1.65                     | 0.79              |
| 1:B:194:ARG:HH22 | 1:B:347:ARG:NH2  | 1.81                     | 0.79              |
| 1:D:247:LEU:CD2  | 1:D:247:LEU:O    | 2.30                     | 0.79              |
| 1:F:288:LEU:HD23 | 1:F:289:LYS:N    | 1.98                     | 0.79              |
| 1:A:287:LEU:CA   | 1:A:288:LEU:HD23 | 2.13                     | 0.78              |
| 1:C:225:ASN:HB3  | 1:C:237:ASN:ND2  | 1.94                     | 0.78              |
| 1:F:282:TRP:HZ3  | 1:F:308:MET:CE   | 1.96                     | 0.78              |
| 1:B:358:LEU:HD12 | 1:B:358:LEU:N    | 1.98                     | 0.78              |
| 1:F:253:THR:O    | 1:F:254:ARG:C    | 2.21                     | 0.78              |
| 1:F:203:LEU:O    | 1:F:206:TYR:N    | 2.17                     | 0.78              |
| 1:G:156:PHE:CE2  | 1:G:158:ASN:HB3  | 2.19                     | 0.78              |
| 1:C:201:PRO:O    | 1:C:204:GLN:CB   | 2.30                     | 0.78              |
| 1:G:366:LEU:HD12 | 1:G:366:LEU:C    | 2.03                     | 0.78              |
| 1:G:155:VAL:CG1  | 1:G:374:THR:HG21 | 2.14                     | 0.78              |
| 1:C:343:VAL:HG12 | 1:C:362:CYS:HB2  | 1.66                     | 0.78              |
| 1:B:193:SER:O    | 1:B:196:VAL:HG22 | 1.81                     | 0.78              |
| 1:A:190:VAL:HG12 | 1:A:211:LEU:HD21 | 1.64                     | 0.78              |
| 1:G:224:LEU:HD21 | 1:G:319:GLN:HB2  | 1.66                     | 0.78              |
| 1:C:197:MET:SD   | 1:C:358:LEU:HD11 | 2.23                     | 0.78              |
| 1:D:194:ARG:CG   | 1:D:195:GLN:H    | 1.94                     | 0.78              |
| 1:E:210:ARG:NH2  | 1:F:153:GLU:CD   | 2.37                     | 0.77              |
| 1:G:156:PHE:CD2  | 1:G:158:ASN:HB3  | 2.18                     | 0.77              |
| 1:A:269:GLU:HB3  | 1:F:217:LEU:CD2  | 2.11                     | 0.77              |
| 1:F:324:PHE:CD2  | 1:F:381:PHE:CE1  | 2.61                     | 0.77              |
| 1:G:138:LEU:CD2  | 1:G:329:PHE:HB3  | 2.14                     | 0.77              |
| 1:E:190:VAL:N    | 1:E:360:ILE:HD11 | 1.98                     | 0.77              |
| 1:B:155:VAL:HG11 | 1:B:374:THR:HB   | 1.64                     | 0.77              |
| 1:E:194:ARG:HG3  | 1:E:358:LEU:HD11 | 1.66                     | 0.77              |
| 1:F:210:ARG:HG2  | 1:F:210:ARG:NH1  | 1.97                     | 0.77              |
| 1:C:346:SER:O    | 1:C:359:THR:CG2  | 2.26                     | 0.77              |
| 1:A:129:LEU:N    | 1:A:129:LEU:HD23 | 2.00                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:129:LEU:HD13 | 1:D:131:ARG:N    | 2.00                     | 0.77              |
| 1:D:131:ARG:HG2  | 1:D:132:LEU:N    | 2.00                     | 0.77              |
| 1:D:356:ASN:CG   | 1:E:178:LYS:HZ1  | 1.87                     | 0.77              |
| 1:G:366:LEU:HD12 | 1:G:367:ALA:N    | 2.00                     | 0.76              |
| 1:C:202:MET:O    | 1:C:203:LEU:C    | 2.23                     | 0.76              |
| 1:E:207:ILE:HA   | 1:E:211:LEU:HB2  | 1.67                     | 0.76              |
| 1:A:155:VAL:HG11 | 1:A:374:THR:OG1  | 1.85                     | 0.76              |
| 1:E:125:ILE:HD13 | 1:E:127:PRO:HD3  | 1.66                     | 0.76              |
| 1:F:207:ILE:HD12 | 1:F:208:ASN:N    | 2.00                     | 0.76              |
| 1:D:158:ASN:H    | 1:D:158:ASN:ND2  | 1.82                     | 0.76              |
| 1:C:213:TYR:CE2  | 1:C:217:LEU:CD2  | 2.68                     | 0.76              |
| 1:D:141:GLY:O    | 1:D:142:ARG:HG2  | 1.85                     | 0.76              |
| 1:A:137:LEU:HD22 | 1:A:329:PHE:HB2  | 1.68                     | 0.76              |
| 1:E:203:LEU:O    | 1:E:204:GLN:C    | 2.23                     | 0.76              |
| 1:C:227:ASP:O    | 1:C:232:ASN:HB2  | 1.86                     | 0.76              |
| 1:C:186:ILE:HD13 | 1:C:222:GLN:HG3  | 1.66                     | 0.76              |
| 1:A:146:ASN:HD22 | 1:G:145:SER:HB2  | 1.50                     | 0.75              |
| 1:F:253:THR:CG2  | 1:F:256:ASP:OD1  | 2.34                     | 0.75              |
| 1:G:183:VAL:HA   | 1:G:367:ALA:HB2  | 1.67                     | 0.75              |
| 1:D:127:PRO:CG   | 1:D:212:MET:HE2  | 2.09                     | 0.75              |
| 1:G:327:GLY:N    | 1:G:329:PHE:HE2  | 1.83                     | 0.75              |
| 1:E:296:ILE:HG23 | 1:E:297:PHE:N    | 2.02                     | 0.75              |
| 1:B:126:MET:SD   | 1:B:126:MET:N    | 2.60                     | 0.75              |
| 1:E:125:ILE:HD11 | 1:E:127:PRO:HD3  | 1.66                     | 0.75              |
| 1:G:145:SER:O    | 1:G:338:ARG:HD3  | 1.85                     | 0.75              |
| 1:E:189:TRP:HE3  | 1:E:189:TRP:O    | 1.70                     | 0.75              |
| 1:B:296:ILE:HD13 | 1:B:296:ILE:N    | 1.98                     | 0.75              |
| 1:B:129:LEU:HD23 | 1:B:129:LEU:C    | 2.07                     | 0.74              |
| 1:A:202:MET:HB2  | 1:B:336:PHE:HE2  | 1.52                     | 0.74              |
| 1:F:226:GLY:H    | 1:F:235:GLY:HA3  | 1.51                     | 0.74              |
| 1:D:191:GLN:NE2  | 1:E:176:PHE:CE2  | 2.53                     | 0.74              |
| 1:B:158:ASN:HB2  | 1:B:172:SER:CA   | 2.16                     | 0.74              |
| 1:A:176:PHE:HE1  | 1:F:190:VAL:HG13 | 1.51                     | 0.74              |
| 1:C:194:ARG:NH1  | 1:C:347:ARG:NH2  | 2.34                     | 0.74              |
| 1:G:196:VAL:HG22 | 1:G:202:MET:CE   | 2.17                     | 0.74              |
| 1:G:199:ASP:C    | 1:G:201:PRO:CD   | 2.56                     | 0.74              |
| 1:B:192:ALA:O    | 1:B:357:MET:HB2  | 1.87                     | 0.74              |
| 1:A:121:ILE:HD12 | 1:A:121:ILE:N    | 2.02                     | 0.74              |
| 1:F:239:VAL:HG12 | 1:F:373:PRO:HB3  | 1.70                     | 0.74              |
| 1:A:287:LEU:CD1  | 1:A:287:LEU:O    | 2.30                     | 0.74              |
| 1:B:130:ARG:NH2  | 1:C:330:ASP:OD2  | 2.20                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:ALA:O    | 1:C:357:MET:HB3  | 1.87                     | 0.74              |
| 1:G:285:ILE:HA   | 1:G:288:LEU:HG   | 1.70                     | 0.74              |
| 1:C:187:ALA:CB   | 1:C:363:GLU:HA   | 2.15                     | 0.74              |
| 1:C:130:ARG:CB   | 1:D:271:SER:CB   | 2.66                     | 0.74              |
| 1:G:327:GLY:O    | 1:G:329:PHE:HD2  | 1.71                     | 0.74              |
| 1:E:316:THR:HG22 | 1:E:318:ALA:H    | 1.53                     | 0.74              |
| 1:E:216:ALA:C    | 1:E:218:LYS:N    | 2.36                     | 0.74              |
| 1:E:156:PHE:HD2  | 1:E:158:ASN:N    | 1.86                     | 0.74              |
| 1:B:210:ARG:HH22 | 1:C:153:GLU:HG3  | 1.52                     | 0.74              |
| 1:C:146:ASN:ND2  | 1:C:365:ARG:NH2  | 2.36                     | 0.73              |
| 1:G:193:SER:O    | 1:G:196:VAL:HB   | 1.87                     | 0.73              |
| 1:B:201:PRO:CB   | 1:B:204:GLN:HB2  | 2.18                     | 0.73              |
| 1:F:203:LEU:HD22 | 1:F:204:GLN:CA   | 2.19                     | 0.73              |
| 1:E:123:GLY:C    | 1:E:124:ILE:HG13 | 2.07                     | 0.73              |
| 1:G:203:LEU:O    | 1:G:205:SER:N    | 2.21                     | 0.73              |
| 1:F:342:THR:O    | 1:F:362:CYS:HA   | 1.88                     | 0.73              |
| 1:E:153:GLU:N    | 1:E:371:TYR:O    | 2.21                     | 0.73              |
| 1:F:158:ASN:H    | 1:F:158:ASN:ND2  | 1.83                     | 0.73              |
| 1:B:258:ILE:HD12 | 1:B:258:ILE:H    | 1.54                     | 0.73              |
| 1:A:195:GLN:NE2  | 1:B:149:GLU:OE2  | 2.21                     | 0.73              |
| 1:B:276:VAL:C    | 1:B:277:LEU:HD23 | 2.07                     | 0.73              |
| 1:G:327:GLY:O    | 1:G:329:PHE:CE2  | 2.42                     | 0.73              |
| 1:C:194:ARG:O    | 1:C:196:VAL:CG2  | 2.36                     | 0.73              |
| 1:A:284:ASN:O    | 1:A:288:LEU:HD22 | 1.88                     | 0.73              |
| 1:B:203:LEU:O    | 1:B:207:ILE:HG13 | 1.88                     | 0.73              |
| 1:F:200:ALA:O    | 1:F:201:PRO:C    | 2.26                     | 0.73              |
| 1:G:200:ALA:O    | 1:G:204:GLN:CB   | 2.37                     | 0.73              |
| 1:F:343:VAL:HG12 | 1:F:362:CYS:CB   | 2.11                     | 0.73              |
| 1:E:304:THR:HG21 | 1:F:309:TRP:O    | 1.88                     | 0.73              |
| 1:A:197:MET:C    | 1:A:197:MET:SD   | 2.67                     | 0.73              |
| 1:B:296:ILE:O    | 1:B:298:GLY:N    | 2.22                     | 0.73              |
| 1:B:295:TYR:HB3  | 1:B:298:GLY:O    | 1.89                     | 0.73              |
| 1:C:265:VAL:HG22 | 1:C:377:ILE:HD13 | 1.71                     | 0.73              |
| 1:E:207:ILE:HG22 | 1:E:211:LEU:HD22 | 1.68                     | 0.72              |
| 1:A:155:VAL:HG13 | 1:A:374:THR:HG21 | 1.71                     | 0.72              |
| 1:C:357:MET:CE   | 1:D:178:LYS:HG2  | 2.19                     | 0.72              |
| 1:A:349:ASP:OD1  | 1:A:350:ARG:HG3  | 1.89                     | 0.72              |
| 1:C:347:ARG:C    | 1:C:349:ASP:H    | 1.88                     | 0.72              |
| 1:A:207:ILE:HG13 | 1:A:211:LEU:HD12 | 1.71                     | 0.72              |
| 1:F:358:LEU:HD23 | 1:F:359:THR:N    | 2.04                     | 0.72              |
| 1:E:125:ILE:HG13 | 1:E:212:MET:HB3  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:203:LEU:C    | 1:E:205:SER:N    | 2.40                     | 0.72              |
| 1:G:278:ASN:OD1  | 1:G:279:PRO:CD   | 2.30                     | 0.72              |
| 1:D:247:LEU:CD2  | 1:D:260:HIS:HB3  | 2.20                     | 0.72              |
| 1:D:349:ASP:OD1  | 1:D:350:ARG:HG3  | 1.89                     | 0.72              |
| 1:D:193:SER:O    | 1:D:194:ARG:HB3  | 1.89                     | 0.72              |
| 1:E:130:ARG:HB3  | 1:F:271:SER:OG   | 1.89                     | 0.72              |
| 1:C:210:ARG:NH2  | 1:D:153:GLU:OE2  | 2.22                     | 0.72              |
| 1:A:207:ILE:HD12 | 1:A:207:ILE:H    | 1.55                     | 0.72              |
| 1:D:156:PHE:HD2  | 1:D:158:ASN:N    | 1.88                     | 0.72              |
| 1:D:132:LEU:H    | 1:D:132:LEU:CD2  | 2.02                     | 0.72              |
| 1:F:198:ASP:C    | 1:F:200:ALA:N    | 2.38                     | 0.71              |
| 1:B:296:ILE:C    | 1:B:298:GLY:H    | 1.91                     | 0.71              |
| 1:E:159:ALA:HB1  | 1:E:160:PRO:HD2  | 1.70                     | 0.71              |
| 1:C:195:GLN:O    | 1:C:196:VAL:C    | 2.28                     | 0.71              |
| 1:G:200:ALA:N    | 1:G:201:PRO:HD2  | 2.04                     | 0.71              |
| 1:G:199:ASP:O    | 1:G:202:MET:N    | 2.23                     | 0.71              |
| 1:E:127:PRO:O    | 1:E:129:LEU:HD22 | 1.90                     | 0.71              |
| 1:B:250:THR:CB   | 1:B:251:GLY:CA   | 2.49                     | 0.71              |
| 1:G:303:PHE:CD2  | 1:G:304:THR:N    | 2.57                     | 0.71              |
| 1:G:132:LEU:HB2  | 1:G:136:ASP:CG   | 2.11                     | 0.71              |
| 1:E:125:ILE:HG12 | 1:E:126:MET:N    | 2.05                     | 0.71              |
| 1:B:156:PHE:HD2  | 1:B:158:ASN:N    | 1.88                     | 0.71              |
| 1:E:333:SER:HB2  | 1:E:369:ALA:O    | 1.91                     | 0.71              |
| 1:G:290:ASP:C    | 1:G:292:GLU:H    | 1.92                     | 0.71              |
| 1:F:282:TRP:CZ3  | 1:F:308:MET:CE   | 2.74                     | 0.71              |
| 1:E:137:LEU:CD2  | 1:E:329:PHE:HB2  | 2.20                     | 0.71              |
| 1:F:206:TYR:O    | 1:F:208:ASN:N    | 2.24                     | 0.71              |
| 1:B:195:GLN:O    | 1:B:196:VAL:C    | 2.29                     | 0.71              |
| 1:B:134:ILE:HD13 | 1:B:220:GLU:HG3  | 1.72                     | 0.71              |
| 1:A:195:GLN:HG3  | 1:A:196:VAL:N    | 2.06                     | 0.71              |
| 1:A:153:GLU:CD   | 1:A:372:ARG:HH21 | 1.93                     | 0.71              |
| 1:A:366:LEU:C    | 1:A:366:LEU:HD12 | 2.11                     | 0.71              |
| 1:E:123:GLY:O    | 1:E:124:ILE:HG13 | 1.91                     | 0.71              |
| 1:G:297:PHE:H    | 1:G:297:PHE:HD2  | 1.38                     | 0.71              |
| 1:B:158:ASN:ND2  | 1:B:172:SER:HB2  | 2.04                     | 0.71              |
| 1:E:158:ASN:H    | 1:E:158:ASN:ND2  | 1.86                     | 0.71              |
| 1:C:195:GLN:O    | 1:C:198:ASP:N    | 2.22                     | 0.71              |
| 1:F:192:ALA:O    | 1:F:357:MET:SD   | 2.49                     | 0.71              |
| 1:B:131:ARG:HH21 | 1:B:220:GLU:CD   | 1.94                     | 0.71              |
| 1:C:146:ASN:HD21 | 1:C:365:ARG:NH2  | 1.89                     | 0.71              |
| 1:C:203:LEU:O    | 1:C:206:TYR:HB3  | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:203:LEU:C    | 1:G:205:SER:H    | 1.93                     | 0.71              |
| 1:F:282:TRP:CZ3  | 1:F:308:MET:HE3  | 2.26                     | 0.71              |
| 1:E:142:ARG:HA   | 1:E:337:ASP:H    | 1.54                     | 0.70              |
| 1:D:347:ARG:HB2  | 1:D:358:LEU:HG   | 1.71                     | 0.70              |
| 1:F:206:TYR:HD2  | 1:F:207:ILE:N    | 1.89                     | 0.70              |
| 1:G:278:ASN:O    | 1:G:280:ARG:N    | 2.24                     | 0.70              |
| 1:A:273:SER:OG   | 1:A:330:ASP:HB2  | 1.91                     | 0.70              |
| 1:D:307:ILE:O    | 1:D:307:ILE:HD12 | 1.92                     | 0.70              |
| 1:E:126:MET:CE   | 1:E:129:LEU:HD21 | 2.21                     | 0.70              |
| 1:B:211:LEU:O    | 1:B:211:LEU:CD1  | 2.24                     | 0.70              |
| 1:E:194:ARG:CA   | 1:E:358:LEU:CD1  | 2.67                     | 0.70              |
| 1:F:329:PHE:H    | 1:F:329:PHE:HD1  | 0.82                     | 0.70              |
| 1:C:196:VAL:HG12 | 1:C:203:LEU:HD11 | 0.72                     | 0.70              |
| 1:G:200:ALA:O    | 1:G:204:GLN:HB3  | 1.92                     | 0.70              |
| 1:G:196:VAL:HG22 | 1:G:202:MET:HE2  | 1.73                     | 0.70              |
| 1:B:249:ALA:CB   | 1:B:252:ASP:OD2  | 2.40                     | 0.70              |
| 1:F:327:GLY:N    | 1:F:329:PHE:CE1  | 2.59                     | 0.70              |
| 1:A:207:ILE:N    | 1:A:207:ILE:HD12 | 2.05                     | 0.70              |
| 1:B:288:LEU:O    | 1:B:296:ILE:HD13 | 1.91                     | 0.70              |
| 1:G:296:ILE:HG22 | 1:G:297:PHE:H    | 1.54                     | 0.70              |
| 1:A:194:ARG:HB2  | 1:A:358:LEU:HD23 | 1.71                     | 0.70              |
| 1:D:122:PRO:CG   | 1:D:343:VAL:HG23 | 2.21                     | 0.70              |
| 1:G:185:THR:OG1  | 1:G:365:ARG:HG2  | 1.90                     | 0.70              |
| 1:D:129:LEU:HD13 | 1:D:130:ARG:N    | 2.07                     | 0.70              |
| 1:A:194:ARG:O    | 1:A:198:ASP:CB   | 2.39                     | 0.69              |
| 1:A:125:ILE:HG21 | 1:A:204:GLN:HE21 | 1.55                     | 0.69              |
| 1:F:275:ILE:HD12 | 1:F:275:ILE:N    | 2.06                     | 0.69              |
| 1:C:194:ARG:O    | 1:C:195:GLN:C    | 2.30                     | 0.69              |
| 1:F:159:ALA:HB1  | 1:F:160:PRO:HD2  | 1.73                     | 0.69              |
| 1:F:329:PHE:CD1  | 1:F:329:PHE:N    | 2.35                     | 0.69              |
| 1:F:156:PHE:HD2  | 1:F:158:ASN:N    | 1.89                     | 0.69              |
| 1:C:292:GLU:HG2  | 1:C:294:ARG:NE   | 2.06                     | 0.69              |
| 1:G:296:ILE:CG2  | 1:G:297:PHE:N    | 2.48                     | 0.69              |
| 1:B:134:ILE:H    | 1:B:134:ILE:HD12 | 1.58                     | 0.69              |
| 1:A:127:PRO:HB3  | 1:A:212:MET:CB   | 2.20                     | 0.69              |
| 1:D:209:ASN:O    | 1:D:213:TYR:CB   | 2.40                     | 0.69              |
| 1:G:155:VAL:CG1  | 1:G:374:THR:CG2  | 2.70                     | 0.69              |
| 1:B:200:ALA:HB1  | 1:B:201:PRO:CD   | 2.23                     | 0.69              |
| 1:B:155:VAL:CG1  | 1:B:374:THR:OG1  | 2.41                     | 0.69              |
| 1:D:356:ASN:OD1  | 1:E:178:LYS:NZ   | 2.19                     | 0.69              |
| 1:E:382:SER:O    | 1:E:383:SER:HB2  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:156:PHE:O    | 1:B:158:ASN:ND2  | 2.25                     | 0.69              |
| 1:E:258:ILE:HD11 | 1:E:381:PHE:HZ   | 1.58                     | 0.69              |
| 1:G:297:PHE:CG   | 1:G:298:GLY:N    | 2.61                     | 0.68              |
| 1:C:323:THR:HA   | 1:C:380:THR:HG22 | 1.75                     | 0.68              |
| 1:A:125:ILE:N    | 1:A:125:ILE:HD12 | 2.08                     | 0.68              |
| 1:D:148:LEU:HD12 | 1:D:181:ALA:HB3  | 1.74                     | 0.68              |
| 1:G:198:ASP:O    | 1:G:199:ASP:CB   | 2.40                     | 0.68              |
| 1:E:203:LEU:O    | 1:E:205:SER:N    | 2.27                     | 0.68              |
| 1:E:184:LYS:HD2  | 1:E:231:ASP:HA   | 1.76                     | 0.68              |
| 1:D:247:LEU:CD2  | 1:D:247:LEU:C    | 2.60                     | 0.68              |
| 1:B:125:ILE:HG12 | 1:B:127:PRO:CD   | 2.22                     | 0.68              |
| 1:B:162:ASP:O    | 1:B:172:SER:C    | 2.30                     | 0.68              |
| 1:D:333:SER:HB3  | 1:D:369:ALA:O    | 1.92                     | 0.68              |
| 1:B:212:MET:O    | 1:B:213:TYR:C    | 2.28                     | 0.68              |
| 1:C:155:VAL:HG23 | 1:C:174:ILE:HG22 | 1.75                     | 0.68              |
| 1:C:213:TYR:CZ   | 1:C:217:LEU:CD1  | 2.59                     | 0.68              |
| 1:F:132:LEU:CD2  | 1:F:136:ASP:HB2  | 2.24                     | 0.68              |
| 1:F:202:MET:HG3  | 1:F:203:LEU:N    | 2.08                     | 0.68              |
| 1:B:275:ILE:HD11 | 1:B:313:VAL:HG22 | 1.75                     | 0.68              |
| 1:A:307:ILE:C    | 1:A:307:ILE:HD12 | 2.14                     | 0.68              |
| 1:B:296:ILE:C    | 1:B:298:GLY:N    | 2.45                     | 0.68              |
| 1:B:341:ALA:HA   | 1:B:363:GLU:O    | 1.94                     | 0.68              |
| 1:F:142:ARG:NH2  | 1:F:340:ASP:OD1  | 2.27                     | 0.68              |
| 1:C:130:ARG:CB   | 1:D:271:SER:HB2  | 2.24                     | 0.68              |
| 1:C:153:GLU:OE2  | 1:C:372:ARG:NH2  | 2.27                     | 0.68              |
| 1:E:220:GLU:HG2  | 1:E:316:THR:HG21 | 1.77                     | 0.67              |
| 1:B:201:PRO:C    | 1:B:204:GLN:N    | 2.33                     | 0.67              |
| 1:A:300:PRO:HA   | 1:A:303:PHE:CB   | 2.24                     | 0.67              |
| 1:G:158:ASN:ND2  | 1:G:159:ALA:H    | 1.92                     | 0.67              |
| 1:B:275:ILE:HG22 | 1:B:326:VAL:HG22 | 1.76                     | 0.67              |
| 1:C:194:ARG:C    | 1:C:196:VAL:N    | 2.41                     | 0.67              |
| 1:C:197:MET:SD   | 1:C:197:MET:N    | 2.65                     | 0.67              |
| 1:G:187:ALA:HB2  | 1:G:363:GLU:HA   | 1.76                     | 0.67              |
| 1:B:131:ARG:NH2  | 1:B:220:GLU:OE2  | 2.27                     | 0.67              |
| 1:C:131:ARG:HH22 | 1:C:220:GLU:CD   | 1.97                     | 0.67              |
| 1:F:198:ASP:OD2  | 1:F:198:ASP:C    | 2.30                     | 0.67              |
| 1:C:188:HIS:O    | 1:C:361:LEU:HA   | 1.95                     | 0.67              |
| 1:A:194:ARG:O    | 1:A:198:ASP:OD2  | 2.12                     | 0.67              |
| 1:E:219:GLU:OE2  | 1:E:364:GLU:OE1  | 2.11                     | 0.67              |
| 1:G:158:ASN:HD22 | 1:G:159:ALA:H    | 1.41                     | 0.67              |
| 1:F:282:TRP:HZ3  | 1:F:308:MET:HE3  | 1.57                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:ALA:HB1  | 1:D:151:VAL:HG11 | 1.76                     | 0.67              |
| 1:F:194:ARG:HB2  | 1:F:356:ASN:OD1  | 1.95                     | 0.67              |
| 1:E:194:ARG:NH1  | 1:E:347:ARG:NH2  | 2.43                     | 0.67              |
| 1:E:224:LEU:HD11 | 1:E:319:GLN:OE1  | 1.94                     | 0.67              |
| 1:C:207:ILE:O    | 1:C:212:MET:HB2  | 1.95                     | 0.67              |
| 1:F:198:ASP:C    | 1:F:200:ALA:H    | 1.95                     | 0.67              |
| 1:C:361:LEU:O    | 1:C:361:LEU:HD12 | 1.95                     | 0.67              |
| 1:C:227:ASP:O    | 1:C:229:THR:N    | 2.28                     | 0.67              |
| 1:G:199:ASP:O    | 1:G:202:MET:HB3  | 1.94                     | 0.67              |
| 1:B:208:ASN:O    | 1:B:212:MET:HG2  | 1.95                     | 0.67              |
| 1:C:192:ALA:CB   | 1:D:151:VAL:HG11 | 2.25                     | 0.67              |
| 1:C:244:ASP:H    | 1:C:264:GLN:HE22 | 1.42                     | 0.67              |
| 1:A:280:ARG:HG3  | 1:A:281:ASP:N    | 2.07                     | 0.67              |
| 1:B:188:HIS:CD2  | 1:B:214:GLY:HA3  | 2.30                     | 0.67              |
| 1:G:329:PHE:CD2  | 1:G:329:PHE:N    | 2.48                     | 0.67              |
| 1:D:295:TYR:CD1  | 1:D:299:GLY:HA2  | 2.28                     | 0.67              |
| 1:C:174:ILE:H    | 1:C:174:ILE:HD13 | 1.60                     | 0.67              |
| 1:D:174:ILE:HG12 | 1:D:176:PHE:HE2  | 1.59                     | 0.67              |
| 1:D:209:ASN:O    | 1:D:213:TYR:HB2  | 1.95                     | 0.67              |
| 1:A:345:VAL:HG22 | 1:A:360:ILE:HA   | 1.76                     | 0.67              |
| 1:G:200:ALA:HB3  | 1:G:201:PRO:HD3  | 1.76                     | 0.66              |
| 1:C:129:LEU:H    | 1:C:129:LEU:HD22 | 1.60                     | 0.66              |
| 1:B:125:ILE:C    | 1:B:127:PRO:HD3  | 2.14                     | 0.66              |
| 1:A:195:GLN:CG   | 1:A:196:VAL:H    | 2.06                     | 0.66              |
| 1:D:301:GLN:O    | 1:D:306:ASN:HB2  | 1.95                     | 0.66              |
| 1:E:188:HIS:NE2  | 1:E:190:VAL:HG13 | 2.11                     | 0.66              |
| 1:F:249:ALA:O    | 1:F:250:THR:C    | 2.32                     | 0.66              |
| 1:D:339:MET:HB3  | 1:D:365:ARG:HB2  | 1.77                     | 0.66              |
| 1:B:199:ASP:C    | 1:B:199:ASP:OD2  | 2.34                     | 0.66              |
| 1:F:206:TYR:CD2  | 1:F:207:ILE:N    | 2.64                     | 0.66              |
| 1:C:347:ARG:C    | 1:C:349:ASP:N    | 2.43                     | 0.66              |
| 1:E:227:ASP:CB   | 1:E:229:THR:CG2  | 2.56                     | 0.66              |
| 1:D:174:ILE:HG12 | 1:D:176:PHE:CE2  | 2.30                     | 0.66              |
| 1:C:233:LEU:HD12 | 1:C:366:LEU:HD11 | 1.76                     | 0.66              |
| 1:B:158:ASN:CB   | 1:B:172:SER:HA   | 2.18                     | 0.66              |
| 1:D:270:PHE:HE2  | 1:D:331:MET:HB3  | 1.61                     | 0.66              |
| 1:B:125:ILE:N    | 1:B:208:ASN:HB3  | 2.11                     | 0.66              |
| 1:A:203:LEU:O    | 1:A:204:GLN:C    | 2.32                     | 0.66              |
| 1:D:187:ALA:HB2  | 1:D:363:GLU:HB3  | 1.76                     | 0.66              |
| 1:G:227:ASP:C    | 1:G:227:ASP:OD1  | 2.34                     | 0.66              |
| 1:G:270:PHE:CE1  | 1:G:372:ARG:CZ   | 2.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:184:LYS:HG3  | 1:D:233:LEU:HD23 | 1.77                     | 0.66              |
| 1:C:307:ILE:O    | 1:C:307:ILE:HG13 | 1.95                     | 0.66              |
| 1:B:125:ILE:HG12 | 1:B:127:PRO:CG   | 2.25                     | 0.66              |
| 1:F:370:HIS:HB3  | 1:F:373:PRO:HG3  | 1.78                     | 0.66              |
| 1:A:191:GLN:HE21 | 1:A:191:GLN:H    | 1.41                     | 0.66              |
| 1:C:198:ASP:O    | 1:C:199:ASP:CG   | 2.34                     | 0.66              |
| 1:D:155:VAL:HG11 | 1:D:374:THR:CB   | 2.26                     | 0.66              |
| 1:E:236:LEU:HD23 | 1:E:370:HIS:HE1  | 1.61                     | 0.66              |
| 1:F:132:LEU:HD22 | 1:F:136:ASP:HB2  | 1.76                     | 0.66              |
| 1:B:199:ASP:O    | 1:B:200:ALA:HB2  | 1.95                     | 0.65              |
| 1:B:126:MET:HE3  | 1:B:212:MET:HG3  | 1.77                     | 0.65              |
| 1:E:296:ILE:HG23 | 1:E:297:PHE:H    | 1.61                     | 0.65              |
| 1:A:350:ARG:O    | 1:A:351:ASP:CG   | 2.35                     | 0.65              |
| 1:F:141:GLY:O    | 1:F:336:PHE:HA   | 1.95                     | 0.65              |
| 1:C:203:LEU:O    | 1:C:204:GLN:C    | 2.33                     | 0.65              |
| 1:C:233:LEU:HD11 | 1:C:366:LEU:HD12 | 1.78                     | 0.65              |
| 1:F:275:ILE:HG23 | 1:F:326:VAL:HG12 | 1.78                     | 0.65              |
| 1:C:194:ARG:C    | 1:C:196:VAL:H    | 1.99                     | 0.65              |
| 1:B:126:MET:N    | 1:B:127:PRO:HD3  | 2.11                     | 0.65              |
| 1:G:345:VAL:HG11 | 1:G:358:LEU:HD21 | 1.78                     | 0.65              |
| 1:B:194:ARG:HD2  | 1:B:357:MET:HA   | 1.78                     | 0.65              |
| 1:F:198:ASP:O    | 1:F:200:ALA:N    | 2.29                     | 0.65              |
| 1:G:279:PRO:O    | 1:G:282:TRP:HB3  | 1.96                     | 0.65              |
| 1:C:368:LEU:HD21 | 1:C:370:HIS:NE2  | 2.12                     | 0.65              |
| 1:E:212:MET:O    | 1:E:215:LEU:N    | 2.30                     | 0.65              |
| 1:D:125:ILE:HD12 | 1:D:208:ASN:OD1  | 1.91                     | 0.65              |
| 1:C:200:ALA:C    | 1:C:202:MET:H    | 2.00                     | 0.65              |
| 1:D:127:PRO:CB   | 1:D:212:MET:HB3  | 2.26                     | 0.65              |
| 1:B:215:LEU:CD2  | 1:B:215:LEU:O    | 2.30                     | 0.65              |
| 1:D:304:THR:OG1  | 1:D:315:PRO:HG3  | 1.97                     | 0.65              |
| 1:G:290:ASP:C    | 1:G:292:GLU:N    | 2.47                     | 0.65              |
| 1:F:258:ILE:HD11 | 1:F:275:ILE:HG21 | 1.77                     | 0.65              |
| 1:B:194:ARG:HA   | 1:B:358:LEU:HD11 | 1.77                     | 0.65              |
| 1:D:341:ALA:HA   | 1:D:363:GLU:O    | 1.96                     | 0.65              |
| 1:E:200:ALA:O    | 1:E:202:MET:N    | 2.30                     | 0.65              |
| 1:G:194:ARG:C    | 1:G:197:MET:H    | 2.00                     | 0.65              |
| 1:F:197:MET:C    | 1:F:197:MET:SD   | 2.74                     | 0.65              |
| 1:C:135:ARG:NH2  | 1:C:337:ASP:OD2  | 2.29                     | 0.65              |
| 1:G:261:ALA:O    | 1:G:265:VAL:HG23 | 1.97                     | 0.65              |
| 1:D:129:LEU:HD13 | 1:D:131:ARG:H    | 1.61                     | 0.64              |
| 1:D:129:LEU:CD1  | 1:D:131:ARG:H    | 2.10                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:277:LEU:O    | 1:D:315:PRO:HA   | 1.98                     | 0.64              |
| 1:G:265:VAL:HG22 | 1:G:377:ILE:HD13 | 1.78                     | 0.64              |
| 1:D:224:LEU:HD12 | 1:D:225:ASN:ND2  | 2.12                     | 0.64              |
| 1:F:200:ALA:CB   | 1:F:201:PRO:CD   | 2.57                     | 0.64              |
| 1:E:200:ALA:O    | 1:E:201:PRO:C    | 2.33                     | 0.64              |
| 1:D:162:ASP:C    | 1:D:173:ASP:H    | 2.01                     | 0.64              |
| 1:C:275:ILE:N    | 1:C:275:ILE:HD12 | 2.13                     | 0.64              |
| 1:C:224:LEU:CD1  | 1:C:225:ASN:CG   | 2.66                     | 0.64              |
| 1:F:361:LEU:C    | 1:F:361:LEU:HD13 | 2.17                     | 0.64              |
| 1:B:155:VAL:HG12 | 1:B:374:THR:OG1  | 1.98                     | 0.64              |
| 1:A:123:GLY:C    | 1:A:124:ILE:HG12 | 2.15                     | 0.64              |
| 1:F:273:SER:O    | 1:F:312:PRO:HD2  | 1.98                     | 0.64              |
| 1:G:345:VAL:HG12 | 1:G:358:LEU:HD11 | 1.80                     | 0.64              |
| 1:G:159:ALA:HB1  | 1:G:160:PRO:HD2  | 1.80                     | 0.64              |
| 1:B:146:ASN:HD22 | 1:B:146:ASN:N    | 1.95                     | 0.64              |
| 1:E:258:ILE:HD11 | 1:E:381:PHE:CZ   | 2.33                     | 0.64              |
| 1:B:216:ALA:O    | 1:B:217:LEU:C    | 2.34                     | 0.64              |
| 1:F:148:LEU:O    | 1:F:180:THR:HG23 | 1.97                     | 0.64              |
| 1:C:189:TRP:HA   | 1:C:360:ILE:O    | 1.97                     | 0.64              |
| 1:F:211:LEU:O    | 1:F:214:GLY:N    | 2.28                     | 0.64              |
| 1:E:157:THR:HG22 | 1:E:267:GLU:HG2  | 1.80                     | 0.64              |
| 1:C:268:SER:O    | 1:C:372:ARG:NH1  | 2.27                     | 0.64              |
| 1:E:289:LYS:HD3  | 1:E:293:GLY:HA2  | 1.77                     | 0.64              |
| 1:D:193:SER:O    | 1:D:194:ARG:CB   | 2.46                     | 0.64              |
| 1:A:275:ILE:HG23 | 1:A:326:VAL:HG22 | 1.80                     | 0.64              |
| 1:D:270:PHE:CE2  | 1:D:331:MET:HB3  | 2.33                     | 0.64              |
| 1:E:194:ARG:HD2  | 1:E:347:ARG:CZ   | 2.28                     | 0.64              |
| 1:F:327:GLY:C    | 1:F:329:PHE:CE1  | 2.72                     | 0.64              |
| 1:E:254:ARG:HG2  | 1:E:381:PHE:HE2  | 1.63                     | 0.64              |
| 1:F:134:ILE:O    | 1:F:137:LEU:N    | 2.24                     | 0.64              |
| 1:D:265:VAL:HG22 | 1:D:377:ILE:HD13 | 1.80                     | 0.64              |
| 1:G:244:ASP:OD2  | 1:G:246:SER:HB3  | 1.98                     | 0.64              |
| 1:F:224:LEU:HD13 | 1:F:237:ASN:ND2  | 2.13                     | 0.63              |
| 1:C:195:GLN:NE2  | 1:C:198:ASP:CB   | 2.46                     | 0.63              |
| 1:E:226:GLY:H    | 1:E:235:GLY:HA3  | 1.63                     | 0.63              |
| 1:C:341:ALA:HB1  | 1:C:362:CYS:SG   | 2.39                     | 0.63              |
| 1:G:155:VAL:HG22 | 1:G:156:PHE:N    | 2.12                     | 0.63              |
| 1:F:131:ARG:NH2  | 1:F:220:GLU:CD   | 2.51                     | 0.63              |
| 1:E:229:THR:H    | 1:E:232:ASN:HB2  | 1.64                     | 0.63              |
| 1:B:215:LEU:HD22 | 1:B:216:ALA:N    | 2.12                     | 0.63              |
| 1:D:129:LEU:HD11 | 1:D:131:ARG:HD3  | 1.79                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:301:GLN:HG3  | 1:F:302:ALA:N    | 2.13                     | 0.63              |
| 1:E:127:PRO:HG2  | 1:E:129:LEU:HD13 | 1.78                     | 0.63              |
| 1:E:216:ALA:C    | 1:E:218:LYS:H    | 1.99                     | 0.63              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:CG   | 2.72                     | 0.63              |
| 1:C:278:ASN:ND2  | 1:C:280:ARG:HB3  | 2.14                     | 0.63              |
| 1:C:287:LEU:CD2  | 1:C:300:PRO:HA   | 2.29                     | 0.63              |
| 1:B:289:LYS:HD2  | 1:B:293:GLY:HA2  | 1.80                     | 0.63              |
| 1:G:134:ILE:HG12 | 1:G:220:GLU:HG3  | 1.79                     | 0.63              |
| 1:E:254:ARG:CG   | 1:E:381:PHE:HE2  | 2.10                     | 0.63              |
| 1:F:202:MET:O    | 1:F:205:SER:HB3  | 1.97                     | 0.63              |
| 1:E:244:ASP:OD1  | 1:E:247:LEU:HG   | 1.98                     | 0.63              |
| 1:A:237:ASN:HB3  | 1:A:378:LYS:HD3  | 1.79                     | 0.63              |
| 1:C:194:ARG:C    | 1:C:196:VAL:HG23 | 2.18                     | 0.63              |
| 1:G:199:ASP:CB   | 1:G:202:MET:HB3  | 2.29                     | 0.63              |
| 1:E:296:ILE:CG2  | 1:E:297:PHE:N    | 2.61                     | 0.63              |
| 1:B:201:PRO:HB3  | 1:B:204:GLN:HB2  | 1.79                     | 0.63              |
| 1:G:275:ILE:HG23 | 1:G:326:VAL:HG22 | 1.79                     | 0.63              |
| 1:D:300:PRO:HG2  | 1:E:301:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:273:SER:HB3  | 1:D:328:GLY:HA2  | 1.81                     | 0.62              |
| 1:A:186:ILE:N    | 1:A:186:ILE:HD12 | 2.14                     | 0.62              |
| 1:D:307:ILE:CG2  | 1:D:312:PRO:HA   | 2.29                     | 0.62              |
| 1:B:195:GLN:HA   | 1:B:197:MET:HG2  | 1.80                     | 0.62              |
| 1:D:342:THR:O    | 1:D:362:CYS:HA   | 1.99                     | 0.62              |
| 1:D:279:PRO:HG3  | 1:D:315:PRO:HB2  | 1.81                     | 0.62              |
| 1:G:135:ARG:NH2  | 1:G:219:GLU:OE2  | 2.33                     | 0.62              |
| 1:G:145:SER:O    | 1:G:338:ARG:CD   | 2.47                     | 0.62              |
| 1:G:157:THR:O    | 1:G:158:ASN:ND2  | 2.32                     | 0.62              |
| 1:F:211:LEU:HD23 | 1:F:211:LEU:C    | 2.20                     | 0.62              |
| 1:B:148:LEU:HD23 | 1:B:148:LEU:O    | 1.99                     | 0.62              |
| 1:C:287:LEU:CD2  | 1:C:300:PRO:CA   | 2.78                     | 0.62              |
| 1:F:345:VAL:CG1  | 1:F:358:LEU:HD11 | 2.29                     | 0.62              |
| 1:A:156:PHE:C    | 1:A:158:ASN:H    | 2.03                     | 0.62              |
| 1:A:158:ASN:ND2  | 1:A:172:SER:HA   | 2.14                     | 0.62              |
| 1:A:280:ARG:CG   | 1:A:281:ASP:N    | 2.62                     | 0.62              |
| 1:C:194:ARG:CZ   | 1:C:347:ARG:NH2  | 2.62                     | 0.62              |
| 1:B:201:PRO:C    | 1:B:204:GLN:HB2  | 2.20                     | 0.62              |
| 1:D:196:VAL:O    | 1:D:199:ASP:OD1  | 2.18                     | 0.62              |
| 1:G:129:LEU:O    | 1:G:129:LEU:HD23 | 1.98                     | 0.62              |
| 1:A:349:ASP:OD1  | 1:A:350:ARG:N    | 2.33                     | 0.62              |
| 1:E:189:TRP:CE3  | 1:E:189:TRP:O    | 2.52                     | 0.62              |
| 1:G:129:LEU:C    | 1:G:131:ARG:H    | 2.02                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:282:TRP:NE1  | 1:D:304:THR:HA   | 2.11                     | 0.62              |
| 1:F:308:MET:HG2  | 1:F:309:TRP:CE3  | 2.35                     | 0.62              |
| 1:D:184:LYS:HZ3  | 1:D:184:LYS:HA   | 1.65                     | 0.62              |
| 1:E:268:SER:HB2  | 1:E:372:ARG:HD3  | 1.82                     | 0.62              |
| 1:F:202:MET:SD   | 1:F:203:LEU:HA   | 2.40                     | 0.62              |
| 1:A:156:PHE:O    | 1:A:158:ASN:ND2  | 2.33                     | 0.62              |
| 1:F:150:TYR:CE1  | 1:F:179:GLN:HB2  | 2.35                     | 0.62              |
| 1:D:122:PRO:CG   | 1:D:343:VAL:O    | 2.39                     | 0.61              |
| 1:E:174:ILE:CD1  | 1:E:174:ILE:H    | 2.12                     | 0.61              |
| 1:G:257:ILE:HA   | 1:G:260:HIS:HD2  | 1.65                     | 0.61              |
| 1:E:125:ILE:HG13 | 1:E:212:MET:CB   | 2.30                     | 0.61              |
| 1:F:203:LEU:O    | 1:F:206:TYR:CA   | 2.47                     | 0.61              |
| 1:B:138:LEU:HD23 | 1:B:329:PHE:HB3  | 1.80                     | 0.61              |
| 1:D:121:ILE:C    | 1:D:121:ILE:HD13 | 2.20                     | 0.61              |
| 1:E:126:MET:HE3  | 1:E:129:LEU:HD21 | 1.82                     | 0.61              |
| 1:F:194:ARG:NH2  | 1:G:363:GLU:OE1  | 2.33                     | 0.61              |
| 1:E:233:LEU:HD13 | 1:E:366:LEU:CD1  | 2.25                     | 0.61              |
| 1:A:240:ALA:HB1  | 1:A:376:ILE:HG22 | 1.82                     | 0.61              |
| 1:D:303:PHE:CD1  | 1:D:303:PHE:N    | 2.67                     | 0.61              |
| 1:A:134:ILE:HD13 | 1:A:314:VAL:HG11 | 1.83                     | 0.61              |
| 1:D:194:ARG:O    | 1:D:197:MET:N    | 2.27                     | 0.61              |
| 1:A:207:ILE:H    | 1:A:207:ILE:CD1  | 2.12                     | 0.61              |
| 1:B:284:ASN:O    | 1:B:288:LEU:HB2  | 2.00                     | 0.61              |
| 1:D:130:ARG:CZ   | 1:D:131:ARG:CB   | 2.79                     | 0.61              |
| 1:E:296:ILE:HG23 | 1:E:297:PHE:CD1  | 2.36                     | 0.61              |
| 1:C:357:MET:CE   | 1:D:178:LYS:CG   | 2.78                     | 0.61              |
| 1:D:191:GLN:N    | 1:D:191:GLN:OE1  | 2.30                     | 0.61              |
| 1:F:206:TYR:C    | 1:F:208:ASN:N    | 2.52                     | 0.61              |
| 1:G:199:ASP:CA   | 1:G:201:PRO:HD2  | 2.30                     | 0.61              |
| 1:D:249:ALA:C    | 1:D:252:ASP:OD2  | 2.38                     | 0.61              |
| 1:A:332:ALA:O    | 1:A:371:TYR:HB2  | 2.00                     | 0.61              |
| 1:B:258:ILE:N    | 1:B:258:ILE:HD12 | 2.16                     | 0.61              |
| 1:F:177:SER:HB3  | 1:F:179:GLN:HE21 | 1.66                     | 0.61              |
| 1:C:194:ARG:O    | 1:C:196:VAL:CA   | 2.48                     | 0.61              |
| 1:C:213:TYR:CD2  | 1:C:217:LEU:HD11 | 2.36                     | 0.61              |
| 1:C:277:LEU:O    | 1:C:315:PRO:HA   | 2.00                     | 0.61              |
| 1:F:210:ARG:O    | 1:F:210:ARG:HD3  | 2.00                     | 0.61              |
| 1:B:173:ASP:OD1  | 1:B:174:ILE:HD13 | 2.00                     | 0.61              |
| 1:F:195:GLN:OE1  | 1:F:195:GLN:HA   | 2.01                     | 0.61              |
| 1:E:360:ILE:HD12 | 1:E:360:ILE:O    | 2.00                     | 0.61              |
| 1:G:155:VAL:HG13 | 1:G:374:THR:HG21 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:210:ARG:C    | 1:F:210:ARG:HD3  | 2.21                     | 0.61              |
| 1:F:224:LEU:HD13 | 1:F:237:ASN:HD21 | 1.65                     | 0.61              |
| 1:G:194:ARG:O    | 1:G:197:MET:N    | 2.34                     | 0.61              |
| 1:B:209:ASN:O    | 1:C:331:MET:HE2  | 2.01                     | 0.61              |
| 1:E:134:ILE:HD12 | 1:E:134:ILE:H    | 1.64                     | 0.61              |
| 1:E:258:ILE:HD12 | 1:E:258:ILE:H    | 1.66                     | 0.61              |
| 1:B:184:LYS:HD2  | 1:B:231:ASP:HA   | 1.82                     | 0.61              |
| 1:E:207:ILE:HG22 | 1:E:211:LEU:CD2  | 2.31                     | 0.61              |
| 1:G:158:ASN:ND2  | 1:G:159:ALA:O    | 2.34                     | 0.61              |
| 1:D:275:ILE:HG22 | 1:D:277:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:191:GLN:OE1  | 1:A:350:ARG:NH2  | 2.33                     | 0.61              |
| 1:D:295:TYR:HE1  | 1:D:300:PRO:HD3  | 1.66                     | 0.61              |
| 1:D:307:ILE:HG21 | 1:D:312:PRO:HA   | 1.81                     | 0.61              |
| 1:G:368:LEU:HD23 | 1:G:368:LEU:H    | 1.66                     | 0.61              |
| 1:C:296:ILE:HG23 | 1:C:297:PHE:CD2  | 2.36                     | 0.61              |
| 1:B:360:ILE:HG22 | 1:B:361:LEU:N    | 2.16                     | 0.60              |
| 1:F:344:GLU:HB2  | 1:F:361:LEU:HD11 | 1.82                     | 0.60              |
| 1:F:327:GLY:CA   | 1:F:329:PHE:HE1  | 2.14                     | 0.60              |
| 1:F:266:THR:HA   | 1:F:270:PHE:O    | 2.02                     | 0.60              |
| 1:C:343:VAL:HG12 | 1:C:362:CYS:CB   | 2.31                     | 0.60              |
| 1:F:225:ASN:HD22 | 1:F:225:ASN:N    | 1.97                     | 0.60              |
| 1:E:278:ASN:HB3  | 1:E:281:ASP:OD2  | 2.01                     | 0.60              |
| 1:F:343:VAL:HA   | 1:F:361:LEU:O    | 2.01                     | 0.60              |
| 1:A:296:ILE:HG23 | 1:A:297:PHE:CE2  | 2.35                     | 0.60              |
| 1:E:258:ILE:HD12 | 1:E:258:ILE:N    | 2.15                     | 0.60              |
| 1:A:133:THR:HG22 | 1:A:135:ARG:H    | 1.66                     | 0.60              |
| 1:E:273:SER:N    | 1:E:328:GLY:HA2  | 2.15                     | 0.60              |
| 1:F:202:MET:SD   | 1:F:203:LEU:CA   | 2.88                     | 0.60              |
| 1:A:368:LEU:HD23 | 1:A:370:HIS:NE2  | 2.12                     | 0.60              |
| 1:C:224:LEU:HD12 | 1:C:225:ASN:ND2  | 2.16                     | 0.60              |
| 1:A:194:ARG:HB2  | 1:A:358:LEU:CD2  | 2.30                     | 0.60              |
| 1:A:233:LEU:HD11 | 1:A:366:LEU:CD1  | 2.26                     | 0.60              |
| 1:A:285:ILE:HA   | 1:A:288:LEU:HD11 | 1.82                     | 0.60              |
| 1:C:275:ILE:HG22 | 1:C:277:LEU:HD11 | 1.83                     | 0.60              |
| 1:E:131:ARG:NH1  | 1:E:316:THR:HA   | 2.16                     | 0.60              |
| 1:C:192:ALA:HB1  | 1:D:151:VAL:CG1  | 2.31                     | 0.60              |
| 1:C:239:VAL:HG12 | 1:C:373:PRO:HB3  | 1.84                     | 0.60              |
| 1:E:335:VAL:HG22 | 1:E:368:LEU:HD13 | 1.83                     | 0.60              |
| 1:E:199:ASP:CB   | 1:E:202:MET:HE2  | 2.31                     | 0.60              |
| 1:C:130:ARG:CB   | 1:D:271:SER:OG   | 2.50                     | 0.60              |
| 1:D:184:LYS:NZ   | 1:D:231:ASP:HA   | 2.17                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:201:PRO:CA   | 1:B:204:GLN:HB2  | 2.32                     | 0.60              |
| 1:F:203:LEU:HD22 | 1:F:204:GLN:HA   | 1.83                     | 0.60              |
| 1:A:206:TYR:O    | 1:A:210:ARG:HB3  | 2.01                     | 0.60              |
| 1:A:158:ASN:ND2  | 1:A:158:ASN:H    | 2.00                     | 0.60              |
| 1:A:297:PHE:CE2  | 1:A:309:TRP:CZ2  | 2.89                     | 0.60              |
| 1:E:204:GLN:O    | 1:E:208:ASN:HB2  | 2.01                     | 0.60              |
| 1:B:125:ILE:HG12 | 1:B:127:PRO:HG3  | 1.84                     | 0.60              |
| 1:B:134:ILE:N    | 1:B:134:ILE:HD12 | 2.16                     | 0.60              |
| 1:D:130:ARG:CZ   | 1:D:131:ARG:HB2  | 2.31                     | 0.60              |
| 1:A:124:ILE:O    | 1:A:126:MET:SD   | 2.59                     | 0.60              |
| 1:E:194:ARG:HH11 | 1:E:347:ARG:CZ   | 2.15                     | 0.60              |
| 1:C:190:VAL:HG22 | 1:D:176:PHE:CE1  | 2.36                     | 0.60              |
| 1:A:146:ASN:ND2  | 1:G:145:SER:HB2  | 2.17                     | 0.60              |
| 1:G:376:ILE:HD12 | 1:G:376:ILE:N    | 2.16                     | 0.60              |
| 1:F:327:GLY:O    | 1:F:329:PHE:CE1  | 2.53                     | 0.60              |
| 1:D:303:PHE:HD1  | 1:D:303:PHE:N    | 1.99                     | 0.60              |
| 1:F:346:SER:HB3  | 1:F:348:GLU:HG3  | 1.84                     | 0.60              |
| 1:C:224:LEU:HD13 | 1:C:237:ASN:ND2  | 2.16                     | 0.60              |
| 1:C:130:ARG:CG   | 1:D:271:SER:CB   | 2.69                     | 0.60              |
| 1:E:155:VAL:CG1  | 1:E:374:THR:HB   | 2.32                     | 0.60              |
| 1:B:217:LEU:C    | 1:B:217:LEU:HD12 | 2.21                     | 0.59              |
| 1:A:189:TRP:HB3  | 1:A:361:LEU:HD13 | 1.84                     | 0.59              |
| 1:C:155:VAL:CG2  | 1:C:174:ILE:HG22 | 2.31                     | 0.59              |
| 1:C:247:LEU:HB3  | 1:C:260:HIS:HD2  | 1.66                     | 0.59              |
| 1:D:261:ALA:O    | 1:D:265:VAL:HG23 | 2.02                     | 0.59              |
| 1:C:129:LEU:N    | 1:C:129:LEU:HD22 | 2.15                     | 0.59              |
| 1:D:201:PRO:O    | 1:D:204:GLN:N    | 2.34                     | 0.59              |
| 1:G:174:ILE:H    | 1:G:174:ILE:CD1  | 2.12                     | 0.59              |
| 1:F:292:GLU:O    | 1:F:294:ARG:HG2  | 2.02                     | 0.59              |
| 1:D:155:VAL:HG11 | 1:D:374:THR:HB   | 1.83                     | 0.59              |
| 1:B:194:ARG:HA   | 1:B:358:LEU:CD1  | 2.32                     | 0.59              |
| 1:A:285:ILE:O    | 1:A:288:LEU:CG   | 2.49                     | 0.59              |
| 1:G:345:VAL:HG22 | 1:G:360:ILE:HG22 | 1.84                     | 0.59              |
| 1:B:341:ALA:HB1  | 1:B:362:CYS:SG   | 2.43                     | 0.59              |
| 1:D:296:ILE:C    | 1:D:298:GLY:H    | 2.06                     | 0.59              |
| 1:B:236:LEU:HD23 | 1:B:370:HIS:HE1  | 1.66                     | 0.59              |
| 1:C:203:LEU:O    | 1:C:206:TYR:CA   | 2.50                     | 0.59              |
| 1:D:155:VAL:CG1  | 1:D:374:THR:HG21 | 2.32                     | 0.59              |
| 1:E:194:ARG:HA   | 1:E:358:LEU:HD11 | 1.82                     | 0.59              |
| 1:C:187:ALA:HB2  | 1:C:363:GLU:CA   | 2.23                     | 0.59              |
| 1:E:300:PRO:HB2  | 1:F:309:TRP:CE2  | 2.37                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:PHE:CE1  | 1:F:190:VAL:HG13 | 2.37                     | 0.59              |
| 1:A:191:GLN:N    | 1:A:191:GLN:HE21 | 1.98                     | 0.59              |
| 1:D:289:LYS:HD2  | 1:D:289:LYS:N    | 2.17                     | 0.59              |
| 1:F:202:MET:SD   | 1:F:202:MET:C    | 2.80                     | 0.59              |
| 1:G:196:VAL:C    | 1:G:198:ASP:H    | 2.06                     | 0.59              |
| 1:E:366:LEU:C    | 1:E:366:LEU:HD12 | 2.23                     | 0.59              |
| 1:E:182:ASN:HB2  | 1:E:184:LYS:NZ   | 2.17                     | 0.59              |
| 1:F:254:ARG:HG2  | 1:F:381:PHE:CD2  | 2.38                     | 0.59              |
| 1:C:330:ASP:OD1  | 1:C:331:MET:N    | 2.35                     | 0.59              |
| 1:D:241:THR:O    | 1:D:377:ILE:HA   | 2.03                     | 0.59              |
| 1:B:194:ARG:CZ   | 1:B:347:ARG:NH2  | 2.66                     | 0.59              |
| 1:F:142:ARG:HG3  | 1:F:337:ASP:CB   | 2.11                     | 0.59              |
| 1:B:180:THR:HG22 | 1:B:181:ALA:N    | 2.18                     | 0.59              |
| 1:A:155:VAL:CG1  | 1:A:374:THR:HG21 | 2.32                     | 0.59              |
| 1:B:158:ASN:ND2  | 1:B:158:ASN:N    | 2.48                     | 0.59              |
| 1:F:327:GLY:CA   | 1:F:329:PHE:CE1  | 2.85                     | 0.59              |
| 1:G:351:ASP:O    | 1:G:355:LYS:CG   | 2.48                     | 0.59              |
| 1:A:277:LEU:O    | 1:A:315:PRO:HA   | 2.03                     | 0.59              |
| 1:F:227:ASP:O    | 1:F:232:ASN:HB2  | 2.03                     | 0.59              |
| 1:D:186:ILE:N    | 1:D:186:ILE:HD12 | 2.17                     | 0.59              |
| 1:E:382:SER:O    | 1:E:383:SER:CB   | 2.49                     | 0.59              |
| 1:B:262:ILE:H    | 1:B:262:ILE:HD12 | 1.66                     | 0.59              |
| 1:E:218:LYS:HG3  | 1:E:218:LYS:O    | 2.03                     | 0.59              |
| 1:F:175:THR:HG22 | 1:F:176:PHE:H    | 1.67                     | 0.59              |
| 1:G:155:VAL:HG23 | 1:G:174:ILE:HG22 | 1.83                     | 0.59              |
| 1:A:155:VAL:CG1  | 1:A:374:THR:OG1  | 2.50                     | 0.59              |
| 1:D:132:LEU:HD23 | 1:D:132:LEU:N    | 2.16                     | 0.59              |
| 1:B:142:ARG:HG3  | 1:B:337:ASP:HB2  | 1.85                     | 0.59              |
| 1:C:347:ARG:O    | 1:C:352:ASN:HB2  | 2.02                     | 0.59              |
| 1:G:189:TRP:HB3  | 1:G:361:LEU:HD13 | 1.84                     | 0.59              |
| 1:E:202:MET:SD   | 1:E:203:LEU:N    | 2.76                     | 0.59              |
| 1:A:265:VAL:HG11 | 1:A:327:GLY:HA2  | 1.85                     | 0.59              |
| 1:A:224:LEU:HD12 | 1:A:225:ASN:ND2  | 2.17                     | 0.59              |
| 1:F:202:MET:O    | 1:F:205:SER:CB   | 2.51                     | 0.58              |
| 1:D:207:ILE:HD12 | 1:D:207:ILE:N    | 2.18                     | 0.58              |
| 1:E:200:ALA:HB3  | 1:E:201:PRO:CD   | 2.33                     | 0.58              |
| 1:G:280:ARG:C    | 1:G:282:TRP:N    | 2.56                     | 0.58              |
| 1:A:183:VAL:HG22 | 1:A:367:ALA:HB2  | 1.83                     | 0.58              |
| 1:A:343:VAL:HG12 | 1:A:362:CYS:CB   | 2.31                     | 0.58              |
| 1:A:187:ALA:HB1  | 1:A:361:LEU:HD11 | 1.85                     | 0.58              |
| 1:A:237:ASN:ND2  | 1:A:325:THR:HG21 | 2.18                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:358:LEU:HD12 | 1:D:358:LEU:N    | 2.18                     | 0.58              |
| 1:B:358:LEU:CD1  | 1:B:358:LEU:N    | 2.66                     | 0.58              |
| 1:C:227:ASP:O    | 1:C:232:ASN:CB   | 2.51                     | 0.58              |
| 1:C:133:THR:HG22 | 1:C:135:ARG:H    | 1.68                     | 0.58              |
| 1:C:376:ILE:N    | 1:C:376:ILE:HD12 | 2.18                     | 0.58              |
| 1:E:335:VAL:HG22 | 1:E:368:LEU:CD1  | 2.33                     | 0.58              |
| 1:C:194:ARG:O    | 1:C:196:VAL:CB   | 2.52                     | 0.58              |
| 1:F:210:ARG:CG   | 1:F:210:ARG:HH11 | 2.02                     | 0.58              |
| 1:A:153:GLU:CD   | 1:F:210:ARG:NH2  | 2.51                     | 0.58              |
| 1:C:244:ASP:H    | 1:C:264:GLN:NE2  | 2.01                     | 0.58              |
| 1:B:368:LEU:HD23 | 1:B:369:ALA:N    | 2.18                     | 0.58              |
| 1:E:194:ARG:NH1  | 1:E:347:ARG:CZ   | 2.67                     | 0.58              |
| 1:G:285:ILE:HA   | 1:G:288:LEU:CG   | 2.34                     | 0.58              |
| 1:D:244:ASP:O    | 1:D:247:LEU:HB3  | 2.03                     | 0.58              |
| 1:F:210:ARG:NH1  | 1:F:210:ARG:CG   | 2.65                     | 0.58              |
| 1:A:345:VAL:HG13 | 1:A:359:THR:O    | 2.04                     | 0.58              |
| 1:G:150:TYR:HE2  | 1:G:181:ALA:HB2  | 1.67                     | 0.58              |
| 1:D:290:ASP:OD2  | 1:D:294:ARG:HB3  | 2.03                     | 0.58              |
| 1:A:244:ASP:OD2  | 1:A:246:SER:HB3  | 2.02                     | 0.58              |
| 1:C:344:GLU:H    | 1:C:361:LEU:HD12 | 1.69                     | 0.58              |
| 1:C:224:LEU:HD12 | 1:C:225:ASN:CG   | 2.24                     | 0.58              |
| 1:A:224:LEU:HD21 | 1:A:276:VAL:HG11 | 1.84                     | 0.58              |
| 1:F:375:ALA:C    | 1:F:376:ILE:HD12 | 2.24                     | 0.58              |
| 1:F:195:GLN:CA   | 1:F:195:GLN:OE1  | 2.50                     | 0.58              |
| 1:F:155:VAL:O    | 1:F:155:VAL:HG13 | 2.03                     | 0.58              |
| 1:F:211:LEU:HD22 | 1:F:212:MET:HE3  | 1.85                     | 0.58              |
| 1:G:310:GLY:C    | 1:G:311:LEU:HD22 | 2.24                     | 0.58              |
| 1:G:226:GLY:H    | 1:G:235:GLY:HA3  | 1.68                     | 0.58              |
| 1:C:201:PRO:O    | 1:C:204:GLN:CA   | 2.51                     | 0.58              |
| 1:C:207:ILE:H    | 1:C:207:ILE:HD13 | 1.68                     | 0.58              |
| 1:G:199:ASP:HB3  | 1:G:202:MET:CB   | 2.31                     | 0.58              |
| 1:E:210:ARG:NH2  | 1:F:153:GLU:OE2  | 2.35                     | 0.58              |
| 1:F:175:THR:HG22 | 1:F:176:PHE:N    | 2.19                     | 0.58              |
| 1:B:253:THR:HG22 | 1:B:254:ARG:N    | 2.19                     | 0.58              |
| 1:G:135:ARG:HH21 | 1:G:219:GLU:CD   | 2.06                     | 0.58              |
| 1:E:193:SER:O    | 1:E:195:GLN:N    | 2.36                     | 0.58              |
| 1:E:212:MET:C    | 1:E:214:GLY:N    | 2.55                     | 0.58              |
| 1:A:190:VAL:HG21 | 1:A:210:ARG:NH1  | 2.19                     | 0.58              |
| 1:C:138:LEU:HD23 | 1:C:329:PHE:HB3  | 1.84                     | 0.58              |
| 1:G:175:THR:HG22 | 1:G:176:PHE:N    | 2.18                     | 0.58              |
| 1:F:331:MET:O    | 1:F:331:MET:HG2  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:282:TRP:CZ3  | 1:F:308:MET:HE1  | 2.39                     | 0.58              |
| 1:D:155:VAL:HG13 | 1:D:155:VAL:O    | 2.03                     | 0.58              |
| 1:C:190:VAL:N    | 1:C:360:ILE:O    | 2.31                     | 0.58              |
| 1:G:354:VAL:O    | 1:G:356:ASN:N    | 2.37                     | 0.58              |
| 1:C:244:ASP:OD2  | 1:C:247:LEU:HG   | 2.04                     | 0.58              |
| 1:C:306:ASN:HB3  | 1:C:313:VAL:HB   | 1.85                     | 0.58              |
| 1:F:153:GLU:CD   | 1:F:372:ARG:HH21 | 2.08                     | 0.57              |
| 1:B:149:GLU:HG2  | 1:B:180:THR:OG1  | 2.04                     | 0.57              |
| 1:A:345:VAL:HA   | 1:A:359:THR:O    | 2.05                     | 0.57              |
| 1:C:200:ALA:HB1  | 1:C:201:PRO:HD2  | 1.86                     | 0.57              |
| 1:G:281:ASP:O    | 1:G:285:ILE:CD1  | 2.52                     | 0.57              |
| 1:F:211:LEU:CD2  | 1:F:212:MET:HE3  | 2.34                     | 0.57              |
| 1:A:155:VAL:HG23 | 1:A:174:ILE:CG2  | 2.30                     | 0.57              |
| 1:B:148:LEU:O    | 1:B:180:THR:HG23 | 2.04                     | 0.57              |
| 1:E:158:ASN:N    | 1:E:158:ASN:ND2  | 2.50                     | 0.57              |
| 1:C:155:VAL:HA   | 1:C:174:ILE:HA   | 1.86                     | 0.57              |
| 1:C:184:LYS:HB2  | 1:C:233:LEU:HD21 | 1.86                     | 0.57              |
| 1:E:253:THR:HB   | 1:E:256:ASP:OD1  | 2.04                     | 0.57              |
| 1:E:148:LEU:N    | 1:E:148:LEU:HD23 | 2.20                     | 0.57              |
| 1:D:239:VAL:HG12 | 1:D:373:PRO:HB3  | 1.86                     | 0.57              |
| 1:E:207:ILE:CG1  | 1:E:208:ASN:H    | 2.12                     | 0.57              |
| 1:E:185:THR:HG22 | 1:E:365:ARG:HG2  | 1.87                     | 0.57              |
| 1:A:174:ILE:H    | 1:A:174:ILE:CD1  | 2.11                     | 0.57              |
| 1:B:279:PRO:HD3  | 1:B:316:THR:O    | 2.04                     | 0.57              |
| 1:D:356:ASN:ND2  | 1:E:178:LYS:NZ   | 2.53                     | 0.57              |
| 1:E:185:THR:O    | 1:E:186:ILE:HD13 | 2.03                     | 0.57              |
| 1:E:155:VAL:HG23 | 1:E:174:ILE:CG2  | 2.32                     | 0.57              |
| 1:D:158:ASN:N    | 1:D:158:ASN:ND2  | 2.48                     | 0.57              |
| 1:F:143:THR:OG1  | 1:F:144:SER:N    | 2.37                     | 0.57              |
| 1:C:152:ARG:HB3  | 1:C:177:SER:HB2  | 1.86                     | 0.57              |
| 1:D:125:ILE:HD13 | 1:D:208:ASN:OD1  | 1.97                     | 0.57              |
| 1:C:184:LYS:HG3  | 1:C:233:LEU:CD2  | 2.35                     | 0.57              |
| 1:A:191:GLN:N    | 1:A:191:GLN:NE2  | 2.53                     | 0.57              |
| 1:E:273:SER:H    | 1:E:328:GLY:HA2  | 1.70                     | 0.57              |
| 1:G:175:THR:HG22 | 1:G:176:PHE:H    | 1.69                     | 0.57              |
| 1:A:339:MET:HB3  | 1:A:365:ARG:HB2  | 1.87                     | 0.57              |
| 1:A:197:MET:C    | 1:A:199:ASP:H    | 2.06                     | 0.57              |
| 1:B:162:ASP:C    | 1:B:173:ASP:N    | 2.55                     | 0.57              |
| 1:A:183:VAL:HA   | 1:A:367:ALA:HB2  | 1.87                     | 0.57              |
| 1:D:346:SER:O    | 1:D:347:ARG:HB3  | 2.05                     | 0.57              |
| 1:C:292:GLU:HG2  | 1:C:294:ARG:HE   | 1.66                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:TYR:CE1  | 1:C:179:GLN:HB2  | 2.40                     | 0.57              |
| 1:F:347:ARG:O    | 1:F:352:ASN:HB2  | 2.04                     | 0.57              |
| 1:G:196:VAL:C    | 1:G:198:ASP:N    | 2.58                     | 0.57              |
| 1:F:174:ILE:N    | 1:F:174:ILE:HD13 | 2.14                     | 0.57              |
| 1:G:295:TYR:HB2  | 1:G:298:GLY:O    | 2.05                     | 0.57              |
| 1:D:127:PRO:HB3  | 1:D:212:MET:HB3  | 1.85                     | 0.57              |
| 1:B:134:ILE:HD13 | 1:B:220:GLU:CG   | 2.35                     | 0.57              |
| 1:B:342:THR:O    | 1:B:362:CYS:CA   | 2.49                     | 0.57              |
| 1:B:342:THR:OG1  | 1:B:363:GLU:HB2  | 2.05                     | 0.57              |
| 1:E:194:ARG:CZ   | 1:E:347:ARG:NH2  | 2.68                     | 0.56              |
| 1:B:129:LEU:C    | 1:B:131:ARG:N    | 2.57                     | 0.56              |
| 1:F:212:MET:CE   | 1:F:212:MET:HA   | 2.34                     | 0.56              |
| 1:C:202:MET:CE   | 1:C:203:LEU:HD23 | 2.35                     | 0.56              |
| 1:E:199:ASP:O    | 1:E:202:MET:CE   | 2.53                     | 0.56              |
| 1:E:206:TYR:C    | 1:E:206:TYR:CD2  | 2.75                     | 0.56              |
| 1:B:127:PRO:C    | 1:B:129:LEU:N    | 2.51                     | 0.56              |
| 1:C:131:ARG:HH11 | 1:C:131:ARG:HB2  | 1.70                     | 0.56              |
| 1:B:162:ASP:HB3  | 1:B:173:ASP:HB2  | 1.86                     | 0.56              |
| 1:C:266:THR:HA   | 1:C:270:PHE:O    | 2.05                     | 0.56              |
| 1:D:302:ALA:O    | 1:D:304:THR:N    | 2.38                     | 0.56              |
| 1:D:309:TRP:HE3  | 1:D:309:TRP:H    | 1.53                     | 0.56              |
| 1:E:222:GLN:OE1  | 1:E:232:ASN:HA   | 2.05                     | 0.56              |
| 1:A:368:LEU:CD2  | 1:A:370:HIS:CD2  | 2.89                     | 0.56              |
| 1:A:368:LEU:HD21 | 1:A:370:HIS:CD2  | 2.36                     | 0.56              |
| 1:B:217:LEU:HD12 | 1:B:218:LYS:N    | 2.20                     | 0.56              |
| 1:B:252:ASP:HB3  | 1:B:256:ASP:HB2  | 1.87                     | 0.56              |
| 1:A:190:VAL:CG1  | 1:A:211:LEU:HD21 | 2.35                     | 0.56              |
| 1:G:304:THR:HG22 | 1:G:305:SER:N    | 2.14                     | 0.56              |
| 1:E:261:ALA:O    | 1:E:265:VAL:HG23 | 2.06                     | 0.56              |
| 1:E:151:VAL:O    | 1:E:151:VAL:HG23 | 2.06                     | 0.56              |
| 1:C:288:LEU:HD23 | 1:C:289:LYS:O    | 2.04                     | 0.56              |
| 1:E:203:LEU:HD12 | 1:E:206:TYR:HB3  | 1.87                     | 0.56              |
| 1:B:126:MET:CE   | 1:B:212:MET:HG3  | 2.36                     | 0.56              |
| 1:B:134:ILE:H    | 1:B:134:ILE:CD1  | 2.19                     | 0.56              |
| 1:F:142:ARG:HA   | 1:F:337:ASP:H    | 1.71                     | 0.56              |
| 1:B:276:VAL:C    | 1:B:277:LEU:CD2  | 2.70                     | 0.56              |
| 1:E:134:ILE:HD12 | 1:E:134:ILE:N    | 2.21                     | 0.56              |
| 1:D:254:ARG:O    | 1:D:258:ILE:HD13 | 2.06                     | 0.56              |
| 1:C:177:SER:O    | 1:C:179:GLN:HG2  | 2.05                     | 0.56              |
| 1:D:358:LEU:CD1  | 1:D:358:LEU:H    | 2.19                     | 0.56              |
| 1:E:190:VAL:HG12 | 1:F:176:PHE:CZ   | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:343:VAL:HG12 | 1:D:362:CYS:SG   | 2.45                     | 0.56              |
| 1:E:157:THR:CG2  | 1:E:267:GLU:CG   | 2.78                     | 0.56              |
| 1:G:366:LEU:CD1  | 1:G:367:ALA:N    | 2.68                     | 0.56              |
| 1:F:277:LEU:HD12 | 1:F:277:LEU:N    | 2.21                     | 0.56              |
| 1:E:224:LEU:HD12 | 1:E:225:ASN:OD1  | 2.05                     | 0.56              |
| 1:G:311:LEU:N    | 1:G:311:LEU:HD22 | 2.20                     | 0.56              |
| 1:C:276:VAL:HG22 | 1:C:314:VAL:CG2  | 2.36                     | 0.56              |
| 1:A:240:ALA:CB   | 1:A:376:ILE:HG22 | 2.36                     | 0.56              |
| 1:A:158:ASN:ND2  | 1:A:158:ASN:N    | 2.54                     | 0.56              |
| 1:A:276:VAL:HB   | 1:A:325:THR:OG1  | 2.06                     | 0.56              |
| 1:A:207:ILE:HG23 | 1:A:211:LEU:HD12 | 1.86                     | 0.56              |
| 1:E:155:VAL:O    | 1:E:155:VAL:HG13 | 2.06                     | 0.56              |
| 1:B:155:VAL:HG13 | 1:B:374:THR:CB   | 2.35                     | 0.56              |
| 1:A:129:LEU:CD2  | 1:A:129:LEU:N    | 2.69                     | 0.56              |
| 1:E:225:ASN:HA   | 1:E:235:GLY:HA3  | 1.88                     | 0.56              |
| 1:D:377:ILE:N    | 1:D:377:ILE:HD12 | 2.21                     | 0.56              |
| 1:E:193:SER:O    | 1:E:196:VAL:HG23 | 2.06                     | 0.56              |
| 1:A:185:THR:HG22 | 1:A:365:ARG:HG2  | 1.88                     | 0.56              |
| 1:B:261:ALA:O    | 1:B:265:VAL:HG23 | 2.06                     | 0.56              |
| 1:A:184:LYS:HE3  | 1:A:230:GLY:O    | 2.05                     | 0.56              |
| 1:C:213:TYR:CD2  | 1:C:217:LEU:CD1  | 2.89                     | 0.56              |
| 1:G:377:ILE:N    | 1:G:377:ILE:HD12 | 2.21                     | 0.56              |
| 1:D:209:ASN:O    | 1:D:213:TYR:HB3  | 2.06                     | 0.56              |
| 1:E:127:PRO:HG2  | 1:E:129:LEU:CD1  | 2.35                     | 0.56              |
| 1:C:196:VAL:CG1  | 1:C:203:LEU:HD13 | 2.32                     | 0.56              |
| 1:C:207:ILE:HG22 | 1:C:211:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:287:LEU:N    | 1:A:288:LEU:CD2  | 2.69                     | 0.56              |
| 1:F:253:THR:HG23 | 1:F:256:ASP:CG   | 2.25                     | 0.56              |
| 1:C:357:MET:HE2  | 1:D:178:LYS:CG   | 2.35                     | 0.56              |
| 1:A:275:ILE:CD1  | 1:A:308:MET:SD   | 2.94                     | 0.56              |
| 1:B:255:ALA:HA   | 1:B:258:ILE:HD13 | 1.88                     | 0.56              |
| 1:C:200:ALA:C    | 1:C:202:MET:N    | 2.58                     | 0.56              |
| 1:B:202:MET:C    | 1:B:204:GLN:N    | 2.50                     | 0.56              |
| 1:E:200:ALA:N    | 1:E:201:PRO:HD2  | 2.20                     | 0.56              |
| 1:E:202:MET:HE1  | 1:E:203:LEU:HB2  | 1.88                     | 0.56              |
| 1:F:254:ARG:HB3  | 1:F:285:ILE:CD1  | 2.37                     | 0.56              |
| 1:G:291:ASN:C    | 1:G:293:GLY:H    | 2.09                     | 0.56              |
| 1:G:196:VAL:O    | 1:G:198:ASP:N    | 2.39                     | 0.55              |
| 1:D:190:VAL:HG11 | 1:D:211:LEU:HD21 | 1.84                     | 0.55              |
| 1:E:354:VAL:O    | 1:E:356:ASN:N    | 2.40                     | 0.55              |
| 1:B:194:ARG:O    | 1:B:195:GLN:HB2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:349:ASP:OD1  | 1:A:350:ARG:CG   | 2.55                     | 0.55              |
| 1:E:135:ARG:NH2  | 1:E:337:ASP:OD2  | 2.34                     | 0.55              |
| 1:D:154:GLU:HB3  | 1:D:175:THR:HB   | 1.87                     | 0.55              |
| 1:G:152:ARG:HG3  | 1:G:371:TYR:O    | 2.06                     | 0.55              |
| 1:E:128:GLY:O    | 1:E:129:LEU:HB2  | 2.05                     | 0.55              |
| 1:D:244:ASP:HB2  | 1:D:264:GLN:NE2  | 2.21                     | 0.55              |
| 1:E:305:SER:HB2  | 1:E:307:ILE:HG12 | 1.87                     | 0.55              |
| 1:F:377:ILE:N    | 1:F:377:ILE:HD12 | 2.21                     | 0.55              |
| 1:F:192:ALA:O    | 1:F:357:MET:HA   | 2.05                     | 0.55              |
| 1:B:125:ILE:CD1  | 1:B:127:PRO:HG3  | 2.37                     | 0.55              |
| 1:E:236:LEU:HD23 | 1:E:370:HIS:CE1  | 2.41                     | 0.55              |
| 1:B:132:LEU:N    | 1:B:132:LEU:HD23 | 2.18                     | 0.55              |
| 1:C:284:ASN:O    | 1:C:288:LEU:HB2  | 2.07                     | 0.55              |
| 1:C:268:SER:O    | 1:C:269:GLU:HB2  | 2.06                     | 0.55              |
| 1:F:203:LEU:HD23 | 1:F:206:TYR:HB3  | 1.89                     | 0.55              |
| 1:E:227:ASP:O    | 1:E:229:THR:HG22 | 2.07                     | 0.55              |
| 1:D:257:ILE:HA   | 1:D:260:HIS:HD2  | 1.71                     | 0.55              |
| 1:B:250:THR:HG22 | 1:B:251:GLY:N    | 2.18                     | 0.55              |
| 1:C:225:ASN:HD22 | 1:C:225:ASN:N    | 2.02                     | 0.55              |
| 1:D:295:TYR:CE1  | 1:D:300:PRO:HD3  | 2.41                     | 0.55              |
| 1:A:297:PHE:HD2  | 1:A:297:PHE:N    | 2.04                     | 0.55              |
| 1:C:297:PHE:HE1  | 1:C:308:MET:HE3  | 1.71                     | 0.55              |
| 1:F:376:ILE:HD12 | 1:F:376:ILE:N    | 2.22                     | 0.55              |
| 1:G:278:ASN:O    | 1:G:281:ASP:N    | 2.40                     | 0.55              |
| 1:B:129:LEU:CD2  | 1:B:129:LEU:C    | 2.74                     | 0.55              |
| 1:E:297:PHE:CD2  | 1:E:298:GLY:N    | 2.75                     | 0.55              |
| 1:E:132:LEU:H    | 1:E:132:LEU:CD2  | 2.17                     | 0.55              |
| 1:D:356:ASN:HD21 | 1:E:178:LYS:NZ   | 2.04                     | 0.55              |
| 1:A:175:THR:HG22 | 1:A:176:PHE:N    | 2.22                     | 0.55              |
| 1:E:194:ARG:HH11 | 1:E:347:ARG:NH1  | 2.04                     | 0.55              |
| 1:E:296:ILE:HG22 | 1:E:298:GLY:H    | 1.71                     | 0.55              |
| 1:C:357:MET:SD   | 1:D:178:LYS:HD3  | 2.47                     | 0.55              |
| 1:G:372:ARG:HH11 | 1:G:372:ARG:HG2  | 1.72                     | 0.55              |
| 1:G:372:ARG:HG2  | 1:G:372:ARG:NH1  | 2.22                     | 0.55              |
| 1:G:335:VAL:HG12 | 1:G:368:LEU:HB3  | 1.89                     | 0.55              |
| 1:C:157:THR:OG1  | 1:C:158:ASN:N    | 2.38                     | 0.55              |
| 1:F:260:HIS:O    | 1:F:263:TYR:HB3  | 2.07                     | 0.55              |
| 1:C:194:ARG:HB2  | 1:C:358:LEU:HG   | 1.88                     | 0.55              |
| 1:B:148:LEU:C    | 1:B:180:THR:HG23 | 2.28                     | 0.55              |
| 1:B:296:ILE:O    | 1:B:296:ILE:HG12 | 2.06                     | 0.55              |
| 1:F:376:ILE:C    | 1:F:377:ILE:HD12 | 2.27                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:359:THR:O    | 1:E:359:THR:HG22 | 2.07                     | 0.55              |
| 1:G:282:TRP:CZ3  | 1:G:313:VAL:HG21 | 2.41                     | 0.55              |
| 1:B:144:SER:HA   | 1:B:338:ARG:NH1  | 2.22                     | 0.55              |
| 1:F:206:TYR:O    | 1:F:207:ILE:C    | 2.45                     | 0.54              |
| 1:F:194:ARG:NH1  | 1:F:347:ARG:CZ   | 2.69                     | 0.54              |
| 1:B:194:ARG:HD2  | 1:B:358:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:278:ASN:HD21 | 1:C:280:ARG:HB3  | 1.70                     | 0.54              |
| 1:C:146:ASN:HD21 | 1:C:365:ARG:HH22 | 1.54                     | 0.54              |
| 1:G:270:PHE:HE1  | 1:G:372:ARG:CZ   | 2.19                     | 0.54              |
| 1:E:215:LEU:O    | 1:E:218:LYS:CA   | 2.55                     | 0.54              |
| 1:C:196:VAL:HG11 | 1:C:203:LEU:CD1  | 2.29                     | 0.54              |
| 1:A:127:PRO:HD3  | 1:A:212:MET:CE   | 2.38                     | 0.54              |
| 1:D:129:LEU:CD1  | 1:D:131:ARG:N    | 2.67                     | 0.54              |
| 1:E:262:ILE:N    | 1:E:262:ILE:HD12 | 2.22                     | 0.54              |
| 1:F:207:ILE:HD12 | 1:F:207:ILE:C    | 2.28                     | 0.54              |
| 1:G:203:LEU:C    | 1:G:205:SER:N    | 2.57                     | 0.54              |
| 1:B:289:LYS:HD2  | 1:B:293:GLY:CA   | 2.37                     | 0.54              |
| 1:D:343:VAL:HA   | 1:D:361:LEU:O    | 2.06                     | 0.54              |
| 1:E:227:ASP:C    | 1:E:229:THR:HG23 | 2.28                     | 0.54              |
| 1:C:275:ILE:HG13 | 1:C:326:VAL:HG12 | 1.89                     | 0.54              |
| 1:D:244:ASP:HB2  | 1:D:264:GLN:HE22 | 1.72                     | 0.54              |
| 1:D:343:VAL:HG12 | 1:D:362:CYS:HB2  | 1.89                     | 0.54              |
| 1:B:153:GLU:HB2  | 1:B:371:TYR:O    | 2.08                     | 0.54              |
| 1:B:258:ILE:CD1  | 1:B:258:ILE:H    | 2.20                     | 0.54              |
| 1:C:132:LEU:CD2  | 1:C:136:ASP:HB2  | 2.38                     | 0.54              |
| 1:A:202:MET:CG   | 1:A:203:LEU:N    | 2.71                     | 0.54              |
| 1:A:377:ILE:N    | 1:A:377:ILE:HD12 | 2.22                     | 0.54              |
| 1:G:316:THR:HG22 | 1:G:318:ALA:N    | 2.17                     | 0.54              |
| 1:D:191:GLN:HB2  | 1:E:151:VAL:HG21 | 1.88                     | 0.54              |
| 1:B:329:PHE:O    | 1:B:330:ASP:C    | 2.45                     | 0.54              |
| 1:B:368:LEU:C    | 1:B:368:LEU:HD23 | 2.28                     | 0.54              |
| 1:B:344:GLU:N    | 1:B:361:LEU:O    | 2.38                     | 0.54              |
| 1:F:344:GLU:H    | 1:F:361:LEU:CD1  | 2.21                     | 0.54              |
| 1:B:161:GLY:O    | 1:B:172:SER:N    | 2.41                     | 0.54              |
| 1:G:355:LYS:O    | 1:G:356:ASN:C    | 2.46                     | 0.54              |
| 1:B:144:SER:HA   | 1:B:338:ARG:HH11 | 1.71                     | 0.54              |
| 1:F:281:ASP:O    | 1:F:285:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:121:ILE:HG23 | 1:A:343:VAL:O    | 2.08                     | 0.54              |
| 1:A:297:PHE:CD2  | 1:A:297:PHE:N    | 2.74                     | 0.54              |
| 1:B:210:ARG:HH22 | 1:C:153:GLU:CG   | 2.18                     | 0.54              |
| 1:E:191:GLN:HB3  | 1:E:359:THR:HA   | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:131:ARG:O    | 1:G:133:THR:N    | 2.33                     | 0.54              |
| 1:B:161:GLY:O    | 1:B:162:ASP:C    | 2.45                     | 0.54              |
| 1:F:225:ASN:HA   | 1:F:235:GLY:HA3  | 1.88                     | 0.54              |
| 1:F:158:ASN:N    | 1:F:158:ASN:HD22 | 2.04                     | 0.54              |
| 1:B:278:ASN:HB3  | 1:B:281:ASP:OD2  | 2.08                     | 0.54              |
| 1:F:211:LEU:CD2  | 1:F:362:CYS:SG   | 2.93                     | 0.54              |
| 1:G:128:GLY:O    | 1:G:130:ARG:HG2  | 2.08                     | 0.54              |
| 1:E:277:LEU:HD23 | 1:E:277:LEU:N    | 2.23                     | 0.54              |
| 1:E:287:LEU:HD12 | 1:E:295:TYR:HE1  | 1.73                     | 0.54              |
| 1:E:155:VAL:CG1  | 1:E:374:THR:CB   | 2.85                     | 0.54              |
| 1:F:199:ASP:O    | 1:F:200:ALA:C    | 2.47                     | 0.53              |
| 1:B:195:GLN:CA   | 1:B:197:MET:HG2  | 2.38                     | 0.53              |
| 1:D:174:ILE:HD13 | 1:D:174:ILE:H    | 1.72                     | 0.53              |
| 1:G:285:ILE:CA   | 1:G:288:LEU:HG   | 2.37                     | 0.53              |
| 1:B:344:GLU:O    | 1:B:361:LEU:N    | 2.42                     | 0.53              |
| 1:D:148:LEU:O    | 1:D:148:LEU:HD12 | 2.06                     | 0.53              |
| 1:C:281:ASP:O    | 1:C:285:ILE:HG12 | 2.08                     | 0.53              |
| 1:D:138:LEU:HD12 | 1:D:138:LEU:N    | 2.22                     | 0.53              |
| 1:E:217:LEU:HD11 | 1:F:269:GLU:HB3  | 1.89                     | 0.53              |
| 1:G:194:ARG:C    | 1:G:196:VAL:N    | 2.51                     | 0.53              |
| 1:D:174:ILE:O    | 1:D:174:ILE:CG1  | 2.56                     | 0.53              |
| 1:G:278:ASN:O    | 1:G:279:PRO:C    | 2.46                     | 0.53              |
| 1:C:366:LEU:HD13 | 1:C:367:ALA:N    | 2.22                     | 0.53              |
| 1:E:215:LEU:HD23 | 1:E:215:LEU:C    | 2.28                     | 0.53              |
| 1:C:345:VAL:HG13 | 1:C:360:ILE:HD13 | 1.91                     | 0.53              |
| 1:G:281:ASP:O    | 1:G:285:ILE:HD12 | 2.07                     | 0.53              |
| 1:E:199:ASP:O    | 1:E:202:MET:HE3  | 2.08                     | 0.53              |
| 1:D:174:ILE:HG12 | 1:D:174:ILE:O    | 2.07                     | 0.53              |
| 1:D:247:LEU:HD21 | 1:D:260:HIS:CB   | 2.32                     | 0.53              |
| 1:C:227:ASP:C    | 1:C:229:THR:N    | 2.61                     | 0.53              |
| 1:F:275:ILE:HG23 | 1:F:326:VAL:CG1  | 2.38                     | 0.53              |
| 1:G:239:VAL:HG12 | 1:G:373:PRO:HB3  | 1.91                     | 0.53              |
| 1:B:304:THR:HG21 | 1:C:309:TRP:O    | 2.07                     | 0.53              |
| 1:F:204:GLN:HA   | 1:F:207:ILE:HG13 | 1.90                     | 0.53              |
| 1:B:149:GLU:HA   | 1:B:180:THR:HA   | 1.91                     | 0.53              |
| 1:A:366:LEU:CD1  | 1:A:366:LEU:C    | 2.76                     | 0.53              |
| 1:A:366:LEU:O    | 1:A:366:LEU:HD12 | 2.08                     | 0.53              |
| 1:D:301:GLN:O    | 1:D:302:ALA:C    | 2.47                     | 0.53              |
| 1:D:307:ILE:HB   | 1:D:311:LEU:O    | 2.09                     | 0.53              |
| 1:C:243:TYR:OH   | 1:C:260:HIS:HB2  | 2.08                     | 0.53              |
| 1:C:132:LEU:HD23 | 1:C:136:ASP:OD2  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:175:THR:HG22 | 1:B:176:PHE:H    | 1.73                     | 0.53              |
| 1:B:202:MET:O    | 1:B:203:LEU:C    | 2.47                     | 0.53              |
| 1:G:200:ALA:O    | 1:G:204:GLN:CA   | 2.57                     | 0.53              |
| 1:C:287:LEU:HD23 | 1:C:300:PRO:HA   | 1.89                     | 0.53              |
| 1:E:307:ILE:HG22 | 1:E:312:PRO:HA   | 1.91                     | 0.53              |
| 1:D:356:ASN:ND2  | 1:E:178:LYS:HZ1  | 2.05                     | 0.53              |
| 1:E:187:ALA:HB2  | 1:E:363:GLU:HA   | 1.90                     | 0.53              |
| 1:E:199:ASP:HB3  | 1:E:202:MET:HE2  | 1.91                     | 0.53              |
| 1:E:206:TYR:HD2  | 1:E:206:TYR:C    | 2.11                     | 0.53              |
| 1:A:125:ILE:CG2  | 1:A:204:GLN:HE21 | 2.09                     | 0.53              |
| 1:F:253:THR:O    | 1:F:256:ASP:N    | 2.42                     | 0.53              |
| 1:E:157:THR:CG2  | 1:E:267:GLU:HG2  | 2.38                     | 0.53              |
| 1:F:206:TYR:C    | 1:F:208:ASN:H    | 2.10                     | 0.53              |
| 1:B:158:ASN:ND2  | 1:B:172:SER:CB   | 2.72                     | 0.53              |
| 1:B:153:GLU:OE1  | 1:B:371:TYR:O    | 2.27                     | 0.53              |
| 1:F:314:VAL:O    | 1:F:314:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:252:ASP:HB3  | 1:E:256:ASP:HB2  | 1.90                     | 0.53              |
| 1:C:152:ARG:O    | 1:C:176:PHE:HA   | 2.09                     | 0.53              |
| 1:D:309:TRP:CE3  | 1:D:309:TRP:N    | 2.77                     | 0.53              |
| 1:E:282:TRP:CE3  | 1:E:282:TRP:HA   | 2.44                     | 0.53              |
| 1:C:194:ARG:HA   | 1:C:358:LEU:CD1  | 2.39                     | 0.53              |
| 1:E:207:ILE:O    | 1:E:211:LEU:N    | 2.39                     | 0.53              |
| 1:B:194:ARG:HG2  | 1:B:356:ASN:O    | 2.08                     | 0.53              |
| 1:E:158:ASN:N    | 1:E:158:ASN:HD22 | 2.06                     | 0.53              |
| 1:D:158:ASN:N    | 1:D:158:ASN:HD22 | 2.05                     | 0.53              |
| 1:E:196:VAL:O    | 1:E:196:VAL:HG12 | 2.09                     | 0.53              |
| 1:F:268:SER:O    | 1:F:269:GLU:HB2  | 2.09                     | 0.53              |
| 1:D:124:ILE:CG2  | 1:D:125:ILE:N    | 2.72                     | 0.53              |
| 1:F:155:VAL:HG23 | 1:F:174:ILE:CG2  | 2.33                     | 0.53              |
| 1:G:278:ASN:HD22 | 1:G:321:ALA:CA   | 2.22                     | 0.53              |
| 1:B:150:TYR:HE2  | 1:B:181:ALA:HB2  | 1.73                     | 0.53              |
| 1:E:220:GLU:CG   | 1:E:316:THR:HG21 | 2.39                     | 0.53              |
| 1:E:220:GLU:OE2  | 1:E:316:THR:OG1  | 2.22                     | 0.53              |
| 1:D:356:ASN:CG   | 1:E:178:LYS:NZ   | 2.62                     | 0.53              |
| 1:A:289:LYS:N    | 1:A:289:LYS:HD2  | 2.23                     | 0.53              |
| 1:C:202:MET:HE1  | 1:C:203:LEU:HD23 | 1.90                     | 0.52              |
| 1:B:148:LEU:CD2  | 1:B:181:ALA:HB3  | 2.40                     | 0.52              |
| 1:G:137:LEU:HD11 | 1:G:314:VAL:HG21 | 1.91                     | 0.52              |
| 1:C:155:VAL:CB   | 1:C:174:ILE:HG22 | 2.39                     | 0.52              |
| 1:F:292:GLU:O    | 1:F:294:ARG:N    | 2.42                     | 0.52              |
| 1:E:282:TRP:HA   | 1:E:282:TRP:HE3  | 1.74                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:213:TYR:O    | 1:C:217:LEU:HD13 | 2.08                     | 0.52              |
| 1:C:190:VAL:HG22 | 1:D:176:PHE:CZ   | 2.44                     | 0.52              |
| 1:F:342:THR:O    | 1:F:363:GLU:N    | 2.42                     | 0.52              |
| 1:A:240:ALA:HB2  | 1:A:376:ILE:HG21 | 1.89                     | 0.52              |
| 1:E:287:LEU:HD22 | 1:E:287:LEU:N    | 2.24                     | 0.52              |
| 1:B:155:VAL:HG13 | 1:B:155:VAL:O    | 2.09                     | 0.52              |
| 1:C:349:ASP:O    | 1:C:352:ASN:OD1  | 2.27                     | 0.52              |
| 1:B:129:LEU:C    | 1:B:131:ARG:H    | 2.12                     | 0.52              |
| 1:A:194:ARG:HG2  | 1:A:195:GLN:N    | 2.23                     | 0.52              |
| 1:B:148:LEU:N    | 1:B:148:LEU:CD2  | 2.72                     | 0.52              |
| 1:D:210:ARG:NH1  | 1:E:371:TYR:CE2  | 2.77                     | 0.52              |
| 1:F:156:PHE:HD2  | 1:F:158:ASN:CA   | 2.22                     | 0.52              |
| 1:G:189:TRP:HZ3  | 1:G:350:ARG:HH22 | 1.55                     | 0.52              |
| 1:B:206:TYR:HD2  | 1:B:210:ARG:HB2  | 1.74                     | 0.52              |
| 1:D:184:LYS:NZ   | 1:D:184:LYS:HA   | 2.25                     | 0.52              |
| 1:E:207:ILE:CA   | 1:E:211:LEU:HB2  | 2.38                     | 0.52              |
| 1:G:280:ARG:O    | 1:G:283:HIS:N    | 2.42                     | 0.52              |
| 1:F:327:GLY:C    | 1:F:329:PHE:CD1  | 2.83                     | 0.52              |
| 1:F:158:ASN:ND2  | 1:F:172:SER:HA   | 2.25                     | 0.52              |
| 1:E:262:ILE:H    | 1:E:262:ILE:HD12 | 1.73                     | 0.52              |
| 1:A:340:ASP:O    | 1:A:342:THR:HG23 | 2.09                     | 0.52              |
| 1:G:268:SER:O    | 1:G:269:GLU:CB   | 2.58                     | 0.52              |
| 1:G:268:SER:O    | 1:G:269:GLU:HB3  | 2.10                     | 0.52              |
| 1:F:153:GLU:OE2  | 1:F:372:ARG:NH2  | 2.42                     | 0.52              |
| 1:F:343:VAL:HA   | 1:F:362:CYS:HA   | 1.91                     | 0.52              |
| 1:C:287:LEU:HD21 | 1:C:300:PRO:CB   | 2.36                     | 0.52              |
| 1:G:156:PHE:O    | 1:G:158:ASN:OD1  | 2.28                     | 0.52              |
| 1:C:130:ARG:HB3  | 1:D:271:SER:OG   | 2.10                     | 0.52              |
| 1:E:156:PHE:HD2  | 1:E:158:ASN:CA   | 2.22                     | 0.52              |
| 1:F:276:VAL:HG22 | 1:F:314:VAL:CG2  | 2.40                     | 0.52              |
| 1:B:175:THR:HG22 | 1:B:176:PHE:N    | 2.25                     | 0.52              |
| 1:D:155:VAL:CG1  | 1:D:374:THR:HB   | 2.38                     | 0.52              |
| 1:A:304:THR:O    | 1:A:306:ASN:N    | 2.43                     | 0.52              |
| 1:D:303:PHE:O    | 1:D:306:ASN:HB3  | 2.10                     | 0.52              |
| 1:B:205:SER:O    | 1:B:206:TYR:C    | 2.46                     | 0.52              |
| 1:B:206:TYR:HE2  | 1:B:210:ARG:HE   | 1.58                     | 0.52              |
| 1:F:188:HIS:O    | 1:F:361:LEU:HA   | 2.10                     | 0.52              |
| 1:C:287:LEU:HD21 | 1:C:300:PRO:HB2  | 1.92                     | 0.52              |
| 1:C:130:ARG:HB3  | 1:D:271:SER:CB   | 2.40                     | 0.52              |
| 1:B:329:PHE:HA   | 1:B:332:ALA:HB3  | 1.91                     | 0.52              |
| 1:E:135:ARG:HD2  | 1:E:219:GLU:OE1  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:204:GLN:OE1  | 1:B:204:GLN:HA   | 2.09                     | 0.52              |
| 1:F:202:MET:O    | 1:F:205:SER:CA   | 2.57                     | 0.52              |
| 1:C:275:ILE:HG23 | 1:C:326:VAL:HG12 | 1.91                     | 0.52              |
| 1:G:128:GLY:C    | 1:G:130:ARG:N    | 2.60                     | 0.52              |
| 1:D:284:ASN:O    | 1:D:287:LEU:HD12 | 2.10                     | 0.52              |
| 1:B:251:GLY:O    | 1:B:252:ASP:CG   | 2.49                     | 0.52              |
| 1:G:155:VAL:HA   | 1:G:174:ILE:HG22 | 1.90                     | 0.52              |
| 1:B:156:PHE:HD2  | 1:B:158:ASN:CA   | 2.23                     | 0.52              |
| 1:G:324:PHE:CZ   | 1:G:379:GLY:HA3  | 2.45                     | 0.52              |
| 1:E:127:PRO:HB2  | 1:E:213:TYR:CE1  | 2.25                     | 0.51              |
| 1:C:277:LEU:HD12 | 1:C:277:LEU:N    | 2.25                     | 0.51              |
| 1:B:208:ASN:HD22 | 1:B:208:ASN:N    | 2.07                     | 0.51              |
| 1:D:156:PHE:HD2  | 1:D:158:ASN:CA   | 2.23                     | 0.51              |
| 1:F:158:ASN:N    | 1:F:158:ASN:ND2  | 2.49                     | 0.51              |
| 1:B:307:ILE:HG22 | 1:B:312:PRO:HA   | 1.91                     | 0.51              |
| 1:F:145:SER:O    | 1:F:338:ARG:HD3  | 2.09                     | 0.51              |
| 1:A:155:VAL:HG13 | 1:A:155:VAL:O    | 2.10                     | 0.51              |
| 1:G:376:ILE:C    | 1:G:377:ILE:HD12 | 2.30                     | 0.51              |
| 1:F:249:ALA:C    | 1:F:250:THR:O    | 2.41                     | 0.51              |
| 1:F:138:LEU:CD2  | 1:F:329:PHE:HB3  | 2.39                     | 0.51              |
| 1:D:224:LEU:O    | 1:D:237:ASN:OD1  | 2.29                     | 0.51              |
| 1:G:150:TYR:CE2  | 1:G:369:ALA:HB1  | 2.45                     | 0.51              |
| 1:E:193:SER:C    | 1:E:195:GLN:H    | 2.12                     | 0.51              |
| 1:A:202:MET:CG   | 1:A:203:LEU:H    | 2.23                     | 0.51              |
| 1:E:329:PHE:HD1  | 1:E:329:PHE:H    | 1.57                     | 0.51              |
| 1:G:216:ALA:HA   | 1:G:219:GLU:HG2  | 1.91                     | 0.51              |
| 1:B:317:LYS:O    | 1:B:317:LYS:HG2  | 2.11                     | 0.51              |
| 1:A:331:MET:HE3  | 1:F:209:ASN:O    | 2.10                     | 0.51              |
| 1:D:155:VAL:CG1  | 1:D:374:THR:CG2  | 2.89                     | 0.51              |
| 1:A:240:ALA:HB2  | 1:A:376:ILE:CG2  | 2.40                     | 0.51              |
| 1:D:300:PRO:HG2  | 1:E:301:GLN:NE2  | 2.25                     | 0.51              |
| 1:E:134:ILE:H    | 1:E:134:ILE:CD1  | 2.24                     | 0.51              |
| 1:C:296:ILE:C    | 1:C:297:PHE:HD2  | 2.13                     | 0.51              |
| 1:D:293:GLY:H    | 1:F:294:ARG:HB2  | 1.75                     | 0.51              |
| 1:B:299:GLY:O    | 1:B:302:ALA:N    | 2.44                     | 0.51              |
| 1:C:195:GLN:O    | 1:C:197:MET:N    | 2.43                     | 0.51              |
| 1:F:193:SER:HA   | 1:F:357:MET:HA   | 1.92                     | 0.51              |
| 1:G:343:VAL:HG22 | 1:G:362:CYS:SG   | 2.50                     | 0.51              |
| 1:B:289:LYS:HD2  | 1:B:293:GLY:C    | 2.30                     | 0.51              |
| 1:G:155:VAL:HG22 | 1:G:156:PHE:H    | 1.74                     | 0.51              |
| 1:G:158:ASN:OD1  | 1:G:172:SER:CA   | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:210:ARG:NH1  | 1:E:371:TYR:CD2  | 2.79                     | 0.51              |
| 1:D:290:ASP:CG   | 1:D:294:ARG:HB3  | 2.30                     | 0.51              |
| 1:B:308:MET:HG3  | 1:B:309:TRP:HD1  | 1.75                     | 0.51              |
| 1:E:199:ASP:HB3  | 1:E:202:MET:HB3  | 1.92                     | 0.51              |
| 1:B:209:ASN:C    | 1:C:331:MET:CE   | 2.79                     | 0.51              |
| 1:A:156:PHE:C    | 1:A:158:ASN:N    | 2.64                     | 0.51              |
| 1:G:237:ASN:HD21 | 1:G:319:GLN:HE22 | 1.57                     | 0.51              |
| 1:B:137:LEU:CD2  | 1:B:329:PHE:HB2  | 2.40                     | 0.51              |
| 1:E:150:TYR:CE1  | 1:E:179:GLN:HB2  | 2.45                     | 0.51              |
| 1:D:175:THR:HG22 | 1:D:176:PHE:N    | 2.25                     | 0.51              |
| 1:A:203:LEU:HD12 | 1:A:207:ILE:HD11 | 1.92                     | 0.51              |
| 1:A:153:GLU:OE2  | 1:A:372:ARG:NH2  | 2.43                     | 0.51              |
| 1:D:146:ASN:O    | 1:D:147:ALA:HB2  | 2.10                     | 0.51              |
| 1:G:343:VAL:HG13 | 1:G:361:LEU:O    | 2.10                     | 0.51              |
| 1:A:254:ARG:O    | 1:A:258:ILE:HD13 | 2.11                     | 0.51              |
| 1:F:193:SER:O    | 1:F:196:VAL:HG13 | 2.11                     | 0.51              |
| 1:E:349:ASP:O    | 1:E:352:ASN:OD1  | 2.29                     | 0.51              |
| 1:E:190:VAL:HG12 | 1:F:176:PHE:CE1  | 2.46                     | 0.51              |
| 1:G:131:ARG:HD3  | 1:G:306:ASN:HD21 | 1.76                     | 0.51              |
| 1:F:138:LEU:HD23 | 1:F:329:PHE:HB3  | 1.93                     | 0.51              |
| 1:E:158:ASN:ND2  | 1:E:172:SER:HA   | 2.26                     | 0.51              |
| 1:A:138:LEU:N    | 1:A:138:LEU:HD12 | 2.26                     | 0.51              |
| 1:E:224:LEU:HD11 | 1:E:319:GLN:CD   | 2.31                     | 0.51              |
| 1:E:281:ASP:O    | 1:E:285:ILE:HG13 | 2.11                     | 0.51              |
| 1:G:371:TYR:O    | 1:G:373:PRO:HD3  | 2.10                     | 0.51              |
| 1:C:132:LEU:HD21 | 1:C:136:ASP:CB   | 2.40                     | 0.51              |
| 1:C:129:LEU:CD1  | 1:D:331:MET:CE   | 2.69                     | 0.50              |
| 1:A:287:LEU:C    | 1:A:288:LEU:HD22 | 2.24                     | 0.50              |
| 1:B:162:ASP:O    | 1:B:173:ASP:N    | 2.44                     | 0.50              |
| 1:A:308:MET:C    | 1:A:310:GLY:H    | 2.14                     | 0.50              |
| 1:G:211:LEU:HD21 | 1:G:362:CYS:HB2  | 1.93                     | 0.50              |
| 1:C:224:LEU:HD13 | 1:C:225:ASN:CG   | 2.31                     | 0.50              |
| 1:G:302:ALA:O    | 1:G:303:PHE:HB2  | 2.11                     | 0.50              |
| 1:E:236:LEU:HD13 | 1:E:329:PHE:HE2  | 1.75                     | 0.50              |
| 1:D:349:ASP:OD1  | 1:D:349:ASP:C    | 2.49                     | 0.50              |
| 1:F:184:LYS:HB2  | 1:F:233:LEU:HD21 | 1.92                     | 0.50              |
| 1:C:207:ILE:HD13 | 1:C:207:ILE:N    | 2.25                     | 0.50              |
| 1:D:358:LEU:CD1  | 1:D:358:LEU:N    | 2.74                     | 0.50              |
| 1:B:212:MET:O    | 1:B:214:GLY:N    | 2.45                     | 0.50              |
| 1:B:158:ASN:CB   | 1:B:172:SER:HB2  | 2.41                     | 0.50              |
| 1:G:301:GLN:CG   | 1:G:302:ALA:H    | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:191:GLN:O    | 1:C:191:GLN:OE1  | 2.30                     | 0.50              |
| 1:C:204:GLN:O    | 1:C:207:ILE:HD13 | 2.11                     | 0.50              |
| 1:F:195:GLN:C    | 1:F:197:MET:N    | 2.65                     | 0.50              |
| 1:E:360:ILE:HD12 | 1:E:360:ILE:C    | 2.32                     | 0.50              |
| 1:E:361:LEU:HG   | 1:E:362:CYS:N    | 2.26                     | 0.50              |
| 1:A:285:ILE:C    | 1:A:288:LEU:CD2  | 2.62                     | 0.50              |
| 1:B:216:ALA:O    | 1:B:217:LEU:O    | 2.29                     | 0.50              |
| 1:C:366:LEU:C    | 1:C:366:LEU:CD1  | 2.75                     | 0.50              |
| 1:F:142:ARG:HG2  | 1:F:337:ASP:HB2  | 1.81                     | 0.50              |
| 1:B:289:LYS:HD2  | 1:B:294:ARG:N    | 2.26                     | 0.50              |
| 1:G:327:GLY:C    | 1:G:329:PHE:CD2  | 2.85                     | 0.50              |
| 1:G:366:LEU:CD1  | 1:G:366:LEU:C    | 2.74                     | 0.50              |
| 1:D:376:ILE:C    | 1:D:377:ILE:HD12 | 2.32                     | 0.50              |
| 1:B:354:VAL:C    | 1:B:356:ASN:N    | 2.63                     | 0.50              |
| 1:A:131:ARG:HH21 | 1:A:316:THR:HB   | 1.75                     | 0.50              |
| 1:A:145:SER:H    | 1:A:338:ARG:HD3  | 1.77                     | 0.50              |
| 1:B:129:LEU:O    | 1:B:131:ARG:N    | 2.44                     | 0.50              |
| 1:C:130:ARG:HB2  | 1:D:271:SER:OG   | 2.12                     | 0.50              |
| 1:E:264:GLN:O    | 1:E:267:GLU:HB2  | 2.12                     | 0.50              |
| 1:D:303:PHE:CA   | 1:D:306:ASN:HB3  | 2.38                     | 0.50              |
| 1:B:258:ILE:HD11 | 1:B:381:PHE:CZ   | 2.46                     | 0.50              |
| 1:B:282:TRP:HE3  | 1:B:282:TRP:HA   | 1.76                     | 0.50              |
| 1:A:151:VAL:HG22 | 1:A:152:ARG:N    | 2.27                     | 0.50              |
| 1:E:126:MET:HE1  | 1:E:129:LEU:HD21 | 1.91                     | 0.50              |
| 1:E:214:GLY:O    | 1:E:217:LEU:HB3  | 2.11                     | 0.50              |
| 1:C:206:TYR:O    | 1:C:210:ARG:N    | 2.36                     | 0.50              |
| 1:B:199:ASP:O    | 1:B:200:ALA:CB   | 2.59                     | 0.50              |
| 1:B:188:HIS:O    | 1:B:361:LEU:HD12 | 2.12                     | 0.50              |
| 1:D:129:LEU:CD1  | 1:D:131:ARG:HD3  | 2.42                     | 0.50              |
| 1:F:129:LEU:HD12 | 1:F:129:LEU:N    | 2.22                     | 0.50              |
| 1:E:226:GLY:N    | 1:E:235:GLY:HA3  | 2.27                     | 0.50              |
| 1:G:134:ILE:CG1  | 1:G:220:GLU:HG3  | 2.42                     | 0.50              |
| 1:G:352:ASN:O    | 1:G:355:LYS:O    | 2.29                     | 0.50              |
| 1:E:137:LEU:HD22 | 1:E:329:PHE:CB   | 2.36                     | 0.50              |
| 1:B:137:LEU:HD22 | 1:B:329:PHE:HB2  | 1.93                     | 0.50              |
| 1:B:282:TRP:CE3  | 1:B:282:TRP:HA   | 2.47                     | 0.50              |
| 1:A:348:GLU:CG   | 1:A:348:GLU:O    | 2.60                     | 0.50              |
| 1:D:266:THR:HA   | 1:D:270:PHE:O    | 2.11                     | 0.50              |
| 1:A:286:ALA:C    | 1:A:288:LEU:CD2  | 2.79                     | 0.50              |
| 1:C:276:VAL:C    | 1:C:277:LEU:HD12 | 2.32                     | 0.50              |
| 1:C:184:LYS:HB3  | 1:C:231:ASP:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:174:ILE:O    | 1:G:174:ILE:HG12 | 2.12                     | 0.50              |
| 1:B:158:ASN:CG   | 1:B:172:SER:O    | 2.50                     | 0.50              |
| 1:F:327:GLY:O    | 1:F:329:PHE:HE1  | 1.95                     | 0.50              |
| 1:E:141:GLY:C    | 1:E:336:PHE:HA   | 2.32                     | 0.50              |
| 1:D:152:ARG:HB3  | 1:D:177:SER:HB2  | 1.94                     | 0.50              |
| 1:C:195:GLN:NE2  | 1:C:198:ASP:O    | 2.45                     | 0.49              |
| 1:C:202:MET:O    | 1:C:205:SER:CA   | 2.60                     | 0.49              |
| 1:F:212:MET:HE2  | 1:F:212:MET:HA   | 1.94                     | 0.49              |
| 1:B:148:LEU:N    | 1:B:148:LEU:HD22 | 2.26                     | 0.49              |
| 1:B:158:ASN:OD1  | 1:B:172:SER:O    | 2.29                     | 0.49              |
| 1:F:327:GLY:C    | 1:F:329:PHE:HE1  | 2.12                     | 0.49              |
| 1:E:307:ILE:HG13 | 1:E:307:ILE:O    | 2.12                     | 0.49              |
| 1:B:368:LEU:HD21 | 1:B:370:HIS:CE1  | 2.46                     | 0.49              |
| 1:B:319:GLN:HE22 | 1:B:324:PHE:HA   | 1.76                     | 0.49              |
| 1:E:206:TYR:HD2  | 1:E:210:ARG:HB2  | 1.77                     | 0.49              |
| 1:A:190:VAL:HG21 | 1:A:210:ARG:HH12 | 1.77                     | 0.49              |
| 1:A:296:ILE:O    | 1:A:297:PHE:HB2  | 2.12                     | 0.49              |
| 1:A:309:TRP:CE3  | 1:A:309:TRP:HA   | 2.47                     | 0.49              |
| 1:F:129:LEU:O    | 1:F:130:ARG:HB2  | 2.11                     | 0.49              |
| 1:D:349:ASP:OD1  | 1:D:350:ARG:CG   | 2.58                     | 0.49              |
| 1:F:132:LEU:CD2  | 1:F:136:ASP:CB   | 2.90                     | 0.49              |
| 1:G:244:ASP:CG   | 1:G:246:SER:HB3  | 2.33                     | 0.49              |
| 1:D:290:ASP:C    | 1:D:292:GLU:H    | 2.15                     | 0.49              |
| 1:D:197:MET:CE   | 1:D:203:LEU:HA   | 2.42                     | 0.49              |
| 1:E:296:ILE:O    | 1:E:297:PHE:C    | 2.49                     | 0.49              |
| 1:D:277:LEU:HD13 | 1:D:324:PHE:HB3  | 1.93                     | 0.49              |
| 1:G:192:ALA:O    | 1:G:357:MET:SD   | 2.70                     | 0.49              |
| 1:D:155:VAL:HG13 | 1:D:374:THR:HG21 | 1.94                     | 0.49              |
| 1:F:200:ALA:O    | 1:F:203:LEU:N    | 2.44                     | 0.49              |
| 1:B:288:LEU:C    | 1:B:296:ILE:HD11 | 2.30                     | 0.49              |
| 1:F:280:ARG:O    | 1:F:283:HIS:HB3  | 2.12                     | 0.49              |
| 1:B:268:SER:HB3  | 1:B:374:THR:HG22 | 1.93                     | 0.49              |
| 1:F:258:ILE:CD1  | 1:F:275:ILE:HG21 | 2.42                     | 0.49              |
| 1:B:280:ARG:O    | 1:B:283:HIS:N    | 2.45                     | 0.49              |
| 1:B:151:VAL:HG13 | 1:B:151:VAL:O    | 2.12                     | 0.49              |
| 1:G:197:MET:C    | 1:G:198:ASP:OD1  | 2.51                     | 0.49              |
| 1:C:343:VAL:HA   | 1:C:362:CYS:HA   | 1.95                     | 0.49              |
| 1:A:286:ALA:C    | 1:A:288:LEU:HD21 | 2.33                     | 0.49              |
| 1:D:131:ARG:HG2  | 1:D:132:LEU:O    | 2.12                     | 0.49              |
| 1:E:287:LEU:HD12 | 1:E:295:TYR:CE1  | 2.48                     | 0.49              |
| 1:A:267:GLU:OE1  | 1:F:317:LYS:NZ   | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:279:PRO:HG3  | 1:E:315:PRO:O    | 2.12                     | 0.49              |
| 1:E:273:SER:HB2  | 1:E:330:ASP:OD1  | 2.12                     | 0.49              |
| 1:G:273:SER:O    | 1:G:311:LEU:HD12 | 2.13                     | 0.49              |
| 1:B:280:ARG:O    | 1:B:281:ASP:C    | 2.51                     | 0.49              |
| 1:E:191:GLN:C    | 1:E:191:GLN:HE21 | 2.15                     | 0.49              |
| 1:F:212:MET:O    | 1:F:215:LEU:N    | 2.46                     | 0.49              |
| 1:E:300:PRO:HG2  | 1:F:309:TRP:NE1  | 2.27                     | 0.49              |
| 1:F:206:TYR:CD2  | 1:F:206:TYR:C    | 2.86                     | 0.49              |
| 1:C:217:LEU:HD23 | 1:D:269:GLU:HB3  | 1.95                     | 0.49              |
| 1:E:184:LYS:HG3  | 1:E:232:ASN:O    | 2.12                     | 0.49              |
| 1:D:162:ASP:OD1  | 1:D:173:ASP:HB2  | 2.12                     | 0.49              |
| 1:G:303:PHE:CD2  | 1:G:304:THR:O    | 2.66                     | 0.49              |
| 1:F:327:GLY:O    | 1:F:329:PHE:CD1  | 2.66                     | 0.49              |
| 1:F:226:GLY:N    | 1:F:235:GLY:HA3  | 2.25                     | 0.49              |
| 1:A:308:MET:C    | 1:A:310:GLY:N    | 2.66                     | 0.49              |
| 1:C:215:LEU:C    | 1:C:215:LEU:HD23 | 2.32                     | 0.49              |
| 1:E:125:ILE:CG1  | 1:E:126:MET:N    | 2.73                     | 0.49              |
| 1:A:201:PRO:O    | 1:A:202:MET:C    | 2.49                     | 0.49              |
| 1:A:174:ILE:HG12 | 1:A:174:ILE:O    | 2.13                     | 0.49              |
| 1:F:358:LEU:C    | 1:F:358:LEU:HD23 | 2.32                     | 0.49              |
| 1:F:225:ASN:N    | 1:F:225:ASN:ND2  | 2.60                     | 0.49              |
| 1:A:263:TYR:CZ   | 1:A:267:GLU:OE2  | 2.66                     | 0.49              |
| 1:G:239:VAL:HG12 | 1:G:239:VAL:O    | 2.13                     | 0.49              |
| 1:E:182:ASN:HB2  | 1:E:184:LYS:HZ2  | 1.78                     | 0.49              |
| 1:D:343:VAL:HG12 | 1:D:362:CYS:CB   | 2.43                     | 0.49              |
| 1:C:155:VAL:HB   | 1:C:174:ILE:HG22 | 1.94                     | 0.49              |
| 1:C:305:SER:O    | 1:C:307:ILE:HG23 | 2.13                     | 0.49              |
| 1:D:290:ASP:O    | 1:D:291:ASN:HB2  | 2.11                     | 0.49              |
| 1:F:192:ALA:O    | 1:F:357:MET:CA   | 2.60                     | 0.49              |
| 1:G:210:ARG:O    | 1:G:211:LEU:C    | 2.49                     | 0.49              |
| 1:E:194:ARG:NH1  | 1:E:347:ARG:NH1  | 2.61                     | 0.49              |
| 1:B:360:ILE:CG2  | 1:B:361:LEU:N    | 2.75                     | 0.49              |
| 1:A:263:TYR:OH   | 1:F:280:ARG:NE   | 2.25                     | 0.49              |
| 1:A:254:ARG:HA   | 1:A:257:ILE:HD12 | 1.95                     | 0.49              |
| 1:C:148:LEU:HB2  | 1:C:181:ALA:HB3  | 1.94                     | 0.49              |
| 1:C:129:LEU:HD11 | 1:D:331:MET:HE3  | 1.86                     | 0.48              |
| 1:D:199:ASP:OD1  | 1:D:200:ALA:N    | 2.46                     | 0.48              |
| 1:G:158:ASN:CG   | 1:G:172:SER:HA   | 2.31                     | 0.48              |
| 1:C:330:ASP:C    | 1:C:330:ASP:OD1  | 2.52                     | 0.48              |
| 1:A:266:THR:HG21 | 1:F:279:PRO:CB   | 2.39                     | 0.48              |
| 1:E:155:VAL:HG11 | 1:E:374:THR:HB   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:153:GLU:OE1  | 1:B:371:TYR:HB3  | 2.12                     | 0.48              |
| 1:B:135:ARG:HH11 | 1:B:135:ARG:HG3  | 1.77                     | 0.48              |
| 1:F:198:ASP:OD2  | 1:F:198:ASP:O    | 2.30                     | 0.48              |
| 1:F:204:GLN:O    | 1:F:206:TYR:N    | 2.45                     | 0.48              |
| 1:C:343:VAL:HA   | 1:C:361:LEU:O    | 2.13                     | 0.48              |
| 1:C:258:ILE:CD1  | 1:C:275:ILE:HG21 | 2.42                     | 0.48              |
| 1:C:131:ARG:HH21 | 1:C:316:THR:HB   | 1.78                     | 0.48              |
| 1:D:131:ARG:HH21 | 1:D:133:THR:HG22 | 1.78                     | 0.48              |
| 1:E:134:ILE:HD12 | 1:E:314:VAL:HG11 | 1.95                     | 0.48              |
| 1:B:155:VAL:HG12 | 1:B:374:THR:CB   | 2.39                     | 0.48              |
| 1:A:308:MET:O    | 1:A:310:GLY:N    | 2.45                     | 0.48              |
| 1:B:244:ASP:OD1  | 1:B:247:LEU:HG   | 2.12                     | 0.48              |
| 1:F:146:ASN:OD1  | 1:F:146:ASN:N    | 2.46                     | 0.48              |
| 1:G:199:ASP:O    | 1:G:203:LEU:N    | 2.45                     | 0.48              |
| 1:E:191:GLN:C    | 1:E:191:GLN:NE2  | 2.66                     | 0.48              |
| 1:C:342:THR:O    | 1:C:363:GLU:N    | 2.43                     | 0.48              |
| 1:A:302:ALA:HA   | 1:A:306:ASN:HD22 | 1.77                     | 0.48              |
| 1:B:249:ALA:N    | 1:B:252:ASP:OD2  | 2.46                     | 0.48              |
| 1:A:127:PRO:HD3  | 1:A:212:MET:HE2  | 1.94                     | 0.48              |
| 1:A:202:MET:HG3  | 1:A:203:LEU:N    | 2.28                     | 0.48              |
| 1:D:129:LEU:C    | 1:D:129:LEU:HD13 | 2.33                     | 0.48              |
| 1:G:132:LEU:HG   | 1:G:136:ASP:OD1  | 2.13                     | 0.48              |
| 1:D:224:LEU:C    | 1:D:224:LEU:HD13 | 2.33                     | 0.48              |
| 1:G:142:ARG:HG2  | 1:G:142:ARG:HH11 | 1.78                     | 0.48              |
| 1:E:216:ALA:O    | 1:E:218:LYS:N    | 2.46                     | 0.48              |
| 1:E:189:TRP:HA   | 1:E:360:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:309:TRP:HE3  | 1:A:309:TRP:HA   | 1.78                     | 0.48              |
| 1:D:158:ASN:HD22 | 1:D:158:ASN:H    | 1.58                     | 0.48              |
| 1:A:137:LEU:HD22 | 1:A:329:PHE:CB   | 2.40                     | 0.48              |
| 1:C:245:THR:HA   | 1:C:248:ASN:ND2  | 2.28                     | 0.48              |
| 1:F:195:GLN:O    | 1:F:197:MET:N    | 2.47                     | 0.48              |
| 1:D:194:ARG:HA   | 1:D:358:LEU:HD22 | 1.94                     | 0.48              |
| 1:D:202:MET:O    | 1:D:203:LEU:C    | 2.51                     | 0.48              |
| 1:A:303:PHE:CD2  | 1:A:304:THR:N    | 2.82                     | 0.48              |
| 1:E:296:ILE:O    | 1:E:298:GLY:O    | 2.31                     | 0.48              |
| 1:F:249:ALA:N    | 1:F:252:ASP:OD2  | 2.44                     | 0.48              |
| 1:D:302:ALA:O    | 1:D:305:SER:N    | 2.46                     | 0.48              |
| 1:B:146:ASN:ND2  | 1:B:146:ASN:N    | 2.62                     | 0.48              |
| 1:A:258:ILE:HD12 | 1:A:258:ILE:N    | 2.29                     | 0.48              |
| 1:B:349:ASP:O    | 1:B:352:ASN:HB2  | 2.13                     | 0.48              |
| 1:B:155:VAL:HG13 | 1:B:374:THR:OG1  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:175:THR:C    | 1:G:176:PHE:HD2  | 2.16                     | 0.48              |
| 1:E:280:ARG:HH11 | 1:E:280:ARG:HG2  | 1.79                     | 0.48              |
| 1:C:210:ARG:HH21 | 1:D:153:GLU:CD   | 1.77                     | 0.48              |
| 1:G:343:VAL:HA   | 1:G:361:LEU:O    | 2.13                     | 0.48              |
| 1:C:345:VAL:HA   | 1:C:359:THR:O    | 2.12                     | 0.48              |
| 1:D:303:PHE:HA   | 1:D:306:ASN:CB   | 2.39                     | 0.48              |
| 1:A:266:THR:C    | 1:A:268:SER:N    | 2.67                     | 0.48              |
| 1:E:195:GLN:OE1  | 1:E:195:GLN:HA   | 2.14                     | 0.48              |
| 1:E:154:GLU:OE2  | 1:E:177:SER:OG   | 2.23                     | 0.48              |
| 1:D:125:ILE:CG1  | 1:D:208:ASN:HD21 | 2.26                     | 0.48              |
| 1:C:194:ARG:HA   | 1:C:358:LEU:HD12 | 1.96                     | 0.48              |
| 1:D:201:PRO:O    | 1:D:202:MET:C    | 2.52                     | 0.48              |
| 1:G:156:PHE:CZ   | 1:G:158:ASN:HB3  | 2.49                     | 0.48              |
| 1:E:130:ARG:CB   | 1:F:271:SER:OG   | 2.59                     | 0.48              |
| 1:B:262:ILE:HD12 | 1:B:262:ILE:N    | 2.27                     | 0.48              |
| 1:C:339:MET:HG2  | 1:C:340:ASP:N    | 2.28                     | 0.48              |
| 1:C:129:LEU:CD1  | 1:D:331:MET:HE1  | 2.15                     | 0.48              |
| 1:D:155:VAL:HG11 | 1:D:374:THR:HG21 | 1.95                     | 0.48              |
| 1:E:199:ASP:HB2  | 1:E:202:MET:HE2  | 1.96                     | 0.48              |
| 1:A:285:ILE:O    | 1:A:288:LEU:HD11 | 2.14                     | 0.48              |
| 1:A:303:PHE:CD2  | 1:A:303:PHE:C    | 2.87                     | 0.48              |
| 1:A:300:PRO:CA   | 1:A:303:PHE:HB3  | 2.39                     | 0.48              |
| 1:D:245:THR:C    | 1:D:247:LEU:H    | 2.17                     | 0.48              |
| 1:D:302:ALA:HB3  | 1:D:305:SER:OG   | 2.13                     | 0.48              |
| 1:D:355:LYS:O    | 1:E:178:LYS:NZ   | 2.45                     | 0.48              |
| 1:E:224:LEU:C    | 1:E:224:LEU:HD13 | 2.33                     | 0.48              |
| 1:C:296:ILE:HG13 | 1:C:297:PHE:CE2  | 2.48                     | 0.48              |
| 1:F:222:GLN:HE22 | 1:F:232:ASN:HB3  | 1.79                     | 0.48              |
| 1:B:262:ILE:H    | 1:B:262:ILE:CD1  | 2.27                     | 0.48              |
| 1:G:148:LEU:HB2  | 1:G:181:ALA:HB3  | 1.95                     | 0.48              |
| 1:E:309:TRP:HE3  | 1:E:309:TRP:HA   | 1.79                     | 0.48              |
| 1:A:283:HIS:HA   | 1:A:303:PHE:HE1  | 1.79                     | 0.48              |
| 1:C:275:ILE:CG2  | 1:C:277:LEU:HD11 | 2.43                     | 0.48              |
| 1:B:249:ALA:HB3  | 1:B:252:ASP:CG   | 2.33                     | 0.48              |
| 1:F:361:LEU:CD1  | 1:F:361:LEU:O    | 2.55                     | 0.48              |
| 1:F:265:VAL:HG22 | 1:F:377:ILE:HD13 | 1.94                     | 0.48              |
| 1:E:309:TRP:CE3  | 1:E:309:TRP:HA   | 2.49                     | 0.48              |
| 1:B:354:VAL:O    | 1:B:356:ASN:N    | 2.47                     | 0.47              |
| 1:F:142:ARG:CG   | 1:F:337:ASP:CB   | 2.72                     | 0.47              |
| 1:A:132:LEU:O    | 1:A:314:VAL:HG13 | 2.13                     | 0.47              |
| 1:A:179:GLN:HG3  | 1:A:180:THR:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:345:VAL:CG2  | 1:G:360:ILE:HG22 | 2.43                     | 0.47              |
| 1:B:125:ILE:CG1  | 1:B:127:PRO:HG3  | 2.44                     | 0.47              |
| 1:B:253:THR:HB   | 1:B:256:ASP:OD1  | 2.13                     | 0.47              |
| 1:D:158:ASN:ND2  | 1:D:172:SER:HA   | 2.29                     | 0.47              |
| 1:G:280:ARG:C    | 1:G:282:TRP:H    | 2.16                     | 0.47              |
| 1:A:287:LEU:N    | 1:A:288:LEU:HD23 | 2.29                     | 0.47              |
| 1:G:156:PHE:CE2  | 1:G:158:ASN:CB   | 2.94                     | 0.47              |
| 1:A:264:GLN:OE1  | 1:A:377:ILE:HG21 | 2.14                     | 0.47              |
| 1:G:329:PHE:HA   | 1:G:332:ALA:HB2  | 1.90                     | 0.47              |
| 1:B:158:ASN:HD22 | 1:B:158:ASN:H    | 1.56                     | 0.47              |
| 1:B:158:ASN:CG   | 1:B:172:SER:HB2  | 2.35                     | 0.47              |
| 1:G:356:ASN:ND2  | 1:G:356:ASN:C    | 2.67                     | 0.47              |
| 1:C:174:ILE:N    | 1:C:174:ILE:HD13 | 2.28                     | 0.47              |
| 1:B:307:ILE:HA   | 1:B:313:VAL:HG23 | 1.96                     | 0.47              |
| 1:C:132:LEU:HD21 | 1:C:136:ASP:HB2  | 1.95                     | 0.47              |
| 1:C:347:ARG:O    | 1:C:348:GLU:C    | 2.51                     | 0.47              |
| 1:D:155:VAL:HG12 | 1:D:374:THR:CB   | 2.39                     | 0.47              |
| 1:B:204:GLN:O    | 1:B:207:ILE:HB   | 2.15                     | 0.47              |
| 1:B:194:ARG:NH1  | 1:B:347:ARG:NH2  | 2.62                     | 0.47              |
| 1:B:212:MET:O    | 1:B:215:LEU:CA   | 2.59                     | 0.47              |
| 1:D:307:ILE:HD13 | 1:D:310:GLY:O    | 2.15                     | 0.47              |
| 1:A:266:THR:C    | 1:A:268:SER:H    | 2.18                     | 0.47              |
| 1:A:263:TYR:O    | 1:A:266:THR:HB   | 2.14                     | 0.47              |
| 1:B:236:LEU:HD13 | 1:B:329:PHE:HE2  | 1.80                     | 0.47              |
| 1:A:184:LYS:HD2  | 1:A:231:ASP:HA   | 1.97                     | 0.47              |
| 1:E:162:ASP:OD1  | 1:E:173:ASP:HB2  | 2.15                     | 0.47              |
| 1:G:196:VAL:HG22 | 1:G:202:MET:HE1  | 1.93                     | 0.47              |
| 1:G:342:THR:O    | 1:G:363:GLU:N    | 2.47                     | 0.47              |
| 1:E:190:VAL:HG22 | 1:E:211:LEU:HD11 | 1.95                     | 0.47              |
| 1:C:189:TRP:HB3  | 1:C:361:LEU:HB3  | 1.96                     | 0.47              |
| 1:C:258:ILE:HD12 | 1:C:275:ILE:HG21 | 1.97                     | 0.47              |
| 1:B:128:GLY:O    | 1:B:213:TYR:OH   | 2.30                     | 0.47              |
| 1:D:129:LEU:CD2  | 1:D:130:ARG:H    | 2.07                     | 0.47              |
| 1:G:138:LEU:HD21 | 1:G:329:PHE:HB3  | 1.94                     | 0.47              |
| 1:B:140:GLN:OE1  | 1:B:140:GLN:N    | 2.47                     | 0.47              |
| 1:E:216:ALA:O    | 1:E:217:LEU:C    | 2.53                     | 0.47              |
| 1:B:125:ILE:CD1  | 1:B:127:PRO:CG   | 2.93                     | 0.47              |
| 1:B:158:ASN:CG   | 1:B:172:SER:CA   | 2.83                     | 0.47              |
| 1:B:158:ASN:HD22 | 1:B:172:SER:HB2  | 1.77                     | 0.47              |
| 1:D:142:ARG:HA   | 1:D:337:ASP:H    | 1.79                     | 0.47              |
| 1:A:224:LEU:HD13 | 1:A:237:ASN:OD1  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:SER:C    | 1:E:195:GLN:N    | 2.68                     | 0.47              |
| 1:F:304:THR:HG22 | 1:F:305:SER:N    | 2.30                     | 0.47              |
| 1:E:249:ALA:O    | 1:E:250:THR:C    | 2.51                     | 0.47              |
| 1:C:195:GLN:OE1  | 1:C:195:GLN:HA   | 2.15                     | 0.47              |
| 1:D:155:VAL:HG11 | 1:D:374:THR:CG2  | 2.45                     | 0.47              |
| 1:C:191:GLN:HA   | 1:C:358:LEU:O    | 2.15                     | 0.47              |
| 1:D:197:MET:HE1  | 1:D:203:LEU:HA   | 1.95                     | 0.47              |
| 1:E:201:PRO:HG2  | 1:E:202:MET:H    | 1.79                     | 0.47              |
| 1:B:194:ARG:CD   | 1:B:357:MET:HA   | 2.43                     | 0.47              |
| 1:C:335:VAL:HG13 | 1:C:366:LEU:CD2  | 2.45                     | 0.47              |
| 1:G:174:ILE:N    | 1:G:174:ILE:HD13 | 2.14                     | 0.47              |
| 1:A:265:VAL:HG12 | 1:A:265:VAL:O    | 2.14                     | 0.47              |
| 1:E:296:ILE:CG2  | 1:E:297:PHE:CD1  | 2.97                     | 0.47              |
| 1:B:156:PHE:HB3  | 1:B:158:ASN:CG   | 2.34                     | 0.47              |
| 1:B:158:ASN:CG   | 1:B:172:SER:C    | 2.74                     | 0.47              |
| 1:E:301:GLN:OE1  | 1:E:304:THR:HB   | 2.14                     | 0.47              |
| 1:E:131:ARG:HH12 | 1:E:316:THR:HA   | 1.78                     | 0.47              |
| 1:F:301:GLN:O    | 1:F:302:ALA:C    | 2.53                     | 0.47              |
| 1:B:190:VAL:HG23 | 1:B:190:VAL:O    | 2.15                     | 0.47              |
| 1:F:189:TRP:HA   | 1:F:360:ILE:O    | 2.15                     | 0.47              |
| 1:A:245:THR:HG23 | 1:A:248:ASN:HD21 | 1.80                     | 0.47              |
| 1:G:200:ALA:N    | 1:G:201:PRO:HD3  | 2.29                     | 0.47              |
| 1:G:360:ILE:HG13 | 1:G:360:ILE:O    | 2.14                     | 0.47              |
| 1:B:159:ALA:HB1  | 1:B:160:PRO:CD   | 2.39                     | 0.47              |
| 1:E:155:VAL:CG2  | 1:E:174:ILE:HG22 | 2.35                     | 0.47              |
| 1:E:130:ARG:HG2  | 1:F:271:SER:OG   | 2.15                     | 0.47              |
| 1:A:331:MET:CE   | 1:F:209:ASN:O    | 2.63                     | 0.47              |
| 1:A:179:GLN:HA   | 1:A:179:GLN:NE2  | 2.30                     | 0.47              |
| 1:A:150:TYR:HE1  | 1:A:181:ALA:HB2  | 1.79                     | 0.47              |
| 1:D:194:ARG:O    | 1:D:195:GLN:C    | 2.54                     | 0.47              |
| 1:E:186:ILE:HD11 | 1:E:222:GLN:HG3  | 1.96                     | 0.47              |
| 1:C:225:ASN:ND2  | 1:C:225:ASN:N    | 2.62                     | 0.47              |
| 1:B:156:PHE:CD2  | 1:B:158:ASN:HB3  | 2.50                     | 0.47              |
| 1:G:299:GLY:O    | 1:G:300:PRO:C    | 2.52                     | 0.47              |
| 1:E:329:PHE:N    | 1:E:329:PHE:CD1  | 2.82                     | 0.47              |
| 1:C:146:ASN:ND2  | 1:C:365:ARG:HH21 | 2.11                     | 0.47              |
| 1:D:124:ILE:O    | 1:D:125:ILE:HG22 | 2.15                     | 0.47              |
| 1:C:206:TYR:CE2  | 1:C:210:ARG:HD3  | 2.50                     | 0.47              |
| 1:E:352:ASN:O    | 1:E:355:LYS:O    | 2.32                     | 0.47              |
| 1:C:275:ILE:HG22 | 1:C:277:LEU:CD1  | 2.45                     | 0.47              |
| 1:F:361:LEU:CD1  | 1:F:361:LEU:C    | 2.83                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:155:VAL:CG1  | 1:A:374:THR:CG2  | 2.92                     | 0.47              |
| 1:E:295:TYR:O    | 1:E:296:ILE:O    | 2.33                     | 0.47              |
| 1:C:297:PHE:N    | 1:C:297:PHE:CD2  | 2.83                     | 0.47              |
| 1:F:322:GLY:O    | 1:F:380:THR:HG22 | 2.14                     | 0.47              |
| 1:D:217:LEU:O    | 1:D:217:LEU:HD23 | 2.15                     | 0.47              |
| 1:D:301:GLN:C    | 1:D:303:PHE:N    | 2.66                     | 0.46              |
| 1:E:220:GLU:OE2  | 1:E:316:THR:HG23 | 2.13                     | 0.46              |
| 1:A:158:ASN:N    | 1:A:158:ASN:HD22 | 2.12                     | 0.46              |
| 1:B:306:ASN:HD22 | 1:B:315:PRO:HG2  | 1.80                     | 0.46              |
| 1:C:200:ALA:O    | 1:C:202:MET:N    | 2.48                     | 0.46              |
| 1:B:211:LEU:HA   | 1:B:211:LEU:HD13 | 1.64                     | 0.46              |
| 1:E:356:ASN:O    | 1:E:357:MET:HB3  | 2.16                     | 0.46              |
| 1:C:342:THR:O    | 1:C:362:CYS:HA   | 2.16                     | 0.46              |
| 1:C:227:ASP:C    | 1:C:229:THR:H    | 2.19                     | 0.46              |
| 1:A:202:MET:HB2  | 1:B:336:PHE:CE2  | 2.41                     | 0.46              |
| 1:C:133:THR:HA   | 1:C:220:GLU:OE2  | 2.14                     | 0.46              |
| 1:A:240:ALA:CB   | 1:A:376:ILE:CG2  | 2.93                     | 0.46              |
| 1:B:161:GLY:C    | 1:B:172:SER:N    | 2.68                     | 0.46              |
| 1:B:209:ASN:HB3  | 1:C:331:MET:CE   | 2.45                     | 0.46              |
| 1:E:325:THR:HG22 | 1:E:329:PHE:HZ   | 1.79                     | 0.46              |
| 1:C:377:ILE:N    | 1:C:377:ILE:HD12 | 2.31                     | 0.46              |
| 1:F:137:LEU:O    | 1:F:137:LEU:HD23 | 2.15                     | 0.46              |
| 1:D:174:ILE:CD1  | 1:D:174:ILE:H    | 2.27                     | 0.46              |
| 1:A:207:ILE:O    | 1:A:211:LEU:HB2  | 2.16                     | 0.46              |
| 1:E:301:GLN:O    | 1:E:304:THR:N    | 2.48                     | 0.46              |
| 1:G:132:LEU:HG   | 1:G:136:ASP:CG   | 2.35                     | 0.46              |
| 1:E:128:GLY:N    | 1:E:213:TYR:CD1  | 2.81                     | 0.46              |
| 1:D:346:SER:O    | 1:D:348:GLU:HG3  | 2.16                     | 0.46              |
| 1:E:358:LEU:HD12 | 1:E:358:LEU:N    | 2.30                     | 0.46              |
| 1:A:196:VAL:O    | 1:A:199:ASP:HB2  | 2.16                     | 0.46              |
| 1:E:302:ALA:HA   | 1:E:305:SER:OG   | 2.16                     | 0.46              |
| 1:D:349:ASP:O    | 1:D:350:ARG:C    | 2.54                     | 0.46              |
| 1:F:295:TYR:CE2  | 1:F:300:PRO:HG3  | 2.51                     | 0.46              |
| 1:B:354:VAL:C    | 1:B:356:ASN:H    | 2.18                     | 0.46              |
| 1:F:342:THR:O    | 1:F:362:CYS:CA   | 2.62                     | 0.46              |
| 1:A:358:LEU:C    | 1:A:358:LEU:HD12 | 2.36                     | 0.46              |
| 1:B:148:LEU:HD21 | 1:B:181:ALA:HB3  | 1.97                     | 0.46              |
| 1:G:155:VAL:CG2  | 1:G:156:PHE:N    | 2.78                     | 0.46              |
| 1:G:156:PHE:CG   | 1:G:158:ASN:HB3  | 2.49                     | 0.46              |
| 1:D:122:PRO:CB   | 1:D:343:VAL:HG23 | 2.45                     | 0.46              |
| 1:D:224:LEU:HD12 | 1:D:225:ASN:CG   | 2.36                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:150:TYR:OH   | 1:D:152:ARG:NH2  | 2.49                     | 0.46              |
| 1:C:201:PRO:O    | 1:C:202:MET:C    | 2.54                     | 0.46              |
| 1:C:211:LEU:C    | 1:C:211:LEU:HD23 | 2.35                     | 0.46              |
| 1:F:198:ASP:O    | 1:F:199:ASP:C    | 2.54                     | 0.46              |
| 1:F:202:MET:O    | 1:F:203:LEU:C    | 2.53                     | 0.46              |
| 1:A:195:GLN:CG   | 1:A:196:VAL:N    | 2.69                     | 0.46              |
| 1:G:153:GLU:OE1  | 1:G:372:ARG:NE   | 2.48                     | 0.46              |
| 1:G:273:SER:H    | 1:G:328:GLY:HA2  | 1.81                     | 0.46              |
| 1:D:149:GLU:HA   | 1:D:180:THR:HA   | 1.98                     | 0.46              |
| 1:G:217:LEU:HD12 | 1:G:217:LEU:N    | 2.31                     | 0.46              |
| 1:A:321:ALA:C    | 1:A:323:THR:H    | 2.18                     | 0.46              |
| 1:G:197:MET:SD   | 1:G:197:MET:O    | 2.73                     | 0.46              |
| 1:F:151:VAL:HG13 | 1:F:151:VAL:O    | 2.16                     | 0.46              |
| 1:C:184:LYS:CB   | 1:C:233:LEU:HD21 | 2.46                     | 0.46              |
| 1:A:196:VAL:O    | 1:A:199:ASP:N    | 2.47                     | 0.46              |
| 1:B:209:ASN:O    | 1:C:331:MET:CE   | 2.63                     | 0.46              |
| 1:E:302:ALA:HA   | 1:E:305:SER:HG   | 1.80                     | 0.46              |
| 1:E:300:PRO:HG2  | 1:F:309:TRP:HE1  | 1.81                     | 0.46              |
| 1:A:309:TRP:CH2  | 1:F:301:GLN:HB3  | 2.51                     | 0.46              |
| 1:C:296:ILE:O    | 1:C:297:PHE:HD2  | 1.98                     | 0.46              |
| 1:F:292:GLU:HB2  | 1:F:294:ARG:HD3  | 1.96                     | 0.46              |
| 1:B:190:VAL:HG12 | 1:C:176:PHE:HZ   | 1.79                     | 0.46              |
| 1:G:152:ARG:HH21 | 1:G:370:HIS:HB2  | 1.79                     | 0.46              |
| 1:A:256:ASP:O    | 1:A:259:ALA:HB3  | 2.16                     | 0.46              |
| 1:F:162:ASP:OD1  | 1:F:173:ASP:CG   | 2.54                     | 0.46              |
| 1:C:207:ILE:H    | 1:C:207:ILE:CD1  | 2.28                     | 0.46              |
| 1:D:127:PRO:CD   | 1:D:212:MET:HE3  | 2.30                     | 0.46              |
| 1:A:206:TYR:HB3  | 1:A:207:ILE:HD12 | 1.98                     | 0.46              |
| 1:B:266:THR:HA   | 1:B:270:PHE:O    | 2.16                     | 0.46              |
| 1:A:158:ASN:ND2  | 1:A:172:SER:CA   | 2.79                     | 0.46              |
| 1:A:343:VAL:HA   | 1:A:361:LEU:O    | 2.16                     | 0.46              |
| 1:G:366:LEU:HD12 | 1:G:367:ALA:CA   | 2.46                     | 0.46              |
| 1:G:217:LEU:HD12 | 1:G:217:LEU:H    | 1.80                     | 0.46              |
| 1:D:174:ILE:HD13 | 1:D:174:ILE:O    | 2.16                     | 0.46              |
| 1:A:155:VAL:CG2  | 1:A:174:ILE:HG22 | 2.37                     | 0.46              |
| 1:G:327:GLY:N    | 1:G:329:PHE:CE2  | 2.74                     | 0.46              |
| 1:D:299:GLY:O    | 1:D:301:GLN:HG2  | 2.16                     | 0.46              |
| 1:F:224:LEU:CD1  | 1:F:237:ASN:HD21 | 2.29                     | 0.46              |
| 1:E:174:ILE:O    | 1:E:174:ILE:HG12 | 2.15                     | 0.46              |
| 1:A:289:LYS:H    | 1:A:289:LYS:HD2  | 1.80                     | 0.46              |
| 1:A:149:GLU:OE1  | 1:F:195:GLN:CG   | 2.64                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:200:ALA:O    | 1:G:201:PRO:C    | 2.53                     | 0.46              |
| 1:G:202:MET:HG2  | 1:G:203:LEU:N    | 2.31                     | 0.46              |
| 1:D:190:VAL:HG11 | 1:D:211:LEU:CD2  | 2.41                     | 0.46              |
| 1:F:254:ARG:HG2  | 1:F:381:PHE:HD2  | 1.81                     | 0.46              |
| 1:B:174:ILE:O    | 1:B:174:ILE:HD13 | 2.15                     | 0.46              |
| 1:D:153:GLU:O    | 1:D:155:VAL:N    | 2.49                     | 0.45              |
| 1:C:217:LEU:CD2  | 1:D:269:GLU:HB3  | 2.46                     | 0.45              |
| 1:A:131:ARG:HH21 | 1:A:316:THR:CB   | 2.29                     | 0.45              |
| 1:A:290:ASP:C    | 1:A:292:GLU:N    | 2.69                     | 0.45              |
| 1:G:134:ILE:O    | 1:G:137:LEU:HB2  | 2.15                     | 0.45              |
| 1:A:263:TYR:CE2  | 1:F:280:ARG:NE   | 2.84                     | 0.45              |
| 1:E:215:LEU:C    | 1:E:218:LYS:H    | 2.17                     | 0.45              |
| 1:C:283:HIS:HE1  | 1:D:260:HIS:HA   | 1.81                     | 0.45              |
| 1:B:180:THR:CG2  | 1:B:181:ALA:N    | 2.80                     | 0.45              |
| 1:B:158:ASN:OD1  | 1:B:172:SER:C    | 2.55                     | 0.45              |
| 1:E:157:THR:HB   | 1:E:267:GLU:OE1  | 2.15                     | 0.45              |
| 1:E:132:LEU:O    | 1:E:132:LEU:HG   | 2.15                     | 0.45              |
| 1:C:186:ILE:CD1  | 1:C:222:GLN:HG3  | 2.41                     | 0.45              |
| 1:B:299:GLY:O    | 1:B:300:PRO:C    | 2.55                     | 0.45              |
| 1:E:141:GLY:O    | 1:E:336:PHE:HA   | 2.17                     | 0.45              |
| 1:E:280:ARG:O    | 1:E:283:HIS:HB3  | 2.17                     | 0.45              |
| 1:C:361:LEU:C    | 1:C:361:LEU:HD12 | 2.36                     | 0.45              |
| 1:A:286:ALA:CB   | 1:A:303:PHE:HD1  | 2.29                     | 0.45              |
| 1:A:194:ARG:O    | 1:A:198:ASP:N    | 2.44                     | 0.45              |
| 1:C:130:ARG:O    | 1:C:131:ARG:O    | 2.34                     | 0.45              |
| 1:B:326:VAL:HG12 | 1:B:327:GLY:N    | 2.32                     | 0.45              |
| 1:C:296:ILE:C    | 1:C:297:PHE:CD2  | 2.90                     | 0.45              |
| 1:F:290:ASP:CG   | 1:F:291:ASN:H    | 2.20                     | 0.45              |
| 1:D:290:ASP:C    | 1:D:292:GLU:N    | 2.70                     | 0.45              |
| 1:A:282:TRP:HA   | 1:A:282:TRP:CE3  | 2.51                     | 0.45              |
| 1:F:153:GLU:O    | 1:F:155:VAL:N    | 2.50                     | 0.45              |
| 1:C:227:ASP:O    | 1:C:232:ASN:ND2  | 2.50                     | 0.45              |
| 1:B:158:ASN:HD22 | 1:B:158:ASN:N    | 2.13                     | 0.45              |
| 1:D:156:PHE:CD2  | 1:D:158:ASN:N    | 2.78                     | 0.45              |
| 1:F:291:ASN:CG   | 1:F:292:GLU:H    | 2.20                     | 0.45              |
| 1:F:192:ALA:O    | 1:F:357:MET:CB   | 2.64                     | 0.45              |
| 1:F:253:THR:O    | 1:F:255:ALA:N    | 2.48                     | 0.45              |
| 1:E:258:ILE:CD1  | 1:E:258:ILE:H    | 2.30                     | 0.45              |
| 1:A:307:ILE:C    | 1:A:307:ILE:CD1  | 2.82                     | 0.45              |
| 1:B:323:THR:HG22 | 1:B:324:PHE:N    | 2.32                     | 0.45              |
| 1:F:322:GLY:O    | 1:F:380:THR:HB   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:236:LEU:O    | 1:F:240:ALA:N    | 2.50                     | 0.45              |
| 1:D:223:LEU:N    | 1:D:223:LEU:HD12 | 2.32                     | 0.45              |
| 1:A:139:ALA:O    | 1:A:335:VAL:HG12 | 2.16                     | 0.45              |
| 1:G:197:MET:HE3  | 1:G:345:VAL:HG11 | 1.99                     | 0.45              |
| 1:D:194:ARG:HG3  | 1:D:358:LEU:HD21 | 1.98                     | 0.45              |
| 1:E:227:ASP:C    | 1:E:229:THR:CG2  | 2.85                     | 0.45              |
| 1:G:129:LEU:C    | 1:G:131:ARG:N    | 2.69                     | 0.45              |
| 1:G:129:LEU:O    | 1:G:130:ARG:HB2  | 2.17                     | 0.45              |
| 1:A:155:VAL:HA   | 1:A:174:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:267:GLU:OE1  | 1:F:317:LYS:CE   | 2.65                     | 0.45              |
| 1:A:296:ILE:C    | 1:A:297:PHE:CD2  | 2.90                     | 0.45              |
| 1:B:227:ASP:O    | 1:B:229:THR:HG23 | 2.17                     | 0.45              |
| 1:G:187:ALA:HB1  | 1:G:362:CYS:O    | 2.17                     | 0.45              |
| 1:B:209:ASN:C    | 1:C:331:MET:HE2  | 2.37                     | 0.45              |
| 1:A:123:GLY:O    | 1:A:124:ILE:CG2  | 2.59                     | 0.45              |
| 1:F:275:ILE:HG22 | 1:F:276:VAL:N    | 2.32                     | 0.45              |
| 1:E:341:ALA:HA   | 1:E:363:GLU:O    | 2.16                     | 0.45              |
| 1:A:290:ASP:OD1  | 1:A:294:ARG:HB3  | 2.17                     | 0.45              |
| 1:G:236:LEU:N    | 1:G:236:LEU:HD12 | 2.32                     | 0.45              |
| 1:E:126:MET:HE3  | 1:E:129:LEU:CD2  | 2.45                     | 0.45              |
| 1:E:194:ARG:HE   | 1:E:356:ASN:ND2  | 2.15                     | 0.45              |
| 1:E:202:MET:CE   | 1:E:203:LEU:HB2  | 2.47                     | 0.45              |
| 1:A:197:MET:C    | 1:A:199:ASP:N    | 2.70                     | 0.45              |
| 1:A:207:ILE:HG22 | 1:A:212:MET:HG2  | 1.98                     | 0.45              |
| 1:F:244:ASP:OD2  | 1:F:246:SER:HB3  | 2.17                     | 0.45              |
| 1:G:329:PHE:O    | 1:G:330:ASP:C    | 2.56                     | 0.45              |
| 1:A:361:LEU:HD12 | 1:A:362:CYS:H    | 1.82                     | 0.45              |
| 1:G:270:PHE:CE1  | 1:G:372:ARG:NE   | 2.85                     | 0.45              |
| 1:E:290:ASP:C    | 1:E:292:GLU:H    | 2.21                     | 0.45              |
| 1:A:282:TRP:HA   | 1:A:282:TRP:HE3  | 1.82                     | 0.45              |
| 1:A:219:GLU:O    | 1:A:223:LEU:HD13 | 2.17                     | 0.45              |
| 1:D:201:PRO:C    | 1:D:203:LEU:N    | 2.68                     | 0.44              |
| 1:E:191:GLN:HB2  | 1:E:358:LEU:O    | 2.17                     | 0.44              |
| 1:E:203:LEU:HD12 | 1:E:206:TYR:CB   | 2.47                     | 0.44              |
| 1:E:206:TYR:O    | 1:E:206:TYR:HD2  | 2.00                     | 0.44              |
| 1:E:347:ARG:C    | 1:E:349:ASP:H    | 2.20                     | 0.44              |
| 1:A:197:MET:SD   | 1:A:198:ASP:N    | 2.90                     | 0.44              |
| 1:B:289:LYS:HA   | 1:B:296:ILE:CD1  | 2.47                     | 0.44              |
| 1:D:305:SER:O    | 1:D:307:ILE:N    | 2.45                     | 0.44              |
| 1:E:301:GLN:O    | 1:E:301:GLN:OE1  | 2.35                     | 0.44              |
| 1:E:156:PHE:O    | 1:E:158:ASN:ND2  | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:224:LEU:HD13 | 1:D:237:ASN:OD1  | 2.17                     | 0.44              |
| 1:G:150:TYR:CE1  | 1:G:179:GLN:HB3  | 2.52                     | 0.44              |
| 1:E:262:ILE:CD1  | 1:E:262:ILE:H    | 2.30                     | 0.44              |
| 1:A:179:GLN:HA   | 1:A:179:GLN:HE21 | 1.82                     | 0.44              |
| 1:F:323:THR:HA   | 1:F:380:THR:HG22 | 1.98                     | 0.44              |
| 1:F:378:LYS:CG   | 1:F:379:GLY:N    | 2.79                     | 0.44              |
| 1:F:264:GLN:HA   | 1:F:267:GLU:HG2  | 1.98                     | 0.44              |
| 1:E:125:ILE:HG23 | 1:E:126:MET:H    | 1.82                     | 0.44              |
| 1:E:194:ARG:NH1  | 1:E:347:ARG:HH22 | 2.12                     | 0.44              |
| 1:F:174:ILE:H    | 1:F:174:ILE:CD1  | 2.17                     | 0.44              |
| 1:A:239:VAL:HG21 | 1:A:370:HIS:HD1  | 1.82                     | 0.44              |
| 1:F:142:ARG:NH2  | 1:F:340:ASP:CG   | 2.71                     | 0.44              |
| 1:A:273:SER:O    | 1:A:312:PRO:HD2  | 2.17                     | 0.44              |
| 1:C:247:LEU:HB3  | 1:C:260:HIS:CD2  | 2.51                     | 0.44              |
| 1:B:329:PHE:N    | 1:B:329:PHE:CD1  | 2.81                     | 0.44              |
| 1:B:333:SER:HB2  | 1:B:369:ALA:O    | 2.17                     | 0.44              |
| 1:C:245:THR:HG23 | 1:C:248:ASN:HD22 | 1.81                     | 0.44              |
| 1:F:347:ARG:O    | 1:F:349:ASP:N    | 2.50                     | 0.44              |
| 1:E:211:LEU:HG   | 1:E:362:CYS:SG   | 2.56                     | 0.44              |
| 1:C:359:THR:HG23 | 1:C:359:THR:O    | 2.18                     | 0.44              |
| 1:A:236:LEU:HD23 | 1:A:370:HIS:CE1  | 2.53                     | 0.44              |
| 1:B:173:ASP:OD1  | 1:B:174:ILE:N    | 2.50                     | 0.44              |
| 1:F:257:ILE:C    | 1:F:259:ALA:N    | 2.69                     | 0.44              |
| 1:F:275:ILE:CG2  | 1:F:277:LEU:HD11 | 2.47                     | 0.44              |
| 1:C:285:ILE:HG21 | 1:C:308:MET:HE1  | 1.99                     | 0.44              |
| 1:D:202:MET:CA   | 1:D:205:SER:OG   | 2.61                     | 0.44              |
| 1:D:247:LEU:HD21 | 1:D:260:HIS:CG   | 2.53                     | 0.44              |
| 1:C:142:ARG:CB   | 1:C:337:ASP:O    | 2.66                     | 0.44              |
| 1:F:288:LEU:HD23 | 1:F:289:LYS:O    | 2.18                     | 0.44              |
| 1:C:156:PHE:HD2  | 1:C:156:PHE:HA   | 1.72                     | 0.44              |
| 1:B:129:LEU:O    | 1:B:129:LEU:HD23 | 2.17                     | 0.44              |
| 1:A:374:THR:C    | 1:A:376:ILE:H    | 2.21                     | 0.44              |
| 1:A:188:HIS:O    | 1:A:361:LEU:HD12 | 2.17                     | 0.44              |
| 1:D:258:ILE:O    | 1:D:261:ALA:HB3  | 2.17                     | 0.44              |
| 1:A:224:LEU:HD12 | 1:A:225:ASN:CG   | 2.38                     | 0.44              |
| 1:A:295:TYR:HD2  | 1:A:295:TYR:HA   | 1.69                     | 0.44              |
| 1:C:203:LEU:O    | 1:C:206:TYR:HB2  | 2.16                     | 0.44              |
| 1:G:290:ASP:O    | 1:G:292:GLU:N    | 2.50                     | 0.44              |
| 1:D:191:GLN:NE2  | 1:E:176:PHE:CD2  | 2.85                     | 0.44              |
| 1:C:185:THR:HA   | 1:C:365:ARG:HA   | 1.99                     | 0.44              |
| 1:C:234:GLU:O    | 1:C:368:LEU:HD23 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:297:PHE:CD2  | 1:D:308:MET:HB2  | 2.52                     | 0.44              |
| 1:G:254:ARG:HD3  | 1:G:381:PHE:CE1  | 2.52                     | 0.44              |
| 1:F:349:ASP:O    | 1:F:352:ASN:OD1  | 2.35                     | 0.44              |
| 1:F:356:ASN:O    | 1:F:357:MET:HG2  | 2.18                     | 0.44              |
| 1:B:194:ARG:NH2  | 1:B:347:ARG:CZ   | 2.80                     | 0.44              |
| 1:A:269:GLU:CB   | 1:F:217:LEU:HD21 | 2.16                     | 0.44              |
| 1:G:155:VAL:HG11 | 1:G:374:THR:CG2  | 2.47                     | 0.44              |
| 1:A:241:THR:O    | 1:A:377:ILE:HA   | 2.17                     | 0.44              |
| 1:A:121:ILE:C    | 1:A:123:GLY:H    | 2.20                     | 0.44              |
| 1:D:280:ARG:HG3  | 1:E:309:TRP:HB3  | 2.00                     | 0.44              |
| 1:B:237:ASN:N    | 1:B:237:ASN:HD22 | 2.15                     | 0.44              |
| 1:G:197:MET:HE1  | 1:G:358:LEU:HD23 | 1.85                     | 0.44              |
| 1:F:194:ARG:HH22 | 1:G:363:GLU:CD   | 2.22                     | 0.44              |
| 1:G:327:GLY:H    | 1:G:329:PHE:HE2  | 1.63                     | 0.44              |
| 1:G:355:LYS:O    | 1:G:357:MET:HB2  | 2.17                     | 0.44              |
| 1:E:156:PHE:CD2  | 1:E:158:ASN:N    | 2.77                     | 0.44              |
| 1:A:330:ASP:OD2  | 1:F:130:ARG:NH2  | 2.43                     | 0.44              |
| 1:B:224:LEU:HD13 | 1:B:224:LEU:C    | 2.38                     | 0.44              |
| 1:E:219:GLU:HG2  | 1:E:223:LEU:HD11 | 1.99                     | 0.44              |
| 1:B:200:ALA:HB1  | 1:B:201:PRO:HD2  | 1.98                     | 0.44              |
| 1:D:194:ARG:HB2  | 1:D:358:LEU:CD1  | 2.48                     | 0.44              |
| 1:D:194:ARG:HB2  | 1:D:358:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:161:GLY:O    | 1:D:162:ASP:C    | 2.56                     | 0.44              |
| 1:E:254:ARG:CG   | 1:E:381:PHE:CE2  | 2.98                     | 0.44              |
| 1:B:142:ARG:HG2  | 1:B:337:ASP:O    | 2.18                     | 0.44              |
| 1:A:154:GLU:OE2  | 1:A:177:SER:HB2  | 2.18                     | 0.44              |
| 1:A:223:LEU:N    | 1:A:223:LEU:HD12 | 2.32                     | 0.44              |
| 1:A:217:LEU:HD23 | 1:A:217:LEU:C    | 2.38                     | 0.44              |
| 1:E:366:LEU:HD12 | 1:E:367:ALA:N    | 2.32                     | 0.43              |
| 1:E:190:VAL:CG2  | 1:E:360:ILE:HD11 | 2.48                     | 0.43              |
| 1:C:301:GLN:HG2  | 1:C:302:ALA:N    | 2.32                     | 0.43              |
| 1:F:324:PHE:HD2  | 1:F:381:PHE:HE1  | 0.86                     | 0.43              |
| 1:A:263:TYR:HB2  | 1:F:303:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:345:VAL:HG22 | 1:A:360:ILE:HG23 | 2.00                     | 0.43              |
| 1:B:142:ARG:HA   | 1:B:337:ASP:H    | 1.83                     | 0.43              |
| 1:F:204:GLN:O    | 1:F:208:ASN:HB2  | 2.18                     | 0.43              |
| 1:F:213:TYR:O    | 1:F:217:LEU:HB2  | 2.17                     | 0.43              |
| 1:C:335:VAL:HG13 | 1:C:366:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:194:ARG:CA   | 1:A:198:ASP:OD2  | 2.66                     | 0.43              |
| 1:G:184:LYS:HD2  | 1:G:231:ASP:HA   | 1.98                     | 0.43              |
| 1:E:220:GLU:CD   | 1:E:316:THR:HG21 | 2.35                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:254:ARG:HG3  | 1:E:381:PHE:HE2  | 1.83                     | 0.43              |
| 1:B:273:SER:HB2  | 1:B:330:ASP:H    | 1.82                     | 0.43              |
| 1:D:195:GLN:HA   | 1:D:195:GLN:OE1  | 2.18                     | 0.43              |
| 1:E:345:VAL:HG13 | 1:E:359:THR:O    | 2.18                     | 0.43              |
| 1:G:288:LEU:HD12 | 1:G:296:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:283:HIS:CE1  | 1:D:260:HIS:HA   | 2.53                     | 0.43              |
| 1:B:208:ASN:ND2  | 1:B:208:ASN:N    | 2.66                     | 0.43              |
| 1:G:155:VAL:CG1  | 1:G:374:THR:OG1  | 2.58                     | 0.43              |
| 1:E:288:LEU:O    | 1:E:295:TYR:HA   | 2.18                     | 0.43              |
| 1:D:296:ILE:C    | 1:D:298:GLY:N    | 2.70                     | 0.43              |
| 1:A:292:GLU:C    | 1:A:294:ARG:H    | 2.22                     | 0.43              |
| 1:E:186:ILE:CD1  | 1:E:222:GLN:HG3  | 2.48                     | 0.43              |
| 1:F:215:LEU:C    | 1:F:215:LEU:HD23 | 2.38                     | 0.43              |
| 1:B:288:LEU:C    | 1:B:288:LEU:HD23 | 2.39                     | 0.43              |
| 1:E:296:ILE:HA   | 1:E:296:ILE:HD13 | 1.88                     | 0.43              |
| 1:B:158:ASN:CB   | 1:B:172:SER:CA   | 2.86                     | 0.43              |
| 1:E:311:LEU:HA   | 1:E:312:PRO:HD3  | 1.92                     | 0.43              |
| 1:B:155:VAL:HG13 | 1:B:374:THR:HG21 | 2.00                     | 0.43              |
| 1:E:258:ILE:O    | 1:E:261:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:329:PHE:HA   | 1:A:332:ALA:HB3  | 2.01                     | 0.43              |
| 1:B:206:TYR:O    | 1:B:210:ARG:HB2  | 2.19                     | 0.43              |
| 1:E:191:GLN:CB   | 1:E:359:THR:HA   | 2.47                     | 0.43              |
| 1:F:174:ILE:HG12 | 1:F:174:ILE:O    | 2.18                     | 0.43              |
| 1:B:194:ARG:HH11 | 1:B:356:ASN:HD21 | 1.66                     | 0.43              |
| 1:C:345:VAL:HG12 | 1:C:346:SER:N    | 2.33                     | 0.43              |
| 1:F:343:VAL:CA   | 1:F:361:LEU:O    | 2.66                     | 0.43              |
| 1:G:158:ASN:ND2  | 1:G:172:SER:OG   | 2.46                     | 0.43              |
| 1:G:335:VAL:HA   | 1:G:368:LEU:HA   | 2.00                     | 0.43              |
| 1:A:148:LEU:O    | 1:A:180:THR:HG23 | 2.19                     | 0.43              |
| 1:F:270:PHE:HE1  | 1:F:372:ARG:NH1  | 2.15                     | 0.43              |
| 1:A:202:MET:CB   | 1:B:336:PHE:HE2  | 2.25                     | 0.43              |
| 1:F:322:GLY:O    | 1:F:380:THR:CG2  | 2.67                     | 0.43              |
| 1:G:202:MET:O    | 1:G:205:SER:N    | 2.52                     | 0.43              |
| 1:A:236:LEU:HD23 | 1:A:370:HIS:NE2  | 2.34                     | 0.43              |
| 1:C:229:THR:O    | 1:C:232:ASN:HB2  | 2.19                     | 0.43              |
| 1:F:156:PHE:O    | 1:F:158:ASN:ND2  | 2.52                     | 0.43              |
| 1:F:148:LEU:O    | 1:F:181:ALA:N    | 2.46                     | 0.43              |
| 1:B:182:ASN:HB2  | 1:B:184:LYS:NZ   | 2.33                     | 0.43              |
| 1:D:243:TYR:HE2  | 1:D:248:ASN:HD21 | 1.67                     | 0.43              |
| 1:B:287:LEU:HD22 | 1:B:287:LEU:N    | 2.33                     | 0.43              |
| 1:D:208:ASN:N    | 1:D:208:ASN:HD22 | 2.15                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:314:VAL:O    | 1:C:314:VAL:HG23 | 2.19                     | 0.43              |
| 1:D:130:ARG:CD   | 1:D:131:ARG:N    | 2.82                     | 0.43              |
| 1:E:279:PRO:HD3  | 1:E:316:THR:O    | 2.19                     | 0.43              |
| 1:C:185:THR:OG1  | 1:C:365:ARG:HG2  | 2.18                     | 0.43              |
| 1:C:325:THR:HA   | 1:C:377:ILE:O    | 2.18                     | 0.43              |
| 1:F:222:GLN:HA   | 1:F:222:GLN:HE21 | 1.84                     | 0.43              |
| 1:C:254:ARG:HB3  | 1:C:381:PHE:CE2  | 2.54                     | 0.43              |
| 1:D:278:ASN:HB3  | 1:D:281:ASP:OD2  | 2.19                     | 0.43              |
| 1:C:347:ARG:HG2  | 1:C:348:GLU:N    | 2.34                     | 0.43              |
| 1:G:349:ASP:OD2  | 1:G:350:ARG:HG3  | 2.18                     | 0.43              |
| 1:E:203:LEU:C    | 1:E:206:TYR:H    | 2.09                     | 0.43              |
| 1:B:253:THR:HG22 | 1:B:254:ARG:H    | 1.83                     | 0.43              |
| 1:A:343:VAL:HA   | 1:A:362:CYS:HA   | 2.01                     | 0.43              |
| 1:A:296:ILE:O    | 1:A:297:PHE:CB   | 2.67                     | 0.43              |
| 1:B:238:LYS:HA   | 1:B:238:LYS:HD2  | 1.73                     | 0.43              |
| 1:D:174:ILE:CG1  | 1:D:176:PHE:HE2  | 2.28                     | 0.43              |
| 1:G:282:TRP:CH2  | 1:G:313:VAL:HG21 | 2.54                     | 0.43              |
| 1:F:211:LEU:CD2  | 1:F:212:MET:CE   | 2.97                     | 0.43              |
| 1:F:344:GLU:O    | 1:F:361:LEU:HD12 | 2.19                     | 0.43              |
| 1:E:333:SER:HA   | 1:E:371:TYR:CD1  | 2.53                     | 0.43              |
| 1:D:236:LEU:HD23 | 1:D:370:HIS:CE1  | 2.54                     | 0.43              |
| 1:F:306:ASN:HB3  | 1:F:313:VAL:HB   | 2.00                     | 0.43              |
| 1:E:194:ARG:NE   | 1:E:356:ASN:OD1  | 2.52                     | 0.42              |
| 1:B:194:ARG:HD2  | 1:B:358:LEU:CD1  | 2.49                     | 0.42              |
| 1:G:285:ILE:HA   | 1:G:288:LEU:CD1  | 2.49                     | 0.42              |
| 1:C:274:GLY:C    | 1:C:275:ILE:HD12 | 2.40                     | 0.42              |
| 1:B:215:LEU:HD22 | 1:B:216:ALA:CA   | 2.49                     | 0.42              |
| 1:B:215:LEU:HD22 | 1:B:216:ALA:HA   | 2.00                     | 0.42              |
| 1:C:376:ILE:C    | 1:C:377:ILE:HD12 | 2.39                     | 0.42              |
| 1:G:309:TRP:CE3  | 1:G:309:TRP:HA   | 2.54                     | 0.42              |
| 1:C:195:GLN:C    | 1:C:197:MET:N    | 2.71                     | 0.42              |
| 1:C:207:ILE:CA   | 1:C:211:LEU:HB3  | 2.40                     | 0.42              |
| 1:E:194:ARG:H    | 1:E:357:MET:HA   | 1.84                     | 0.42              |
| 1:A:203:LEU:CD1  | 1:A:207:ILE:HD11 | 2.49                     | 0.42              |
| 1:A:124:ILE:O    | 1:A:126:MET:HE3  | 2.19                     | 0.42              |
| 1:A:137:LEU:HB3  | 1:A:138:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:345:VAL:HG22 | 1:A:360:ILE:HG12 | 2.00                     | 0.42              |
| 1:G:233:LEU:HD13 | 1:G:368:LEU:HD22 | 2.00                     | 0.42              |
| 1:D:280:ARG:HG3  | 1:E:309:TRP:O    | 2.19                     | 0.42              |
| 1:D:195:GLN:HG3  | 1:D:196:VAL:N    | 2.34                     | 0.42              |
| 1:F:344:GLU:H    | 1:F:361:LEU:HD13 | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:203:LEU:O    | 1:A:206:TYR:N    | 2.52                     | 0.42              |
| 1:D:277:LEU:CD1  | 1:D:324:PHE:HB3  | 2.49                     | 0.42              |
| 1:G:355:LYS:HE2  | 1:G:355:LYS:HB3  | 1.61                     | 0.42              |
| 1:G:244:ASP:OD2  | 1:G:247:LEU:HG   | 2.20                     | 0.42              |
| 1:A:277:LEU:HD23 | 1:A:277:LEU:HA   | 1.52                     | 0.42              |
| 1:E:127:PRO:HA   | 1:E:213:TYR:HB2  | 2.01                     | 0.42              |
| 1:G:194:ARG:O    | 1:G:195:GLN:C    | 2.55                     | 0.42              |
| 1:C:280:ARG:O    | 1:C:283:HIS:HB3  | 2.20                     | 0.42              |
| 1:C:227:ASP:HB3  | 1:C:229:THR:HG1  | 1.85                     | 0.42              |
| 1:C:183:VAL:CA   | 1:C:367:ALA:HB2  | 2.35                     | 0.42              |
| 1:E:296:ILE:C    | 1:E:298:GLY:N    | 2.70                     | 0.42              |
| 1:A:132:LEU:N    | 1:A:132:LEU:HD12 | 2.33                     | 0.42              |
| 1:D:258:ILE:HD12 | 1:D:258:ILE:N    | 2.34                     | 0.42              |
| 1:D:258:ILE:HG21 | 1:D:308:MET:HE2  | 2.01                     | 0.42              |
| 1:E:253:THR:HG22 | 1:E:255:ALA:H    | 1.84                     | 0.42              |
| 1:D:236:LEU:HA   | 1:D:370:HIS:CE1  | 2.54                     | 0.42              |
| 1:C:256:ASP:O    | 1:C:259:ALA:HB3  | 2.20                     | 0.42              |
| 1:C:202:MET:O    | 1:C:205:SER:HB3  | 2.19                     | 0.42              |
| 1:D:268:SER:HB3  | 1:D:374:THR:HG22 | 2.01                     | 0.42              |
| 1:A:194:ARG:HA   | 1:A:198:ASP:OD2  | 2.20                     | 0.42              |
| 1:B:209:ASN:HB3  | 1:C:331:MET:HE3  | 2.00                     | 0.42              |
| 1:E:236:LEU:HD13 | 1:E:329:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:158:ASN:HD22 | 1:E:158:ASN:H    | 1.61                     | 0.42              |
| 1:F:129:LEU:O    | 1:F:130:ARG:CB   | 2.66                     | 0.42              |
| 1:B:206:TYR:CD2  | 1:B:210:ARG:HB2  | 2.55                     | 0.42              |
| 1:G:333:SER:HB3  | 1:G:369:ALA:O    | 2.18                     | 0.42              |
| 1:B:217:LEU:O    | 1:B:220:GLU:N    | 2.53                     | 0.42              |
| 1:C:224:LEU:HD13 | 1:C:237:ASN:HD21 | 1.82                     | 0.42              |
| 1:A:195:GLN:HG3  | 1:A:196:VAL:CG2  | 2.35                     | 0.42              |
| 1:A:208:ASN:N    | 1:A:208:ASN:HD22 | 2.17                     | 0.42              |
| 1:E:358:LEU:HB3  | 1:E:359:THR:H    | 1.61                     | 0.42              |
| 1:B:217:LEU:O    | 1:B:218:LYS:C    | 2.57                     | 0.42              |
| 1:G:133:THR:HB   | 1:G:220:GLU:OE2  | 2.19                     | 0.42              |
| 1:A:153:GLU:O    | 1:A:155:VAL:N    | 2.52                     | 0.42              |
| 1:E:301:GLN:O    | 1:E:302:ALA:C    | 2.58                     | 0.42              |
| 1:F:345:VAL:HG13 | 1:F:358:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:349:ASP:OD1  | 1:A:349:ASP:C    | 2.57                     | 0.42              |
| 1:E:275:ILE:HG22 | 1:E:326:VAL:HG13 | 2.02                     | 0.42              |
| 1:G:211:LEU:HD23 | 1:G:211:LEU:C    | 2.40                     | 0.42              |
| 1:C:190:VAL:HG22 | 1:D:176:PHE:HE1  | 1.84                     | 0.42              |
| 1:D:173:ASP:OD1  | 1:D:174:ILE:HD13 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:125:ILE:HD11 | 1:B:127:PRO:HG3  | 2.02                     | 0.42              |
| 1:G:299:GLY:O    | 1:G:303:PHE:HB2  | 2.20                     | 0.42              |
| 1:F:222:GLN:HA   | 1:F:222:GLN:NE2  | 2.35                     | 0.42              |
| 1:B:244:ASP:CG   | 1:B:247:LEU:HG   | 2.40                     | 0.42              |
| 1:B:152:ARG:O    | 1:B:154:GLU:N    | 2.53                     | 0.42              |
| 1:E:125:ILE:HG13 | 1:E:212:MET:CG   | 2.49                     | 0.42              |
| 1:C:198:ASP:CG   | 1:C:198:ASP:O    | 2.57                     | 0.42              |
| 1:F:195:GLN:O    | 1:F:196:VAL:C    | 2.58                     | 0.42              |
| 1:C:224:LEU:CD1  | 1:C:237:ASN:HD21 | 2.33                     | 0.42              |
| 1:F:187:ALA:HB2  | 1:F:363:GLU:HA   | 2.02                     | 0.42              |
| 1:D:343:VAL:CG1  | 1:D:362:CYS:SG   | 3.08                     | 0.42              |
| 1:F:225:ASN:ND2  | 1:F:225:ASN:O    | 2.53                     | 0.42              |
| 1:B:186:ILE:HG22 | 1:B:187:ALA:N    | 2.34                     | 0.42              |
| 1:B:342:THR:O    | 1:B:362:CYS:SG   | 2.77                     | 0.42              |
| 1:D:158:ASN:CG   | 1:D:172:SER:CA   | 2.80                     | 0.42              |
| 1:A:175:THR:HG22 | 1:A:176:PHE:H    | 1.84                     | 0.42              |
| 1:F:227:ASP:C    | 1:F:229:THR:H    | 2.23                     | 0.42              |
| 1:D:292:GLU:O    | 1:D:294:ARG:N    | 2.53                     | 0.42              |
| 1:C:152:ARG:HG3  | 1:C:371:TYR:O    | 2.19                     | 0.42              |
| 1:D:207:ILE:HG13 | 1:D:211:LEU:CD1  | 2.41                     | 0.42              |
| 1:E:189:TRP:O    | 1:E:191:GLN:N    | 2.53                     | 0.42              |
| 1:E:227:ASP:O    | 1:E:229:THR:CG2  | 2.67                     | 0.42              |
| 1:G:280:ARG:C    | 1:G:283:HIS:H    | 2.23                     | 0.42              |
| 1:C:258:ILE:O    | 1:C:261:ALA:HB3  | 2.20                     | 0.42              |
| 1:C:278:ASN:HB3  | 1:C:319:GLN:O    | 2.20                     | 0.42              |
| 1:B:156:PHE:CD2  | 1:B:158:ASN:CA   | 3.01                     | 0.42              |
| 1:C:328:GLY:O    | 1:C:331:MET:N    | 2.45                     | 0.42              |
| 1:G:352:ASN:O    | 1:G:353:PHE:C    | 2.56                     | 0.42              |
| 1:E:254:ARG:HA   | 1:E:257:ILE:CD1  | 2.49                     | 0.42              |
| 1:C:322:GLY:O    | 1:C:380:THR:HA   | 2.20                     | 0.42              |
| 1:F:227:ASP:C    | 1:F:229:THR:N    | 2.73                     | 0.42              |
| 1:D:185:THR:C    | 1:D:186:ILE:HD12 | 2.40                     | 0.42              |
| 1:C:288:LEU:HD23 | 1:C:288:LEU:C    | 2.40                     | 0.42              |
| 1:A:152:ARG:HB3  | 1:A:177:SER:HB3  | 2.02                     | 0.42              |
| 1:E:139:ALA:HB3  | 1:E:334:GLN:HB3  | 2.00                     | 0.42              |
| 1:E:125:ILE:HD11 | 1:E:127:PRO:CD   | 2.42                     | 0.41              |
| 1:D:125:ILE:CG1  | 1:D:208:ASN:ND2  | 2.80                     | 0.41              |
| 1:D:173:ASP:OD1  | 1:D:174:ILE:CD1  | 2.68                     | 0.41              |
| 1:C:227:ASP:O    | 1:C:228:GLY:C    | 2.59                     | 0.41              |
| 1:B:252:ASP:HB3  | 1:B:256:ASP:CB   | 2.49                     | 0.41              |
| 1:A:203:LEU:O    | 1:A:207:ILE:HD13 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:ARG:HG2  | 1:A:210:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:329:PHE:HD1  | 1:A:329:PHE:H    | 1.66                     | 0.41              |
| 1:B:137:LEU:O    | 1:B:137:LEU:HD23 | 2.20                     | 0.41              |
| 1:B:349:ASP:O    | 1:B:352:ASN:CB   | 2.67                     | 0.41              |
| 1:B:351:ASP:HB3  | 1:B:355:LYS:HE3  | 2.02                     | 0.41              |
| 1:B:191:GLN:HA   | 1:B:359:THR:HA   | 2.02                     | 0.41              |
| 1:F:192:ALA:C    | 1:F:357:MET:SD   | 2.97                     | 0.41              |
| 1:E:202:MET:HE3  | 1:E:202:MET:HB3  | 1.73                     | 0.41              |
| 1:D:187:ALA:HB1  | 1:D:361:LEU:HD11 | 2.00                     | 0.41              |
| 1:B:153:GLU:O    | 1:B:155:VAL:N    | 2.54                     | 0.41              |
| 1:B:187:ALA:HB1  | 1:B:362:CYS:O    | 2.20                     | 0.41              |
| 1:A:331:MET:SD   | 1:F:209:ASN:O    | 2.78                     | 0.41              |
| 1:A:131:ARG:HB3  | 1:A:131:ARG:HH11 | 1.85                     | 0.41              |
| 1:D:149:GLU:HG2  | 1:D:180:THR:HG23 | 2.03                     | 0.41              |
| 1:E:190:VAL:HG23 | 1:E:190:VAL:O    | 2.20                     | 0.41              |
| 1:B:296:ILE:O    | 1:B:297:PHE:CG   | 2.73                     | 0.41              |
| 1:D:206:TYR:O    | 1:D:210:ARG:HB3  | 2.20                     | 0.41              |
| 1:E:156:PHE:CD2  | 1:E:158:ASN:CA   | 3.04                     | 0.41              |
| 1:F:257:ILE:O    | 1:F:258:ILE:C    | 2.59                     | 0.41              |
| 1:F:338:ARG:HH11 | 1:F:338:ARG:HG3  | 1.84                     | 0.41              |
| 1:G:199:ASP:O    | 1:G:200:ALA:C    | 2.59                     | 0.41              |
| 1:E:190:VAL:N    | 1:E:360:ILE:CD1  | 2.78                     | 0.41              |
| 1:B:216:ALA:O    | 1:B:219:GLU:HB3  | 2.20                     | 0.41              |
| 1:C:357:MET:CE   | 1:D:178:LYS:HD3  | 2.51                     | 0.41              |
| 1:D:225:ASN:ND2  | 1:D:318:ALA:O    | 2.54                     | 0.41              |
| 1:F:184:LYS:HD2  | 1:F:231:ASP:HA   | 2.02                     | 0.41              |
| 1:F:208:ASN:C    | 1:F:208:ASN:OD1  | 2.58                     | 0.41              |
| 1:F:151:VAL:CG2  | 1:F:176:PHE:HB3  | 2.50                     | 0.41              |
| 1:E:300:PRO:CG   | 1:F:309:TRP:NE1  | 2.83                     | 0.41              |
| 1:A:134:ILE:O    | 1:A:138:LEU:HD13 | 2.20                     | 0.41              |
| 1:C:268:SER:HB2  | 1:C:372:ARG:HD3  | 2.02                     | 0.41              |
| 1:E:235:GLY:O    | 1:E:238:LYS:HB3  | 2.20                     | 0.41              |
| 1:D:221:GLY:O    | 1:D:225:ASN:N    | 2.47                     | 0.41              |
| 1:F:348:GLU:H    | 1:F:348:GLU:HG2  | 1.55                     | 0.41              |
| 1:A:245:THR:O    | 1:A:245:THR:HG22 | 2.21                     | 0.41              |
| 1:A:290:ASP:C    | 1:A:292:GLU:H    | 2.23                     | 0.41              |
| 1:D:207:ILE:CD1  | 1:D:207:ILE:N    | 2.84                     | 0.41              |
| 1:G:282:TRP:CE3  | 1:G:313:VAL:HG11 | 2.55                     | 0.41              |
| 1:D:206:TYR:OH   | 1:D:210:ARG:NH1  | 2.53                     | 0.41              |
| 1:A:345:VAL:CG2  | 1:A:360:ILE:HG12 | 2.51                     | 0.41              |
| 1:A:186:ILE:N    | 1:A:186:ILE:CD1  | 2.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:124:ILE:HG23 | 1:D:125:ILE:N    | 2.34                     | 0.41              |
| 1:D:268:SER:O    | 1:D:270:PHE:HD1  | 2.04                     | 0.41              |
| 1:A:149:GLU:OE1  | 1:F:195:GLN:HG2  | 2.21                     | 0.41              |
| 1:E:347:ARG:O    | 1:E:352:ASN:HB2  | 2.21                     | 0.41              |
| 1:B:125:ILE:CG1  | 1:B:127:PRO:CG   | 2.96                     | 0.41              |
| 1:A:193:SER:OG   | 1:A:195:GLN:HG2  | 2.20                     | 0.41              |
| 1:A:266:THR:O    | 1:A:268:SER:N    | 2.53                     | 0.41              |
| 1:E:325:THR:HA   | 1:E:377:ILE:O    | 2.21                     | 0.41              |
| 1:F:288:LEU:O    | 1:F:295:TYR:HA   | 2.21                     | 0.41              |
| 1:D:233:LEU:HD11 | 1:D:366:LEU:HD11 | 2.03                     | 0.41              |
| 1:G:335:VAL:HG12 | 1:G:368:LEU:CB   | 2.51                     | 0.41              |
| 1:A:316:THR:HG23 | 1:A:319:GLN:H    | 1.85                     | 0.41              |
| 1:F:320:ALA:O    | 1:F:323:THR:HB   | 2.20                     | 0.41              |
| 1:D:217:LEU:C    | 1:D:217:LEU:HD23 | 2.40                     | 0.41              |
| 1:E:237:ASN:HD22 | 1:E:237:ASN:N    | 2.18                     | 0.41              |
| 1:C:207:ILE:CG2  | 1:C:211:LEU:HD13 | 2.50                     | 0.41              |
| 1:G:207:ILE:O    | 1:G:211:LEU:HB3  | 2.21                     | 0.41              |
| 1:G:345:VAL:CG1  | 1:G:358:LEU:HD11 | 2.48                     | 0.41              |
| 1:D:162:ASP:C    | 1:D:173:ASP:N    | 2.70                     | 0.41              |
| 1:C:277:LEU:HA   | 1:C:319:GLN:HG2  | 2.03                     | 0.41              |
| 1:A:125:ILE:N    | 1:A:125:ILE:CD1  | 2.74                     | 0.41              |
| 1:B:143:THR:OG1  | 1:B:144:SER:N    | 2.54                     | 0.41              |
| 1:G:236:LEU:O    | 1:G:240:ALA:N    | 2.54                     | 0.41              |
| 1:D:256:ASP:O    | 1:D:259:ALA:HB3  | 2.19                     | 0.41              |
| 1:F:152:ARG:O    | 1:F:154:GLU:N    | 2.54                     | 0.41              |
| 1:D:208:ASN:N    | 1:D:208:ASN:ND2  | 2.69                     | 0.41              |
| 1:F:193:SER:O    | 1:F:196:VAL:CG1  | 2.69                     | 0.41              |
| 1:D:196:VAL:HA   | 1:D:199:ASP:OD1  | 2.21                     | 0.41              |
| 1:B:253:THR:CG2  | 1:B:254:ARG:N    | 2.83                     | 0.41              |
| 1:C:300:PRO:C    | 1:C:302:ALA:N    | 2.74                     | 0.41              |
| 1:G:128:GLY:C    | 1:G:130:ARG:H    | 2.24                     | 0.41              |
| 1:G:306:ASN:OD1  | 1:G:306:ASN:O    | 2.39                     | 0.41              |
| 1:E:296:ILE:O    | 1:E:298:GLY:N    | 2.53                     | 0.41              |
| 1:F:275:ILE:HG22 | 1:F:277:LEU:HD11 | 2.02                     | 0.41              |
| 1:C:290:ASP:C    | 1:C:292:GLU:N    | 2.74                     | 0.41              |
| 1:D:328:GLY:C    | 1:D:330:ASP:N    | 2.74                     | 0.41              |
| 1:F:331:MET:O    | 1:F:331:MET:CG   | 2.69                     | 0.41              |
| 1:D:309:TRP:HE3  | 1:D:309:TRP:N    | 2.17                     | 0.41              |
| 1:B:324:PHE:N    | 1:B:324:PHE:CD1  | 2.89                     | 0.41              |
| 1:E:154:GLU:OE2  | 1:E:177:SER:CB   | 2.69                     | 0.41              |
| 1:F:178:LYS:HB2  | 1:F:178:LYS:HE3  | 1.80                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:SER:HB3  | 1:A:369:ALA:O    | 2.21                     | 0.41              |
| 1:C:196:VAL:HG11 | 1:C:203:LEU:HD13 | 1.98                     | 0.41              |
| 1:E:194:ARG:HE   | 1:E:356:ASN:HD21 | 1.69                     | 0.41              |
| 1:E:211:LEU:HD12 | 1:E:211:LEU:HA   | 1.65                     | 0.41              |
| 1:C:189:TRP:O    | 1:C:189:TRP:CD2  | 2.74                     | 0.41              |
| 1:C:131:ARG:HB2  | 1:C:131:ARG:NH1  | 2.34                     | 0.41              |
| 1:F:290:ASP:OD1  | 1:F:291:ASN:N    | 2.49                     | 0.41              |
| 1:G:142:ARG:NH1  | 1:G:142:ARG:HG2  | 2.35                     | 0.41              |
| 1:D:236:LEU:HD23 | 1:D:370:HIS:NE2  | 2.35                     | 0.41              |
| 1:C:236:LEU:O    | 1:C:240:ALA:HB2  | 2.21                     | 0.41              |
| 1:E:145:SER:C    | 1:E:147:ALA:H    | 2.23                     | 0.41              |
| 1:G:199:ASP:O    | 1:G:202:MET:CB   | 2.67                     | 0.40              |
| 1:G:188:HIS:N    | 1:G:215:LEU:HD13 | 2.37                     | 0.40              |
| 1:G:346:SER:O    | 1:G:358:LEU:HD12 | 2.20                     | 0.40              |
| 1:B:148:LEU:HD23 | 1:B:181:ALA:HB3  | 2.04                     | 0.40              |
| 1:D:131:ARG:NH2  | 1:D:133:THR:HG22 | 2.36                     | 0.40              |
| 1:A:158:ASN:OD1  | 1:A:172:SER:HA   | 2.21                     | 0.40              |
| 1:E:292:GLU:O    | 1:E:294:ARG:N    | 2.50                     | 0.40              |
| 1:A:152:ARG:O    | 1:A:154:GLU:N    | 2.55                     | 0.40              |
| 1:C:202:MET:O    | 1:C:203:LEU:O    | 2.39                     | 0.40              |
| 1:G:204:GLN:HG2  | 1:G:204:GLN:O    | 2.21                     | 0.40              |
| 1:G:211:LEU:HD12 | 1:G:360:ILE:HD12 | 2.03                     | 0.40              |
| 1:B:196:VAL:H    | 1:B:196:VAL:HG23 | 1.68                     | 0.40              |
| 1:D:127:PRO:HB3  | 1:D:212:MET:CB   | 2.49                     | 0.40              |
| 1:A:195:GLN:O    | 1:A:199:ASP:OD2  | 2.39                     | 0.40              |
| 1:B:342:THR:O    | 1:B:363:GLU:N    | 2.54                     | 0.40              |
| 1:F:143:THR:HG22 | 1:F:336:PHE:HB3  | 2.03                     | 0.40              |
| 1:E:290:ASP:C    | 1:E:292:GLU:N    | 2.74                     | 0.40              |
| 1:A:258:ILE:O    | 1:A:262:ILE:HG13 | 2.21                     | 0.40              |
| 1:E:120:GLN:O    | 1:E:122:PRO:HD3  | 2.22                     | 0.40              |
| 1:E:218:LYS:O    | 1:E:219:GLU:C    | 2.59                     | 0.40              |
| 1:C:204:GLN:HA   | 1:C:207:ILE:CD1  | 2.51                     | 0.40              |
| 1:A:127:PRO:HD3  | 1:A:212:MET:HE3  | 2.03                     | 0.40              |
| 1:G:155:VAL:CG2  | 1:G:156:PHE:H    | 2.35                     | 0.40              |
| 1:G:327:GLY:C    | 1:G:329:PHE:HD2  | 2.21                     | 0.40              |
| 1:B:158:ASN:C    | 1:B:172:SER:HB2  | 2.42                     | 0.40              |
| 1:A:183:VAL:HG13 | 1:A:366:LEU:C    | 2.41                     | 0.40              |
| 1:F:282:TRP:CE3  | 1:F:282:TRP:HA   | 2.57                     | 0.40              |
| 1:A:297:PHE:HE1  | 1:A:308:MET:CE   | 2.34                     | 0.40              |
| 1:E:289:LYS:HA   | 1:E:294:ARG:O    | 2.21                     | 0.40              |
| 1:G:248:ASN:HD22 | 1:G:248:ASN:N    | 2.19                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:339:MET:HB3  | 1:E:339:MET:HE2  | 1.94                     | 0.40              |
| 1:D:347:ARG:O    | 1:D:347:ARG:CG   | 2.69                     | 0.40              |
| 1:E:194:ARG:HD2  | 1:E:347:ARG:NE   | 2.36                     | 0.40              |
| 1:A:285:ILE:HA   | 1:A:288:LEU:CD1  | 2.47                     | 0.40              |
| 1:D:260:HIS:O    | 1:D:263:TYR:HB3  | 2.21                     | 0.40              |
| 1:C:184:LYS:HE3  | 1:C:230:GLY:O    | 2.22                     | 0.40              |
| 1:F:211:LEU:HD23 | 1:F:212:MET:N    | 2.37                     | 0.40              |
| 1:A:260:HIS:O    | 1:A:263:TYR:HB3  | 2.21                     | 0.40              |
| 1:E:134:ILE:HD13 | 1:E:220:GLU:HG3  | 2.02                     | 0.40              |
| 1:C:194:ARG:HA   | 1:C:358:LEU:HG   | 2.02                     | 0.40              |
| 1:G:188:HIS:O    | 1:G:361:LEU:HD12 | 2.22                     | 0.40              |
| 1:F:142:ARG:HH22 | 1:F:340:ASP:CG   | 2.25                     | 0.40              |
| 1:C:224:LEU:HD13 | 1:C:224:LEU:C    | 2.42                     | 0.40              |
| 1:C:224:LEU:O    | 1:C:237:ASN:ND2  | 2.55                     | 0.40              |
| 1:B:288:LEU:HD23 | 1:B:289:LYS:N    | 2.36                     | 0.40              |
| 1:F:252:ASP:HB3  | 1:F:256:ASP:HB2  | 2.04                     | 0.40              |
| 1:B:156:PHE:CD2  | 1:B:158:ASN:CB   | 3.05                     | 0.40              |
| 1:F:282:TRP:HA   | 1:F:282:TRP:HE3  | 1.86                     | 0.40              |
| 1:B:266:THR:C    | 1:B:268:SER:H    | 2.24                     | 0.40              |
| 1:C:244:ASP:OD2  | 1:C:246:SER:HB3  | 2.22                     | 0.40              |
| 1:D:296:ILE:HG22 | 1:D:297:PHE:CD1  | 2.57                     | 0.40              |
| 1:B:349:ASP:O    | 1:B:350:ARG:C    | 2.60                     | 0.40              |
| 1:A:290:ASP:OD2  | 1:A:292:GLU:O    | 2.39                     | 0.40              |
| 1:F:378:LYS:HG3  | 1:F:379:GLY:N    | 2.36                     | 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     | 254/273 (93%) | 195 (77%) | 49 (19%) | 10 (4%)  | <b>4</b> 38 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | B     | 248/273 (91%)   | 189 (76%)  | 48 (19%)  | 11 (4%)  | 3           | 34 |
| 1   | C     | 246/273 (90%)   | 188 (76%)  | 47 (19%)  | 11 (4%)  | 3           | 34 |
| 1   | D     | 252/273 (92%)   | 209 (83%)  | 34 (14%)  | 9 (4%)   | 4           | 41 |
| 1   | E     | 253/273 (93%)   | 190 (75%)  | 49 (19%)  | 14 (6%)  | 2           | 29 |
| 1   | F     | 246/273 (90%)   | 192 (78%)  | 40 (16%)  | 14 (6%)  | 2           | 28 |
| 1   | G     | 245/273 (90%)   | 199 (81%)  | 36 (15%)  | 10 (4%)  | 3           | 37 |
| All | All   | 1744/1911 (91%) | 1362 (78%) | 303 (17%) | 79 (4%)  | 3           | 34 |

All (79) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 124 | ILE  |
| 1   | A     | 208 | ASN  |
| 1   | B     | 200 | ALA  |
| 1   | B     | 297 | PHE  |
| 1   | C     | 131 | ARG  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 306 | ASN  |
| 1   | D     | 194 | ARG  |
| 1   | D     | 195 | GLN  |
| 1   | D     | 303 | PHE  |
| 1   | E     | 296 | ILE  |
| 1   | F     | 200 | ALA  |
| 1   | F     | 201 | PRO  |
| 1   | G     | 199 | ASP  |
| 1   | G     | 204 | GLN  |
| 1   | G     | 279 | PRO  |
| 1   | A     | 304 | THR  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 350 | ARG  |
| 1   | C     | 157 | THR  |
| 1   | C     | 196 | VAL  |
| 1   | C     | 228 | GLY  |
| 1   | C     | 229 | THR  |
| 1   | D     | 154 | GLU  |
| 1   | D     | 293 | GLY  |
| 1   | F     | 128 | GLY  |
| 1   | F     | 293 | GLY  |
| 1   | F     | 348 | GLU  |
| 1   | G     | 132 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 296 | ILE  |
| 1   | G     | 354 | VAL  |
| 1   | A     | 154 | GLU  |
| 1   | A     | 358 | LEU  |
| 1   | B     | 153 | GLU  |
| 1   | C     | 200 | ALA  |
| 1   | D     | 127 | PRO  |
| 1   | D     | 173 | ASP  |
| 1   | E     | 161 | GLY  |
| 1   | E     | 200 | ALA  |
| 1   | E     | 348 | GLU  |
| 1   | F     | 153 | GLU  |
| 1   | F     | 154 | GLU  |
| 1   | F     | 161 | GLY  |
| 1   | F     | 382 | SER  |
| 1   | A     | 309 | TRP  |
| 1   | C     | 348 | GLU  |
| 1   | D     | 160 | PRO  |
| 1   | E     | 194 | ARG  |
| 1   | E     | 213 | TYR  |
| 1   | E     | 354 | VAL  |
| 1   | G     | 197 | MET  |
| 1   | A     | 160 | PRO  |
| 1   | B     | 172 | SER  |
| 1   | B     | 354 | VAL  |
| 1   | B     | 355 | LYS  |
| 1   | D     | 382 | SER  |
| 1   | E     | 125 | ILE  |
| 1   | E     | 190 | VAL  |
| 1   | E     | 357 | MET  |
| 1   | F     | 199 | ASP  |
| 1   | F     | 207 | ILE  |
| 1   | F     | 283 | HIS  |
| 1   | G     | 160 | PRO  |
| 1   | G     | 348 | GLU  |
| 1   | A     | 198 | ASP  |
| 1   | A     | 305 | SER  |
| 1   | B     | 162 | ASP  |
| 1   | C     | 230 | GLY  |
| 1   | E     | 154 | GLU  |
| 1   | E     | 201 | PRO  |
| 1   | F     | 160 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 161 | GLY  |
| 1   | A     | 161 | GLY  |
| 1   | E     | 160 | PRO  |
| 1   | B     | 207 | ILE  |
| 1   | C     | 298 | GLY  |
| 1   | B     | 159 | ALA  |
| 1   | F     | 196 | VAL  |
| 1   | E     | 251 | GLY  |

### 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     | 211/223 (95%)   | 184 (87%)  | 27 (13%)  | 5           | 32 |
| 1   | B     | 206/223 (92%)   | 181 (88%)  | 25 (12%)  | 6           | 34 |
| 1   | C     | 204/223 (92%)   | 184 (90%)  | 20 (10%)  | 10          | 45 |
| 1   | D     | 209/223 (94%)   | 191 (91%)  | 18 (9%)   | 13          | 53 |
| 1   | E     | 210/223 (94%)   | 185 (88%)  | 25 (12%)  | 6           | 35 |
| 1   | F     | 204/223 (92%)   | 173 (85%)  | 31 (15%)  | 3           | 25 |
| 1   | G     | 203/223 (91%)   | 185 (91%)  | 18 (9%)   | 12          | 51 |
| All | All   | 1447/1561 (93%) | 1283 (89%) | 164 (11%) | 7           | 38 |

All (164) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 119 | MET  |
| 1   | A     | 121 | ILE  |
| 1   | A     | 124 | ILE  |
| 1   | A     | 125 | ILE  |
| 1   | A     | 126 | MET  |
| 1   | A     | 129 | LEU  |
| 1   | A     | 131 | ARG  |
| 1   | A     | 137 | LEU  |
| 1   | A     | 157 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 158 | ASN  |
| 1   | A     | 174 | ILE  |
| 1   | A     | 191 | GLN  |
| 1   | A     | 193 | SER  |
| 1   | A     | 194 | ARG  |
| 1   | A     | 209 | ASN  |
| 1   | A     | 266 | THR  |
| 1   | A     | 273 | SER  |
| 1   | A     | 280 | ARG  |
| 1   | A     | 282 | TRP  |
| 1   | A     | 288 | LEU  |
| 1   | A     | 289 | LYS  |
| 1   | A     | 295 | TYR  |
| 1   | A     | 297 | PHE  |
| 1   | A     | 301 | GLN  |
| 1   | A     | 303 | PHE  |
| 1   | A     | 309 | TRP  |
| 1   | A     | 366 | LEU  |
| 1   | B     | 126 | MET  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 132 | LEU  |
| 1   | B     | 140 | GLN  |
| 1   | B     | 142 | ARG  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 148 | LEU  |
| 1   | B     | 158 | ASN  |
| 1   | B     | 174 | ILE  |
| 1   | B     | 178 | LYS  |
| 1   | B     | 199 | ASP  |
| 1   | B     | 211 | LEU  |
| 1   | B     | 213 | TYR  |
| 1   | B     | 215 | LEU  |
| 1   | B     | 217 | LEU  |
| 1   | B     | 256 | ASP  |
| 1   | B     | 270 | PHE  |
| 1   | B     | 271 | SER  |
| 1   | B     | 277 | LEU  |
| 1   | B     | 282 | TRP  |
| 1   | B     | 296 | ILE  |
| 1   | B     | 324 | PHE  |
| 1   | B     | 353 | PHE  |
| 1   | B     | 356 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 358 | LEU  |
| 1   | C     | 129 | LEU  |
| 1   | C     | 132 | LEU  |
| 1   | C     | 156 | PHE  |
| 1   | C     | 174 | ILE  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 191 | GLN  |
| 1   | C     | 193 | SER  |
| 1   | C     | 194 | ARG  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 197 | MET  |
| 1   | C     | 202 | MET  |
| 1   | C     | 207 | ILE  |
| 1   | C     | 225 | ASN  |
| 1   | C     | 233 | LEU  |
| 1   | C     | 282 | TRP  |
| 1   | C     | 301 | GLN  |
| 1   | C     | 331 | MET  |
| 1   | C     | 347 | ARG  |
| 1   | C     | 356 | ASN  |
| 1   | C     | 366 | LEU  |
| 1   | D     | 121 | ILE  |
| 1   | D     | 127 | PRO  |
| 1   | D     | 130 | ARG  |
| 1   | D     | 131 | ARG  |
| 1   | D     | 132 | LEU  |
| 1   | D     | 158 | ASN  |
| 1   | D     | 174 | ILE  |
| 1   | D     | 184 | LYS  |
| 1   | D     | 198 | ASP  |
| 1   | D     | 199 | ASP  |
| 1   | D     | 247 | LEU  |
| 1   | D     | 282 | TRP  |
| 1   | D     | 284 | ASN  |
| 1   | D     | 287 | LEU  |
| 1   | D     | 289 | LYS  |
| 1   | D     | 303 | PHE  |
| 1   | D     | 309 | TRP  |
| 1   | D     | 348 | GLU  |
| 1   | E     | 125 | ILE  |
| 1   | E     | 129 | LEU  |
| 1   | E     | 140 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 158 | ASN  |
| 1   | E     | 173 | ASP  |
| 1   | E     | 174 | ILE  |
| 1   | E     | 189 | TRP  |
| 1   | E     | 191 | GLN  |
| 1   | E     | 199 | ASP  |
| 1   | E     | 202 | MET  |
| 1   | E     | 205 | SER  |
| 1   | E     | 206 | TYR  |
| 1   | E     | 212 | MET  |
| 1   | E     | 217 | LEU  |
| 1   | E     | 220 | GLU  |
| 1   | E     | 229 | THR  |
| 1   | E     | 282 | TRP  |
| 1   | E     | 296 | ILE  |
| 1   | E     | 301 | GLN  |
| 1   | E     | 305 | SER  |
| 1   | E     | 309 | TRP  |
| 1   | E     | 348 | GLU  |
| 1   | E     | 353 | PHE  |
| 1   | E     | 359 | THR  |
| 1   | E     | 382 | SER  |
| 1   | F     | 129 | LEU  |
| 1   | F     | 132 | LEU  |
| 1   | F     | 133 | THR  |
| 1   | F     | 143 | THR  |
| 1   | F     | 145 | SER  |
| 1   | F     | 146 | ASN  |
| 1   | F     | 158 | ASN  |
| 1   | F     | 174 | ILE  |
| 1   | F     | 193 | SER  |
| 1   | F     | 196 | VAL  |
| 1   | F     | 197 | MET  |
| 1   | F     | 198 | ASP  |
| 1   | F     | 202 | MET  |
| 1   | F     | 203 | LEU  |
| 1   | F     | 210 | ARG  |
| 1   | F     | 212 | MET  |
| 1   | F     | 217 | LEU  |
| 1   | F     | 225 | ASN  |
| 1   | F     | 247 | LEU  |
| 1   | F     | 254 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 257 | ILE  |
| 1   | F     | 277 | LEU  |
| 1   | F     | 282 | TRP  |
| 1   | F     | 287 | LEU  |
| 1   | F     | 289 | LYS  |
| 1   | F     | 307 | ILE  |
| 1   | F     | 329 | PHE  |
| 1   | F     | 348 | GLU  |
| 1   | F     | 361 | LEU  |
| 1   | F     | 363 | GLU  |
| 1   | F     | 378 | LYS  |
| 1   | G     | 130 | ARG  |
| 1   | G     | 131 | ARG  |
| 1   | G     | 132 | LEU  |
| 1   | G     | 158 | ASN  |
| 1   | G     | 174 | ILE  |
| 1   | G     | 193 | SER  |
| 1   | G     | 198 | ASP  |
| 1   | G     | 229 | THR  |
| 1   | G     | 245 | THR  |
| 1   | G     | 290 | ASP  |
| 1   | G     | 297 | PHE  |
| 1   | G     | 303 | PHE  |
| 1   | G     | 329 | PHE  |
| 1   | G     | 338 | ARG  |
| 1   | G     | 355 | LYS  |
| 1   | G     | 356 | ASN  |
| 1   | G     | 357 | MET  |
| 1   | G     | 372 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 146 | ASN  |
| 1   | A     | 158 | ASN  |
| 1   | A     | 179 | GLN  |
| 1   | A     | 204 | GLN  |
| 1   | A     | 208 | ASN  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 334 | GLN  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 158 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 208 | ASN  |
| 1   | B     | 209 | ASN  |
| 1   | B     | 284 | ASN  |
| 1   | B     | 319 | GLN  |
| 1   | B     | 334 | GLN  |
| 1   | B     | 352 | ASN  |
| 1   | B     | 356 | ASN  |
| 1   | B     | 370 | HIS  |
| 1   | C     | 146 | ASN  |
| 1   | C     | 191 | GLN  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 204 | GLN  |
| 1   | C     | 222 | GLN  |
| 1   | C     | 225 | ASN  |
| 1   | C     | 232 | ASN  |
| 1   | C     | 237 | ASN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 278 | ASN  |
| 1   | C     | 283 | HIS  |
| 1   | C     | 284 | ASN  |
| 1   | C     | 301 | GLN  |
| 1   | C     | 356 | ASN  |
| 1   | D     | 158 | ASN  |
| 1   | D     | 208 | ASN  |
| 1   | D     | 225 | ASN  |
| 1   | D     | 334 | GLN  |
| 1   | E     | 158 | ASN  |
| 1   | E     | 179 | GLN  |
| 1   | E     | 191 | GLN  |
| 1   | E     | 232 | ASN  |
| 1   | E     | 237 | ASN  |
| 1   | E     | 334 | GLN  |
| 1   | F     | 140 | GLN  |
| 1   | F     | 158 | ASN  |
| 1   | F     | 179 | GLN  |
| 1   | F     | 222 | GLN  |
| 1   | F     | 225 | ASN  |
| 1   | F     | 237 | ASN  |
| 1   | G     | 158 | ASN  |
| 1   | G     | 248 | ASN  |
| 1   | G     | 260 | HIS  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 291 | ASN  |
| 1   | G     | 356 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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     | 256/273 (93%)   | -0.19  | 2 (0%) 87 76  | 1, 28, 53, 72         | 0     |
| 1   | B     | 250/273 (91%)   | -0.13  | 5 (2%) 68 51  | 1, 31, 59, 78         | 0     |
| 1   | C     | 248/273 (90%)   | -0.14  | 1 (0%) 93 88  | 7, 33, 59, 69         | 0     |
| 1   | D     | 254/273 (93%)   | -0.20  | 3 (1%) 81 66  | 1, 32, 54, 79         | 0     |
| 1   | E     | 255/273 (93%)   | -0.19  | 5 (1%) 68 51  | 5, 34, 57, 90         | 0     |
| 1   | F     | 248/273 (90%)   | -0.18  | 1 (0%) 93 88  | 1, 31, 54, 75         | 0     |
| 1   | G     | 247/273 (90%)   | -0.15  | 1 (0%) 93 88  | 3, 31, 57, 87         | 0     |
| All | All   | 1758/1911 (91%) | -0.17  | 18 (1%) 84 71 | 1, 31, 57, 90         | 0     |

All (18) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 162 | ASP  | 4.6  |
| 1   | B     | 383 | SER  | 4.0  |
| 1   | A     | 160 | PRO  | 3.5  |
| 1   | E     | 120 | GLN  | 3.2  |
| 1   | B     | 125 | ILE  | 2.7  |
| 1   | B     | 208 | ASN  | 2.7  |
| 1   | E     | 192 | ALA  | 2.6  |
| 1   | B     | 158 | ASN  | 2.6  |
| 1   | B     | 162 | ASP  | 2.6  |
| 1   | F     | 160 | PRO  | 2.5  |
| 1   | D     | 160 | PRO  | 2.5  |
| 1   | A     | 161 | GLY  | 2.3  |
| 1   | G     | 320 | ALA  | 2.3  |
| 1   | C     | 198 | ASP  | 2.2  |
| 1   | D     | 128 | GLY  | 2.2  |
| 1   | E     | 383 | SER  | 2.2  |
| 1   | D     | 157 | THR  | 2.1  |
| 1   | E     | 125 | 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.