



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 2C9G  
EMDB ID: : EMD-1178  
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON  
BASE DODECAHEDRON  
Authors : Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.;  
Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.  
Deposited on : 2005-12-12  
Resolution : 9.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

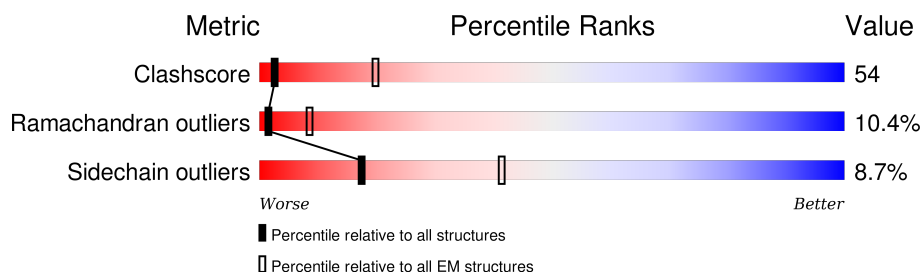
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain      |
|-----|-------|--------|-----------------------|
| 1   | A     | 523    | <br>30% 44% 11% • 14% |
| 1   | B     | 523    | <br>29% 45% 11% • 14% |
| 1   | C     | 523    | <br>30% 45% 11% • 14% |
| 1   | D     | 523    | <br>29% 45% 11% • 14% |
| 1   | E     | 523    | <br>29% 46% 11% • 14% |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PENTON PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 448      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3568  | 2255 | 618 | 683 | 12 |         |       |
| 1   | B     | 448      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3568  | 2255 | 618 | 683 | 12 |         |       |
| 1   | C     | 448      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3568  | 2255 | 618 | 683 | 12 |         |       |
| 1   | D     | 448      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3568  | 2255 | 618 | 683 | 12 |         |       |
| 1   | E     | 448      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3568  | 2255 | 618 | 683 | 12 |         |       |

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

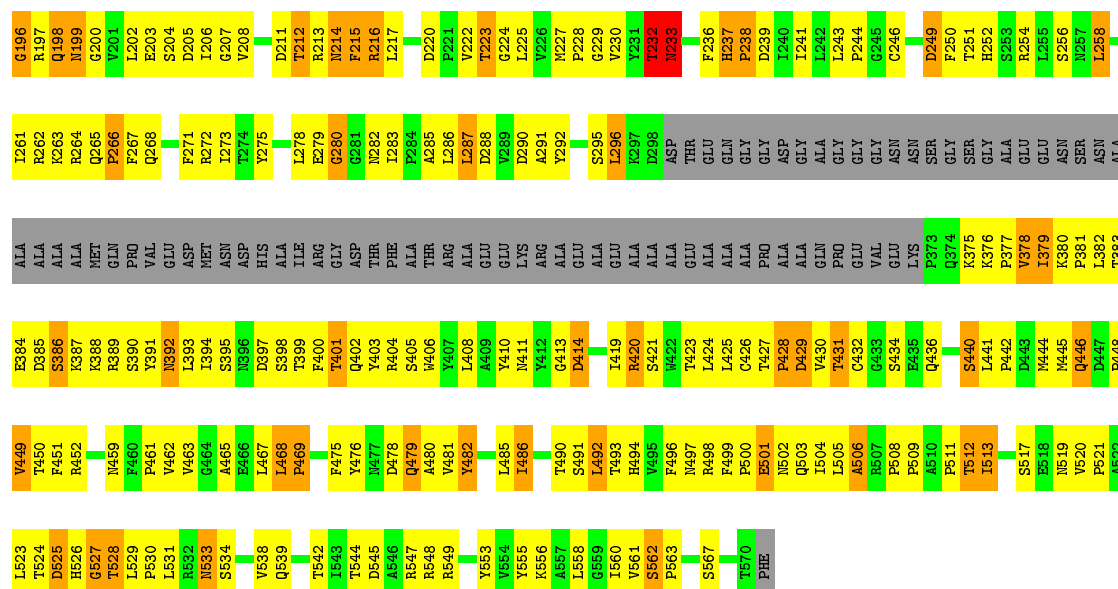
Chain A:  30%  44%  11%  14%

Sequence logo for Chain A, showing amino acid frequencies across 100 positions. The logo is divided into four color-coded regions: green (30%), yellow (44%), red (11%), and black (14%). Amino acids are listed in columns, with their relative frequency indicated by the height of the letters. The sequence is: T528, L529, P530, L531, R532, N533, S534, V535, Q536, L537, T544, D545, A546, R547, R548, R549, Y553, V554, Y555, R556, A557, L558, G559, I560, V561, S562, P563, S567, T570, PHE.

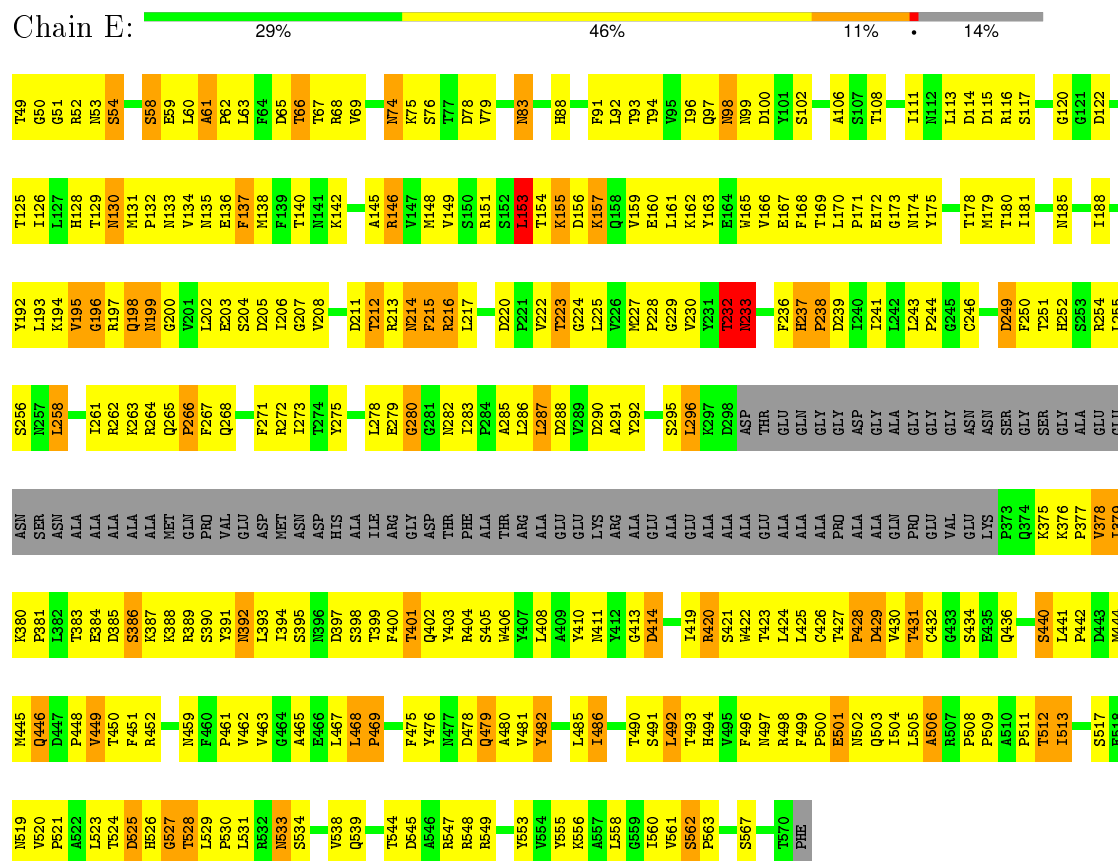
Chain B:

| Item | Category |
|------|----------|
| Y192 | Green    |
| L193 | Green    |
| K194 | Green    |
| V195 | Green    |
| G196 | Green    |
| L197 | Green    |
| Q198 | Green    |
| N199 | Green    |
| G200 | Green    |
| Z201 | Green    |
| L202 | Green    |
| E203 | Green    |
| S204 | Green    |
| D205 | Green    |
| L206 | Green    |
| G207 | Green    |
| V208 | Green    |
| D211 | Green    |
| T212 | Green    |
| R213 | Green    |
| N214 | Green    |
| F215 | Green    |
| R216 | Green    |
| L217 | Green    |
| D220 | Green    |
| P221 | Green    |
| P222 | Green    |
| T223 | Green    |
| G224 | Green    |
| L225 | Green    |
| V226 | Green    |
| M227 | Green    |
| P228 | Green    |
| G229 | Green    |
| Z230 | Green    |
| T231 | Green    |
| T232 | Green    |
| D233 | Green    |
| F236 | Green    |
| E237 | Green    |
| P238 | Green    |
| D239 | Green    |
| L240 | Green    |
| L242 | Green    |
| L243 | Green    |
| P244 | Green    |
| G245 | Green    |
| C246 | Green    |
| D249 | Green    |
| F250 | Green    |
| T251 | Green    |
| E252 | Green    |
| S253 | Green    |
| R254 | Green    |
| T49  | Green    |
| G50  | Green    |
| G51  | Green    |
| R52  | Green    |
| N53  | Green    |
| S54  | Green    |
| S58  | Green    |
| E59  | Green    |
| L60  | Green    |
| A61  | Green    |
| P62  | Green    |
| L63  | Green    |
| F64  | Green    |
| D65  | Green    |
| T66  | Green    |
| T67  | Green    |
| R68  | Green    |
| V69  | Green    |
| A145 | Green    |
| R146 | Green    |
| V147 | Green    |
| M148 | Green    |
| V149 | Green    |
| S150 | Green    |
| R151 | Green    |
| S152 | Green    |
| L153 | Green    |
| T154 | Green    |
| K155 | Green    |
| D156 | Green    |
| K157 | Green    |
| Q158 | Green    |
| V159 | Green    |
| E160 | Green    |
| L161 | Green    |
| K162 | Green    |
| V163 | Green    |
| E164 | Green    |
| V165 | Green    |
| V166 | Green    |
| E167 | Green    |
| F168 | Green    |
| L169 | Green    |
| L170 | Green    |
| P171 | Green    |
| E172 | Green    |
| G173 | Green    |
| M174 | Green    |
| Y175 | Green    |
| T178 | Green    |
| M179 | Green    |
| T180 | Green    |
| L181 | Green    |
| N185 | Green    |
| L188 | Green    |
| M74  | Yellow   |
| K75  | Yellow   |
| S76  | Yellow   |
| T77  | Yellow   |
| D78  | Yellow   |
| V79  | Yellow   |
| N83  | Yellow   |
| H88  | Yellow   |
| F91  | Yellow   |
| L92  | Yellow   |
| T93  | Yellow   |
| T94  | Yellow   |
| P95  | Yellow   |
| L96  | Yellow   |
| Q97  | Yellow   |
| N98  | Yellow   |
| N99  | Yellow   |
| D100 | Yellow   |
| V101 | Yellow   |
| S102 | Yellow   |
| A106 | Yellow   |
| S107 | Yellow   |
| T108 | Yellow   |
| I111 | Yellow   |
| M112 | Yellow   |
| L113 | Yellow   |
| D114 | Yellow   |
| L115 | Yellow   |
| R116 | Yellow   |
| S117 | Yellow   |
| G120 | Yellow   |
| D122 | Yellow   |
| G121 | Yellow   |
| D122 | Yellow   |
| S107 | Orange   |
| T108 | Orange   |
| I111 | Orange   |
| M112 | Orange   |
| L113 | Orange   |
| D114 | Orange   |
| L115 | Orange   |
| R116 | Orange   |
| S117 | Orange   |
| G120 | Orange   |
| D122 | Orange   |
| G121 | Orange   |
| D122 | Orange   |
| S107 | Grey     |
| T108 | Grey     |
| I111 | Grey     |
| M112 | Grey     |
| L113 | Grey     |
| D114 | Grey     |
| L115 | Grey     |
| R116 | Grey     |
| S117 | Grey     |
| G120 | Grey     |
| D122 | Grey     |
| G121 | Grey     |
| D122 | Grey     |





## • Molecule 1: PENTON PROTEIN



## 4 Experimental information

| Property                             | Value            | Source    |
|--------------------------------------|------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE  | Depositor |
| Imposed symmetry                     | POINT, I         | Depositor |
| Number of images                     | Not provided     | Depositor |
| Resolution determination method      | Not provided     | Depositor |
| CTF correction method                | AMPLITUDE, PHASE | Depositor |
| Microscope                           | JEOL 2010F       | Depositor |
| Voltage (kV)                         | 200              | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided     | Depositor |
| Minimum defocus (nm)                 | Not provided     | Depositor |
| Maximum defocus (nm)                 | Not provided     | Depositor |
| Magnification                        | 50000            | Depositor |
| Image detector                       | KODAK SO163 FILM | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 2$ | RMSZ        | $\# Z  > 2$     |
| 1   | A     | 0.57         | 0/3652      | 0.81        | 2/4971 (0.0%)   |
| 1   | B     | 0.57         | 0/3652      | 0.81        | 2/4971 (0.0%)   |
| 1   | C     | 0.57         | 0/3652      | 0.81        | 2/4971 (0.0%)   |
| 1   | D     | 0.57         | 0/3652      | 0.81        | 2/4971 (0.0%)   |
| 1   | E     | 0.57         | 0/3652      | 0.81        | 2/4971 (0.0%)   |
| All | All   | 0.57         | 0/18260     | 0.81        | 10/24855 (0.0%) |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|-----------|------|------------------------|---------------------|
| 1   | E     | 207 | GLY  | N-CA-C    | 5.62 | 127.14                 | 113.10              |
| 1   | D     | 207 | GLY  | N-CA-C    | 5.60 | 127.10                 | 113.10              |
| 1   | A     | 207 | GLY  | N-CA-C    | 5.58 | 127.06                 | 113.10              |
| 1   | C     | 207 | GLY  | N-CA-C    | 5.58 | 127.06                 | 113.10              |
| 1   | B     | 207 | GLY  | N-CA-C    | 5.58 | 127.06                 | 113.10              |
| 1   | C     | 153 | LEU  | CB-CG-CD2 | 5.37 | 120.13                 | 111.00              |
| 1   | D     | 153 | LEU  | CB-CG-CD2 | 5.36 | 120.12                 | 111.00              |
| 1   | A     | 153 | LEU  | CB-CG-CD2 | 5.36 | 120.11                 | 111.00              |
| 1   | B     | 153 | LEU  | CB-CG-CD2 | 5.33 | 120.06                 | 111.00              |
| 1   | E     | 153 | LEU  | CB-CG-CD2 | 5.33 | 120.05                 | 111.00              |

There are no chirality outliers.

There are no planarity outliers.

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

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



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3568  | 0        | 3498     | 414     | 0            |
| 1   | B     | 3568  | 0        | 3498     | 421     | 0            |
| 1   | C     | 3568  | 0        | 3498     | 421     | 0            |
| 1   | D     | 3568  | 0        | 3498     | 424     | 0            |
| 1   | E     | 3568  | 0        | 3498     | 422     | 0            |
| All | All   | 17840 | 0        | 17490    | 1895    | 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 54.

All (1895) 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:B:452:ARG:HH21 | 1:C:99:ASN:HB3   | 1.14                     | 1.13              |
| 1:C:452:ARG:HH21 | 1:D:99:ASN:HB3   | 1.14                     | 1.11              |
| 1:D:452:ARG:HH21 | 1:E:99:ASN:HB3   | 1.14                     | 1.10              |
| 1:A:99:ASN:HB3   | 1:E:452:ARG:HH21 | 1.14                     | 1.07              |
| 1:A:452:ARG:HH21 | 1:B:99:ASN:HB3   | 1.14                     | 1.06              |
| 1:D:68:ARG:HG2   | 1:D:68:ARG:HH11  | 1.25                     | 1.02              |
| 1:A:68:ARG:HG2   | 1:A:68:ARG:HH11  | 1.25                     | 1.01              |
| 1:E:68:ARG:HG2   | 1:E:68:ARG:HH11  | 1.25                     | 0.99              |
| 1:B:68:ARG:HG2   | 1:B:68:ARG:HH11  | 1.25                     | 0.98              |
| 1:C:68:ARG:HG2   | 1:C:68:ARG:HH11  | 1.25                     | 0.97              |
| 1:C:452:ARG:NH2  | 1:D:99:ASN:HB3   | 1.86                     | 0.91              |
| 1:B:278:LEU:HD23 | 1:B:419:ILE:HD12 | 1.53                     | 0.91              |
| 1:A:99:ASN:HB3   | 1:E:452:ARG:NH2  | 1.86                     | 0.91              |
| 1:A:278:LEU:HD23 | 1:A:419:ILE:HD12 | 1.53                     | 0.91              |
| 1:B:292:TYR:HA   | 1:B:377:PRO:CG   | 2.01                     | 0.90              |
| 1:C:292:TYR:HA   | 1:C:377:PRO:CG   | 2.01                     | 0.90              |
| 1:A:452:ARG:NH2  | 1:B:99:ASN:HB3   | 1.86                     | 0.90              |
| 1:E:278:LEU:HD23 | 1:E:419:ILE:HD12 | 1.53                     | 0.90              |
| 1:D:292:TYR:HA   | 1:D:377:PRO:CG   | 2.02                     | 0.90              |
| 1:E:292:TYR:HA   | 1:E:377:PRO:CG   | 2.01                     | 0.90              |
| 1:B:452:ARG:NH2  | 1:C:99:ASN:HB3   | 1.86                     | 0.90              |
| 1:B:295:SER:HB3  | 1:B:377:PRO:HG3  | 1.51                     | 0.90              |
| 1:C:376:LYS:HB3  | 1:C:377:PRO:HD2  | 1.55                     | 0.89              |
| 1:D:451:PHE:HD2  | 1:D:461:PRO:HA   | 1.38                     | 0.89              |
| 1:B:68:ARG:HH12  | 1:B:562:SER:HB3  | 1.38                     | 0.89              |
| 1:C:295:SER:HB3  | 1:C:377:PRO:HG3  | 1.51                     | 0.89              |
| 1:D:452:ARG:NH2  | 1:E:99:ASN:HB3   | 1.86                     | 0.89              |
| 1:D:68:ARG:HH12  | 1:D:562:SER:HB3  | 1.38                     | 0.89              |
| 1:B:376:LYS:HB3  | 1:B:377:PRO:HD2  | 1.55                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:295:SER:HB3  | 1:D:377:PRO:HG3  | 1.51                     | 0.89              |
| 1:D:376:LYS:HB3  | 1:D:377:PRO:HD2  | 1.54                     | 0.89              |
| 1:D:278:LEU:HD23 | 1:D:419:ILE:HD12 | 1.53                     | 0.89              |
| 1:C:451:PHE:HD2  | 1:C:461:PRO:HA   | 1.38                     | 0.89              |
| 1:A:295:SER:HB3  | 1:A:377:PRO:HG3  | 1.51                     | 0.89              |
| 1:E:295:SER:HB3  | 1:E:377:PRO:HG3  | 1.50                     | 0.88              |
| 1:A:451:PHE:HD2  | 1:A:461:PRO:HA   | 1.38                     | 0.88              |
| 1:C:278:LEU:HD23 | 1:C:419:ILE:HD12 | 1.53                     | 0.88              |
| 1:A:292:TYR:HA   | 1:A:377:PRO:CG   | 2.02                     | 0.88              |
| 1:A:68:ARG:HH12  | 1:A:562:SER:HB3  | 1.38                     | 0.88              |
| 1:E:376:LYS:HB3  | 1:E:377:PRO:HD2  | 1.55                     | 0.88              |
| 1:E:451:PHE:HD2  | 1:E:461:PRO:HA   | 1.38                     | 0.88              |
| 1:A:376:LYS:HB3  | 1:A:377:PRO:HD2  | 1.54                     | 0.87              |
| 1:C:68:ARG:HH12  | 1:C:562:SER:HB3  | 1.38                     | 0.87              |
| 1:E:68:ARG:HH12  | 1:E:562:SER:HB3  | 1.38                     | 0.87              |
| 1:B:262:ARG:NH1  | 1:C:130:ASN:HD22 | 1.73                     | 0.87              |
| 1:B:211:ASP:HA   | 1:B:508:PRO:CG   | 2.05                     | 0.87              |
| 1:D:83:ASN:HD22  | 1:D:91:PHE:HB2   | 1.40                     | 0.86              |
| 1:A:52:ARG:HB3   | 1:A:117:SER:OG   | 1.75                     | 0.86              |
| 1:A:130:ASN:HD22 | 1:E:262:ARG:NH1  | 1.73                     | 0.86              |
| 1:D:504:ILE:HG22 | 1:D:505:LEU:HD23 | 1.57                     | 0.86              |
| 1:E:52:ARG:HB3   | 1:E:117:SER:OG   | 1.75                     | 0.86              |
| 1:B:504:ILE:HG22 | 1:B:505:LEU:HD23 | 1.57                     | 0.86              |
| 1:C:211:ASP:HA   | 1:C:508:PRO:CG   | 2.05                     | 0.86              |
| 1:E:504:ILE:HG22 | 1:E:505:LEU:HD23 | 1.57                     | 0.86              |
| 1:E:211:ASP:HA   | 1:E:508:PRO:CG   | 2.05                     | 0.86              |
| 1:D:262:ARG:NH1  | 1:E:130:ASN:HD22 | 1.73                     | 0.86              |
| 1:B:451:PHE:HD2  | 1:B:461:PRO:HA   | 1.38                     | 0.85              |
| 1:A:262:ARG:NH1  | 1:B:130:ASN:HD22 | 1.74                     | 0.85              |
| 1:A:211:ASP:HA   | 1:A:508:PRO:CG   | 2.05                     | 0.85              |
| 1:D:211:ASP:HA   | 1:D:508:PRO:CG   | 2.05                     | 0.85              |
| 1:A:83:ASN:HD22  | 1:A:91:PHE:HB2   | 1.40                     | 0.85              |
| 1:C:52:ARG:HB3   | 1:C:117:SER:OG   | 1.75                     | 0.85              |
| 1:B:193:LEU:HD11 | 1:B:498:ARG:HH12 | 1.41                     | 0.85              |
| 1:C:58:SER:O     | 1:C:60:LEU:N     | 2.09                     | 0.85              |
| 1:B:52:ARG:HB3   | 1:B:117:SER:OG   | 1.75                     | 0.85              |
| 1:C:262:ARG:NH1  | 1:D:130:ASN:HD22 | 1.73                     | 0.85              |
| 1:B:58:SER:O     | 1:B:60:LEU:N     | 2.09                     | 0.85              |
| 1:C:504:ILE:HG22 | 1:C:505:LEU:HD23 | 1.57                     | 0.85              |
| 1:E:83:ASN:HD22  | 1:E:91:PHE:HB2   | 1.40                     | 0.85              |
| 1:B:83:ASN:HD22  | 1:B:91:PHE:HB2   | 1.40                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:504:ILE:HG22 | 1:A:505:LEU:HD23 | 1.58                     | 0.84              |
| 1:C:83:ASN:HD22  | 1:C:91:PHE:HB2   | 1.40                     | 0.84              |
| 1:E:58:SER:O     | 1:E:60:LEU:N     | 2.09                     | 0.84              |
| 1:D:52:ARG:HB3   | 1:D:117:SER:OG   | 1.75                     | 0.84              |
| 1:D:178:THR:HG21 | 1:D:511:PRO:HD2  | 1.60                     | 0.84              |
| 1:D:58:SER:O     | 1:D:60:LEU:N     | 2.09                     | 0.84              |
| 1:E:156:ASP:O    | 1:E:157:LYS:HG3  | 1.78                     | 0.84              |
| 1:D:193:LEU:HD11 | 1:D:498:ARG:HH12 | 1.41                     | 0.84              |
| 1:C:178:THR:HG21 | 1:C:511:PRO:HD2  | 1.60                     | 0.84              |
| 1:A:58:SER:O     | 1:A:60:LEU:N     | 2.09                     | 0.84              |
| 1:C:193:LEU:HD11 | 1:C:498:ARG:HH12 | 1.41                     | 0.83              |
| 1:A:193:LEU:HD11 | 1:A:498:ARG:HH12 | 1.41                     | 0.83              |
| 1:A:156:ASP:O    | 1:A:157:LYS:HG3  | 1.78                     | 0.83              |
| 1:C:156:ASP:O    | 1:C:157:LYS:HG3  | 1.78                     | 0.83              |
| 1:D:468:LEU:HD12 | 1:D:469:PRO:HD2  | 1.59                     | 0.83              |
| 1:C:49:THR:HG23  | 1:C:53:ASN:OD1   | 1.79                     | 0.83              |
| 1:B:178:THR:HG21 | 1:B:511:PRO:HD2  | 1.59                     | 0.83              |
| 1:E:193:LEU:HD11 | 1:E:498:ARG:HH12 | 1.41                     | 0.83              |
| 1:D:156:ASP:O    | 1:D:157:LYS:HG3  | 1.78                     | 0.83              |
| 1:E:49:THR:HG23  | 1:E:53:ASN:OD1   | 1.79                     | 0.83              |
| 1:E:178:THR:HG21 | 1:E:511:PRO:HD2  | 1.60                     | 0.82              |
| 1:E:468:LEU:HD12 | 1:E:469:PRO:HD2  | 1.59                     | 0.82              |
| 1:B:156:ASP:O    | 1:B:157:LYS:HG3  | 1.78                     | 0.82              |
| 1:D:49:THR:HG23  | 1:D:53:ASN:OD1   | 1.79                     | 0.82              |
| 1:B:49:THR:HG23  | 1:B:53:ASN:OD1   | 1.79                     | 0.82              |
| 1:A:49:THR:HG23  | 1:A:53:ASN:OD1   | 1.79                     | 0.82              |
| 1:D:544:THR:CG2  | 1:D:548:ARG:HA   | 2.10                     | 0.82              |
| 1:C:468:LEU:HD12 | 1:C:469:PRO:HD2  | 1.60                     | 0.82              |
| 1:B:468:LEU:HD12 | 1:B:469:PRO:HD2  | 1.60                     | 0.82              |
| 1:A:178:THR:HG21 | 1:A:511:PRO:HD2  | 1.60                     | 0.81              |
| 1:A:468:LEU:HD12 | 1:A:469:PRO:HD2  | 1.59                     | 0.81              |
| 1:B:544:THR:CG2  | 1:B:548:ARG:HA   | 2.10                     | 0.81              |
| 1:A:384:GLU:HG2  | 1:A:390:SER:HA   | 1.62                     | 0.81              |
| 1:C:544:THR:CG2  | 1:C:548:ARG:HA   | 2.10                     | 0.81              |
| 1:C:68:ARG:HG2   | 1:C:68:ARG:NH1   | 1.92                     | 0.81              |
| 1:A:544:THR:CG2  | 1:A:548:ARG:HA   | 2.10                     | 0.81              |
| 1:B:384:GLU:HG2  | 1:B:390:SER:HA   | 1.62                     | 0.80              |
| 1:E:544:THR:CG2  | 1:E:548:ARG:HA   | 2.10                     | 0.80              |
| 1:C:384:GLU:HG2  | 1:C:390:SER:HA   | 1.62                     | 0.80              |
| 1:B:68:ARG:HG2   | 1:B:68:ARG:NH1   | 1.92                     | 0.80              |
| 1:E:384:GLU:HG2  | 1:E:390:SER:HA   | 1.62                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:389:ARG:HD3  | 1:D:502:ASN:HD22 | 1.47                     | 0.79              |
| 1:C:237:HIS:CD2  | 1:C:425:LEU:HD11 | 2.18                     | 0.79              |
| 1:A:68:ARG:HG2   | 1:A:68:ARG:NH1   | 1.92                     | 0.79              |
| 1:D:237:HIS:CD2  | 1:D:425:LEU:HD11 | 2.18                     | 0.79              |
| 1:D:214:ASN:HD22 | 1:D:214:ASN:C    | 1.86                     | 0.79              |
| 1:E:237:HIS:CD2  | 1:E:425:LEU:HD11 | 2.18                     | 0.79              |
| 1:B:237:HIS:CD2  | 1:B:425:LEU:HD11 | 2.17                     | 0.79              |
| 1:D:384:GLU:HG2  | 1:D:390:SER:HA   | 1.62                     | 0.79              |
| 1:A:214:ASN:HD22 | 1:A:214:ASN:C    | 1.86                     | 0.79              |
| 1:A:237:HIS:CD2  | 1:A:425:LEU:HD11 | 2.18                     | 0.78              |
| 1:E:214:ASN:HD22 | 1:E:214:ASN:C    | 1.86                     | 0.78              |
| 1:B:214:ASN:C    | 1:B:214:ASN:HD22 | 1.86                     | 0.78              |
| 1:B:389:ARG:HD3  | 1:B:502:ASN:HD22 | 1.47                     | 0.78              |
| 1:A:154:THR:OG1  | 1:A:160:GLU:HB2  | 1.84                     | 0.77              |
| 1:E:154:THR:OG1  | 1:E:160:GLU:HB2  | 1.84                     | 0.77              |
| 1:B:154:THR:OG1  | 1:B:160:GLU:HB2  | 1.84                     | 0.77              |
| 1:E:389:ARG:HD3  | 1:E:502:ASN:HD22 | 1.47                     | 0.77              |
| 1:C:214:ASN:C    | 1:C:214:ASN:HD22 | 1.86                     | 0.77              |
| 1:C:379:ILE:O    | 1:C:381:PRO:HD3  | 1.85                     | 0.77              |
| 1:A:379:ILE:O    | 1:A:381:PRO:HD3  | 1.85                     | 0.77              |
| 1:D:154:THR:OG1  | 1:D:160:GLU:HB2  | 1.84                     | 0.77              |
| 1:A:389:ARG:HD3  | 1:A:502:ASN:HD22 | 1.48                     | 0.77              |
| 1:C:389:ARG:HD3  | 1:C:502:ASN:HD22 | 1.47                     | 0.77              |
| 1:B:211:ASP:HA   | 1:B:508:PRO:HG3  | 1.67                     | 0.77              |
| 1:C:211:ASP:HA   | 1:C:508:PRO:HG3  | 1.67                     | 0.77              |
| 1:C:154:THR:OG1  | 1:C:160:GLU:HB2  | 1.84                     | 0.77              |
| 1:A:403:TYR:CE1  | 1:A:504:ILE:HG21 | 2.21                     | 0.76              |
| 1:C:403:TYR:CE1  | 1:C:504:ILE:HG21 | 2.21                     | 0.76              |
| 1:D:292:TYR:HA   | 1:D:377:PRO:HG2  | 1.67                     | 0.76              |
| 1:D:403:TYR:CE1  | 1:D:504:ILE:HG21 | 2.21                     | 0.76              |
| 1:E:379:ILE:O    | 1:E:381:PRO:HD3  | 1.85                     | 0.76              |
| 1:B:403:TYR:CE1  | 1:B:504:ILE:HG21 | 2.21                     | 0.76              |
| 1:A:211:ASP:HA   | 1:A:508:PRO:HG3  | 1.67                     | 0.76              |
| 1:C:292:TYR:HA   | 1:C:377:PRO:HG2  | 1.67                     | 0.76              |
| 1:B:379:ILE:O    | 1:B:381:PRO:HD3  | 1.85                     | 0.76              |
| 1:E:292:TYR:HA   | 1:E:377:PRO:HG2  | 1.67                     | 0.76              |
| 1:C:475:PHE:O    | 1:C:513:ILE:HA   | 1.87                     | 0.76              |
| 1:B:292:TYR:HA   | 1:B:377:PRO:HG2  | 1.67                     | 0.75              |
| 1:D:379:ILE:O    | 1:D:381:PRO:HD3  | 1.85                     | 0.75              |
| 1:E:403:TYR:CE1  | 1:E:504:ILE:HG21 | 2.21                     | 0.75              |
| 1:C:68:ARG:NH1   | 1:C:562:SER:HB3  | 2.01                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:452:ARG:HE   | 1:E:98:ASN:HD21  | 1.34                     | 0.75              |
| 1:B:475:PHE:O    | 1:B:513:ILE:HA   | 1.87                     | 0.75              |
| 1:B:451:PHE:CD2  | 1:B:461:PRO:HA   | 2.22                     | 0.75              |
| 1:D:211:ASP:HA   | 1:D:508:PRO:HG3  | 1.67                     | 0.75              |
| 1:E:475:PHE:O    | 1:E:513:ILE:HA   | 1.87                     | 0.75              |
| 1:A:68:ARG:NH1   | 1:A:562:SER:HB3  | 2.01                     | 0.75              |
| 1:E:211:ASP:HA   | 1:E:508:PRO:HG3  | 1.67                     | 0.75              |
| 1:D:68:ARG:NH1   | 1:D:562:SER:HB3  | 2.01                     | 0.74              |
| 1:E:68:ARG:NH1   | 1:E:562:SER:HB3  | 2.01                     | 0.74              |
| 1:D:451:PHE:CD2  | 1:D:461:PRO:HA   | 2.22                     | 0.74              |
| 1:A:292:TYR:HA   | 1:A:377:PRO:HG2  | 1.67                     | 0.74              |
| 1:B:68:ARG:NH1   | 1:B:562:SER:HB3  | 2.01                     | 0.74              |
| 1:E:68:ARG:HG2   | 1:E:68:ARG:NH1   | 1.92                     | 0.74              |
| 1:C:295:SER:O    | 1:C:296:LEU:HB2  | 1.88                     | 0.74              |
| 1:C:451:PHE:CD2  | 1:C:461:PRO:HA   | 2.22                     | 0.74              |
| 1:B:145:ALA:HB3  | 1:B:168:PHE:HE1  | 1.53                     | 0.74              |
| 1:E:403:TYR:HD1  | 1:E:504:ILE:HD13 | 1.52                     | 0.74              |
| 1:A:403:TYR:HD1  | 1:A:504:ILE:HD13 | 1.52                     | 0.74              |
| 1:C:142:LYS:HG2  | 1:C:169:THR:HG22 | 1.70                     | 0.74              |
| 1:D:475:PHE:O    | 1:D:513:ILE:HA   | 1.86                     | 0.74              |
| 1:A:475:PHE:O    | 1:A:513:ILE:HA   | 1.87                     | 0.74              |
| 1:B:295:SER:O    | 1:B:296:LEU:HB2  | 1.88                     | 0.74              |
| 1:E:295:SER:O    | 1:E:296:LEU:HB2  | 1.88                     | 0.74              |
| 1:C:249:ASP:C    | 1:C:249:ASP:OD1  | 2.26                     | 0.74              |
| 1:C:145:ALA:HB3  | 1:C:168:PHE:HE1  | 1.53                     | 0.74              |
| 1:D:142:LYS:HG2  | 1:D:169:THR:HG22 | 1.70                     | 0.74              |
| 1:B:452:ARG:HE   | 1:C:98:ASN:HD21  | 1.34                     | 0.73              |
| 1:D:68:ARG:HG2   | 1:D:68:ARG:NH1   | 1.92                     | 0.73              |
| 1:B:243:LEU:HD21 | 1:B:403:TYR:CE2  | 2.23                     | 0.73              |
| 1:E:451:PHE:CD2  | 1:E:461:PRO:HA   | 2.22                     | 0.73              |
| 1:D:249:ASP:C    | 1:D:249:ASP:OD1  | 2.26                     | 0.73              |
| 1:B:403:TYR:HD1  | 1:B:504:ILE:HD13 | 1.52                     | 0.73              |
| 1:A:145:ALA:HB3  | 1:A:168:PHE:HE1  | 1.53                     | 0.73              |
| 1:D:243:LEU:HD21 | 1:D:403:TYR:CE2  | 2.24                     | 0.73              |
| 1:C:452:ARG:HE   | 1:D:98:ASN:HD21  | 1.34                     | 0.73              |
| 1:A:452:ARG:HE   | 1:B:98:ASN:HD21  | 1.34                     | 0.73              |
| 1:C:403:TYR:HD1  | 1:C:504:ILE:HD13 | 1.52                     | 0.73              |
| 1:D:468:LEU:CD1  | 1:D:469:PRO:HD2  | 2.19                     | 0.73              |
| 1:A:249:ASP:OD1  | 1:A:249:ASP:C    | 2.26                     | 0.73              |
| 1:A:295:SER:O    | 1:A:296:LEU:HB2  | 1.88                     | 0.73              |
| 1:C:243:LEU:HD21 | 1:C:403:TYR:CE2  | 2.23                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:142:LYS:HG2  | 1:A:169:THR:HG22 | 1.70                     | 0.73              |
| 1:A:244:PRO:HA   | 1:A:275:TYR:CD2  | 2.24                     | 0.73              |
| 1:D:295:SER:O    | 1:D:296:LEU:HB2  | 1.88                     | 0.73              |
| 1:D:403:TYR:HD1  | 1:D:504:ILE:HD13 | 1.52                     | 0.73              |
| 1:E:148:MET:HA   | 1:E:163:TYR:HD2  | 1.54                     | 0.73              |
| 1:A:98:ASN:HD21  | 1:E:452:ARG:HE   | 1.34                     | 0.72              |
| 1:D:244:PRO:HA   | 1:D:275:TYR:CD2  | 2.24                     | 0.72              |
| 1:D:544:THR:HG22 | 1:D:548:ARG:HA   | 1.71                     | 0.72              |
| 1:A:468:LEU:CD1  | 1:A:469:PRO:HD2  | 2.19                     | 0.72              |
| 1:B:249:ASP:C    | 1:B:249:ASP:OD1  | 2.27                     | 0.72              |
| 1:E:145:ALA:HB3  | 1:E:168:PHE:HE1  | 1.53                     | 0.72              |
| 1:A:243:LEU:HD21 | 1:A:403:TYR:CE2  | 2.23                     | 0.72              |
| 1:A:197:ARG:HG3  | 1:A:198:GLN:N    | 2.05                     | 0.72              |
| 1:B:544:THR:HG22 | 1:B:548:ARG:HA   | 1.71                     | 0.72              |
| 1:B:148:MET:HA   | 1:B:163:TYR:HD2  | 1.54                     | 0.72              |
| 1:B:142:LYS:HG2  | 1:B:169:THR:HG22 | 1.70                     | 0.72              |
| 1:D:145:ALA:HB3  | 1:D:168:PHE:HE1  | 1.53                     | 0.72              |
| 1:E:142:LYS:HG2  | 1:E:169:THR:HG22 | 1.70                     | 0.72              |
| 1:A:451:PHE:CD2  | 1:A:461:PRO:HA   | 2.22                     | 0.72              |
| 1:E:197:ARG:HG3  | 1:E:198:GLN:N    | 2.05                     | 0.72              |
| 1:E:249:ASP:OD1  | 1:E:249:ASP:C    | 2.26                     | 0.72              |
| 1:B:244:PRO:HA   | 1:B:275:TYR:CD2  | 2.24                     | 0.72              |
| 1:E:243:LEU:HD21 | 1:E:403:TYR:CE2  | 2.23                     | 0.72              |
| 1:E:244:PRO:HA   | 1:E:275:TYR:CD2  | 2.24                     | 0.72              |
| 1:E:468:LEU:CD1  | 1:E:469:PRO:HD2  | 2.19                     | 0.72              |
| 1:B:468:LEU:CD1  | 1:B:469:PRO:HD2  | 2.19                     | 0.72              |
| 1:D:148:MET:HA   | 1:D:163:TYR:HD2  | 1.54                     | 0.72              |
| 1:C:244:PRO:HA   | 1:C:275:TYR:CD2  | 2.24                     | 0.71              |
| 1:C:148:MET:HA   | 1:C:163:TYR:HD2  | 1.54                     | 0.71              |
| 1:C:544:THR:HG22 | 1:C:548:ARG:HA   | 1.70                     | 0.71              |
| 1:A:544:THR:HG22 | 1:A:548:ARG:HA   | 1.70                     | 0.71              |
| 1:E:544:THR:HG22 | 1:E:548:ARG:HA   | 1.71                     | 0.71              |
| 1:D:197:ARG:HG3  | 1:D:198:GLN:N    | 2.05                     | 0.71              |
| 1:C:468:LEU:CD1  | 1:C:469:PRO:HD2  | 2.19                     | 0.71              |
| 1:A:436:GLN:HE22 | 1:B:74:ASN:ND2   | 1.88                     | 0.71              |
| 1:B:419:ILE:HG22 | 1:B:423:THR:CG2  | 2.21                     | 0.71              |
| 1:A:419:ILE:HG22 | 1:A:423:THR:CG2  | 2.21                     | 0.71              |
| 1:C:197:ARG:HG3  | 1:C:198:GLN:N    | 2.05                     | 0.71              |
| 1:D:436:GLN:HE22 | 1:E:74:ASN:ND2   | 1.88                     | 0.71              |
| 1:A:243:LEU:HD21 | 1:A:403:TYR:CD2  | 2.26                     | 0.71              |
| 1:A:74:ASN:ND2   | 1:E:436:GLN:HE22 | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:419:ILE:HG22 | 1:C:423:THR:CG2  | 2.21                     | 0.71              |
| 1:B:197:ARG:HG3  | 1:B:198:GLN:N    | 2.05                     | 0.71              |
| 1:A:148:MET:HA   | 1:A:163:TYR:HD2  | 1.54                     | 0.71              |
| 1:E:419:ILE:HG22 | 1:E:423:THR:CG2  | 2.21                     | 0.71              |
| 1:C:436:GLN:HE22 | 1:D:74:ASN:ND2   | 1.89                     | 0.71              |
| 1:C:243:LEU:HD21 | 1:C:403:TYR:CD2  | 2.26                     | 0.70              |
| 1:E:249:ASP:HB2  | 1:E:272:ARG:HG2  | 1.73                     | 0.70              |
| 1:D:419:ILE:HG22 | 1:D:423:THR:CG2  | 2.21                     | 0.70              |
| 1:E:243:LEU:HD21 | 1:E:403:TYR:CD2  | 2.26                     | 0.70              |
| 1:B:436:GLN:HE22 | 1:C:74:ASN:ND2   | 1.89                     | 0.70              |
| 1:C:122:ASP:OD1  | 1:C:528:THR:HB   | 1.91                     | 0.70              |
| 1:C:217:LEU:HB2  | 1:C:232:THR:HG21 | 1.73                     | 0.70              |
| 1:A:122:ASP:OD1  | 1:A:528:THR:HB   | 1.91                     | 0.70              |
| 1:B:160:GLU:OE2  | 1:B:162:LYS:HE3  | 1.91                     | 0.70              |
| 1:D:249:ASP:HB2  | 1:D:272:ARG:HG2  | 1.73                     | 0.70              |
| 1:B:122:ASP:OD1  | 1:B:528:THR:HB   | 1.91                     | 0.70              |
| 1:D:243:LEU:HD21 | 1:D:403:TYR:CD2  | 2.26                     | 0.70              |
| 1:B:215:PHE:CE1  | 1:B:241:ILE:HD11 | 2.27                     | 0.70              |
| 1:A:160:GLU:OE2  | 1:A:162:LYS:HE3  | 1.91                     | 0.70              |
| 1:E:160:GLU:OE2  | 1:E:162:LYS:HE3  | 1.91                     | 0.70              |
| 1:D:217:LEU:HB2  | 1:D:232:THR:HG21 | 1.73                     | 0.70              |
| 1:C:160:GLU:OE2  | 1:C:162:LYS:HE3  | 1.91                     | 0.70              |
| 1:D:122:ASP:OD1  | 1:D:528:THR:HB   | 1.91                     | 0.70              |
| 1:E:217:LEU:HB2  | 1:E:232:THR:HG21 | 1.73                     | 0.70              |
| 1:B:243:LEU:HD21 | 1:B:403:TYR:CD2  | 2.26                     | 0.69              |
| 1:A:419:ILE:HG22 | 1:A:423:THR:HG21 | 1.75                     | 0.69              |
| 1:B:249:ASP:HB2  | 1:B:272:ARG:HG2  | 1.73                     | 0.69              |
| 1:A:249:ASP:HB2  | 1:A:272:ARG:HG2  | 1.73                     | 0.69              |
| 1:C:444:MET:HG2  | 1:C:444:MET:O    | 1.92                     | 0.69              |
| 1:D:215:PHE:CE1  | 1:D:241:ILE:HD11 | 2.27                     | 0.69              |
| 1:C:215:PHE:CE1  | 1:C:241:ILE:HD11 | 2.27                     | 0.69              |
| 1:C:249:ASP:HB2  | 1:C:272:ARG:HG2  | 1.73                     | 0.69              |
| 1:E:122:ASP:OD1  | 1:E:528:THR:HB   | 1.91                     | 0.69              |
| 1:B:419:ILE:HG22 | 1:B:423:THR:HG21 | 1.75                     | 0.69              |
| 1:D:419:ILE:HG22 | 1:D:423:THR:HG21 | 1.75                     | 0.69              |
| 1:B:444:MET:O    | 1:B:444:MET:HG2  | 1.92                     | 0.69              |
| 1:C:441:LEU:HD12 | 1:C:445:MET:HE1  | 1.75                     | 0.69              |
| 1:A:215:PHE:CE1  | 1:A:241:ILE:HD11 | 2.27                     | 0.69              |
| 1:D:160:GLU:OE2  | 1:D:162:LYS:HE3  | 1.91                     | 0.69              |
| 1:E:512:THR:O    | 1:E:513:ILE:HB   | 1.93                     | 0.69              |
| 1:B:217:LEU:HB2  | 1:B:232:THR:HG21 | 1.73                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:217:LEU:HB2  | 1:A:232:THR:HG21 | 1.73                     | 0.68              |
| 1:D:444:MET:O    | 1:D:444:MET:HG2  | 1.92                     | 0.68              |
| 1:E:215:PHE:CE1  | 1:E:241:ILE:HD11 | 2.27                     | 0.68              |
| 1:A:142:LYS:HD3  | 1:A:167:GLU:OE2  | 1.93                     | 0.68              |
| 1:E:444:MET:O    | 1:E:444:MET:HG2  | 1.92                     | 0.68              |
| 1:D:512:THR:O    | 1:D:513:ILE:HB   | 1.93                     | 0.68              |
| 1:D:142:LYS:HD3  | 1:D:167:GLU:OE2  | 1.93                     | 0.68              |
| 1:E:142:LYS:HD3  | 1:E:167:GLU:OE2  | 1.93                     | 0.68              |
| 1:E:278:LEU:HD22 | 1:E:406:TRP:HA   | 1.76                     | 0.68              |
| 1:A:512:THR:O    | 1:A:513:ILE:HB   | 1.93                     | 0.68              |
| 1:C:419:ILE:HG22 | 1:C:423:THR:HG21 | 1.75                     | 0.68              |
| 1:E:419:ILE:HG22 | 1:E:423:THR:HG21 | 1.75                     | 0.68              |
| 1:B:142:LYS:HD3  | 1:B:167:GLU:OE2  | 1.94                     | 0.68              |
| 1:A:444:MET:O    | 1:A:444:MET:HG2  | 1.92                     | 0.68              |
| 1:A:146:ARG:O    | 1:A:246:CYS:HB2  | 1.94                     | 0.68              |
| 1:B:149:VAL:HG23 | 1:B:195:VAL:HG11 | 1.76                     | 0.68              |
| 1:B:512:THR:O    | 1:B:513:ILE:HB   | 1.93                     | 0.68              |
| 1:D:217:LEU:HB2  | 1:D:232:THR:CG2  | 2.25                     | 0.67              |
| 1:A:386:SER:O    | 1:A:387:LYS:HB2  | 1.94                     | 0.67              |
| 1:E:149:VAL:HG23 | 1:E:195:VAL:HG11 | 1.76                     | 0.67              |
| 1:C:217:LEU:HB2  | 1:C:232:THR:CG2  | 2.25                     | 0.67              |
| 1:E:217:LEU:HB2  | 1:E:232:THR:CG2  | 2.25                     | 0.67              |
| 1:D:149:VAL:HG23 | 1:D:195:VAL:HG11 | 1.76                     | 0.67              |
| 1:A:278:LEU:HD22 | 1:A:406:TRP:HA   | 1.76                     | 0.67              |
| 1:D:278:LEU:HD22 | 1:D:406:TRP:HA   | 1.76                     | 0.67              |
| 1:C:83:ASN:N     | 1:C:83:ASN:OD1   | 2.27                     | 0.67              |
| 1:C:512:THR:O    | 1:C:513:ILE:HB   | 1.93                     | 0.67              |
| 1:C:142:LYS:HD3  | 1:C:167:GLU:OE2  | 1.94                     | 0.67              |
| 1:E:386:SER:O    | 1:E:387:LYS:HB2  | 1.94                     | 0.67              |
| 1:C:227:MET:HB2  | 1:C:228:PRO:HD3  | 1.76                     | 0.67              |
| 1:A:149:VAL:HG23 | 1:A:195:VAL:HG11 | 1.76                     | 0.67              |
| 1:D:386:SER:O    | 1:D:387:LYS:HB2  | 1.94                     | 0.67              |
| 1:B:217:LEU:HB2  | 1:B:232:THR:CG2  | 2.25                     | 0.67              |
| 1:D:227:MET:HB2  | 1:D:228:PRO:HD3  | 1.76                     | 0.67              |
| 1:A:227:MET:HB2  | 1:A:228:PRO:HD3  | 1.76                     | 0.67              |
| 1:B:227:MET:HB2  | 1:B:228:PRO:HD3  | 1.76                     | 0.67              |
| 1:C:452:ARG:HH22 | 1:D:99:ASN:HD22  | 1.43                     | 0.67              |
| 1:D:146:ARG:O    | 1:D:246:CYS:HB2  | 1.94                     | 0.67              |
| 1:D:468:LEU:HD12 | 1:D:469:PRO:CD   | 2.25                     | 0.66              |
| 1:C:146:ARG:O    | 1:C:246:CYS:HB2  | 1.94                     | 0.66              |
| 1:E:146:ARG:O    | 1:E:246:CYS:HB2  | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:426:CYS:HA   | 1:B:132:PRO:HG3  | 1.77                     | 0.66              |
| 1:B:468:LEU:HD12 | 1:B:469:PRO:CD   | 2.26                     | 0.66              |
| 1:C:426:CYS:HA   | 1:D:132:PRO:HG3  | 1.77                     | 0.66              |
| 1:D:452:ARG:HH22 | 1:E:99:ASN:HD22  | 1.43                     | 0.66              |
| 1:C:430:VAL:HG21 | 1:C:517:SER:N    | 2.10                     | 0.66              |
| 1:B:278:LEU:HD22 | 1:B:406:TRP:HA   | 1.76                     | 0.66              |
| 1:C:149:VAL:HG23 | 1:C:195:VAL:HG11 | 1.76                     | 0.66              |
| 1:D:441:LEU:HD12 | 1:D:445:MET:HE1  | 1.77                     | 0.66              |
| 1:B:146:ARG:O    | 1:B:246:CYS:HB2  | 1.94                     | 0.66              |
| 1:B:386:SER:O    | 1:B:387:LYS:HB2  | 1.94                     | 0.66              |
| 1:C:278:LEU:HD22 | 1:C:406:TRP:HA   | 1.76                     | 0.66              |
| 1:A:468:LEU:HD12 | 1:A:469:PRO:CD   | 2.26                     | 0.66              |
| 1:A:217:LEU:HB2  | 1:A:232:THR:CG2  | 2.25                     | 0.66              |
| 1:C:386:SER:O    | 1:C:387:LYS:HB2  | 1.94                     | 0.66              |
| 1:D:430:VAL:HG21 | 1:D:517:SER:N    | 2.11                     | 0.66              |
| 1:A:452:ARG:HH22 | 1:B:99:ASN:HD22  | 1.43                     | 0.66              |
| 1:B:426:CYS:HA   | 1:C:132:PRO:HG3  | 1.77                     | 0.66              |
| 1:C:468:LEU:HD12 | 1:C:469:PRO:CD   | 2.26                     | 0.66              |
| 1:E:227:MET:HB2  | 1:E:228:PRO:HD3  | 1.76                     | 0.66              |
| 1:A:99:ASN:HD22  | 1:E:452:ARG:HH22 | 1.43                     | 0.65              |
| 1:A:132:PRO:HG3  | 1:E:426:CYS:HA   | 1.77                     | 0.65              |
| 1:B:430:VAL:HG21 | 1:B:517:SER:N    | 2.10                     | 0.65              |
| 1:D:60:LEU:O     | 1:D:61:ALA:HB3   | 1.97                     | 0.65              |
| 1:E:430:VAL:HG21 | 1:E:517:SER:N    | 2.11                     | 0.65              |
| 1:B:393:LEU:HD12 | 1:B:393:LEU:N    | 2.12                     | 0.65              |
| 1:D:426:CYS:HA   | 1:E:132:PRO:HG3  | 1.77                     | 0.65              |
| 1:D:193:LEU:HD11 | 1:D:498:ARG:NH1  | 2.12                     | 0.65              |
| 1:B:60:LEU:O     | 1:B:61:ALA:HB3   | 1.97                     | 0.65              |
| 1:C:60:LEU:O     | 1:C:61:ALA:HB3   | 1.97                     | 0.65              |
| 1:A:430:VAL:HG21 | 1:A:517:SER:N    | 2.10                     | 0.65              |
| 1:A:393:LEU:N    | 1:A:393:LEU:HD12 | 2.12                     | 0.65              |
| 1:A:436:GLN:HE22 | 1:B:74:ASN:HD21  | 1.45                     | 0.65              |
| 1:B:452:ARG:HH22 | 1:C:99:ASN:HD22  | 1.43                     | 0.65              |
| 1:D:436:GLN:NE2  | 1:E:74:ASN:HD21  | 1.95                     | 0.65              |
| 1:E:133:ASN:HB2  | 1:E:174:ASN:OD1  | 1.97                     | 0.65              |
| 1:D:393:LEU:N    | 1:D:393:LEU:HD12 | 2.12                     | 0.65              |
| 1:A:211:ASP:O    | 1:A:212:THR:HG22 | 1.97                     | 0.64              |
| 1:C:193:LEU:HD11 | 1:C:498:ARG:NH1  | 2.12                     | 0.64              |
| 1:C:211:ASP:O    | 1:C:212:THR:HG22 | 1.97                     | 0.64              |
| 1:D:436:GLN:HE22 | 1:E:74:ASN:HD21  | 1.45                     | 0.64              |
| 1:E:468:LEU:HD12 | 1:E:469:PRO:CD   | 2.26                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:513:ILE:HG22 | 1:C:513:ILE:O    | 1.97                     | 0.64              |
| 1:E:60:LEU:O     | 1:E:61:ALA:HB3   | 1.97                     | 0.64              |
| 1:C:393:LEU:N    | 1:C:393:LEU:HD12 | 2.12                     | 0.64              |
| 1:B:436:GLN:NE2  | 1:C:74:ASN:HD21  | 1.95                     | 0.64              |
| 1:E:393:LEU:HD12 | 1:E:393:LEU:N    | 2.12                     | 0.64              |
| 1:B:278:LEU:O    | 1:B:404:ARG:HD3  | 1.98                     | 0.64              |
| 1:E:513:ILE:HG22 | 1:E:513:ILE:O    | 1.97                     | 0.64              |
| 1:B:436:GLN:HE22 | 1:C:74:ASN:HD21  | 1.46                     | 0.64              |
| 1:D:513:ILE:O    | 1:D:513:ILE:HG22 | 1.97                     | 0.64              |
| 1:C:436:GLN:NE2  | 1:D:74:ASN:HD21  | 1.96                     | 0.64              |
| 1:E:278:LEU:O    | 1:E:404:ARG:HD3  | 1.98                     | 0.64              |
| 1:A:133:ASN:HB2  | 1:A:174:ASN:OD1  | 1.97                     | 0.64              |
| 1:E:493:THR:HG21 | 1:E:497:ASN:O    | 1.99                     | 0.64              |
| 1:E:499:PHE:N    | 1:E:500:PRO:HD3  | 2.13                     | 0.64              |
| 1:A:74:ASN:HD21  | 1:E:436:GLN:NE2  | 1.95                     | 0.63              |
| 1:C:133:ASN:HB2  | 1:C:174:ASN:OD1  | 1.97                     | 0.63              |
| 1:B:133:ASN:HB2  | 1:B:174:ASN:OD1  | 1.97                     | 0.63              |
| 1:B:513:ILE:HG22 | 1:B:513:ILE:O    | 1.97                     | 0.63              |
| 1:A:436:GLN:NE2  | 1:B:74:ASN:HD21  | 1.95                     | 0.63              |
| 1:C:436:GLN:HE22 | 1:D:74:ASN:HD21  | 1.45                     | 0.63              |
| 1:C:499:PHE:N    | 1:C:500:PRO:HD3  | 2.13                     | 0.63              |
| 1:B:493:THR:HG21 | 1:B:497:ASN:O    | 1.99                     | 0.63              |
| 1:D:278:LEU:O    | 1:D:404:ARG:HD3  | 1.98                     | 0.63              |
| 1:E:441:LEU:HD12 | 1:E:445:MET:HE1  | 1.81                     | 0.63              |
| 1:B:211:ASP:O    | 1:B:212:THR:HG22 | 1.97                     | 0.63              |
| 1:D:211:ASP:O    | 1:D:212:THR:HG22 | 1.97                     | 0.63              |
| 1:B:499:PHE:N    | 1:B:500:PRO:HD3  | 2.13                     | 0.63              |
| 1:D:499:PHE:N    | 1:D:500:PRO:HD3  | 2.13                     | 0.63              |
| 1:A:60:LEU:O     | 1:A:61:ALA:HB3   | 1.97                     | 0.63              |
| 1:E:211:ASP:O    | 1:E:212:THR:HG22 | 1.97                     | 0.63              |
| 1:C:493:THR:HG21 | 1:C:497:ASN:O    | 1.98                     | 0.63              |
| 1:C:278:LEU:O    | 1:C:404:ARG:HD3  | 1.98                     | 0.63              |
| 1:D:133:ASN:HB2  | 1:D:174:ASN:OD1  | 1.97                     | 0.63              |
| 1:A:493:THR:HG21 | 1:A:497:ASN:O    | 1.98                     | 0.63              |
| 1:A:134:VAL:HA   | 1:A:140:THR:OG1  | 1.99                     | 0.63              |
| 1:E:134:VAL:HA   | 1:E:140:THR:OG1  | 1.99                     | 0.63              |
| 1:E:83:ASN:OD1   | 1:E:83:ASN:N     | 2.26                     | 0.63              |
| 1:E:148:MET:HA   | 1:E:163:TYR:CD2  | 2.34                     | 0.63              |
| 1:B:193:LEU:HD11 | 1:B:498:ARG:NH1  | 2.12                     | 0.62              |
| 1:D:134:VAL:HA   | 1:D:140:THR:OG1  | 1.99                     | 0.62              |
| 1:A:499:PHE:N    | 1:A:500:PRO:HD3  | 2.13                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:441:LEU:HD12 | 1:B:445:MET:HE1  | 1.79                     | 0.62              |
| 1:B:134:VAL:HA   | 1:B:140:THR:OG1  | 1.99                     | 0.62              |
| 1:D:544:THR:HG21 | 1:D:548:ARG:HD2  | 1.81                     | 0.62              |
| 1:A:513:ILE:HG22 | 1:A:513:ILE:O    | 1.97                     | 0.62              |
| 1:D:148:MET:HA   | 1:D:163:TYR:CD2  | 2.34                     | 0.62              |
| 1:A:278:LEU:O    | 1:A:404:ARG:HD3  | 1.98                     | 0.62              |
| 1:C:378:VAL:HG12 | 1:C:379:ILE:N    | 2.14                     | 0.62              |
| 1:D:125:THR:HG23 | 1:D:524:THR:CG2  | 2.29                     | 0.62              |
| 1:A:378:VAL:HG12 | 1:A:379:ILE:N    | 2.15                     | 0.62              |
| 1:B:125:THR:HG23 | 1:B:524:THR:CG2  | 2.29                     | 0.62              |
| 1:D:258:LEU:O    | 1:D:258:LEU:HD12 | 2.00                     | 0.62              |
| 1:A:544:THR:HG21 | 1:A:548:ARG:HD2  | 1.81                     | 0.62              |
| 1:E:544:THR:HG21 | 1:E:548:ARG:HD2  | 1.81                     | 0.62              |
| 1:B:178:THR:CG2  | 1:B:511:PRO:HD2  | 2.29                     | 0.62              |
| 1:A:258:LEU:HD12 | 1:A:258:LEU:O    | 2.00                     | 0.62              |
| 1:B:544:THR:HG21 | 1:B:548:ARG:HD2  | 1.81                     | 0.62              |
| 1:A:125:THR:HG23 | 1:A:524:THR:CG2  | 2.29                     | 0.62              |
| 1:B:148:MET:HA   | 1:B:163:TYR:CD2  | 2.34                     | 0.62              |
| 1:A:148:MET:HA   | 1:A:163:TYR:CD2  | 2.34                     | 0.62              |
| 1:D:493:THR:HG21 | 1:D:497:ASN:O    | 1.99                     | 0.62              |
| 1:C:134:VAL:HA   | 1:C:140:THR:OG1  | 1.99                     | 0.62              |
| 1:C:148:MET:HA   | 1:C:163:TYR:CD2  | 2.34                     | 0.62              |
| 1:B:125:THR:CG2  | 1:B:526:HIS:NE2  | 2.63                     | 0.62              |
| 1:C:125:THR:HG23 | 1:C:524:THR:CG2  | 2.29                     | 0.62              |
| 1:E:125:THR:HG23 | 1:E:524:THR:CG2  | 2.29                     | 0.62              |
| 1:B:60:LEU:O     | 1:B:60:LEU:HG    | 2.00                     | 0.62              |
| 1:A:125:THR:CG2  | 1:A:526:HIS:NE2  | 2.63                     | 0.62              |
| 1:E:378:VAL:HG12 | 1:E:379:ILE:N    | 2.15                     | 0.61              |
| 1:D:125:THR:CG2  | 1:D:526:HIS:NE2  | 2.63                     | 0.61              |
| 1:D:60:LEU:HG    | 1:D:60:LEU:O     | 2.00                     | 0.61              |
| 1:E:125:THR:CG2  | 1:E:526:HIS:NE2  | 2.63                     | 0.61              |
| 1:B:394:ILE:HG23 | 1:B:398:SER:HB2  | 1.82                     | 0.61              |
| 1:A:193:LEU:HD11 | 1:A:498:ARG:NH1  | 2.12                     | 0.61              |
| 1:E:220:ASP:OD1  | 1:E:222:VAL:HG12 | 2.00                     | 0.61              |
| 1:A:394:ILE:HG23 | 1:A:398:SER:HB2  | 1.82                     | 0.61              |
| 1:E:60:LEU:O     | 1:E:60:LEU:HG    | 2.00                     | 0.61              |
| 1:B:220:ASP:OD1  | 1:B:222:VAL:HG12 | 2.00                     | 0.61              |
| 1:D:394:ILE:HG23 | 1:D:398:SER:HB2  | 1.82                     | 0.61              |
| 1:B:378:VAL:HG12 | 1:B:379:ILE:N    | 2.15                     | 0.61              |
| 1:E:444:MET:HB2  | 1:E:539:GLN:OE1  | 2.01                     | 0.61              |
| 1:C:220:ASP:OD1  | 1:C:222:VAL:HG12 | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:74:ASN:HD21  | 1:E:436:GLN:HE22 | 1.46                     | 0.61              |
| 1:D:220:ASP:OD1  | 1:D:222:VAL:HG12 | 2.00                     | 0.61              |
| 1:C:258:LEU:O    | 1:C:258:LEU:HD12 | 2.00                     | 0.61              |
| 1:B:258:LEU:O    | 1:B:258:LEU:HD12 | 2.00                     | 0.61              |
| 1:C:444:MET:HB2  | 1:C:539:GLN:OE1  | 2.00                     | 0.61              |
| 1:D:178:THR:CG2  | 1:D:511:PRO:HD2  | 2.30                     | 0.61              |
| 1:E:193:LEU:HD11 | 1:E:498:ARG:NH1  | 2.12                     | 0.61              |
| 1:C:74:ASN:ND2   | 1:C:556:LYS:HZ1  | 1.98                     | 0.61              |
| 1:C:394:ILE:HG23 | 1:C:398:SER:HB2  | 1.82                     | 0.61              |
| 1:B:444:MET:HB2  | 1:B:539:GLN:OE1  | 2.01                     | 0.61              |
| 1:A:220:ASP:OD1  | 1:A:222:VAL:HG12 | 2.00                     | 0.61              |
| 1:C:125:THR:CG2  | 1:C:526:HIS:NE2  | 2.63                     | 0.61              |
| 1:C:544:THR:HG21 | 1:C:548:ARG:HD2  | 1.81                     | 0.61              |
| 1:D:378:VAL:HG12 | 1:D:379:ILE:N    | 2.15                     | 0.61              |
| 1:C:178:THR:CG2  | 1:C:511:PRO:HD2  | 2.30                     | 0.60              |
| 1:E:258:LEU:O    | 1:E:258:LEU:HD12 | 2.00                     | 0.60              |
| 1:D:444:MET:HB2  | 1:D:539:GLN:OE1  | 2.01                     | 0.60              |
| 1:D:440:SER:HB3  | 1:D:461:PRO:O    | 2.01                     | 0.60              |
| 1:C:440:SER:HB3  | 1:C:461:PRO:O    | 2.02                     | 0.60              |
| 1:C:60:LEU:O     | 1:C:60:LEU:HG    | 2.00                     | 0.60              |
| 1:A:383:THR:HG22 | 1:A:384:GLU:HG3  | 1.84                     | 0.60              |
| 1:B:125:THR:HG21 | 1:B:526:HIS:NE2  | 2.17                     | 0.60              |
| 1:B:394:ILE:HG23 | 1:B:395:SER:H    | 1.67                     | 0.60              |
| 1:A:263:LYS:NZ   | 1:A:268:GLN:HB2  | 2.16                     | 0.60              |
| 1:E:263:LYS:NZ   | 1:E:268:GLN:HB2  | 2.16                     | 0.60              |
| 1:B:425:LEU:HD23 | 1:C:172:GLU:HB3  | 1.83                     | 0.60              |
| 1:E:383:THR:HG22 | 1:E:384:GLU:HG3  | 1.83                     | 0.60              |
| 1:D:125:THR:HG21 | 1:D:526:HIS:NE2  | 2.16                     | 0.60              |
| 1:C:383:THR:HG22 | 1:C:384:GLU:HG3  | 1.84                     | 0.60              |
| 1:B:220:ASP:HB2  | 1:B:227:MET:HG2  | 1.84                     | 0.60              |
| 1:A:125:THR:HG21 | 1:A:526:HIS:NE2  | 2.17                     | 0.60              |
| 1:A:394:ILE:HG23 | 1:A:395:SER:H    | 1.67                     | 0.60              |
| 1:E:394:ILE:HG23 | 1:E:395:SER:H    | 1.66                     | 0.60              |
| 1:A:440:SER:HB3  | 1:A:461:PRO:O    | 2.02                     | 0.60              |
| 1:A:60:LEU:O     | 1:A:60:LEU:HG    | 2.00                     | 0.60              |
| 1:D:383:THR:HG22 | 1:D:384:GLU:HG3  | 1.84                     | 0.60              |
| 1:B:278:LEU:CD2  | 1:B:406:TRP:HA   | 2.32                     | 0.60              |
| 1:A:444:MET:HB2  | 1:A:539:GLN:OE1  | 2.01                     | 0.60              |
| 1:D:449:VAL:CG2  | 1:E:67:THR:HG21  | 2.32                     | 0.60              |
| 1:E:125:THR:HG21 | 1:E:526:HIS:NE2  | 2.17                     | 0.60              |
| 1:A:449:VAL:CG2  | 1:B:67:THR:HG21  | 2.32                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:410:TYR:CD1  | 1:C:420:ARG:HA   | 2.37                     | 0.60              |
| 1:A:172:GLU:HB3  | 1:E:425:LEU:HD23 | 1.83                     | 0.60              |
| 1:A:220:ASP:HB2  | 1:A:227:MET:HG2  | 1.84                     | 0.60              |
| 1:C:449:VAL:CG2  | 1:D:67:THR:HG21  | 2.32                     | 0.60              |
| 1:E:278:LEU:CD2  | 1:E:406:TRP:HA   | 2.32                     | 0.60              |
| 1:C:243:LEU:HD11 | 1:C:403:TYR:HE2  | 1.67                     | 0.60              |
| 1:B:214:ASN:C    | 1:B:214:ASN:ND2  | 2.55                     | 0.60              |
| 1:A:436:GLN:NE2  | 1:B:556:LYS:HZ3  | 2.00                     | 0.60              |
| 1:C:394:ILE:HG23 | 1:C:395:SER:H    | 1.67                     | 0.60              |
| 1:D:389:ARG:HG2  | 1:D:389:ARG:NH1  | 2.17                     | 0.59              |
| 1:D:278:LEU:CD2  | 1:D:406:TRP:HA   | 2.32                     | 0.59              |
| 1:C:389:ARG:NH1  | 1:C:389:ARG:HG2  | 2.17                     | 0.59              |
| 1:D:410:TYR:CD1  | 1:D:420:ARG:HA   | 2.37                     | 0.59              |
| 1:D:425:LEU:HD23 | 1:E:172:GLU:HB3  | 1.84                     | 0.59              |
| 1:A:425:LEU:HD23 | 1:B:172:GLU:HB3  | 1.84                     | 0.59              |
| 1:A:67:THR:HG21  | 1:E:449:VAL:CG2  | 2.32                     | 0.59              |
| 1:E:282:ASN:HD21 | 1:E:404:ARG:HE   | 1.51                     | 0.59              |
| 1:E:389:ARG:HG2  | 1:E:389:ARG:NH1  | 2.17                     | 0.59              |
| 1:C:220:ASP:HB2  | 1:C:227:MET:HG2  | 1.84                     | 0.59              |
| 1:A:389:ARG:HG2  | 1:A:389:ARG:NH1  | 2.17                     | 0.59              |
| 1:E:278:LEU:HD23 | 1:E:419:ILE:CD1  | 2.30                     | 0.59              |
| 1:E:440:SER:HB3  | 1:E:461:PRO:O    | 2.01                     | 0.59              |
| 1:B:410:TYR:CD1  | 1:B:420:ARG:HA   | 2.37                     | 0.59              |
| 1:D:214:ASN:C    | 1:D:214:ASN:ND2  | 2.55                     | 0.59              |
| 1:D:220:ASP:HB2  | 1:D:227:MET:HG2  | 1.84                     | 0.59              |
| 1:E:394:ILE:HG23 | 1:E:398:SER:HB2  | 1.82                     | 0.59              |
| 1:B:263:LYS:NZ   | 1:B:268:GLN:HB2  | 2.16                     | 0.59              |
| 1:B:449:VAL:CG2  | 1:C:67:THR:HG21  | 2.32                     | 0.59              |
| 1:E:243:LEU:HD11 | 1:E:403:TYR:HE2  | 1.67                     | 0.59              |
| 1:D:243:LEU:HD11 | 1:D:403:TYR:HE2  | 1.67                     | 0.59              |
| 1:A:410:TYR:CD1  | 1:A:420:ARG:HA   | 2.37                     | 0.59              |
| 1:B:383:THR:HG22 | 1:B:384:GLU:HG3  | 1.83                     | 0.59              |
| 1:E:410:TYR:CD1  | 1:E:420:ARG:HA   | 2.37                     | 0.59              |
| 1:A:378:VAL:O    | 1:A:380:LYS:N    | 2.35                     | 0.59              |
| 1:E:378:VAL:O    | 1:E:380:LYS:N    | 2.36                     | 0.59              |
| 1:B:282:ASN:HD21 | 1:B:404:ARG:HE   | 1.50                     | 0.59              |
| 1:D:243:LEU:CD2  | 1:D:403:TYR:CD2  | 2.86                     | 0.59              |
| 1:C:378:VAL:O    | 1:C:380:LYS:N    | 2.36                     | 0.59              |
| 1:B:243:LEU:CD2  | 1:B:403:TYR:CD2  | 2.86                     | 0.59              |
| 1:C:425:LEU:HD23 | 1:D:172:GLU:HB3  | 1.83                     | 0.59              |
| 1:C:263:LYS:NZ   | 1:C:268:GLN:HB2  | 2.16                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:125:THR:HG21 | 1:C:526:HIS:NE2  | 2.17                     | 0.59              |
| 1:B:224:GLY:O    | 1:B:399:THR:HB   | 2.03                     | 0.59              |
| 1:C:520:VAL:CG2  | 1:C:521:PRO:HD2  | 2.33                     | 0.59              |
| 1:A:278:LEU:CD2  | 1:A:406:TRP:HA   | 2.32                     | 0.59              |
| 1:A:178:THR:CG2  | 1:A:511:PRO:HD2  | 2.30                     | 0.59              |
| 1:C:214:ASN:C    | 1:C:214:ASN:ND2  | 2.55                     | 0.59              |
| 1:E:520:VAL:CG2  | 1:E:521:PRO:HD2  | 2.33                     | 0.59              |
| 1:C:278:LEU:CD2  | 1:C:406:TRP:HA   | 2.32                     | 0.59              |
| 1:D:287:LEU:C    | 1:D:287:LEU:HD23 | 2.24                     | 0.59              |
| 1:B:243:LEU:HD11 | 1:B:403:TYR:HE2  | 1.67                     | 0.58              |
| 1:C:243:LEU:CD2  | 1:C:403:TYR:CD2  | 2.86                     | 0.58              |
| 1:C:282:ASN:HD21 | 1:C:404:ARG:HE   | 1.50                     | 0.58              |
| 1:B:197:ARG:HG3  | 1:B:198:GLN:CG   | 2.33                     | 0.58              |
| 1:A:197:ARG:HG3  | 1:A:198:GLN:CG   | 2.33                     | 0.58              |
| 1:B:389:ARG:HG2  | 1:B:389:ARG:NH1  | 2.17                     | 0.58              |
| 1:B:378:VAL:O    | 1:B:380:LYS:N    | 2.35                     | 0.58              |
| 1:E:220:ASP:HB2  | 1:E:227:MET:HG2  | 1.84                     | 0.58              |
| 1:C:224:GLY:O    | 1:C:399:THR:HB   | 2.03                     | 0.58              |
| 1:E:224:GLY:O    | 1:E:399:THR:HB   | 2.03                     | 0.58              |
| 1:B:278:LEU:HD23 | 1:B:419:ILE:CD1  | 2.30                     | 0.58              |
| 1:E:243:LEU:CD2  | 1:E:403:TYR:CD2  | 2.86                     | 0.58              |
| 1:C:197:ARG:HG3  | 1:C:198:GLN:CG   | 2.33                     | 0.58              |
| 1:D:154:THR:HG22 | 1:D:155:LYS:N    | 2.19                     | 0.58              |
| 1:D:394:ILE:HG23 | 1:D:395:SER:H    | 1.67                     | 0.58              |
| 1:D:263:LYS:NZ   | 1:D:268:GLN:HB2  | 2.16                     | 0.58              |
| 1:A:282:ASN:HD21 | 1:A:404:ARG:HE   | 1.50                     | 0.58              |
| 1:D:282:ASN:HD21 | 1:D:404:ARG:HE   | 1.50                     | 0.58              |
| 1:E:154:THR:HG22 | 1:E:155:LYS:N    | 2.18                     | 0.58              |
| 1:B:154:THR:HG22 | 1:B:155:LYS:N    | 2.19                     | 0.58              |
| 1:A:224:GLY:O    | 1:A:399:THR:HB   | 2.03                     | 0.58              |
| 1:A:243:LEU:CD2  | 1:A:403:TYR:CD2  | 2.86                     | 0.58              |
| 1:C:278:LEU:HD23 | 1:C:419:ILE:CD1  | 2.30                     | 0.58              |
| 1:B:440:SER:HB3  | 1:B:461:PRO:O    | 2.02                     | 0.58              |
| 1:E:178:THR:CG2  | 1:E:511:PRO:HD2  | 2.30                     | 0.58              |
| 1:C:287:LEU:C    | 1:C:287:LEU:HD23 | 2.24                     | 0.58              |
| 1:B:211:ASP:O    | 1:B:212:THR:CG2  | 2.52                     | 0.58              |
| 1:D:211:ASP:O    | 1:D:212:THR:CG2  | 2.52                     | 0.58              |
| 1:C:410:TYR:HE2  | 1:D:172:GLU:OE1  | 1.87                     | 0.58              |
| 1:A:520:VAL:CG2  | 1:A:521:PRO:HD2  | 2.33                     | 0.58              |
| 1:C:211:ASP:O    | 1:C:212:THR:CG2  | 2.52                     | 0.58              |
| 1:A:172:GLU:OE1  | 1:E:410:TYR:HE2  | 1.87                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:214:ASN:ND2  | 1:E:214:ASN:C    | 2.55                     | 0.58              |
| 1:A:278:LEU:HD23 | 1:A:419:ILE:CD1  | 2.30                     | 0.58              |
| 1:E:211:ASP:O    | 1:E:212:THR:CG2  | 2.52                     | 0.58              |
| 1:C:494:HIS:C    | 1:C:496:PHE:H    | 2.07                     | 0.58              |
| 1:A:211:ASP:O    | 1:A:212:THR:CG2  | 2.52                     | 0.58              |
| 1:A:154:THR:HG22 | 1:A:155:LYS:N    | 2.19                     | 0.58              |
| 1:D:378:VAL:O    | 1:D:380:LYS:N    | 2.35                     | 0.58              |
| 1:B:287:LEU:HD23 | 1:B:287:LEU:C    | 2.24                     | 0.58              |
| 1:C:154:THR:HG22 | 1:C:155:LYS:N    | 2.18                     | 0.57              |
| 1:A:287:LEU:C    | 1:A:287:LEU:HD23 | 2.24                     | 0.57              |
| 1:A:243:LEU:HD11 | 1:A:403:TYR:HE2  | 1.67                     | 0.57              |
| 1:A:282:ASN:ND2  | 1:A:404:ARG:HE   | 2.03                     | 0.57              |
| 1:B:410:TYR:HE2  | 1:C:172:GLU:OE1  | 1.87                     | 0.57              |
| 1:A:410:TYR:HE2  | 1:B:172:GLU:OE1  | 1.87                     | 0.57              |
| 1:E:287:LEU:C    | 1:E:287:LEU:HD23 | 2.24                     | 0.57              |
| 1:B:282:ASN:ND2  | 1:B:404:ARG:HE   | 2.03                     | 0.57              |
| 1:D:410:TYR:HE2  | 1:E:172:GLU:OE1  | 1.87                     | 0.57              |
| 1:D:197:ARG:HG3  | 1:D:198:GLN:CG   | 2.33                     | 0.57              |
| 1:D:224:GLY:O    | 1:D:399:THR:HB   | 2.03                     | 0.57              |
| 1:C:479:GLN:O    | 1:C:479:GLN:HG2  | 2.05                     | 0.57              |
| 1:E:197:ARG:HG3  | 1:E:198:GLN:CG   | 2.33                     | 0.57              |
| 1:B:520:VAL:CG2  | 1:B:521:PRO:HD2  | 2.33                     | 0.57              |
| 1:D:403:TYR:CD1  | 1:D:504:ILE:HD13 | 2.39                     | 0.57              |
| 1:D:282:ASN:ND2  | 1:D:404:ARG:HE   | 2.03                     | 0.57              |
| 1:D:482:TYR:CE1  | 1:D:486:ILE:HD12 | 2.40                     | 0.57              |
| 1:D:520:VAL:CG2  | 1:D:521:PRO:HD2  | 2.33                     | 0.57              |
| 1:A:233:ASN:O    | 1:A:233:ASN:CG   | 2.43                     | 0.57              |
| 1:A:441:LEU:HD12 | 1:A:445:MET:HE1  | 1.87                     | 0.57              |
| 1:C:567:SER:HB2  | 1:D:49:THR:HG21  | 1.87                     | 0.57              |
| 1:B:479:GLN:O    | 1:B:479:GLN:HG2  | 2.05                     | 0.57              |
| 1:E:444:MET:HE3  | 1:E:561:VAL:HG21 | 1.87                     | 0.57              |
| 1:B:482:TYR:CE1  | 1:B:486:ILE:HD12 | 2.40                     | 0.57              |
| 1:E:233:ASN:CG   | 1:E:233:ASN:O    | 2.43                     | 0.57              |
| 1:E:282:ASN:ND2  | 1:E:404:ARG:HE   | 2.03                     | 0.56              |
| 1:E:134:VAL:HG22 | 1:E:173:GLY:O    | 2.05                     | 0.56              |
| 1:A:134:VAL:HG22 | 1:A:173:GLY:O    | 2.05                     | 0.56              |
| 1:C:436:GLN:NE2  | 1:D:556:LYS:HZ3  | 2.03                     | 0.56              |
| 1:A:482:TYR:CE1  | 1:A:486:ILE:HD12 | 2.40                     | 0.56              |
| 1:B:233:ASN:O    | 1:B:233:ASN:CG   | 2.43                     | 0.56              |
| 1:C:282:ASN:ND2  | 1:C:404:ARG:HE   | 2.02                     | 0.56              |
| 1:B:134:VAL:HG22 | 1:B:173:GLY:O    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:567:SER:HB2  | 1:B:49:THR:HG21  | 1.87                     | 0.56              |
| 1:B:494:HIS:C    | 1:B:496:PHE:H    | 2.08                     | 0.56              |
| 1:B:392:ASN:HB3  | 1:B:402:GLN:NE2  | 2.21                     | 0.56              |
| 1:E:479:GLN:O    | 1:E:479:GLN:HG2  | 2.05                     | 0.56              |
| 1:B:434:SER:N    | 1:C:555:TYR:HE2  | 2.04                     | 0.56              |
| 1:E:273:ILE:O    | 1:E:273:ILE:HG23 | 2.05                     | 0.56              |
| 1:D:479:GLN:O    | 1:D:479:GLN:HG2  | 2.05                     | 0.56              |
| 1:C:125:THR:CG2  | 1:C:524:THR:HG23 | 2.36                     | 0.56              |
| 1:D:567:SER:HB2  | 1:E:49:THR:HG21  | 1.87                     | 0.56              |
| 1:D:392:ASN:HB3  | 1:D:402:GLN:NE2  | 2.21                     | 0.56              |
| 1:C:392:ASN:HB3  | 1:C:402:GLN:NE2  | 2.21                     | 0.56              |
| 1:E:392:ASN:HB3  | 1:E:402:GLN:NE2  | 2.21                     | 0.56              |
| 1:A:434:SER:N    | 1:B:555:TYR:HE2  | 2.04                     | 0.56              |
| 1:C:233:ASN:O    | 1:C:233:ASN:CG   | 2.43                     | 0.56              |
| 1:B:403:TYR:CD1  | 1:B:504:ILE:HD13 | 2.39                     | 0.56              |
| 1:E:74:ASN:ND2   | 1:E:556:LYS:HZ1  | 2.04                     | 0.56              |
| 1:E:493:THR:HG22 | 1:E:494:HIS:N    | 2.21                     | 0.56              |
| 1:A:125:THR:CG2  | 1:A:524:THR:HG23 | 2.35                     | 0.56              |
| 1:C:482:TYR:CE1  | 1:C:486:ILE:HD12 | 2.40                     | 0.56              |
| 1:D:273:ILE:O    | 1:D:273:ILE:HG23 | 2.05                     | 0.56              |
| 1:A:392:ASN:HB3  | 1:A:402:GLN:NE2  | 2.21                     | 0.56              |
| 1:A:67:THR:O     | 1:A:68:ARG:HG2   | 2.06                     | 0.56              |
| 1:B:419:ILE:O    | 1:B:423:THR:HG22 | 2.06                     | 0.56              |
| 1:D:134:VAL:HG22 | 1:D:173:GLY:O    | 2.05                     | 0.56              |
| 1:B:567:SER:HB2  | 1:C:49:THR:HG21  | 1.87                     | 0.56              |
| 1:C:428:PRO:O    | 1:C:429:ASP:HB3  | 2.06                     | 0.56              |
| 1:D:494:HIS:C    | 1:D:496:PHE:H    | 2.07                     | 0.56              |
| 1:E:482:TYR:CE1  | 1:E:486:ILE:HD12 | 2.40                     | 0.56              |
| 1:B:273:ILE:O    | 1:B:273:ILE:HG23 | 2.05                     | 0.56              |
| 1:E:125:THR:CG2  | 1:E:524:THR:HG23 | 2.35                     | 0.56              |
| 1:A:273:ILE:O    | 1:A:273:ILE:HG23 | 2.05                     | 0.56              |
| 1:A:68:ARG:NH1   | 1:A:68:ARG:CG    | 2.66                     | 0.56              |
| 1:C:403:TYR:CD1  | 1:C:504:ILE:HD13 | 2.39                     | 0.56              |
| 1:A:493:THR:HG22 | 1:A:494:HIS:N    | 2.21                     | 0.56              |
| 1:D:67:THR:O     | 1:D:68:ARG:HG2   | 2.06                     | 0.55              |
| 1:C:283:ILE:O    | 1:C:401:THR:HG23 | 2.07                     | 0.55              |
| 1:A:555:TYR:HE2  | 1:E:434:SER:N    | 2.04                     | 0.55              |
| 1:C:434:SER:N    | 1:D:555:TYR:HE2  | 2.04                     | 0.55              |
| 1:B:403:TYR:HD1  | 1:B:504:ILE:CD1  | 2.20                     | 0.55              |
| 1:A:49:THR:HG21  | 1:E:567:SER:HB2  | 1.87                     | 0.55              |
| 1:A:494:HIS:C    | 1:A:496:PHE:H    | 2.08                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:125:THR:CG2  | 1:B:524:THR:HG23 | 2.36                     | 0.55              |
| 1:B:501:GLU:H    | 1:B:501:GLU:CD   | 2.10                     | 0.55              |
| 1:D:233:ASN:O    | 1:D:233:ASN:CG   | 2.42                     | 0.55              |
| 1:A:479:GLN:HG2  | 1:A:479:GLN:O    | 2.05                     | 0.55              |
| 1:D:68:ARG:HH11  | 1:D:68:ARG:CG    | 2.07                     | 0.55              |
| 1:D:419:ILE:O    | 1:D:423:THR:HG22 | 2.06                     | 0.55              |
| 1:D:403:TYR:HD1  | 1:D:504:ILE:CD1  | 2.19                     | 0.55              |
| 1:C:440:SER:C    | 1:C:442:PRO:HD3  | 2.27                     | 0.55              |
| 1:A:440:SER:C    | 1:A:442:PRO:HD3  | 2.27                     | 0.55              |
| 1:C:197:ARG:HG3  | 1:C:198:GLN:H    | 1.71                     | 0.55              |
| 1:E:283:ILE:O    | 1:E:401:THR:HG23 | 2.06                     | 0.55              |
| 1:A:283:ILE:O    | 1:A:401:THR:HG23 | 2.07                     | 0.55              |
| 1:B:283:ILE:O    | 1:B:401:THR:HG23 | 2.07                     | 0.55              |
| 1:A:428:PRO:O    | 1:A:429:ASP:HB3  | 2.06                     | 0.55              |
| 1:B:493:THR:HG22 | 1:B:494:HIS:N    | 2.21                     | 0.55              |
| 1:C:449:VAL:HG22 | 1:D:67:THR:HG21  | 1.89                     | 0.55              |
| 1:A:419:ILE:O    | 1:A:423:THR:HG22 | 2.06                     | 0.55              |
| 1:C:67:THR:O     | 1:C:68:ARG:HG2   | 2.06                     | 0.55              |
| 1:E:67:THR:O     | 1:E:68:ARG:HG2   | 2.06                     | 0.55              |
| 1:D:440:SER:C    | 1:D:442:PRO:HD3  | 2.27                     | 0.55              |
| 1:A:214:ASN:C    | 1:A:214:ASN:ND2  | 2.55                     | 0.55              |
| 1:B:428:PRO:O    | 1:B:429:ASP:HB3  | 2.06                     | 0.55              |
| 1:E:494:HIS:C    | 1:E:496:PHE:H    | 2.08                     | 0.55              |
| 1:D:125:THR:CG2  | 1:D:524:THR:HG23 | 2.35                     | 0.55              |
| 1:A:501:GLU:CD   | 1:A:501:GLU:H    | 2.10                     | 0.55              |
| 1:E:501:GLU:H    | 1:E:501:GLU:CD   | 2.10                     | 0.55              |
| 1:B:449:VAL:HG22 | 1:C:67:THR:HG21  | 1.88                     | 0.55              |
| 1:D:449:VAL:HG22 | 1:E:67:THR:HG21  | 1.89                     | 0.55              |
| 1:C:134:VAL:HG22 | 1:C:173:GLY:O    | 2.05                     | 0.55              |
| 1:A:444:MET:HE3  | 1:A:561:VAL:HG21 | 1.88                     | 0.55              |
| 1:A:449:VAL:HG22 | 1:B:67:THR:HG21  | 1.89                     | 0.55              |
| 1:B:67:THR:O     | 1:B:68:ARG:HG2   | 2.06                     | 0.55              |
| 1:E:197:ARG:HG3  | 1:E:198:GLN:H    | 1.71                     | 0.55              |
| 1:D:493:THR:HG22 | 1:D:494:HIS:N    | 2.21                     | 0.55              |
| 1:C:136:GLU:O    | 1:C:137:PHE:HB2  | 2.07                     | 0.55              |
| 1:A:197:ARG:HG3  | 1:A:198:GLN:H    | 1.71                     | 0.55              |
| 1:D:215:PHE:HE1  | 1:D:241:ILE:HD11 | 1.71                     | 0.55              |
| 1:C:273:ILE:HG23 | 1:C:273:ILE:O    | 2.05                     | 0.55              |
| 1:A:529:LEU:HD21 | 1:B:68:ARG:NE    | 2.22                     | 0.55              |
| 1:E:419:ILE:O    | 1:E:423:THR:HG22 | 2.06                     | 0.55              |
| 1:D:434:SER:N    | 1:E:555:TYR:HE2  | 2.04                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:136:GLU:O    | 1:B:137:PHE:HB2  | 2.07                     | 0.55              |
| 1:A:403:TYR:CD1  | 1:A:504:ILE:HD13 | 2.39                     | 0.54              |
| 1:C:419:ILE:O    | 1:C:423:THR:HG22 | 2.06                     | 0.54              |
| 1:D:83:ASN:OD1   | 1:D:83:ASN:N     | 2.26                     | 0.54              |
| 1:B:440:SER:C    | 1:B:442:PRO:HD3  | 2.27                     | 0.54              |
| 1:A:74:ASN:ND2   | 1:A:556:LYS:HZ1  | 2.05                     | 0.54              |
| 1:B:525:ASP:C    | 1:B:525:ASP:OD1  | 2.45                     | 0.54              |
| 1:D:278:LEU:HD23 | 1:D:419:ILE:CD1  | 2.30                     | 0.54              |
| 1:C:544:THR:HG21 | 1:C:548:ARG:HA   | 1.89                     | 0.54              |
| 1:D:283:ILE:O    | 1:D:401:THR:HG23 | 2.07                     | 0.54              |
| 1:A:505:LEU:O    | 1:A:506:ALA:O    | 2.26                     | 0.54              |
| 1:E:428:PRO:O    | 1:E:429:ASP:HB3  | 2.07                     | 0.54              |
| 1:B:263:LYS:HZ3  | 1:B:268:GLN:HB2  | 1.73                     | 0.54              |
| 1:D:136:GLU:O    | 1:D:137:PHE:HB2  | 2.07                     | 0.54              |
| 1:B:529:LEU:HD21 | 1:C:68:ARG:NE    | 2.23                     | 0.54              |
| 1:D:428:PRO:O    | 1:D:429:ASP:HB3  | 2.06                     | 0.54              |
| 1:A:263:LYS:HZ3  | 1:A:268:GLN:HB2  | 1.73                     | 0.54              |
| 1:C:501:GLU:H    | 1:C:501:GLU:CD   | 2.10                     | 0.54              |
| 1:D:463:VAL:HB   | 1:D:529:LEU:CD1  | 2.38                     | 0.54              |
| 1:E:440:SER:C    | 1:E:442:PRO:HD3  | 2.27                     | 0.54              |
| 1:C:211:ASP:CG   | 1:C:212:THR:H    | 2.10                     | 0.54              |
| 1:E:211:ASP:CG   | 1:E:212:THR:H    | 2.10                     | 0.54              |
| 1:D:385:ASP:O    | 1:D:386:SER:C    | 2.45                     | 0.54              |
| 1:C:525:ASP:C    | 1:C:525:ASP:OD1  | 2.45                     | 0.54              |
| 1:D:501:GLU:H    | 1:D:501:GLU:CD   | 2.10                     | 0.54              |
| 1:E:215:PHE:HE1  | 1:E:241:ILE:HD11 | 1.71                     | 0.54              |
| 1:D:525:ASP:OD1  | 1:D:525:ASP:C    | 2.45                     | 0.54              |
| 1:E:389:ARG:HG2  | 1:E:389:ARG:HH11 | 1.73                     | 0.54              |
| 1:E:505:LEU:O    | 1:E:506:ALA:O    | 2.26                     | 0.54              |
| 1:E:192:TYR:CZ   | 1:E:197:ARG:HB3  | 2.43                     | 0.54              |
| 1:A:525:ASP:C    | 1:A:525:ASP:OD1  | 2.45                     | 0.54              |
| 1:B:203:GLU:C    | 1:B:205:ASP:H    | 2.11                     | 0.54              |
| 1:E:208:VAL:O    | 1:E:208:VAL:HG23 | 2.08                     | 0.54              |
| 1:E:463:VAL:HB   | 1:E:529:LEU:CD1  | 2.38                     | 0.54              |
| 1:A:68:ARG:NE    | 1:E:529:LEU:HD21 | 2.23                     | 0.54              |
| 1:D:505:LEU:O    | 1:D:506:ALA:O    | 2.26                     | 0.54              |
| 1:C:505:LEU:O    | 1:C:506:ALA:O    | 2.26                     | 0.54              |
| 1:B:192:TYR:CZ   | 1:B:197:ARG:HB3  | 2.43                     | 0.54              |
| 1:D:197:ARG:HG3  | 1:D:198:GLN:H    | 1.71                     | 0.54              |
| 1:E:525:ASP:C    | 1:E:525:ASP:OD1  | 2.45                     | 0.54              |
| 1:A:136:GLU:O    | 1:A:137:PHE:HB2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:192:TYR:CZ   | 1:D:197:ARG:HB3  | 2.43                     | 0.54              |
| 1:C:192:TYR:CZ   | 1:C:197:ARG:HB3  | 2.43                     | 0.54              |
| 1:A:192:TYR:CZ   | 1:A:197:ARG:HB3  | 2.43                     | 0.54              |
| 1:B:385:ASP:O    | 1:B:386:SER:C    | 2.45                     | 0.54              |
| 1:C:385:ASP:O    | 1:C:386:SER:C    | 2.45                     | 0.54              |
| 1:C:493:THR:HG22 | 1:C:494:HIS:N    | 2.21                     | 0.54              |
| 1:B:208:VAL:O    | 1:B:208:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:239:ASP:OD1  | 1:A:239:ASP:C    | 2.46                     | 0.54              |
| 1:A:67:THR:HG21  | 1:E:449:VAL:HG22 | 1.89                     | 0.54              |
| 1:E:136:GLU:O    | 1:E:137:PHE:HB2  | 2.07                     | 0.54              |
| 1:A:203:GLU:C    | 1:A:205:ASP:H    | 2.11                     | 0.54              |
| 1:D:211:ASP:CG   | 1:D:212:THR:H    | 2.10                     | 0.53              |
| 1:B:197:ARG:HG3  | 1:B:198:GLN:H    | 1.71                     | 0.53              |
| 1:E:544:THR:HG21 | 1:E:548:ARG:HA   | 1.89                     | 0.53              |
| 1:A:385:ASP:O    | 1:A:386:SER:C    | 2.45                     | 0.53              |
| 1:E:385:ASP:O    | 1:E:386:SER:C    | 2.46                     | 0.53              |
| 1:C:239:ASP:OD1  | 1:C:239:ASP:C    | 2.45                     | 0.53              |
| 1:E:239:ASP:OD1  | 1:E:239:ASP:C    | 2.46                     | 0.53              |
| 1:D:449:VAL:HG12 | 1:D:450:THR:N    | 2.23                     | 0.53              |
| 1:E:403:TYR:HD1  | 1:E:504:ILE:CD1  | 2.19                     | 0.53              |
| 1:B:544:THR:HG21 | 1:B:548:ARG:HA   | 1.89                     | 0.53              |
| 1:D:478:ASP:C    | 1:D:480:ALA:H    | 2.12                     | 0.53              |
| 1:A:478:ASP:C    | 1:A:480:ALA:H    | 2.12                     | 0.53              |
| 1:C:203:GLU:C    | 1:C:205:ASP:H    | 2.11                     | 0.53              |
| 1:B:215:PHE:HE1  | 1:B:241:ILE:HD11 | 1.71                     | 0.53              |
| 1:B:478:ASP:C    | 1:B:480:ALA:H    | 2.12                     | 0.53              |
| 1:B:389:ARG:HH11 | 1:B:389:ARG:HG2  | 1.73                     | 0.53              |
| 1:B:154:THR:CG2  | 1:B:155:LYS:N    | 2.72                     | 0.53              |
| 1:D:151:ARG:HG3  | 1:D:161:LEU:CD2  | 2.39                     | 0.53              |
| 1:C:478:ASP:C    | 1:C:480:ALA:H    | 2.12                     | 0.53              |
| 1:B:452:ARG:NH2  | 1:C:99:ASN:HD22  | 2.07                     | 0.53              |
| 1:A:463:VAL:HB   | 1:A:529:LEU:CD1  | 2.38                     | 0.53              |
| 1:D:529:LEU:HD21 | 1:E:68:ARG:NE    | 2.23                     | 0.53              |
| 1:A:389:ARG:HG2  | 1:A:389:ARG:HH11 | 1.73                     | 0.53              |
| 1:A:295:SER:HB3  | 1:A:377:PRO:CG   | 2.33                     | 0.53              |
| 1:C:93:THR:HG22  | 1:C:94:THR:N     | 2.23                     | 0.53              |
| 1:D:208:VAL:HG23 | 1:D:208:VAL:O    | 2.08                     | 0.53              |
| 1:A:93:THR:HG22  | 1:A:94:THR:N     | 2.23                     | 0.53              |
| 1:C:403:TYR:HD1  | 1:C:504:ILE:CD1  | 2.19                     | 0.53              |
| 1:C:69:VAL:CG2   | 1:C:561:VAL:HB   | 2.39                     | 0.53              |
| 1:C:529:LEU:HD21 | 1:D:68:ARG:NE    | 2.23                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:154:THR:CG2  | 1:D:155:LYS:N    | 2.72                     | 0.53              |
| 1:E:203:GLU:C    | 1:E:205:ASP:H    | 2.11                     | 0.53              |
| 1:D:389:ARG:HH11 | 1:D:389:ARG:HG2  | 1.73                     | 0.53              |
| 1:B:211:ASP:CG   | 1:B:212:THR:H    | 2.10                     | 0.53              |
| 1:A:236:PHE:O    | 1:A:237:HIS:HB3  | 2.09                     | 0.53              |
| 1:D:69:VAL:CG2   | 1:D:561:VAL:HB   | 2.39                     | 0.53              |
| 1:C:386:SER:O    | 1:C:387:LYS:CB   | 2.57                     | 0.53              |
| 1:D:151:ARG:HG3  | 1:D:161:LEU:HD21 | 1.91                     | 0.53              |
| 1:D:93:THR:HG22  | 1:D:94:THR:N     | 2.23                     | 0.53              |
| 1:B:449:VAL:HG12 | 1:B:450:THR:N    | 2.23                     | 0.53              |
| 1:B:505:LEU:O    | 1:B:506:ALA:O    | 2.26                     | 0.53              |
| 1:E:292:TYR:HA   | 1:E:377:PRO:HG3  | 1.91                     | 0.53              |
| 1:C:236:PHE:O    | 1:C:237:HIS:HB3  | 2.09                     | 0.53              |
| 1:C:154:THR:CG2  | 1:C:155:LYS:N    | 2.72                     | 0.53              |
| 1:E:69:VAL:CG2   | 1:E:561:VAL:HB   | 2.39                     | 0.53              |
| 1:C:151:ARG:HG3  | 1:C:161:LEU:HD21 | 1.91                     | 0.53              |
| 1:B:222:VAL:HG13 | 1:B:223:THR:N    | 2.24                     | 0.53              |
| 1:E:151:ARG:HG3  | 1:E:161:LEU:HD21 | 1.91                     | 0.53              |
| 1:C:295:SER:HB3  | 1:C:377:PRO:CG   | 2.33                     | 0.52              |
| 1:C:197:ARG:CG   | 1:C:198:GLN:N    | 2.72                     | 0.52              |
| 1:A:544:THR:HG21 | 1:A:548:ARG:HA   | 1.89                     | 0.52              |
| 1:C:222:VAL:HG13 | 1:C:223:THR:N    | 2.24                     | 0.52              |
| 1:E:151:ARG:HG3  | 1:E:161:LEU:CD2  | 2.39                     | 0.52              |
| 1:E:120:GLY:O    | 1:E:563:PRO:HA   | 2.10                     | 0.52              |
| 1:C:208:VAL:HG23 | 1:C:208:VAL:O    | 2.08                     | 0.52              |
| 1:A:449:VAL:HG12 | 1:A:450:THR:N    | 2.23                     | 0.52              |
| 1:D:236:PHE:O    | 1:D:237:HIS:HB3  | 2.09                     | 0.52              |
| 1:C:180:THR:HG21 | 1:C:258:LEU:CD2  | 2.40                     | 0.52              |
| 1:A:215:PHE:HE1  | 1:A:241:ILE:HD11 | 1.71                     | 0.52              |
| 1:B:69:VAL:CG2   | 1:B:561:VAL:HB   | 2.39                     | 0.52              |
| 1:D:266:PRO:O    | 1:D:268:GLN:N    | 2.43                     | 0.52              |
| 1:E:93:THR:HG22  | 1:E:94:THR:N     | 2.23                     | 0.52              |
| 1:B:239:ASP:OD1  | 1:B:239:ASP:C    | 2.45                     | 0.52              |
| 1:A:211:ASP:CG   | 1:A:212:THR:H    | 2.10                     | 0.52              |
| 1:D:180:THR:HG21 | 1:D:258:LEU:CD2  | 2.40                     | 0.52              |
| 1:D:53:ASN:O     | 1:D:54:SER:C     | 2.48                     | 0.52              |
| 1:A:154:THR:CG2  | 1:A:155:LYS:N    | 2.72                     | 0.52              |
| 1:A:69:VAL:CG2   | 1:A:561:VAL:HB   | 2.39                     | 0.52              |
| 1:A:386:SER:O    | 1:A:387:LYS:CB   | 2.57                     | 0.52              |
| 1:B:151:ARG:HG3  | 1:B:161:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:151:ARG:HG3  | 1:A:161:LEU:CD2  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:120:GLY:O    | 1:B:563:PRO:HA   | 2.10                     | 0.52              |
| 1:B:463:VAL:HB   | 1:B:529:LEU:CD1  | 2.38                     | 0.52              |
| 1:C:449:VAL:HG12 | 1:C:450:THR:N    | 2.23                     | 0.52              |
| 1:A:452:ARG:NH2  | 1:B:99:ASN:HD22  | 2.06                     | 0.52              |
| 1:C:389:ARG:HH11 | 1:C:389:ARG:HG2  | 1.73                     | 0.52              |
| 1:B:180:THR:HG21 | 1:B:258:LEU:CD2  | 2.40                     | 0.52              |
| 1:E:180:THR:HG21 | 1:E:258:LEU:CD2  | 2.40                     | 0.52              |
| 1:E:236:PHE:O    | 1:E:237:HIS:HB3  | 2.09                     | 0.52              |
| 1:B:266:PRO:O    | 1:B:268:GLN:N    | 2.43                     | 0.52              |
| 1:C:151:ARG:HG3  | 1:C:161:LEU:CD2  | 2.39                     | 0.52              |
| 1:E:171:PRO:O    | 1:E:175:TYR:OH   | 2.25                     | 0.52              |
| 1:E:449:VAL:HG12 | 1:E:450:THR:N    | 2.23                     | 0.52              |
| 1:D:441:LEU:N    | 1:D:442:PRO:HD3  | 2.24                     | 0.52              |
| 1:B:197:ARG:CG   | 1:B:198:GLN:N    | 2.72                     | 0.52              |
| 1:D:197:ARG:CG   | 1:D:198:GLN:N    | 2.72                     | 0.52              |
| 1:E:154:THR:CG2  | 1:E:155:LYS:N    | 2.71                     | 0.52              |
| 1:C:403:TYR:CD1  | 1:C:504:ILE:HG21 | 2.45                     | 0.52              |
| 1:A:211:ASP:HA   | 1:A:508:PRO:HG2  | 1.89                     | 0.52              |
| 1:E:197:ARG:CG   | 1:E:198:GLN:N    | 2.72                     | 0.52              |
| 1:D:386:SER:O    | 1:D:387:LYS:CB   | 2.57                     | 0.52              |
| 1:C:520:VAL:HG23 | 1:C:521:PRO:HD2  | 1.92                     | 0.52              |
| 1:E:520:VAL:HG23 | 1:E:521:PRO:HD2  | 1.92                     | 0.52              |
| 1:E:478:ASP:C    | 1:E:480:ALA:H    | 2.12                     | 0.52              |
| 1:A:208:VAL:O    | 1:A:208:VAL:HG23 | 2.08                     | 0.52              |
| 1:C:463:VAL:HB   | 1:C:529:LEU:CD1  | 2.38                     | 0.52              |
| 1:A:403:TYR:HD1  | 1:A:504:ILE:CD1  | 2.20                     | 0.52              |
| 1:C:211:ASP:HA   | 1:C:508:PRO:HG2  | 1.89                     | 0.52              |
| 1:C:262:ARG:HH11 | 1:D:130:ASN:HD22 | 1.55                     | 0.52              |
| 1:A:171:PRO:O    | 1:A:175:TYR:OH   | 2.25                     | 0.52              |
| 1:C:74:ASN:HD22  | 1:C:556:LYS:HZ1  | 1.58                     | 0.52              |
| 1:E:386:SER:O    | 1:E:387:LYS:CB   | 2.57                     | 0.52              |
| 1:E:222:VAL:HG13 | 1:E:223:THR:N    | 2.24                     | 0.52              |
| 1:A:266:PRO:O    | 1:A:268:GLN:N    | 2.43                     | 0.52              |
| 1:B:93:THR:HG22  | 1:B:94:THR:N     | 2.23                     | 0.52              |
| 1:A:99:ASN:HD22  | 1:E:452:ARG:NH2  | 2.07                     | 0.52              |
| 1:B:403:TYR:CD1  | 1:B:504:ILE:HG21 | 2.45                     | 0.52              |
| 1:A:197:ARG:CG   | 1:A:198:GLN:N    | 2.72                     | 0.52              |
| 1:D:222:VAL:HG13 | 1:D:223:THR:N    | 2.24                     | 0.52              |
| 1:A:222:VAL:HG13 | 1:A:223:THR:N    | 2.24                     | 0.52              |
| 1:B:125:THR:HG22 | 1:B:524:THR:HG23 | 1.92                     | 0.52              |
| 1:B:151:ARG:HG3  | 1:B:161:LEU:CD2  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:120:GLY:O    | 1:D:563:PRO:HA   | 2.10                     | 0.52              |
| 1:A:180:THR:HG21 | 1:A:258:LEU:CD2  | 2.40                     | 0.52              |
| 1:D:125:THR:CG2  | 1:D:524:THR:CG2  | 2.88                     | 0.52              |
| 1:D:151:ARG:HB3  | 1:D:200:GLY:O    | 2.10                     | 0.52              |
| 1:E:403:TYR:CD1  | 1:E:504:ILE:HG21 | 2.45                     | 0.52              |
| 1:E:295:SER:HB3  | 1:E:377:PRO:CG   | 2.33                     | 0.52              |
| 1:C:263:LYS:HZ3  | 1:C:268:GLN:HB2  | 1.74                     | 0.52              |
| 1:D:452:ARG:NH2  | 1:E:99:ASN:HD22  | 2.06                     | 0.51              |
| 1:A:441:LEU:N    | 1:A:442:PRO:HD3  | 2.24                     | 0.51              |
| 1:C:125:THR:CG2  | 1:C:524:THR:CG2  | 2.88                     | 0.51              |
| 1:C:295:SER:OG   | 1:C:377:PRO:HD3  | 2.10                     | 0.51              |
| 1:A:53:ASN:O     | 1:A:54:SER:C     | 2.48                     | 0.51              |
| 1:C:215:PHE:HE1  | 1:C:241:ILE:HD11 | 1.71                     | 0.51              |
| 1:C:151:ARG:HB3  | 1:C:200:GLY:O    | 2.10                     | 0.51              |
| 1:E:151:ARG:HB3  | 1:E:200:GLY:O    | 2.10                     | 0.51              |
| 1:D:295:SER:OG   | 1:D:377:PRO:HD3  | 2.10                     | 0.51              |
| 1:B:441:LEU:N    | 1:B:442:PRO:HD3  | 2.24                     | 0.51              |
| 1:C:436:GLN:CD   | 1:D:556:LYS:HZ3  | 2.14                     | 0.51              |
| 1:A:125:THR:CG2  | 1:A:524:THR:CG2  | 2.88                     | 0.51              |
| 1:E:125:THR:CG2  | 1:E:524:THR:CG2  | 2.88                     | 0.51              |
| 1:D:138:MET:HB3  | 1:D:254:ARG:NH1  | 2.26                     | 0.51              |
| 1:D:239:ASP:C    | 1:D:239:ASP:OD1  | 2.45                     | 0.51              |
| 1:C:171:PRO:O    | 1:C:175:TYR:OH   | 2.25                     | 0.51              |
| 1:C:132:PRO:HD3  | 1:C:553:TYR:CE2  | 2.46                     | 0.51              |
| 1:D:425:LEU:HD12 | 1:D:426:CYS:N    | 2.26                     | 0.51              |
| 1:E:132:PRO:HD3  | 1:E:553:TYR:CE2  | 2.46                     | 0.51              |
| 1:E:53:ASN:O     | 1:E:54:SER:C     | 2.48                     | 0.51              |
| 1:B:53:ASN:O     | 1:B:54:SER:C     | 2.48                     | 0.51              |
| 1:E:494:HIS:C    | 1:E:496:PHE:N    | 2.64                     | 0.51              |
| 1:C:125:THR:HG22 | 1:C:524:THR:HG23 | 1.92                     | 0.51              |
| 1:A:151:ARG:HB3  | 1:A:200:GLY:O    | 2.10                     | 0.51              |
| 1:A:151:ARG:HG3  | 1:A:161:LEU:HD21 | 1.91                     | 0.51              |
| 1:A:295:SER:OG   | 1:A:377:PRO:HD3  | 2.10                     | 0.51              |
| 1:B:211:ASP:HA   | 1:B:508:PRO:HG2  | 1.89                     | 0.51              |
| 1:B:444:MET:HE3  | 1:B:561:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:125:THR:HG22 | 1:D:524:THR:HG23 | 1.92                     | 0.51              |
| 1:B:125:THR:CG2  | 1:B:524:THR:CG2  | 2.88                     | 0.51              |
| 1:D:203:GLU:C    | 1:D:205:ASP:H    | 2.11                     | 0.51              |
| 1:A:120:GLY:O    | 1:A:563:PRO:HA   | 2.10                     | 0.51              |
| 1:E:264:ARG:NH1  | 1:E:424:LEU:HD13 | 2.26                     | 0.51              |
| 1:B:295:SER:OG   | 1:B:377:PRO:HD3  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:451:PHE:CE1  | 1:D:97:GLN:HB2   | 2.46                     | 0.51              |
| 1:B:132:PRO:HD3  | 1:B:553:TYR:CE2  | 2.46                     | 0.51              |
| 1:D:132:PRO:HD3  | 1:D:553:TYR:CE2  | 2.46                     | 0.51              |
| 1:D:547:ARG:O    | 1:D:548:ARG:HB2  | 2.11                     | 0.51              |
| 1:E:425:LEU:HD12 | 1:E:426:CYS:N    | 2.25                     | 0.51              |
| 1:A:520:VAL:HG23 | 1:A:521:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:151:ARG:HB3  | 1:B:200:GLY:O    | 2.10                     | 0.51              |
| 1:B:138:MET:HB3  | 1:B:254:ARG:NH1  | 2.26                     | 0.51              |
| 1:B:264:ARG:NH1  | 1:B:424:LEU:HD13 | 2.26                     | 0.51              |
| 1:C:120:GLY:O    | 1:C:563:PRO:HA   | 2.10                     | 0.51              |
| 1:B:295:SER:HB3  | 1:B:377:PRO:CG   | 2.33                     | 0.51              |
| 1:E:403:TYR:CD1  | 1:E:504:ILE:HD13 | 2.39                     | 0.51              |
| 1:D:295:SER:HB3  | 1:D:377:PRO:CG   | 2.33                     | 0.51              |
| 1:C:441:LEU:N    | 1:C:442:PRO:HD3  | 2.24                     | 0.51              |
| 1:A:60:LEU:O     | 1:A:61:ALA:CB    | 2.59                     | 0.51              |
| 1:C:60:LEU:O     | 1:C:61:ALA:CB    | 2.59                     | 0.51              |
| 1:D:544:THR:HG21 | 1:D:548:ARG:HA   | 1.89                     | 0.51              |
| 1:A:556:LYS:HZ3  | 1:E:436:GLN:NE2  | 2.08                     | 0.51              |
| 1:C:494:HIS:C    | 1:C:496:PHE:N    | 2.64                     | 0.51              |
| 1:D:494:HIS:C    | 1:D:496:PHE:N    | 2.64                     | 0.51              |
| 1:E:125:THR:HG22 | 1:E:524:THR:HG23 | 1.92                     | 0.51              |
| 1:C:395:SER:C    | 1:C:397:ASP:H    | 2.14                     | 0.51              |
| 1:E:263:LYS:HZ3  | 1:E:268:GLN:HB2  | 1.75                     | 0.51              |
| 1:C:138:MET:HB3  | 1:C:254:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:403:TYR:CD1  | 1:A:504:ILE:HG21 | 2.45                     | 0.51              |
| 1:D:403:TYR:CD1  | 1:D:504:ILE:HG21 | 2.45                     | 0.51              |
| 1:A:97:GLN:HB2   | 1:E:451:PHE:CE1  | 2.46                     | 0.51              |
| 1:B:451:PHE:CE1  | 1:C:97:GLN:HB2   | 2.46                     | 0.51              |
| 1:C:53:ASN:O     | 1:C:54:SER:C     | 2.48                     | 0.51              |
| 1:E:197:ARG:HG3  | 1:E:198:GLN:HG2  | 1.93                     | 0.51              |
| 1:D:430:VAL:HG23 | 1:D:517:SER:HB2  | 1.93                     | 0.51              |
| 1:B:520:VAL:HG23 | 1:B:521:PRO:HD2  | 1.92                     | 0.51              |
| 1:A:264:ARG:NH1  | 1:A:424:LEU:HD13 | 2.26                     | 0.51              |
| 1:C:491:SER:O    | 1:C:492:LEU:O    | 2.29                     | 0.51              |
| 1:E:295:SER:OG   | 1:E:377:PRO:HD3  | 2.10                     | 0.51              |
| 1:E:441:LEU:N    | 1:E:442:PRO:HD3  | 2.24                     | 0.51              |
| 1:C:425:LEU:HD12 | 1:C:426:CYS:N    | 2.25                     | 0.51              |
| 1:D:264:ARG:NH1  | 1:D:424:LEU:HD13 | 2.26                     | 0.51              |
| 1:C:452:ARG:NH2  | 1:D:99:ASN:HD22  | 2.07                     | 0.51              |
| 1:D:451:PHE:CE1  | 1:E:97:GLN:HB2   | 2.46                     | 0.51              |
| 1:A:451:PHE:CE1  | 1:B:97:GLN:HB2   | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:236:PHE:O    | 1:B:237:HIS:HB3  | 2.09                     | 0.51              |
| 1:C:547:ARG:O    | 1:C:548:ARG:HB2  | 2.11                     | 0.51              |
| 1:A:132:PRO:HD3  | 1:A:553:TYR:CE2  | 2.46                     | 0.51              |
| 1:C:264:ARG:NH1  | 1:C:424:LEU:HD13 | 2.26                     | 0.51              |
| 1:A:138:MET:HB3  | 1:A:254:ARG:NH1  | 2.26                     | 0.51              |
| 1:B:135:ASN:HA   | 1:B:172:GLU:HG2  | 1.93                     | 0.50              |
| 1:A:494:HIS:C    | 1:A:496:PHE:N    | 2.64                     | 0.50              |
| 1:A:125:THR:HG22 | 1:A:524:THR:HG23 | 1.92                     | 0.50              |
| 1:A:98:ASN:ND2   | 1:E:452:ARG:HE   | 2.08                     | 0.50              |
| 1:D:451:PHE:HE1  | 1:E:97:GLN:HG3   | 1.76                     | 0.50              |
| 1:B:451:PHE:CE1  | 1:C:97:GLN:HG3   | 2.47                     | 0.50              |
| 1:C:567:SER:CB   | 1:D:49:THR:HG21  | 2.41                     | 0.50              |
| 1:A:556:LYS:HZ3  | 1:E:436:GLN:CD   | 2.14                     | 0.50              |
| 1:B:427:THR:HG23 | 1:B:428:PRO:HD2  | 1.94                     | 0.50              |
| 1:E:430:VAL:HG23 | 1:E:517:SER:HB2  | 1.93                     | 0.50              |
| 1:C:266:PRO:C    | 1:C:268:GLN:H    | 2.15                     | 0.50              |
| 1:D:520:VAL:HG23 | 1:D:521:PRO:HD2  | 1.92                     | 0.50              |
| 1:D:233:ASN:O    | 1:D:233:ASN:OD1  | 2.30                     | 0.50              |
| 1:D:243:LEU:CD2  | 1:D:403:TYR:HD2  | 2.24                     | 0.50              |
| 1:D:197:ARG:HG3  | 1:D:198:GLN:HG2  | 1.93                     | 0.50              |
| 1:A:547:ARG:O    | 1:A:548:ARG:HB2  | 2.11                     | 0.50              |
| 1:E:138:MET:HB3  | 1:E:254:ARG:NH1  | 2.26                     | 0.50              |
| 1:D:60:LEU:O     | 1:D:61:ALA:CB    | 2.59                     | 0.50              |
| 1:B:60:LEU:O     | 1:B:61:ALA:CB    | 2.59                     | 0.50              |
| 1:A:451:PHE:HE1  | 1:B:97:GLN:HG3   | 1.76                     | 0.50              |
| 1:E:192:TYR:CD2  | 1:E:193:LEU:HD23 | 2.47                     | 0.50              |
| 1:D:436:GLN:CD   | 1:E:556:LYS:HZ3  | 2.14                     | 0.50              |
| 1:A:233:ASN:O    | 1:A:233:ASN:OD1  | 2.30                     | 0.50              |
| 1:E:243:LEU:CD2  | 1:E:403:TYR:HD2  | 2.24                     | 0.50              |
| 1:C:451:PHE:CE1  | 1:D:97:GLN:HG3   | 2.47                     | 0.50              |
| 1:A:451:PHE:CE1  | 1:B:97:GLN:HG3   | 2.47                     | 0.50              |
| 1:C:135:ASN:HA   | 1:C:172:GLU:HG2  | 1.94                     | 0.50              |
| 1:E:211:ASP:HA   | 1:E:508:PRO:HG2  | 1.89                     | 0.50              |
| 1:A:197:ARG:HG3  | 1:A:198:GLN:HG2  | 1.93                     | 0.50              |
| 1:D:567:SER:CB   | 1:E:49:THR:HG21  | 2.41                     | 0.50              |
| 1:C:544:THR:HG22 | 1:C:545:ASP:N    | 2.27                     | 0.50              |
| 1:C:266:PRO:O    | 1:C:268:GLN:N    | 2.43                     | 0.50              |
| 1:A:243:LEU:CD2  | 1:A:403:TYR:HD2  | 2.24                     | 0.50              |
| 1:E:243:LEU:CD2  | 1:E:244:PRO:HD3  | 2.42                     | 0.50              |
| 1:A:97:GLN:HG3   | 1:E:451:PHE:CE1  | 2.47                     | 0.50              |
| 1:D:192:TYR:CD2  | 1:D:193:LEU:HD23 | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:178:THR:O    | 1:C:181:ILE:N    | 2.45                     | 0.50              |
| 1:C:192:TYR:CD2  | 1:C:193:LEU:HD23 | 2.47                     | 0.50              |
| 1:D:427:THR:HG23 | 1:D:428:PRO:HD2  | 1.94                     | 0.50              |
| 1:E:427:THR:HG23 | 1:E:428:PRO:HD2  | 1.94                     | 0.50              |
| 1:A:266:PRO:C    | 1:A:268:GLN:H    | 2.15                     | 0.50              |
| 1:A:491:SER:O    | 1:A:492:LEU:O    | 2.29                     | 0.50              |
| 1:C:451:PHE:HE1  | 1:D:97:GLN:HG3   | 1.77                     | 0.50              |
| 1:B:61:ALA:HB1   | 1:B:62:PRO:CD    | 2.42                     | 0.50              |
| 1:D:237:HIS:ND1  | 1:D:238:PRO:O    | 2.45                     | 0.50              |
| 1:B:567:SER:CB   | 1:C:49:THR:HG21  | 2.41                     | 0.50              |
| 1:A:567:SER:CB   | 1:B:49:THR:HG21  | 2.41                     | 0.50              |
| 1:A:178:THR:O    | 1:A:181:ILE:N    | 2.45                     | 0.50              |
| 1:B:544:THR:HG22 | 1:B:545:ASP:N    | 2.26                     | 0.50              |
| 1:B:547:ARG:O    | 1:B:548:ARG:HB2  | 2.11                     | 0.50              |
| 1:A:544:THR:HG22 | 1:A:545:ASP:N    | 2.27                     | 0.50              |
| 1:B:491:SER:O    | 1:B:492:LEU:O    | 2.29                     | 0.50              |
| 1:B:243:LEU:CD2  | 1:B:244:PRO:HD3  | 2.42                     | 0.50              |
| 1:D:451:PHE:CE1  | 1:E:97:GLN:HG3   | 2.47                     | 0.50              |
| 1:E:61:ALA:HB1   | 1:E:62:PRO:CD    | 2.42                     | 0.50              |
| 1:A:61:ALA:HB1   | 1:A:62:PRO:CD    | 2.42                     | 0.50              |
| 1:B:425:LEU:HD12 | 1:B:426:CYS:N    | 2.26                     | 0.50              |
| 1:C:61:ALA:HB1   | 1:C:62:PRO:CD    | 2.42                     | 0.50              |
| 1:D:135:ASN:HA   | 1:D:172:GLU:HG2  | 1.94                     | 0.50              |
| 1:B:395:SER:C    | 1:B:397:ASP:H    | 2.14                     | 0.50              |
| 1:B:266:PRO:C    | 1:B:268:GLN:H    | 2.15                     | 0.50              |
| 1:C:233:ASN:O    | 1:C:233:ASN:OD1  | 2.30                     | 0.50              |
| 1:D:114:ASP:OD1  | 1:D:115:ASP:N    | 2.45                     | 0.50              |
| 1:D:491:SER:O    | 1:D:492:LEU:O    | 2.29                     | 0.50              |
| 1:C:243:LEU:CD2  | 1:C:244:PRO:HD3  | 2.42                     | 0.50              |
| 1:A:192:TYR:CD2  | 1:A:193:LEU:HD23 | 2.47                     | 0.50              |
| 1:E:178:THR:O    | 1:E:181:ILE:N    | 2.45                     | 0.50              |
| 1:E:547:ARG:O    | 1:E:548:ARG:HB2  | 2.11                     | 0.50              |
| 1:B:436:GLN:CD   | 1:C:556:LYS:HZ3  | 2.16                     | 0.50              |
| 1:B:386:SER:O    | 1:B:387:LYS:CB   | 2.57                     | 0.50              |
| 1:D:395:SER:C    | 1:D:397:ASP:H    | 2.14                     | 0.50              |
| 1:E:266:PRO:O    | 1:E:268:GLN:N    | 2.43                     | 0.50              |
| 1:E:266:PRO:C    | 1:E:268:GLN:H    | 2.14                     | 0.50              |
| 1:B:233:ASN:OD1  | 1:B:233:ASN:O    | 2.30                     | 0.50              |
| 1:C:114:ASP:OD1  | 1:C:115:ASP:N    | 2.45                     | 0.50              |
| 1:A:425:LEU:HD12 | 1:A:426:CYS:N    | 2.26                     | 0.49              |
| 1:D:178:THR:O    | 1:D:181:ILE:N    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:197:ARG:HG3  | 1:D:198:GLN:HG3  | 1.94                     | 0.49              |
| 1:B:178:THR:O    | 1:B:181:ILE:N    | 2.45                     | 0.49              |
| 1:A:49:THR:HG21  | 1:E:567:SER:CB   | 2.42                     | 0.49              |
| 1:E:544:THR:HG22 | 1:E:545:ASP:N    | 2.26                     | 0.49              |
| 1:B:494:HIS:C    | 1:B:496:PHE:N    | 2.64                     | 0.49              |
| 1:D:243:LEU:HD22 | 1:D:244:PRO:CD   | 2.43                     | 0.49              |
| 1:C:197:ARG:HG3  | 1:C:198:GLN:HG2  | 1.93                     | 0.49              |
| 1:D:436:GLN:NE2  | 1:E:556:LYS:HZ3  | 2.09                     | 0.49              |
| 1:A:394:ILE:HG22 | 1:A:400:PHE:O    | 2.12                     | 0.49              |
| 1:D:266:PRO:C    | 1:D:268:GLN:H    | 2.15                     | 0.49              |
| 1:B:481:VAL:HG21 | 1:C:482:TYR:OH   | 2.12                     | 0.49              |
| 1:A:486:ILE:HD11 | 1:E:485:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:126:ILE:HG23 | 1:A:523:LEU:HD23 | 1.94                     | 0.49              |
| 1:D:243:LEU:CD2  | 1:D:244:PRO:HD3  | 2.42                     | 0.49              |
| 1:B:212:THR:HG23 | 1:B:508:PRO:HB3  | 1.94                     | 0.49              |
| 1:D:212:THR:HG23 | 1:D:508:PRO:HB3  | 1.94                     | 0.49              |
| 1:D:544:THR:HG22 | 1:D:545:ASP:N    | 2.26                     | 0.49              |
| 1:C:444:MET:HE3  | 1:C:561:VAL:HG21 | 1.94                     | 0.49              |
| 1:D:126:ILE:HG23 | 1:D:523:LEU:HD23 | 1.94                     | 0.49              |
| 1:E:114:ASP:OD1  | 1:E:115:ASP:N    | 2.45                     | 0.49              |
| 1:B:171:PRO:O    | 1:B:175:TYR:OH   | 2.25                     | 0.49              |
| 1:A:243:LEU:CD2  | 1:A:244:PRO:HD3  | 2.42                     | 0.49              |
| 1:D:61:ALA:HB1   | 1:D:62:PRO:CD    | 2.42                     | 0.49              |
| 1:B:129:THR:HG22 | 1:B:553:TYR:O    | 2.13                     | 0.49              |
| 1:E:444:MET:CE   | 1:E:561:VAL:HG21 | 2.43                     | 0.49              |
| 1:A:430:VAL:HG23 | 1:A:517:SER:HB2  | 1.93                     | 0.49              |
| 1:A:395:SER:C    | 1:A:397:ASP:H    | 2.14                     | 0.49              |
| 1:E:491:SER:O    | 1:E:492:LEU:O    | 2.29                     | 0.49              |
| 1:E:67:THR:OG1   | 1:E:68:ARG:N     | 2.45                     | 0.49              |
| 1:C:243:LEU:HD22 | 1:C:244:PRO:CD   | 2.43                     | 0.49              |
| 1:C:237:HIS:ND1  | 1:C:238:PRO:O    | 2.45                     | 0.49              |
| 1:C:91:PHE:N     | 1:C:91:PHE:CD2   | 2.81                     | 0.49              |
| 1:A:129:THR:HG22 | 1:A:553:TYR:O    | 2.13                     | 0.49              |
| 1:A:436:GLN:CD   | 1:B:556:LYS:HZ3  | 2.15                     | 0.49              |
| 1:A:481:VAL:HG21 | 1:B:482:TYR:OH   | 2.13                     | 0.49              |
| 1:A:485:LEU:HD11 | 1:B:486:ILE:HD11 | 1.95                     | 0.49              |
| 1:B:243:LEU:CD2  | 1:B:403:TYR:HD2  | 2.24                     | 0.49              |
| 1:E:60:LEU:O     | 1:E:61:ALA:CB    | 2.59                     | 0.49              |
| 1:B:262:ARG:HH11 | 1:C:130:ASN:HD22 | 1.55                     | 0.49              |
| 1:C:212:THR:HG23 | 1:C:508:PRO:HB3  | 1.94                     | 0.49              |
| 1:E:135:ASN:HA   | 1:E:172:GLU:HG2  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:125:THR:HG22 | 1:E:526:HIS:NE2  | 2.28                     | 0.49              |
| 1:E:394:ILE:HG22 | 1:E:400:PHE:O    | 2.12                     | 0.49              |
| 1:B:114:ASP:OD1  | 1:B:115:ASP:N    | 2.45                     | 0.49              |
| 1:E:243:LEU:HD22 | 1:E:244:PRO:CD   | 2.43                     | 0.49              |
| 1:E:129:THR:HG22 | 1:E:553:TYR:O    | 2.13                     | 0.49              |
| 1:A:262:ARG:HH11 | 1:B:130:ASN:HD22 | 1.56                     | 0.49              |
| 1:B:197:ARG:HG3  | 1:B:198:GLN:HG2  | 1.93                     | 0.49              |
| 1:D:444:MET:CE   | 1:D:561:VAL:HG21 | 2.43                     | 0.49              |
| 1:B:394:ILE:HG22 | 1:B:400:PHE:O    | 2.12                     | 0.49              |
| 1:C:394:ILE:HG22 | 1:C:400:PHE:O    | 2.13                     | 0.49              |
| 1:A:114:ASP:OD1  | 1:A:115:ASP:N    | 2.45                     | 0.49              |
| 1:D:67:THR:OG1   | 1:D:68:ARG:N     | 2.45                     | 0.49              |
| 1:A:452:ARG:HE   | 1:B:98:ASN:ND2   | 2.08                     | 0.49              |
| 1:A:97:GLN:HG3   | 1:E:451:PHE:HE1  | 1.77                     | 0.49              |
| 1:E:211:ASP:OD1  | 1:E:213:ARG:HG2  | 2.13                     | 0.49              |
| 1:B:451:PHE:HE1  | 1:C:97:GLN:HG3   | 1.76                     | 0.49              |
| 1:E:233:ASN:OD1  | 1:E:233:ASN:O    | 2.30                     | 0.49              |
| 1:E:126:ILE:HG23 | 1:E:523:LEU:HD23 | 1.94                     | 0.49              |
| 1:E:449:VAL:HG12 | 1:E:450:THR:HG23 | 1.95                     | 0.49              |
| 1:B:243:LEU:HD22 | 1:B:244:PRO:CD   | 2.43                     | 0.49              |
| 1:C:197:ARG:HG3  | 1:C:198:GLN:HG3  | 1.94                     | 0.49              |
| 1:C:430:VAL:HG23 | 1:C:517:SER:HB2  | 1.93                     | 0.49              |
| 1:B:430:VAL:HG23 | 1:B:517:SER:HB2  | 1.93                     | 0.49              |
| 1:B:452:ARG:HE   | 1:C:98:ASN:ND2   | 2.08                     | 0.49              |
| 1:A:451:PHE:HE2  | 1:A:462:VAL:HG23 | 1.78                     | 0.49              |
| 1:B:192:TYR:CD2  | 1:B:193:LEU:HD23 | 2.47                     | 0.49              |
| 1:D:129:THR:HG22 | 1:D:553:TYR:O    | 2.13                     | 0.49              |
| 1:A:197:ARG:HG3  | 1:A:198:GLN:HG3  | 1.94                     | 0.49              |
| 1:C:427:THR:HG23 | 1:C:428:PRO:HD2  | 1.94                     | 0.49              |
| 1:D:125:THR:HG22 | 1:D:526:HIS:NE2  | 2.28                     | 0.49              |
| 1:D:481:VAL:HG21 | 1:E:482:TYR:OH   | 2.13                     | 0.49              |
| 1:C:243:LEU:CD2  | 1:C:403:TYR:HD2  | 2.24                     | 0.48              |
| 1:A:212:THR:HG23 | 1:A:508:PRO:HB3  | 1.94                     | 0.48              |
| 1:D:214:ASN:HD21 | 1:D:216:ARG:HG2  | 1.78                     | 0.48              |
| 1:B:444:MET:CE   | 1:B:561:VAL:HG21 | 2.43                     | 0.48              |
| 1:D:69:VAL:HG22  | 1:D:561:VAL:HB   | 1.95                     | 0.48              |
| 1:D:444:MET:HE3  | 1:D:561:VAL:HG21 | 1.94                     | 0.48              |
| 1:A:427:THR:HG23 | 1:A:428:PRO:HD2  | 1.94                     | 0.48              |
| 1:D:203:GLU:O    | 1:D:205:ASP:N    | 2.46                     | 0.48              |
| 1:C:449:VAL:HG12 | 1:C:450:THR:HG23 | 1.95                     | 0.48              |
| 1:B:98:ASN:HD22  | 1:B:99:ASN:N     | 2.11                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:441:LEU:HB2  | 1:A:445:MET:HE2  | 1.95                     | 0.48              |
| 1:D:211:ASP:HA   | 1:D:508:PRO:HG2  | 1.89                     | 0.48              |
| 1:B:545:ASP:OD1  | 1:B:549:ARG:HG2  | 2.13                     | 0.48              |
| 1:C:69:VAL:HG22  | 1:C:561:VAL:HB   | 1.95                     | 0.48              |
| 1:A:482:TYR:OH   | 1:E:481:VAL:HG21 | 2.12                     | 0.48              |
| 1:C:203:GLU:O    | 1:C:205:ASP:N    | 2.46                     | 0.48              |
| 1:E:203:GLU:O    | 1:E:205:ASP:N    | 2.46                     | 0.48              |
| 1:D:66:THR:HA    | 1:D:563:PRO:O    | 2.13                     | 0.48              |
| 1:A:449:VAL:HG12 | 1:A:450:THR:HG23 | 1.95                     | 0.48              |
| 1:B:67:THR:OG1   | 1:B:68:ARG:N     | 2.45                     | 0.48              |
| 1:A:243:LEU:HD22 | 1:A:244:PRO:CD   | 2.43                     | 0.48              |
| 1:C:292:TYR:HA   | 1:C:377:PRO:HG3  | 1.90                     | 0.48              |
| 1:C:389:ARG:CD   | 1:C:502:ASN:HD22 | 2.23                     | 0.48              |
| 1:B:237:HIS:ND1  | 1:B:238:PRO:O    | 2.45                     | 0.48              |
| 1:D:91:PHE:CD2   | 1:D:91:PHE:N     | 2.81                     | 0.48              |
| 1:C:211:ASP:OD1  | 1:C:213:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:125:THR:HG22 | 1:A:526:HIS:NE2  | 2.28                     | 0.48              |
| 1:C:451:PHE:HE2  | 1:C:462:VAL:HG23 | 1.78                     | 0.48              |
| 1:A:91:PHE:CD2   | 1:A:91:PHE:N     | 2.81                     | 0.48              |
| 1:D:545:ASP:OD1  | 1:D:549:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:214:ASN:HD21 | 1:A:216:ARG:HG2  | 1.78                     | 0.48              |
| 1:D:476:TYR:HD1  | 1:D:513:ILE:HD12 | 1.79                     | 0.48              |
| 1:C:444:MET:CE   | 1:C:561:VAL:HG21 | 2.43                     | 0.48              |
| 1:C:481:VAL:HG21 | 1:D:482:TYR:OH   | 2.12                     | 0.48              |
| 1:C:452:ARG:HE   | 1:D:98:ASN:ND2   | 2.08                     | 0.48              |
| 1:D:452:ARG:HE   | 1:E:98:ASN:ND2   | 2.08                     | 0.48              |
| 1:E:451:PHE:HE2  | 1:E:462:VAL:HG23 | 1.78                     | 0.48              |
| 1:E:212:THR:HG23 | 1:E:508:PRO:HB3  | 1.94                     | 0.48              |
| 1:A:545:ASP:OD1  | 1:A:549:ARG:HG2  | 2.13                     | 0.48              |
| 1:E:69:VAL:HG22  | 1:E:561:VAL:HB   | 1.95                     | 0.48              |
| 1:D:394:ILE:HG22 | 1:D:400:PHE:O    | 2.13                     | 0.48              |
| 1:B:485:LEU:HD11 | 1:C:486:ILE:HD11 | 1.94                     | 0.48              |
| 1:A:66:THR:HA    | 1:A:563:PRO:O    | 2.14                     | 0.48              |
| 1:C:66:THR:HA    | 1:C:563:PRO:O    | 2.13                     | 0.48              |
| 1:C:126:ILE:HG23 | 1:C:523:LEU:HD23 | 1.94                     | 0.48              |
| 1:A:67:THR:OG1   | 1:A:68:ARG:N     | 2.45                     | 0.48              |
| 1:B:292:TYR:HA   | 1:B:377:PRO:HG3  | 1.90                     | 0.48              |
| 1:C:129:THR:HG22 | 1:C:553:TYR:O    | 2.13                     | 0.48              |
| 1:B:211:ASP:OD1  | 1:B:213:ARG:HG2  | 2.13                     | 0.48              |
| 1:B:197:ARG:HG3  | 1:B:198:GLN:HG3  | 1.94                     | 0.48              |
| 1:D:485:LEU:HD11 | 1:E:486:ILE:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:98:ASN:HD22  | 1:C:99:ASN:N     | 2.11                     | 0.48              |
| 1:A:111:ILE:HD13 | 1:E:449:VAL:HG11 | 1.96                     | 0.48              |
| 1:A:243:LEU:CD2  | 1:A:403:TYR:CE2  | 2.96                     | 0.48              |
| 1:D:243:LEU:HD22 | 1:D:244:PRO:HD2  | 1.96                     | 0.48              |
| 1:B:197:ARG:C    | 1:B:199:ASN:H    | 2.17                     | 0.48              |
| 1:C:545:ASP:OD1  | 1:C:549:ARG:HG2  | 2.13                     | 0.48              |
| 1:E:237:HIS:ND1  | 1:E:238:PRO:O    | 2.45                     | 0.48              |
| 1:E:214:ASN:HD21 | 1:E:216:ARG:HG2  | 1.78                     | 0.48              |
| 1:A:444:MET:CE   | 1:A:561:VAL:HG21 | 2.43                     | 0.48              |
| 1:C:125:THR:HG22 | 1:C:526:HIS:NE2  | 2.28                     | 0.48              |
| 1:B:66:THR:HA    | 1:B:563:PRO:O    | 2.13                     | 0.48              |
| 1:D:538:VAL:HG23 | 1:D:538:VAL:O    | 2.14                     | 0.48              |
| 1:E:98:ASN:HD22  | 1:E:99:ASN:N     | 2.11                     | 0.48              |
| 1:A:243:LEU:HD22 | 1:A:244:PRO:HD2  | 1.96                     | 0.48              |
| 1:E:243:LEU:HD22 | 1:E:244:PRO:HD2  | 1.96                     | 0.48              |
| 1:A:135:ASN:HA   | 1:A:172:GLU:HG2  | 1.94                     | 0.48              |
| 1:A:431:THR:O    | 1:A:432:CYS:HB2  | 2.14                     | 0.48              |
| 1:B:126:ILE:HG23 | 1:B:523:LEU:HD23 | 1.94                     | 0.48              |
| 1:A:389:ARG:CD   | 1:A:502:ASN:HD22 | 2.23                     | 0.48              |
| 1:D:171:PRO:O    | 1:D:175:TYR:OH   | 2.25                     | 0.48              |
| 1:B:476:TYR:HD1  | 1:B:513:ILE:HD12 | 1.79                     | 0.48              |
| 1:E:395:SER:C    | 1:E:397:ASP:H    | 2.14                     | 0.48              |
| 1:B:538:VAL:HG23 | 1:B:538:VAL:O    | 2.14                     | 0.48              |
| 1:C:243:LEU:CD2  | 1:C:403:TYR:CE2  | 2.96                     | 0.48              |
| 1:D:211:ASP:OD1  | 1:D:213:ARG:HG2  | 2.13                     | 0.48              |
| 1:E:91:PHE:N     | 1:E:91:PHE:CD2   | 2.81                     | 0.48              |
| 1:B:214:ASN:HD21 | 1:B:216:ARG:HG2  | 1.79                     | 0.48              |
| 1:B:125:THR:HG22 | 1:B:526:HIS:NE2  | 2.28                     | 0.48              |
| 1:B:203:GLU:O    | 1:B:205:ASP:N    | 2.46                     | 0.48              |
| 1:B:203:GLU:HA   | 1:B:206:ILE:HG13 | 1.96                     | 0.48              |
| 1:E:75:LYS:HZ2   | 1:E:94:THR:HG23  | 1.79                     | 0.48              |
| 1:A:130:ASN:HD22 | 1:E:262:ARG:HH11 | 1.55                     | 0.47              |
| 1:A:197:ARG:C    | 1:A:199:ASN:H    | 2.17                     | 0.47              |
| 1:E:197:ARG:HG3  | 1:E:198:GLN:HG3  | 1.94                     | 0.47              |
| 1:E:410:TYR:O    | 1:E:420:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:203:GLU:O    | 1:A:205:ASP:N    | 2.46                     | 0.47              |
| 1:E:538:VAL:HG23 | 1:E:538:VAL:O    | 2.14                     | 0.47              |
| 1:A:538:VAL:HG23 | 1:A:538:VAL:O    | 2.14                     | 0.47              |
| 1:A:449:VAL:HG11 | 1:B:111:ILE:HD13 | 1.96                     | 0.47              |
| 1:D:449:VAL:HG12 | 1:D:450:THR:HG23 | 1.95                     | 0.47              |
| 1:D:508:PRO:HA   | 1:D:509:PRO:HD3  | 1.73                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:83:ASN:OD1   | 1:A:83:ASN:N     | 2.26                     | 0.47              |
| 1:C:410:TYR:O    | 1:C:420:ARG:HD3  | 2.14                     | 0.47              |
| 1:E:545:ASP:OD1  | 1:E:549:ARG:HG2  | 2.13                     | 0.47              |
| 1:C:214:ASN:HD21 | 1:C:216:ARG:HG2  | 1.78                     | 0.47              |
| 1:A:436:GLN:N    | 1:A:436:GLN:OE1  | 2.38                     | 0.47              |
| 1:D:430:VAL:CG2  | 1:D:431:THR:N    | 2.77                     | 0.47              |
| 1:B:499:PHE:N    | 1:B:500:PRO:CD   | 2.77                     | 0.47              |
| 1:D:499:PHE:N    | 1:D:500:PRO:CD   | 2.78                     | 0.47              |
| 1:B:243:LEU:HD22 | 1:B:244:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:243:LEU:HD22 | 1:C:244:PRO:HD2  | 1.96                     | 0.47              |
| 1:B:451:PHE:HE2  | 1:B:462:VAL:HG23 | 1.78                     | 0.47              |
| 1:A:410:TYR:O    | 1:A:420:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:211:ASP:OD1  | 1:A:213:ARG:HG2  | 2.13                     | 0.47              |
| 1:B:431:THR:O    | 1:B:432:CYS:HB2  | 2.14                     | 0.47              |
| 1:D:98:ASN:HD22  | 1:D:99:ASN:N     | 2.12                     | 0.47              |
| 1:E:476:TYR:HD1  | 1:E:513:ILE:HD12 | 1.79                     | 0.47              |
| 1:B:430:VAL:CG2  | 1:B:431:THR:N    | 2.77                     | 0.47              |
| 1:D:263:LYS:HZ3  | 1:D:268:GLN:HB2  | 1.77                     | 0.47              |
| 1:A:203:GLU:HA   | 1:A:206:ILE:HG13 | 1.96                     | 0.47              |
| 1:E:66:THR:HA    | 1:E:563:PRO:O    | 2.14                     | 0.47              |
| 1:A:405:SER:HB3  | 1:A:408:LEU:HB2  | 1.97                     | 0.47              |
| 1:E:243:LEU:CD2  | 1:E:403:TYR:CE2  | 2.96                     | 0.47              |
| 1:D:216:ARG:O    | 1:D:216:ARG:HG3  | 2.15                     | 0.47              |
| 1:E:216:ARG:O    | 1:E:216:ARG:HG3  | 2.15                     | 0.47              |
| 1:C:431:THR:O    | 1:C:432:CYS:HB2  | 2.14                     | 0.47              |
| 1:C:149:VAL:CG2  | 1:C:195:VAL:HG11 | 2.45                     | 0.47              |
| 1:E:431:THR:O    | 1:E:432:CYS:HB2  | 2.14                     | 0.47              |
| 1:A:430:VAL:CG2  | 1:A:431:THR:N    | 2.77                     | 0.47              |
| 1:A:499:PHE:N    | 1:A:500:PRO:CD   | 2.78                     | 0.47              |
| 1:C:485:LEU:HD11 | 1:D:486:ILE:HD11 | 1.94                     | 0.47              |
| 1:C:413:GLY:O    | 1:C:414:ASP:C    | 2.53                     | 0.47              |
| 1:A:98:ASN:HD22  | 1:A:99:ASN:N     | 2.11                     | 0.47              |
| 1:A:216:ARG:HG3  | 1:A:216:ARG:O    | 2.15                     | 0.47              |
| 1:A:476:TYR:HD1  | 1:A:513:ILE:HD12 | 1.79                     | 0.47              |
| 1:C:558:LEU:HD23 | 1:C:558:LEU:HA   | 1.62                     | 0.47              |
| 1:A:69:VAL:HG22  | 1:A:561:VAL:HB   | 1.95                     | 0.47              |
| 1:A:78:ASP:OD1   | 1:A:94:THR:HG22  | 2.15                     | 0.47              |
| 1:D:405:SER:HB3  | 1:D:408:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:413:GLY:O    | 1:D:414:ASP:C    | 2.53                     | 0.47              |
| 1:B:449:VAL:HG11 | 1:C:111:ILE:HD13 | 1.95                     | 0.47              |
| 1:B:449:VAL:HG12 | 1:B:450:THR:HG23 | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:449:VAL:HG11 | 1:D:111:ILE:HD13 | 1.96                     | 0.47              |
| 1:B:410:TYR:O    | 1:B:420:ARG:HD3  | 2.14                     | 0.47              |
| 1:C:131:MET:HA   | 1:C:553:TYR:CD2  | 2.50                     | 0.47              |
| 1:D:410:TYR:O    | 1:D:420:ARG:HD3  | 2.14                     | 0.47              |
| 1:D:131:MET:HA   | 1:D:553:TYR:CD2  | 2.50                     | 0.47              |
| 1:E:197:ARG:C    | 1:E:199:ASN:H    | 2.17                     | 0.47              |
| 1:E:180:THR:HG21 | 1:E:258:LEU:HD23 | 1.97                     | 0.47              |
| 1:B:216:ARG:O    | 1:B:216:ARG:HG3  | 2.15                     | 0.47              |
| 1:E:74:ASN:HD22  | 1:E:556:LYS:HZ1  | 1.61                     | 0.47              |
| 1:B:69:VAL:HG22  | 1:B:561:VAL:HB   | 1.95                     | 0.47              |
| 1:B:413:GLY:O    | 1:B:414:ASP:C    | 2.53                     | 0.47              |
| 1:D:449:VAL:HG11 | 1:E:111:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:261:ILE:HD12 | 1:E:406:TRP:CE3  | 2.50                     | 0.47              |
| 1:E:131:MET:HA   | 1:E:553:TYR:CD2  | 2.50                     | 0.47              |
| 1:C:197:ARG:C    | 1:C:199:ASN:H    | 2.17                     | 0.47              |
| 1:A:74:ASN:HD22  | 1:A:556:LYS:HZ1  | 1.62                     | 0.47              |
| 1:A:261:ILE:HD12 | 1:A:406:TRP:CE3  | 2.50                     | 0.47              |
| 1:E:389:ARG:CG   | 1:E:389:ARG:HH11 | 2.28                     | 0.47              |
| 1:D:451:PHE:HE2  | 1:D:462:VAL:HG23 | 1.78                     | 0.47              |
| 1:C:389:ARG:CG   | 1:C:389:ARG:HH11 | 2.28                     | 0.47              |
| 1:A:60:LEU:HD21  | 1:E:451:PHE:O    | 2.15                     | 0.47              |
| 1:E:430:VAL:CG2  | 1:E:431:THR:N    | 2.77                     | 0.47              |
| 1:D:389:ARG:CG   | 1:D:389:ARG:HH11 | 2.28                     | 0.47              |
| 1:B:91:PHE:CD2   | 1:B:91:PHE:N     | 2.81                     | 0.47              |
| 1:C:430:VAL:CG2  | 1:C:431:THR:N    | 2.78                     | 0.47              |
| 1:C:265:GLN:HA   | 1:C:266:PRO:HD2  | 1.57                     | 0.47              |
| 1:B:233:ASN:OD1  | 1:B:233:ASN:C    | 2.54                     | 0.47              |
| 1:D:203:GLU:HA   | 1:D:206:ILE:HG13 | 1.96                     | 0.47              |
| 1:C:78:ASP:OD1   | 1:C:94:THR:HG22  | 2.14                     | 0.47              |
| 1:E:405:SER:HB3  | 1:E:408:LEU:HB2  | 1.97                     | 0.47              |
| 1:B:261:ILE:HD12 | 1:B:406:TRP:CE3  | 2.50                     | 0.46              |
| 1:B:130:ASN:HA   | 1:B:519:ASN:CG   | 2.36                     | 0.46              |
| 1:B:131:MET:HA   | 1:B:553:TYR:CD2  | 2.50                     | 0.46              |
| 1:C:203:GLU:HA   | 1:C:206:ILE:HG13 | 1.96                     | 0.46              |
| 1:B:405:SER:HB3  | 1:B:408:LEU:HB2  | 1.97                     | 0.46              |
| 1:A:450:THR:HG21 | 1:B:96:ILE:CD1   | 2.46                     | 0.46              |
| 1:D:292:TYR:HA   | 1:D:377:PRO:HG3  | 1.90                     | 0.46              |
| 1:A:451:PHE:O    | 1:B:60:LEU:HD21  | 2.16                     | 0.46              |
| 1:A:130:ASN:HA   | 1:A:519:ASN:CG   | 2.36                     | 0.46              |
| 1:A:237:HIS:ND1  | 1:A:238:PRO:O    | 2.45                     | 0.46              |
| 1:D:197:ARG:O    | 1:D:199:ASN:N    | 2.43                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:MET:HA   | 1:A:553:TYR:CD2  | 2.50                     | 0.46              |
| 1:C:476:TYR:HD1  | 1:C:513:ILE:HD12 | 1.79                     | 0.46              |
| 1:D:138:MET:HB3  | 1:D:254:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:413:GLY:O    | 1:A:414:ASP:C    | 2.53                     | 0.46              |
| 1:A:389:ARG:CG   | 1:A:389:ARG:HH11 | 2.29                     | 0.46              |
| 1:D:261:ILE:HD12 | 1:D:406:TRP:CE3  | 2.50                     | 0.46              |
| 1:B:508:PRO:HA   | 1:B:509:PRO:HD3  | 1.73                     | 0.46              |
| 1:B:83:ASN:N     | 1:B:83:ASN:OD1   | 2.26                     | 0.46              |
| 1:C:180:THR:HG21 | 1:C:258:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:180:THR:HG21 | 1:A:258:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:436:GLN:HE22 | 1:B:556:LYS:HZ3  | 1.63                     | 0.46              |
| 1:E:138:MET:HB3  | 1:E:254:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:96:ILE:CD1   | 1:E:450:THR:HG21 | 2.46                     | 0.46              |
| 1:C:130:ASN:HA   | 1:C:519:ASN:CG   | 2.36                     | 0.46              |
| 1:B:441:LEU:HB2  | 1:B:445:MET:HE2  | 1.98                     | 0.46              |
| 1:C:215:PHE:O    | 1:C:216:ARG:HB3  | 2.15                     | 0.46              |
| 1:E:203:GLU:HA   | 1:E:206:ILE:HG13 | 1.96                     | 0.46              |
| 1:D:78:ASP:OD1   | 1:D:94:THR:HG22  | 2.14                     | 0.46              |
| 1:C:113:LEU:HD23 | 1:C:113:LEU:HA   | 1.71                     | 0.46              |
| 1:B:68:ARG:CG    | 1:B:68:ARG:NH1   | 2.66                     | 0.46              |
| 1:D:450:THR:HG21 | 1:E:96:ILE:CD1   | 2.46                     | 0.46              |
| 1:B:376:LYS:CB   | 1:B:377:PRO:HD2  | 2.32                     | 0.46              |
| 1:D:451:PHE:O    | 1:E:60:LEU:HD21  | 2.16                     | 0.46              |
| 1:C:451:PHE:O    | 1:D:60:LEU:HD21  | 2.16                     | 0.46              |
| 1:B:211:ASP:C    | 1:B:212:THR:CG2  | 2.84                     | 0.46              |
| 1:E:211:ASP:C    | 1:E:212:THR:CG2  | 2.84                     | 0.46              |
| 1:D:410:TYR:CE2  | 1:E:172:GLU:OE1  | 2.69                     | 0.46              |
| 1:A:513:ILE:HD12 | 1:A:513:ILE:N    | 2.31                     | 0.46              |
| 1:D:146:ARG:HE   | 1:D:246:CYS:HA   | 1.80                     | 0.46              |
| 1:E:146:ARG:HE   | 1:E:246:CYS:HA   | 1.79                     | 0.46              |
| 1:E:413:GLY:O    | 1:E:414:ASP:C    | 2.53                     | 0.46              |
| 1:A:51:GLY:HA3   | 1:A:116:ARG:HH12 | 1.81                     | 0.46              |
| 1:C:244:PRO:HA   | 1:C:275:TYR:CE2  | 2.51                     | 0.46              |
| 1:D:211:ASP:C    | 1:D:212:THR:CG2  | 2.84                     | 0.46              |
| 1:B:180:THR:HG21 | 1:B:258:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:427:THR:HA   | 1:A:428:PRO:HD3  | 1.75                     | 0.46              |
| 1:B:202:LEU:O    | 1:B:205:ASP:OD1  | 2.34                     | 0.46              |
| 1:E:78:ASP:OD1   | 1:E:94:THR:HG22  | 2.14                     | 0.46              |
| 1:B:78:ASP:OD1   | 1:B:94:THR:HG22  | 2.15                     | 0.46              |
| 1:B:51:GLY:HA3   | 1:B:116:ARG:HH12 | 1.81                     | 0.46              |
| 1:C:538:VAL:O    | 1:C:538:VAL:HG23 | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:GLY:HA3   | 1:C:116:ARG:HH12 | 1.81                     | 0.46              |
| 1:B:450:THR:HG21 | 1:C:96:ILE:CD1   | 2.45                     | 0.46              |
| 1:D:130:ASN:HA   | 1:D:519:ASN:CG   | 2.36                     | 0.46              |
| 1:D:178:THR:O    | 1:D:180:THR:N    | 2.49                     | 0.46              |
| 1:C:178:THR:O    | 1:C:180:THR:N    | 2.49                     | 0.46              |
| 1:A:178:THR:O    | 1:A:180:THR:N    | 2.49                     | 0.46              |
| 1:A:544:THR:HG23 | 1:A:549:ARG:N    | 2.31                     | 0.46              |
| 1:E:215:PHE:O    | 1:E:216:ARG:HB3  | 2.15                     | 0.46              |
| 1:C:216:ARG:O    | 1:C:216:ARG:HG3  | 2.15                     | 0.46              |
| 1:B:436:GLN:NE2  | 1:C:556:LYS:HZ3  | 2.14                     | 0.46              |
| 1:A:146:ARG:HE   | 1:A:246:CYS:HA   | 1.80                     | 0.46              |
| 1:C:146:ARG:HE   | 1:C:246:CYS:HA   | 1.80                     | 0.46              |
| 1:C:138:MET:HB3  | 1:C:254:ARG:HH11 | 1.80                     | 0.46              |
| 1:E:295:SER:CB   | 1:E:377:PRO:HG3  | 2.36                     | 0.46              |
| 1:C:261:ILE:HD12 | 1:C:406:TRP:CE3  | 2.50                     | 0.46              |
| 1:B:135:ASN:HB2  | 1:B:172:GLU:OE2  | 2.16                     | 0.46              |
| 1:C:544:THR:HG23 | 1:C:549:ARG:N    | 2.31                     | 0.46              |
| 1:A:132:PRO:HD3  | 1:A:553:TYR:CD2  | 2.51                     | 0.46              |
| 1:B:215:PHE:O    | 1:B:216:ARG:HB3  | 2.15                     | 0.46              |
| 1:A:233:ASN:C    | 1:A:233:ASN:OD1  | 2.54                     | 0.46              |
| 1:B:151:ARG:NH1  | 1:B:205:ASP:OD2  | 2.49                     | 0.46              |
| 1:A:73:ASP:OD1   | 1:A:73:ASP:N     | 2.42                     | 0.46              |
| 1:B:244:PRO:HA   | 1:B:275:TYR:CE2  | 2.51                     | 0.46              |
| 1:D:295:SER:CB   | 1:D:377:PRO:HG3  | 2.36                     | 0.46              |
| 1:C:211:ASP:C    | 1:C:212:THR:CG2  | 2.84                     | 0.46              |
| 1:A:211:ASP:C    | 1:A:212:THR:CG2  | 2.84                     | 0.46              |
| 1:D:132:PRO:HD3  | 1:D:553:TYR:CD2  | 2.51                     | 0.46              |
| 1:A:468:LEU:HA   | 1:A:469:PRO:HD3  | 1.76                     | 0.46              |
| 1:D:215:PHE:O    | 1:D:216:ARG:HB3  | 2.15                     | 0.46              |
| 1:A:135:ASN:HB2  | 1:A:172:GLU:OE2  | 2.16                     | 0.46              |
| 1:A:215:PHE:O    | 1:A:216:ARG:HB3  | 2.15                     | 0.46              |
| 1:C:513:ILE:N    | 1:C:513:ILE:HD12 | 2.31                     | 0.46              |
| 1:B:146:ARG:HE   | 1:B:246:CYS:HA   | 1.80                     | 0.46              |
| 1:E:202:LEU:O    | 1:E:205:ASP:OD1  | 2.34                     | 0.46              |
| 1:A:138:MET:HB3  | 1:A:254:ARG:HH11 | 1.80                     | 0.46              |
| 1:D:51:GLY:HA3   | 1:D:116:ARG:HH12 | 1.81                     | 0.46              |
| 1:B:382:LEU:HA   | 1:B:382:LEU:HD12 | 1.75                     | 0.46              |
| 1:B:389:ARG:HH11 | 1:B:389:ARG:CG   | 2.28                     | 0.46              |
| 1:B:237:HIS:CD2  | 1:B:425:LEU:CD1  | 2.97                     | 0.46              |
| 1:D:135:ASN:HB2  | 1:D:172:GLU:OE2  | 2.16                     | 0.46              |
| 1:B:178:THR:O    | 1:B:180:THR:N    | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:178:THR:O    | 1:E:180:THR:N    | 2.49                     | 0.46              |
| 1:C:499:PHE:N    | 1:C:500:PRO:CD   | 2.77                     | 0.46              |
| 1:B:225:LEU:HD22 | 1:B:285:ALA:O    | 2.16                     | 0.46              |
| 1:C:233:ASN:C    | 1:C:233:ASN:OD1  | 2.54                     | 0.46              |
| 1:D:202:LEU:O    | 1:D:205:ASP:OD1  | 2.34                     | 0.46              |
| 1:C:405:SER:HB3  | 1:C:408:LEU:HB2  | 1.97                     | 0.46              |
| 1:C:67:THR:OG1   | 1:C:68:ARG:N     | 2.45                     | 0.45              |
| 1:C:450:THR:HG21 | 1:D:96:ILE:CD1   | 2.46                     | 0.45              |
| 1:C:295:SER:CB   | 1:C:377:PRO:HG3  | 2.36                     | 0.45              |
| 1:D:244:PRO:HA   | 1:D:275:TYR:CE2  | 2.51                     | 0.45              |
| 1:B:132:PRO:HD3  | 1:B:553:TYR:CD2  | 2.51                     | 0.45              |
| 1:D:197:ARG:CG   | 1:D:198:GLN:H    | 2.29                     | 0.45              |
| 1:B:513:ILE:HD12 | 1:B:513:ILE:N    | 2.31                     | 0.45              |
| 1:B:493:THR:CG2  | 1:B:494:HIS:N    | 2.79                     | 0.45              |
| 1:A:225:LEU:HD22 | 1:A:285:ALA:O    | 2.16                     | 0.45              |
| 1:C:151:ARG:NH1  | 1:C:205:ASP:OD2  | 2.49                     | 0.45              |
| 1:E:244:PRO:HA   | 1:E:275:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:135:ASN:HA   | 1:C:172:GLU:CG   | 2.46                     | 0.45              |
| 1:B:451:PHE:O    | 1:C:60:LEU:HD21  | 2.16                     | 0.45              |
| 1:D:544:THR:HG23 | 1:D:549:ARG:N    | 2.31                     | 0.45              |
| 1:E:544:THR:HG23 | 1:E:549:ARG:N    | 2.31                     | 0.45              |
| 1:D:431:THR:O    | 1:D:432:CYS:HB2  | 2.14                     | 0.45              |
| 1:E:493:THR:HG22 | 1:E:494:HIS:O    | 2.16                     | 0.45              |
| 1:A:493:THR:HG22 | 1:A:494:HIS:O    | 2.16                     | 0.45              |
| 1:E:233:ASN:OD1  | 1:E:233:ASN:C    | 2.54                     | 0.45              |
| 1:A:151:ARG:NH1  | 1:A:205:ASP:OD2  | 2.49                     | 0.45              |
| 1:A:93:THR:HG22  | 1:A:94:THR:O     | 2.16                     | 0.45              |
| 1:E:441:LEU:HB2  | 1:E:445:MET:HE2  | 1.97                     | 0.45              |
| 1:E:135:ASN:HA   | 1:E:172:GLU:CG   | 2.46                     | 0.45              |
| 1:B:135:ASN:HA   | 1:B:172:GLU:CG   | 2.47                     | 0.45              |
| 1:A:410:TYR:CE2  | 1:B:172:GLU:OE1  | 2.69                     | 0.45              |
| 1:D:197:ARG:C    | 1:D:199:ASN:H    | 2.17                     | 0.45              |
| 1:D:436:GLN:HE21 | 1:E:558:LEU:HD11 | 1.81                     | 0.45              |
| 1:C:436:GLN:HE21 | 1:D:558:LEU:HD11 | 1.81                     | 0.45              |
| 1:D:195:VAL:HG12 | 1:D:196:GLY:N    | 2.32                     | 0.45              |
| 1:C:493:THR:HG22 | 1:C:494:HIS:O    | 2.16                     | 0.45              |
| 1:C:493:THR:CG2  | 1:C:494:HIS:N    | 2.80                     | 0.45              |
| 1:D:493:THR:CG2  | 1:D:494:HIS:N    | 2.80                     | 0.45              |
| 1:A:382:LEU:HD12 | 1:A:382:LEU:HA   | 1.75                     | 0.45              |
| 1:C:197:ARG:CG   | 1:C:198:GLN:H    | 2.29                     | 0.45              |
| 1:A:558:LEU:HD11 | 1:E:436:GLN:HE21 | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:146:ARG:HB2  | 1:C:165:TRP:CD2  | 2.52                     | 0.45              |
| 1:E:93:THR:HG22  | 1:E:94:THR:O     | 2.16                     | 0.45              |
| 1:E:51:GLY:HA3   | 1:E:116:ARG:HH12 | 1.81                     | 0.45              |
| 1:C:68:ARG:CG    | 1:C:68:ARG:NH1   | 2.66                     | 0.45              |
| 1:A:295:SER:CB   | 1:A:377:PRO:HG3  | 2.36                     | 0.45              |
| 1:E:130:ASN:HA   | 1:E:519:ASN:CG   | 2.36                     | 0.45              |
| 1:B:135:ASN:N    | 1:B:140:THR:OG1  | 2.47                     | 0.45              |
| 1:C:237:HIS:CD2  | 1:C:425:LEU:CD1  | 2.97                     | 0.45              |
| 1:D:135:ASN:HA   | 1:D:172:GLU:CG   | 2.47                     | 0.45              |
| 1:D:170:LEU:HB3  | 1:D:171:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:135:ASN:HA   | 1:A:172:GLU:CG   | 2.47                     | 0.45              |
| 1:B:436:GLN:HE21 | 1:C:558:LEU:HD11 | 1.81                     | 0.45              |
| 1:E:195:VAL:HG12 | 1:E:196:GLY:N    | 2.32                     | 0.45              |
| 1:D:146:ARG:HB2  | 1:D:165:TRP:CD2  | 2.52                     | 0.45              |
| 1:B:265:GLN:HA   | 1:B:266:PRO:HD2  | 1.57                     | 0.45              |
| 1:D:225:LEU:HD22 | 1:D:285:ALA:O    | 2.16                     | 0.45              |
| 1:C:225:LEU:HD22 | 1:C:285:ALA:O    | 2.16                     | 0.45              |
| 1:E:225:LEU:HD22 | 1:E:285:ALA:O    | 2.16                     | 0.45              |
| 1:C:202:LEU:O    | 1:C:205:ASP:OD1  | 2.34                     | 0.45              |
| 1:E:170:LEU:HB3  | 1:E:171:PRO:HD2  | 1.99                     | 0.45              |
| 1:D:446:GLN:O    | 1:D:448:PRO:HD3  | 2.17                     | 0.45              |
| 1:B:529:LEU:HD21 | 1:C:68:ARG:HE    | 1.82                     | 0.45              |
| 1:B:243:LEU:CD2  | 1:B:403:TYR:CE2  | 2.96                     | 0.45              |
| 1:D:441:LEU:HB2  | 1:D:445:MET:HE2  | 1.99                     | 0.45              |
| 1:E:135:ASN:HB2  | 1:E:172:GLU:OE2  | 2.16                     | 0.45              |
| 1:A:146:ARG:HB2  | 1:A:165:TRP:CD2  | 2.52                     | 0.45              |
| 1:A:202:LEU:O    | 1:A:205:ASP:OD1  | 2.34                     | 0.45              |
| 1:D:151:ARG:NH1  | 1:D:205:ASP:OD2  | 2.49                     | 0.45              |
| 1:B:93:THR:HG22  | 1:B:94:THR:O     | 2.16                     | 0.45              |
| 1:B:527:GLY:HA3  | 1:C:68:ARG:NH2   | 2.32                     | 0.45              |
| 1:C:463:VAL:HB   | 1:C:529:LEU:HD13 | 1.99                     | 0.45              |
| 1:D:243:LEU:HD23 | 1:D:244:PRO:HD3  | 1.99                     | 0.45              |
| 1:C:132:PRO:HD3  | 1:C:553:TYR:CD2  | 2.51                     | 0.45              |
| 1:E:132:PRO:HD3  | 1:E:553:TYR:CD2  | 2.51                     | 0.45              |
| 1:D:180:THR:HG21 | 1:D:258:LEU:HD23 | 1.97                     | 0.45              |
| 1:D:513:ILE:N    | 1:D:513:ILE:HD12 | 2.31                     | 0.45              |
| 1:A:436:GLN:HE21 | 1:B:558:LEU:HD11 | 1.81                     | 0.45              |
| 1:D:74:ASN:ND2   | 1:D:556:LYS:HZ1  | 2.13                     | 0.45              |
| 1:E:499:PHE:N    | 1:E:500:PRO:CD   | 2.77                     | 0.45              |
| 1:E:202:LEU:O    | 1:E:203:GLU:C    | 2.55                     | 0.45              |
| 1:E:446:GLN:O    | 1:E:448:PRO:HD3  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:135:ASN:HB2  | 1:C:172:GLU:OE2  | 2.16                     | 0.45              |
| 1:B:197:ARG:CG   | 1:B:198:GLN:H    | 2.30                     | 0.45              |
| 1:E:258:LEU:C    | 1:E:258:LEU:HD12 | 2.37                     | 0.45              |
| 1:B:544:THR:HG23 | 1:B:549:ARG:N    | 2.31                     | 0.45              |
| 1:E:513:ILE:HD12 | 1:E:513:ILE:N    | 2.31                     | 0.45              |
| 1:C:436:GLN:N    | 1:C:436:GLN:OE1  | 2.38                     | 0.45              |
| 1:E:525:ASP:O    | 1:E:525:ASP:OD1  | 2.35                     | 0.45              |
| 1:A:446:GLN:O    | 1:A:448:PRO:HD3  | 2.17                     | 0.45              |
| 1:D:250:PHE:O    | 1:D:252:HIS:N    | 2.50                     | 0.45              |
| 1:D:63:LEU:HD12  | 1:D:63:LEU:HA    | 1.82                     | 0.45              |
| 1:A:243:LEU:HD23 | 1:A:244:PRO:HD3  | 1.99                     | 0.45              |
| 1:A:292:TYR:HA   | 1:A:377:PRO:HG3  | 1.91                     | 0.45              |
| 1:B:195:VAL:HG12 | 1:B:196:GLY:N    | 2.32                     | 0.45              |
| 1:E:493:THR:CG2  | 1:E:494:HIS:N    | 2.80                     | 0.45              |
| 1:D:525:ASP:OD1  | 1:D:525:ASP:O    | 2.35                     | 0.45              |
| 1:D:233:ASN:C    | 1:D:233:ASN:OD1  | 2.54                     | 0.45              |
| 1:D:529:LEU:HD21 | 1:E:68:ARG:HE    | 1.82                     | 0.45              |
| 1:B:129:THR:HB   | 1:B:130:ASN:H    | 1.65                     | 0.45              |
| 1:E:476:TYR:HD1  | 1:E:513:ILE:CD1  | 2.30                     | 0.45              |
| 1:B:149:VAL:CG2  | 1:B:195:VAL:HG11 | 2.45                     | 0.45              |
| 1:C:195:VAL:HG12 | 1:C:196:GLY:N    | 2.32                     | 0.45              |
| 1:C:225:LEU:HD13 | 1:C:287:LEU:HA   | 1.99                     | 0.45              |
| 1:B:138:MET:HB3  | 1:B:254:ARG:HH11 | 1.80                     | 0.45              |
| 1:C:533:ASN:OD1  | 1:C:533:ASN:N    | 2.50                     | 0.45              |
| 1:B:295:SER:CB   | 1:B:377:PRO:HG3  | 2.36                     | 0.44              |
| 1:A:197:ARG:O    | 1:A:199:ASN:N    | 2.43                     | 0.44              |
| 1:A:74:ASN:ND2   | 1:A:556:LYS:NZ   | 2.66                     | 0.44              |
| 1:C:217:LEU:CB   | 1:C:232:THR:HG21 | 2.46                     | 0.44              |
| 1:B:146:ARG:HB2  | 1:B:165:TRP:CD2  | 2.52                     | 0.44              |
| 1:B:493:THR:HG22 | 1:B:494:HIS:O    | 2.16                     | 0.44              |
| 1:A:525:ASP:O    | 1:A:525:ASP:OD1  | 2.35                     | 0.44              |
| 1:C:525:ASP:O    | 1:C:525:ASP:OD1  | 2.35                     | 0.44              |
| 1:B:203:GLU:C    | 1:B:205:ASP:N    | 2.71                     | 0.44              |
| 1:A:75:LYS:NZ    | 1:A:94:THR:HG23  | 2.33                     | 0.44              |
| 1:E:151:ARG:NH1  | 1:E:205:ASP:OD2  | 2.49                     | 0.44              |
| 1:B:170:LEU:HB3  | 1:B:171:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:250:PHE:O    | 1:A:252:HIS:N    | 2.50                     | 0.44              |
| 1:E:389:ARG:CD   | 1:E:502:ASN:HD22 | 2.23                     | 0.44              |
| 1:D:258:LEU:C    | 1:D:258:LEU:HD12 | 2.37                     | 0.44              |
| 1:A:172:GLU:OE1  | 1:E:410:TYR:CE2  | 2.68                     | 0.44              |
| 1:E:420:ARG:O    | 1:E:420:ARG:HG3  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:493:THR:HG22 | 1:D:494:HIS:O    | 2.16                     | 0.44              |
| 1:C:229:GLY:O    | 1:C:286:LEU:HD13 | 2.18                     | 0.44              |
| 1:E:250:PHE:O    | 1:E:252:HIS:N    | 2.50                     | 0.44              |
| 1:E:533:ASN:OD1  | 1:E:533:ASN:N    | 2.50                     | 0.44              |
| 1:A:529:LEU:HD21 | 1:B:68:ARG:HE    | 1.82                     | 0.44              |
| 1:E:68:ARG:NH1   | 1:E:68:ARG:CG    | 2.66                     | 0.44              |
| 1:E:243:LEU:HD23 | 1:E:244:PRO:HD3  | 1.99                     | 0.44              |
| 1:D:389:ARG:CD   | 1:D:502:ASN:HD22 | 2.23                     | 0.44              |
| 1:A:476:TYR:HD1  | 1:A:513:ILE:CD1  | 2.30                     | 0.44              |
| 1:D:217:LEU:CB   | 1:D:232:THR:HG21 | 2.46                     | 0.44              |
| 1:B:225:LEU:HD13 | 1:B:287:LEU:HA   | 2.00                     | 0.44              |
| 1:D:75:LYS:NZ    | 1:D:94:THR:HG23  | 2.32                     | 0.44              |
| 1:E:75:LYS:NZ    | 1:E:94:THR:HG23  | 2.32                     | 0.44              |
| 1:B:229:GLY:O    | 1:B:286:LEU:HD13 | 2.18                     | 0.44              |
| 1:C:527:GLY:HA3  | 1:D:68:ARG:NH2   | 2.32                     | 0.44              |
| 1:B:243:LEU:HD23 | 1:B:244:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:441:LEU:HD12 | 1:A:445:MET:CE   | 2.48                     | 0.44              |
| 1:C:262:ARG:NH1  | 1:D:130:ASN:ND2  | 2.55                     | 0.44              |
| 1:C:410:TYR:CE2  | 1:D:172:GLU:OE1  | 2.68                     | 0.44              |
| 1:B:476:TYR:HD1  | 1:B:513:ILE:CD1  | 2.30                     | 0.44              |
| 1:D:265:GLN:HA   | 1:D:266:PRO:HD2  | 1.57                     | 0.44              |
| 1:C:203:GLU:C    | 1:C:205:ASP:N    | 2.70                     | 0.44              |
| 1:D:203:GLU:C    | 1:D:205:ASP:N    | 2.70                     | 0.44              |
| 1:C:75:LYS:NZ    | 1:C:94:THR:HG23  | 2.32                     | 0.44              |
| 1:C:93:THR:HG22  | 1:C:94:THR:O     | 2.17                     | 0.44              |
| 1:A:533:ASN:OD1  | 1:A:533:ASN:N    | 2.50                     | 0.44              |
| 1:E:63:LEU:HD12  | 1:E:63:LEU:HA    | 1.82                     | 0.44              |
| 1:A:229:GLY:O    | 1:A:286:LEU:HD13 | 2.18                     | 0.44              |
| 1:D:295:SER:O    | 1:D:296:LEU:CB   | 2.64                     | 0.44              |
| 1:E:441:LEU:HD12 | 1:E:445:MET:CE   | 2.48                     | 0.44              |
| 1:C:468:LEU:C    | 1:C:468:LEU:HD12 | 2.38                     | 0.44              |
| 1:B:74:ASN:ND2   | 1:B:556:LYS:NZ   | 2.65                     | 0.44              |
| 1:A:195:VAL:HG12 | 1:A:196:GLY:N    | 2.32                     | 0.44              |
| 1:E:146:ARG:HB2  | 1:E:165:TRP:CD2  | 2.52                     | 0.44              |
| 1:D:429:ASP:OD1  | 1:D:432:CYS:N    | 2.51                     | 0.44              |
| 1:A:429:ASP:OD1  | 1:A:432:CYS:N    | 2.51                     | 0.44              |
| 1:A:203:GLU:C    | 1:A:205:ASP:N    | 2.70                     | 0.44              |
| 1:D:93:THR:HG22  | 1:D:94:THR:O     | 2.17                     | 0.44              |
| 1:B:75:LYS:NZ    | 1:B:94:THR:HG23  | 2.32                     | 0.44              |
| 1:E:229:GLY:O    | 1:E:286:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:250:PHE:O    | 1:B:252:HIS:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:GLN:O    | 1:B:448:PRO:HD3  | 2.17                     | 0.44              |
| 1:C:250:PHE:O    | 1:C:252:HIS:N    | 2.50                     | 0.44              |
| 1:C:63:LEU:HA    | 1:C:63:LEU:HD12  | 1.82                     | 0.44              |
| 1:C:243:LEU:HD23 | 1:C:244:PRO:HD3  | 1.99                     | 0.44              |
| 1:B:558:LEU:HD23 | 1:B:558:LEU:HA   | 1.62                     | 0.44              |
| 1:B:463:VAL:HB   | 1:B:529:LEU:HD13 | 1.99                     | 0.44              |
| 1:B:261:ILE:HD12 | 1:B:406:TRP:CZ3  | 2.53                     | 0.44              |
| 1:B:258:LEU:HD12 | 1:B:258:LEU:C    | 2.38                     | 0.44              |
| 1:E:468:LEU:HD12 | 1:E:468:LEU:C    | 2.38                     | 0.44              |
| 1:B:436:GLN:OE1  | 1:B:436:GLN:N    | 2.39                     | 0.44              |
| 1:E:128:HIS:HD2  | 1:E:555:TYR:HD2  | 1.66                     | 0.44              |
| 1:C:264:ARG:O    | 1:C:264:ARG:HG3  | 2.18                     | 0.44              |
| 1:A:560:ILE:HD11 | 1:E:465:ALA:HB3  | 2.00                     | 0.44              |
| 1:A:68:ARG:HE    | 1:E:529:LEU:HD21 | 1.82                     | 0.44              |
| 1:E:261:ILE:HD12 | 1:E:406:TRP:CZ3  | 2.53                     | 0.44              |
| 1:B:420:ARG:HG3  | 1:B:420:ARG:O    | 2.17                     | 0.44              |
| 1:A:83:ASN:ND2   | 1:A:92:LEU:O     | 2.51                     | 0.44              |
| 1:C:420:ARG:HG3  | 1:C:420:ARG:O    | 2.17                     | 0.44              |
| 1:C:83:ASN:ND2   | 1:C:92:LEU:O     | 2.51                     | 0.44              |
| 1:A:197:ARG:CG   | 1:A:198:GLN:H    | 2.30                     | 0.44              |
| 1:E:225:LEU:HD13 | 1:E:287:LEU:HA   | 1.99                     | 0.44              |
| 1:C:128:HIS:HD2  | 1:C:555:TYR:HD2  | 1.66                     | 0.44              |
| 1:A:391:TYR:O    | 1:A:392:ASN:C    | 2.57                     | 0.44              |
| 1:D:533:ASN:OD1  | 1:D:533:ASN:N    | 2.50                     | 0.44              |
| 1:A:68:ARG:NH2   | 1:E:527:GLY:HA3  | 2.32                     | 0.44              |
| 1:C:170:LEU:HB3  | 1:C:171:PRO:HD2  | 1.99                     | 0.44              |
| 1:E:83:ASN:ND2   | 1:E:92:LEU:O     | 2.51                     | 0.44              |
| 1:A:170:LEU:HB3  | 1:A:171:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:525:ASP:OD1  | 1:B:525:ASP:O    | 2.35                     | 0.44              |
| 1:C:446:GLN:O    | 1:C:448:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:527:GLY:HA3  | 1:B:68:ARG:NH2   | 2.32                     | 0.43              |
| 1:C:261:ILE:HD12 | 1:C:406:TRP:CZ3  | 2.53                     | 0.43              |
| 1:D:83:ASN:ND2   | 1:D:92:LEU:O     | 2.51                     | 0.43              |
| 1:A:130:ASN:ND2  | 1:E:262:ARG:NH1  | 2.55                     | 0.43              |
| 1:D:420:ARG:HG3  | 1:D:420:ARG:O    | 2.17                     | 0.43              |
| 1:A:420:ARG:O    | 1:A:420:ARG:HG3  | 2.17                     | 0.43              |
| 1:D:135:ASN:N    | 1:D:140:THR:OG1  | 2.47                     | 0.43              |
| 1:C:258:LEU:HD12 | 1:C:258:LEU:C    | 2.37                     | 0.43              |
| 1:E:436:GLN:OE1  | 1:E:436:GLN:N    | 2.39                     | 0.43              |
| 1:A:493:THR:CG2  | 1:A:494:HIS:N    | 2.79                     | 0.43              |
| 1:C:202:LEU:O    | 1:C:203:GLU:C    | 2.55                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:467:LEU:HD12 | 1:B:467:LEU:HA   | 1.83                     | 0.43              |
| 1:D:106:ALA:C    | 1:D:108:THR:N    | 2.71                     | 0.43              |
| 1:D:527:GLY:HA3  | 1:E:68:ARG:NH2   | 2.33                     | 0.43              |
| 1:D:261:ILE:HD12 | 1:D:406:TRP:CZ3  | 2.53                     | 0.43              |
| 1:D:468:LEU:HD12 | 1:D:468:LEU:C    | 2.38                     | 0.43              |
| 1:A:258:LEU:HD12 | 1:A:258:LEU:C    | 2.37                     | 0.43              |
| 1:A:468:LEU:C    | 1:A:468:LEU:HD12 | 2.38                     | 0.43              |
| 1:E:74:ASN:ND2   | 1:E:556:LYS:NZ   | 2.66                     | 0.43              |
| 1:D:444:MET:HB2  | 1:D:539:GLN:CD   | 2.39                     | 0.43              |
| 1:A:225:LEU:HD13 | 1:A:287:LEU:HA   | 1.99                     | 0.43              |
| 1:A:202:LEU:O    | 1:A:203:GLU:C    | 2.55                     | 0.43              |
| 1:A:264:ARG:O    | 1:A:264:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:533:ASN:N    | 1:B:533:ASN:OD1  | 2.50                     | 0.43              |
| 1:A:244:PRO:HA   | 1:A:275:TYR:CE2  | 2.51                     | 0.43              |
| 1:B:83:ASN:ND2   | 1:B:92:LEU:O     | 2.51                     | 0.43              |
| 1:C:429:ASP:OD1  | 1:C:432:CYS:N    | 2.51                     | 0.43              |
| 1:A:393:LEU:N    | 1:A:393:LEU:CD1  | 2.81                     | 0.43              |
| 1:C:524:THR:OG1  | 1:C:525:ASP:N    | 2.52                     | 0.43              |
| 1:E:264:ARG:HG3  | 1:E:264:ARG:O    | 2.18                     | 0.43              |
| 1:A:467:LEU:HD13 | 1:B:126:ILE:HG21 | 2.01                     | 0.43              |
| 1:A:106:ALA:C    | 1:A:108:THR:H    | 2.22                     | 0.43              |
| 1:A:463:VAL:HB   | 1:A:529:LEU:HD13 | 1.99                     | 0.43              |
| 1:D:262:ARG:HH11 | 1:E:130:ASN:HD22 | 1.55                     | 0.43              |
| 1:E:197:ARG:CG   | 1:E:198:GLN:H    | 2.29                     | 0.43              |
| 1:E:444:MET:HB2  | 1:E:539:GLN:CD   | 2.39                     | 0.43              |
| 1:D:225:LEU:HD13 | 1:D:287:LEU:HA   | 1.99                     | 0.43              |
| 1:C:391:TYR:O    | 1:C:392:ASN:C    | 2.57                     | 0.43              |
| 1:B:202:LEU:O    | 1:B:203:GLU:C    | 2.55                     | 0.43              |
| 1:C:419:ILE:C    | 1:C:421:SER:N    | 2.72                     | 0.43              |
| 1:B:411:ASN:OD1  | 1:C:172:GLU:N    | 2.52                     | 0.43              |
| 1:A:237:HIS:CD2  | 1:A:425:LEU:CD1  | 2.97                     | 0.43              |
| 1:C:74:ASN:ND2   | 1:C:556:LYS:NZ   | 2.66                     | 0.43              |
| 1:B:497:ASN:O    | 1:B:500:PRO:HD3  | 2.19                     | 0.43              |
| 1:C:395:SER:C    | 1:C:397:ASP:N    | 2.71                     | 0.43              |
| 1:B:467:LEU:HD13 | 1:C:126:ILE:HG21 | 2.00                     | 0.43              |
| 1:D:229:GLY:O    | 1:D:286:LEU:HD13 | 2.18                     | 0.43              |
| 1:C:527:GLY:HA3  | 1:D:68:ARG:HH21  | 1.84                     | 0.43              |
| 1:A:527:GLY:HA3  | 1:B:68:ARG:HH21  | 1.84                     | 0.43              |
| 1:B:419:ILE:C    | 1:B:421:SER:N    | 2.72                     | 0.43              |
| 1:A:419:ILE:C    | 1:A:421:SER:N    | 2.72                     | 0.43              |
| 1:C:476:TYR:HD1  | 1:C:513:ILE:CD1  | 2.30                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:74:ASN:ND2   | 1:D:556:LYS:NZ   | 2.66                     | 0.43              |
| 1:E:149:VAL:CG2  | 1:E:195:VAL:HG11 | 2.45                     | 0.43              |
| 1:B:393:LEU:CD1  | 1:B:393:LEU:N    | 2.81                     | 0.43              |
| 1:A:497:ASN:O    | 1:A:500:PRO:HD3  | 2.19                     | 0.43              |
| 1:A:524:THR:OG1  | 1:A:525:ASP:N    | 2.52                     | 0.43              |
| 1:A:481:VAL:O    | 1:A:482:TYR:C    | 2.57                     | 0.43              |
| 1:B:465:ALA:HB3  | 1:C:560:ILE:HD11 | 2.00                     | 0.43              |
| 1:C:106:ALA:C    | 1:C:108:THR:N    | 2.71                     | 0.43              |
| 1:A:68:ARG:NH1   | 1:A:562:SER:CB   | 2.79                     | 0.43              |
| 1:D:463:VAL:HB   | 1:D:529:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:419:ILE:O    | 1:A:421:SER:N    | 2.52                     | 0.43              |
| 1:B:262:ARG:NH1  | 1:C:130:ASN:ND2  | 2.55                     | 0.43              |
| 1:A:508:PRO:HA   | 1:A:509:PRO:HD3  | 1.73                     | 0.43              |
| 1:C:444:MET:HB2  | 1:C:539:GLN:CD   | 2.39                     | 0.43              |
| 1:B:429:ASP:OD1  | 1:B:432:CYS:N    | 2.51                     | 0.43              |
| 1:E:427:THR:HA   | 1:E:428:PRO:HD3  | 1.75                     | 0.43              |
| 1:E:391:TYR:O    | 1:E:392:ASN:C    | 2.57                     | 0.43              |
| 1:C:529:LEU:HD21 | 1:D:68:ARG:HE    | 1.82                     | 0.43              |
| 1:D:243:LEU:CD2  | 1:D:403:TYR:CE2  | 2.96                     | 0.43              |
| 1:C:441:LEU:HB2  | 1:C:445:MET:HE2  | 2.00                     | 0.43              |
| 1:D:436:GLN:N    | 1:D:436:GLN:OE1  | 2.38                     | 0.43              |
| 1:A:126:ILE:HG21 | 1:E:467:LEU:HD13 | 2.00                     | 0.43              |
| 1:E:106:ALA:C    | 1:E:108:THR:H    | 2.22                     | 0.43              |
| 1:C:465:ALA:HB3  | 1:D:560:ILE:HD11 | 2.00                     | 0.43              |
| 1:E:463:VAL:HB   | 1:E:529:LEU:HD13 | 1.99                     | 0.43              |
| 1:D:74:ASN:HD22  | 1:D:556:LYS:HZ1  | 1.67                     | 0.43              |
| 1:E:217:LEU:CB   | 1:E:232:THR:HG21 | 2.46                     | 0.43              |
| 1:D:393:LEU:N    | 1:D:393:LEU:CD1  | 2.81                     | 0.43              |
| 1:C:481:VAL:O    | 1:C:482:TYR:C    | 2.57                     | 0.43              |
| 1:E:68:ARG:NH1   | 1:E:562:SER:CB   | 2.79                     | 0.43              |
| 1:A:261:ILE:HD12 | 1:A:406:TRP:CZ3  | 2.53                     | 0.43              |
| 1:E:275:TYR:CE1  | 1:E:404:ARG:HD2  | 2.54                     | 0.43              |
| 1:E:419:ILE:O    | 1:E:421:SER:N    | 2.52                     | 0.43              |
| 1:C:197:ARG:O    | 1:C:199:ASN:N    | 2.43                     | 0.43              |
| 1:A:214:ASN:O    | 1:A:216:ARG:N    | 2.50                     | 0.43              |
| 1:A:444:MET:HB2  | 1:A:539:GLN:CD   | 2.39                     | 0.43              |
| 1:B:524:THR:OG1  | 1:B:525:ASP:N    | 2.52                     | 0.43              |
| 1:A:128:HIS:HD2  | 1:A:555:TYR:HD2  | 1.66                     | 0.43              |
| 1:B:264:ARG:O    | 1:B:264:ARG:HG3  | 2.18                     | 0.43              |
| 1:D:264:ARG:O    | 1:D:264:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:527:GLY:HA3  | 1:C:68:ARG:HH21  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:419:ILE:O    | 1:C:421:SER:N    | 2.52                     | 0.42              |
| 1:E:497:ASN:O    | 1:E:500:PRO:HD3  | 2.19                     | 0.42              |
| 1:D:394:ILE:HG23 | 1:D:395:SER:N    | 2.34                     | 0.42              |
| 1:E:265:GLN:HA   | 1:E:266:PRO:HD2  | 1.57                     | 0.42              |
| 1:E:481:VAL:O    | 1:E:482:TYR:C    | 2.57                     | 0.42              |
| 1:B:391:TYR:O    | 1:B:392:ASN:C    | 2.57                     | 0.42              |
| 1:D:202:LEU:O    | 1:D:203:GLU:C    | 2.55                     | 0.42              |
| 1:E:65:ASP:O     | 1:E:66:THR:C     | 2.58                     | 0.42              |
| 1:D:65:ASP:O     | 1:D:66:THR:C     | 2.57                     | 0.42              |
| 1:A:279:GLU:O    | 1:A:280:GLY:O    | 2.38                     | 0.42              |
| 1:C:194:LYS:HG2  | 1:C:194:LYS:O    | 2.19                     | 0.42              |
| 1:D:68:ARG:NH1   | 1:D:562:SER:CB   | 2.79                     | 0.42              |
| 1:B:419:ILE:O    | 1:B:421:SER:N    | 2.52                     | 0.42              |
| 1:D:275:TYR:CE1  | 1:D:404:ARG:HD2  | 2.54                     | 0.42              |
| 1:A:451:PHE:CE1  | 1:B:97:GLN:CB    | 3.03                     | 0.42              |
| 1:B:468:LEU:HD12 | 1:B:468:LEU:C    | 2.38                     | 0.42              |
| 1:D:476:TYR:HD1  | 1:D:513:ILE:CD1  | 2.30                     | 0.42              |
| 1:D:441:LEU:HD12 | 1:D:445:MET:CE   | 2.47                     | 0.42              |
| 1:D:278:LEU:CD2  | 1:D:419:ILE:HD12 | 2.38                     | 0.42              |
| 1:C:411:ASN:OD1  | 1:D:172:GLU:N    | 2.51                     | 0.42              |
| 1:C:430:VAL:O    | 1:C:432:CYS:N    | 2.53                     | 0.42              |
| 1:D:128:HIS:HD2  | 1:D:555:TYR:HD2  | 1.66                     | 0.42              |
| 1:D:75:LYS:HZ2   | 1:D:94:THR:HG23  | 1.84                     | 0.42              |
| 1:C:65:ASP:O     | 1:C:66:THR:C     | 2.58                     | 0.42              |
| 1:C:467:LEU:HA   | 1:C:467:LEU:HD12 | 1.83                     | 0.42              |
| 1:D:106:ALA:C    | 1:D:108:THR:H    | 2.22                     | 0.42              |
| 1:E:106:ALA:C    | 1:E:108:THR:N    | 2.71                     | 0.42              |
| 1:B:106:ALA:C    | 1:B:108:THR:H    | 2.22                     | 0.42              |
| 1:B:389:ARG:CD   | 1:B:502:ASN:HD22 | 2.23                     | 0.42              |
| 1:E:419:ILE:C    | 1:E:421:SER:N    | 2.72                     | 0.42              |
| 1:B:410:TYR:CE2  | 1:C:172:GLU:OE1  | 2.68                     | 0.42              |
| 1:D:411:ASN:OD1  | 1:E:172:GLU:N    | 2.52                     | 0.42              |
| 1:A:53:ASN:O     | 1:A:54:SER:O     | 2.38                     | 0.42              |
| 1:B:444:MET:HB2  | 1:B:539:GLN:CD   | 2.39                     | 0.42              |
| 1:D:149:VAL:CG2  | 1:D:195:VAL:HG11 | 2.45                     | 0.42              |
| 1:C:497:ASN:O    | 1:C:500:PRO:HD3  | 2.19                     | 0.42              |
| 1:B:481:VAL:O    | 1:B:482:TYR:C    | 2.57                     | 0.42              |
| 1:B:128:HIS:HD2  | 1:B:555:TYR:HD2  | 1.66                     | 0.42              |
| 1:C:75:LYS:HZ2   | 1:C:94:THR:HG23  | 1.83                     | 0.42              |
| 1:E:203:GLU:HG2  | 1:E:203:GLU:H    | 1.69                     | 0.42              |
| 1:D:419:ILE:O    | 1:D:421:SER:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:451:PHE:CE1  | 1:C:97:GLN:CB    | 3.03                     | 0.42              |
| 1:E:237:HIS:CD2  | 1:E:425:LEU:CD1  | 2.97                     | 0.42              |
| 1:A:172:GLU:N    | 1:E:411:ASN:OD1  | 2.52                     | 0.42              |
| 1:C:393:LEU:CD1  | 1:C:393:LEU:N    | 2.81                     | 0.42              |
| 1:E:203:GLU:C    | 1:E:205:ASP:N    | 2.71                     | 0.42              |
| 1:A:106:ALA:C    | 1:A:108:THR:N    | 2.71                     | 0.42              |
| 1:B:275:TYR:CE1  | 1:B:404:ARG:HD2  | 2.54                     | 0.42              |
| 1:B:295:SER:O    | 1:B:296:LEU:CB   | 2.64                     | 0.42              |
| 1:D:502:ASN:C    | 1:D:504:ILE:H    | 2.23                     | 0.42              |
| 1:C:275:TYR:CE1  | 1:C:404:ARG:HD2  | 2.54                     | 0.42              |
| 1:E:135:ASN:N    | 1:E:140:THR:OG1  | 2.47                     | 0.42              |
| 1:E:53:ASN:O     | 1:E:54:SER:O     | 2.38                     | 0.42              |
| 1:A:558:LEU:HD23 | 1:A:558:LEU:HA   | 1.62                     | 0.42              |
| 1:C:478:ASP:C    | 1:C:480:ALA:N    | 2.73                     | 0.42              |
| 1:D:93:THR:CG2   | 1:D:94:THR:N     | 2.83                     | 0.42              |
| 1:E:93:THR:CG2   | 1:E:94:THR:N     | 2.83                     | 0.42              |
| 1:B:230:VAL:HG13 | 1:B:503:GLN:NE2  | 2.35                     | 0.42              |
| 1:C:230:VAL:HG13 | 1:C:503:GLN:NE2  | 2.35                     | 0.42              |
| 1:D:230:VAL:HG13 | 1:D:503:GLN:NE2  | 2.35                     | 0.42              |
| 1:E:230:VAL:HG13 | 1:E:503:GLN:NE2  | 2.35                     | 0.42              |
| 1:B:194:LYS:HG2  | 1:B:194:LYS:O    | 2.19                     | 0.42              |
| 1:D:527:GLY:HA3  | 1:E:68:ARG:HH21  | 1.84                     | 0.42              |
| 1:C:502:ASN:C    | 1:C:504:ILE:H    | 2.23                     | 0.42              |
| 1:B:237:HIS:NE2  | 1:B:425:LEU:CD1  | 2.83                     | 0.42              |
| 1:B:441:LEU:HD12 | 1:B:445:MET:CE   | 2.47                     | 0.42              |
| 1:E:145:ALA:HB3  | 1:E:168:PHE:CE1  | 2.44                     | 0.42              |
| 1:D:524:THR:OG1  | 1:D:525:ASP:N    | 2.52                     | 0.42              |
| 1:A:395:SER:C    | 1:A:397:ASP:N    | 2.71                     | 0.42              |
| 1:D:467:LEU:HD13 | 1:E:126:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:106:ALA:C    | 1:C:108:THR:H    | 2.22                     | 0.42              |
| 1:A:465:ALA:HB3  | 1:B:560:ILE:HD11 | 2.00                     | 0.42              |
| 1:D:279:GLU:O    | 1:D:280:GLY:O    | 2.37                     | 0.42              |
| 1:A:230:VAL:HG13 | 1:A:503:GLN:NE2  | 2.35                     | 0.42              |
| 1:A:502:ASN:C    | 1:A:504:ILE:H    | 2.23                     | 0.42              |
| 1:D:451:PHE:CE1  | 1:E:97:GLN:CB    | 3.03                     | 0.42              |
| 1:D:406:TRP:HE1  | 1:D:419:ILE:HG21 | 1.85                     | 0.42              |
| 1:A:411:ASN:OD1  | 1:B:172:GLU:N    | 2.52                     | 0.42              |
| 1:E:475:PHE:CD1  | 1:E:475:PHE:N    | 2.88                     | 0.42              |
| 1:A:430:VAL:O    | 1:A:432:CYS:N    | 2.53                     | 0.42              |
| 1:D:497:ASN:O    | 1:D:500:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:65:ASP:O     | 1:A:66:THR:C     | 2.58                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:465:ALA:HB3  | 1:E:560:ILE:HD11 | 2.00                     | 0.42              |
| 1:C:279:GLU:O    | 1:C:280:GLY:O    | 2.38                     | 0.42              |
| 1:A:68:ARG:HH21  | 1:E:527:GLY:HA3  | 1.84                     | 0.42              |
| 1:C:441:LEU:HD12 | 1:C:445:MET:CE   | 2.48                     | 0.42              |
| 1:B:197:ARG:O    | 1:B:199:ASN:N    | 2.43                     | 0.42              |
| 1:E:178:THR:C    | 1:E:180:THR:N    | 2.73                     | 0.42              |
| 1:D:53:ASN:O     | 1:D:54:SER:O     | 2.38                     | 0.42              |
| 1:D:391:TYR:O    | 1:D:392:ASN:C    | 2.57                     | 0.42              |
| 1:B:65:ASP:O     | 1:B:66:THR:C     | 2.57                     | 0.42              |
| 1:B:279:GLU:O    | 1:B:280:GLY:O    | 2.38                     | 0.42              |
| 1:E:194:LYS:HG2  | 1:E:194:LYS:O    | 2.19                     | 0.42              |
| 1:B:68:ARG:NH1   | 1:B:562:SER:CB   | 2.79                     | 0.42              |
| 1:B:502:ASN:C    | 1:B:504:ILE:H    | 2.23                     | 0.42              |
| 1:C:406:TRP:HE1  | 1:C:419:ILE:HG21 | 1.85                     | 0.42              |
| 1:D:237:HIS:NE2  | 1:D:425:LEU:CD1  | 2.83                     | 0.42              |
| 1:A:237:HIS:NE2  | 1:A:425:LEU:CD1  | 2.83                     | 0.42              |
| 1:D:178:THR:C    | 1:D:180:THR:N    | 2.73                     | 0.42              |
| 1:A:180:THR:O    | 1:A:181:ILE:C    | 2.58                     | 0.42              |
| 1:B:475:PHE:CD1  | 1:B:475:PHE:N    | 2.88                     | 0.42              |
| 1:E:430:VAL:O    | 1:E:432:CYS:N    | 2.53                     | 0.42              |
| 1:E:524:THR:OG1  | 1:E:525:ASP:N    | 2.52                     | 0.42              |
| 1:E:501:GLU:O    | 1:E:501:GLU:HG2  | 2.20                     | 0.42              |
| 1:C:467:LEU:HD13 | 1:D:126:ILE:HG21 | 2.01                     | 0.42              |
| 1:D:194:LYS:O    | 1:D:194:LYS:HG2  | 2.19                     | 0.42              |
| 1:D:68:ARG:NH1   | 1:D:68:ARG:CG    | 2.66                     | 0.41              |
| 1:E:131:MET:HA   | 1:E:132:PRO:HD3  | 1.87                     | 0.41              |
| 1:D:129:THR:HB   | 1:D:130:ASN:H    | 1.65                     | 0.41              |
| 1:A:149:VAL:CG2  | 1:A:195:VAL:HG11 | 2.45                     | 0.41              |
| 1:B:406:TRP:HE1  | 1:B:419:ILE:HG21 | 1.85                     | 0.41              |
| 1:E:376:LYS:CB   | 1:E:377:PRO:HD2  | 2.32                     | 0.41              |
| 1:B:211:ASP:C    | 1:B:212:THR:HG23 | 2.41                     | 0.41              |
| 1:C:180:THR:O    | 1:C:181:ILE:C    | 2.58                     | 0.41              |
| 1:B:53:ASN:O     | 1:B:54:SER:O     | 2.38                     | 0.41              |
| 1:B:468:LEU:HA   | 1:B:469:PRO:HD3  | 1.76                     | 0.41              |
| 1:B:154:THR:HG1  | 1:B:160:GLU:HB2  | 1.83                     | 0.41              |
| 1:D:430:VAL:O    | 1:D:432:CYS:N    | 2.53                     | 0.41              |
| 1:B:430:VAL:O    | 1:B:432:CYS:N    | 2.53                     | 0.41              |
| 1:B:394:ILE:HG23 | 1:B:395:SER:N    | 2.34                     | 0.41              |
| 1:B:75:LYS:HZ2   | 1:B:94:THR:HG23  | 1.84                     | 0.41              |
| 1:E:279:GLU:O    | 1:E:280:GLY:O    | 2.38                     | 0.41              |
| 1:A:194:LYS:HG2  | 1:A:194:LYS:O    | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:450:THR:HG21 | 1:C:96:ILE:HD13  | 2.03                     | 0.41              |
| 1:A:275:TYR:CE1  | 1:A:404:ARG:HD2  | 2.54                     | 0.41              |
| 1:E:243:LEU:HD23 | 1:E:243:LEU:HA   | 1.92                     | 0.41              |
| 1:E:406:TRP:HE1  | 1:E:419:ILE:HG21 | 1.85                     | 0.41              |
| 1:C:451:PHE:CE1  | 1:D:97:GLN:CB    | 3.03                     | 0.41              |
| 1:C:419:ILE:HG22 | 1:C:423:THR:HG22 | 2.02                     | 0.41              |
| 1:C:178:THR:C    | 1:C:180:THR:N    | 2.73                     | 0.41              |
| 1:A:178:THR:C    | 1:A:180:THR:N    | 2.73                     | 0.41              |
| 1:D:383:THR:C    | 1:D:384:GLU:HG3  | 2.41                     | 0.41              |
| 1:A:154:THR:HG1  | 1:A:160:GLU:HB2  | 1.81                     | 0.41              |
| 1:C:214:ASN:O    | 1:C:216:ARG:N    | 2.50                     | 0.41              |
| 1:E:149:VAL:HG22 | 1:E:149:VAL:O    | 2.21                     | 0.41              |
| 1:D:481:VAL:O    | 1:D:482:TYR:C    | 2.57                     | 0.41              |
| 1:B:93:THR:CG2   | 1:B:94:THR:N     | 2.83                     | 0.41              |
| 1:C:135:ASN:N    | 1:C:140:THR:OG1  | 2.47                     | 0.41              |
| 1:C:211:ASP:C    | 1:C:212:THR:HG23 | 2.41                     | 0.41              |
| 1:C:237:HIS:NE2  | 1:C:425:LEU:CD1  | 2.83                     | 0.41              |
| 1:B:180:THR:O    | 1:B:181:ILE:C    | 2.58                     | 0.41              |
| 1:E:383:THR:C    | 1:E:384:GLU:HG3  | 2.41                     | 0.41              |
| 1:E:237:HIS:NE2  | 1:E:425:LEU:CD1  | 2.83                     | 0.41              |
| 1:E:287:LEU:HD23 | 1:E:288:ASP:C    | 2.41                     | 0.41              |
| 1:B:88:HIS:CD2   | 1:B:555:TYR:O    | 2.74                     | 0.41              |
| 1:C:501:GLU:O    | 1:C:501:GLU:HG2  | 2.20                     | 0.41              |
| 1:D:501:GLU:HG2  | 1:D:501:GLU:O    | 2.20                     | 0.41              |
| 1:D:530:PRO:HG3  | 1:E:66:THR:O     | 2.21                     | 0.41              |
| 1:E:211:ASP:C    | 1:E:212:THR:HG23 | 2.41                     | 0.41              |
| 1:D:214:ASN:O    | 1:D:216:ARG:N    | 2.50                     | 0.41              |
| 1:A:135:ASN:N    | 1:A:140:THR:OG1  | 2.47                     | 0.41              |
| 1:E:395:SER:C    | 1:E:397:ASP:N    | 2.71                     | 0.41              |
| 1:D:265:GLN:NE2  | 1:D:268:GLN:NE2  | 2.68                     | 0.41              |
| 1:C:88:HIS:CD2   | 1:C:555:TYR:O    | 2.74                     | 0.41              |
| 1:B:106:ALA:C    | 1:B:108:THR:N    | 2.71                     | 0.41              |
| 1:C:382:LEU:HA   | 1:C:382:LEU:HD12 | 1.75                     | 0.41              |
| 1:D:382:LEU:HA   | 1:D:382:LEU:HD12 | 1.75                     | 0.41              |
| 1:E:502:ASN:C    | 1:E:504:ILE:H    | 2.23                     | 0.41              |
| 1:C:211:ASP:OD1  | 1:C:212:THR:N    | 2.35                     | 0.41              |
| 1:E:508:PRO:HA   | 1:E:509:PRO:HD3  | 1.73                     | 0.41              |
| 1:E:197:ARG:O    | 1:E:199:ASN:N    | 2.43                     | 0.41              |
| 1:C:475:PHE:CD1  | 1:C:475:PHE:N    | 2.88                     | 0.41              |
| 1:B:395:SER:C    | 1:B:397:ASP:N    | 2.71                     | 0.41              |
| 1:B:287:LEU:HD23 | 1:B:288:ASP:C    | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:530:PRO:HG3  | 1:C:66:THR:O     | 2.21                     | 0.41              |
| 1:E:255:LEU:HA   | 1:E:255:LEU:HD23 | 1.91                     | 0.41              |
| 1:A:406:TRP:HE1  | 1:A:419:ILE:HG21 | 1.85                     | 0.41              |
| 1:A:419:ILE:HG22 | 1:A:423:THR:HG22 | 2.02                     | 0.41              |
| 1:E:214:ASN:O    | 1:E:216:ARG:N    | 2.50                     | 0.41              |
| 1:C:149:VAL:HG22 | 1:C:149:VAL:O    | 2.21                     | 0.41              |
| 1:E:429:ASP:OD1  | 1:E:432:CYS:N    | 2.51                     | 0.41              |
| 1:A:430:VAL:HG23 | 1:A:431:THR:N    | 2.36                     | 0.41              |
| 1:E:393:LEU:CD1  | 1:E:393:LEU:N    | 2.81                     | 0.41              |
| 1:E:265:GLN:NE2  | 1:E:268:GLN:NE2  | 2.68                     | 0.41              |
| 1:C:265:GLN:NE2  | 1:C:268:GLN:NE2  | 2.68                     | 0.41              |
| 1:A:287:LEU:HD23 | 1:A:288:ASP:C    | 2.41                     | 0.41              |
| 1:A:203:GLU:H    | 1:A:203:GLU:HG2  | 1.69                     | 0.41              |
| 1:D:478:ASP:C    | 1:D:480:ALA:N    | 2.73                     | 0.41              |
| 1:B:478:ASP:C    | 1:B:480:ALA:N    | 2.73                     | 0.41              |
| 1:A:530:PRO:HG3  | 1:B:66:THR:O     | 2.21                     | 0.41              |
| 1:A:153:LEU:HD23 | 1:A:159:VAL:HG12 | 2.03                     | 0.41              |
| 1:C:450:THR:HG21 | 1:D:96:ILE:HD13  | 2.03                     | 0.41              |
| 1:A:97:GLN:CB    | 1:E:451:PHE:CE1  | 3.03                     | 0.41              |
| 1:A:211:ASP:C    | 1:A:212:THR:HG23 | 2.41                     | 0.41              |
| 1:C:180:THR:HG21 | 1:C:258:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:383:THR:C    | 1:B:384:GLU:HG3  | 2.41                     | 0.41              |
| 1:B:214:ASN:O    | 1:B:216:ARG:N    | 2.50                     | 0.41              |
| 1:A:475:PHE:CD1  | 1:A:475:PHE:N    | 2.88                     | 0.41              |
| 1:C:430:VAL:HG23 | 1:C:431:THR:N    | 2.36                     | 0.41              |
| 1:D:395:SER:C    | 1:D:397:ASP:N    | 2.71                     | 0.41              |
| 1:E:478:ASP:C    | 1:E:480:ALA:N    | 2.73                     | 0.41              |
| 1:E:113:LEU:HA   | 1:E:113:LEU:HD23 | 1.71                     | 0.41              |
| 1:C:68:ARG:NH1   | 1:C:562:SER:CB   | 2.79                     | 0.41              |
| 1:A:96:ILE:HD13  | 1:E:450:THR:HG21 | 2.03                     | 0.41              |
| 1:B:243:LEU:CD1  | 1:B:403:TYR:HE2  | 2.33                     | 0.41              |
| 1:C:504:ILE:C    | 1:C:506:ALA:H    | 2.25                     | 0.41              |
| 1:E:129:THR:HB   | 1:E:130:ASN:H    | 1.65                     | 0.41              |
| 1:D:211:ASP:C    | 1:D:212:THR:HG23 | 2.41                     | 0.41              |
| 1:D:134:VAL:HG21 | 1:D:175:TYR:CE2  | 2.56                     | 0.41              |
| 1:D:180:THR:O    | 1:D:181:ILE:C    | 2.58                     | 0.41              |
| 1:E:180:THR:O    | 1:E:181:ILE:C    | 2.58                     | 0.41              |
| 1:B:381:PRO:O    | 1:B:381:PRO:HG2  | 2.21                     | 0.41              |
| 1:D:475:PHE:CD1  | 1:D:475:PHE:N    | 2.88                     | 0.41              |
| 1:D:394:ILE:CG2  | 1:D:398:SER:HB2  | 2.51                     | 0.41              |
| 1:A:265:GLN:NE2  | 1:A:268:GLN:NE2  | 2.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:287:LEU:HD23 | 1:D:288:ASP:C    | 2.41                     | 0.41              |
| 1:A:501:GLU:HG2  | 1:A:501:GLU:O    | 2.20                     | 0.41              |
| 1:E:88:HIS:CD2   | 1:E:555:TYR:O    | 2.74                     | 0.41              |
| 1:A:93:THR:CG2   | 1:A:94:THR:N     | 2.83                     | 0.41              |
| 1:E:153:LEU:HD23 | 1:E:159:VAL:HG12 | 2.03                     | 0.41              |
| 1:B:185:ASN:O    | 1:B:188:ILE:HB   | 2.21                     | 0.41              |
| 1:D:153:LEU:HD23 | 1:D:159:VAL:HG12 | 2.03                     | 0.41              |
| 1:B:113:LEU:HA   | 1:B:113:LEU:HD23 | 1.71                     | 0.41              |
| 1:D:96:ILE:HA    | 1:D:96:ILE:HD13  | 1.87                     | 0.41              |
| 1:E:295:SER:O    | 1:E:296:LEU:CB   | 2.64                     | 0.41              |
| 1:C:131:MET:HA   | 1:C:132:PRO:HD3  | 1.87                     | 0.41              |
| 1:D:131:MET:HA   | 1:D:132:PRO:HD3  | 1.87                     | 0.41              |
| 1:C:53:ASN:O     | 1:C:54:SER:O     | 2.38                     | 0.41              |
| 1:B:178:THR:C    | 1:B:180:THR:N    | 2.73                     | 0.41              |
| 1:A:217:LEU:CB   | 1:A:232:THR:HG21 | 2.46                     | 0.41              |
| 1:D:149:VAL:HG22 | 1:D:149:VAL:O    | 2.21                     | 0.41              |
| 1:B:430:VAL:HG23 | 1:B:431:THR:N    | 2.36                     | 0.41              |
| 1:A:66:THR:O     | 1:E:530:PRO:HG3  | 2.21                     | 0.41              |
| 1:D:290:ASP:O    | 1:D:291:ALA:C    | 2.60                     | 0.41              |
| 1:C:96:ILE:HG22  | 1:C:98:ASN:H     | 1.86                     | 0.40              |
| 1:D:96:ILE:HG22  | 1:D:98:ASN:H     | 1.86                     | 0.40              |
| 1:E:468:LEU:HA   | 1:E:469:PRO:HD3  | 1.76                     | 0.40              |
| 1:A:383:THR:C    | 1:A:384:GLU:HG3  | 2.41                     | 0.40              |
| 1:D:430:VAL:HG23 | 1:D:431:THR:N    | 2.36                     | 0.40              |
| 1:B:501:GLU:HG2  | 1:B:501:GLU:O    | 2.20                     | 0.40              |
| 1:C:93:THR:CG2   | 1:C:94:THR:N     | 2.83                     | 0.40              |
| 1:B:153:LEU:HD23 | 1:B:159:VAL:HG12 | 2.03                     | 0.40              |
| 1:B:63:LEU:HD12  | 1:B:63:LEU:HA    | 1.82                     | 0.40              |
| 1:D:542:THR:O    | 1:D:542:THR:HG22 | 2.21                     | 0.40              |
| 1:D:419:ILE:C    | 1:D:421:SER:N    | 2.72                     | 0.40              |
| 1:C:129:THR:HB   | 1:C:130:ASN:H    | 1.65                     | 0.40              |
| 1:D:180:THR:HG21 | 1:D:258:LEU:HD21 | 2.03                     | 0.40              |
| 1:D:198:GLN:HG3  | 1:D:198:GLN:H    | 1.63                     | 0.40              |
| 1:C:383:THR:C    | 1:C:384:GLU:HG3  | 2.41                     | 0.40              |
| 1:A:220:ASP:HA   | 1:A:221:PRO:HD2  | 1.89                     | 0.40              |
| 1:C:153:LEU:HD23 | 1:C:159:VAL:HG12 | 2.03                     | 0.40              |
| 1:C:508:PRO:HA   | 1:C:509:PRO:HD3  | 1.73                     | 0.40              |
| 1:B:132:PRO:HD2  | 1:B:135:ASN:HD22 | 1.86                     | 0.40              |
| 1:A:180:THR:HG21 | 1:A:258:LEU:HD21 | 2.03                     | 0.40              |
| 1:D:75:LYS:HB3   | 1:D:78:ASP:OD2   | 2.22                     | 0.40              |
| 1:C:530:PRO:HG3  | 1:D:66:THR:O     | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:185:ASN:O    | 1:E:188:ILE:HB   | 2.21                     | 0.40              |
| 1:B:96:ILE:HG22  | 1:B:98:ASN:H     | 1.86                     | 0.40              |
| 1:E:243:LEU:CG   | 1:E:403:TYR:CE2  | 3.05                     | 0.40              |
| 1:E:419:ILE:HA   | 1:E:422:TRP:NE1  | 2.37                     | 0.40              |
| 1:C:134:VAL:HG21 | 1:C:175:TYR:CE2  | 2.56                     | 0.40              |
| 1:D:145:ALA:HB3  | 1:D:168:PHE:CE1  | 2.44                     | 0.40              |
| 1:B:265:GLN:NE2  | 1:B:268:GLN:NE2  | 2.68                     | 0.40              |
| 1:B:75:LYS:HB3   | 1:B:78:ASP:OD2   | 2.22                     | 0.40              |
| 1:C:73:ASP:OD1   | 1:C:73:ASP:N     | 2.42                     | 0.40              |
| 1:B:278:LEU:CD2  | 1:B:419:ILE:HD12 | 2.38                     | 0.40              |
| 1:A:211:ASP:OD1  | 1:A:212:THR:N    | 2.35                     | 0.40              |
| 1:E:468:LEU:HD12 | 1:E:469:PRO:N    | 2.37                     | 0.40              |
| 1:A:134:VAL:HG21 | 1:A:175:TYR:CE2  | 2.56                     | 0.40              |
| 1:C:381:PRO:HG2  | 1:C:381:PRO:O    | 2.21                     | 0.40              |
| 1:D:154:THR:HG1  | 1:D:160:GLU:HB2  | 1.83                     | 0.40              |
| 1:A:149:VAL:HG22 | 1:A:149:VAL:O    | 2.21                     | 0.40              |
| 1:E:394:ILE:HG23 | 1:E:395:SER:N    | 2.34                     | 0.40              |
| 1:B:481:VAL:HG13 | 1:B:482:TYR:N    | 2.37                     | 0.40              |
| 1:D:88:HIS:CD2   | 1:D:555:TYR:O    | 2.74                     | 0.40              |
| 1:E:290:ASP:O    | 1:E:291:ALA:C    | 2.60                     | 0.40              |
| 1:D:113:LEU:HA   | 1:D:113:LEU:HD23 | 1.71                     | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 444/523 (85%) | 324 (73%) | 74 (17%) | 46 (10%) | 1           | 12 |
| 1   | B     | 444/523 (85%) | 324 (73%) | 74 (17%) | 46 (10%) | 1           | 12 |
| 1   | C     | 444/523 (85%) | 324 (73%) | 74 (17%) | 46 (10%) | 1           | 12 |
| 1   | D     | 444/523 (85%) | 323 (73%) | 75 (17%) | 46 (10%) | 1           | 12 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1   | E     | 444/523 (85%)   | 324 (73%)  | 74 (17%)  | 46 (10%)  | 1           | 12 |
| All | All   | 2220/2615 (85%) | 1619 (73%) | 371 (17%) | 230 (10%) | 1           | 12 |

All (230) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | SER  |
| 1   | A     | 59  | GLU  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 137 | PHE  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 375 | LYS  |
| 1   | A     | 378 | VAL  |
| 1   | A     | 379 | ILE  |
| 1   | A     | 449 | VAL  |
| 1   | A     | 469 | PRO  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 506 | ALA  |
| 1   | B     | 54  | SER  |
| 1   | B     | 59  | GLU  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 137 | PHE  |
| 1   | B     | 296 | LEU  |
| 1   | B     | 375 | LYS  |
| 1   | B     | 378 | VAL  |
| 1   | B     | 379 | ILE  |
| 1   | B     | 449 | VAL  |
| 1   | B     | 469 | PRO  |
| 1   | B     | 492 | LEU  |
| 1   | B     | 506 | ALA  |
| 1   | C     | 54  | SER  |
| 1   | C     | 59  | GLU  |
| 1   | C     | 130 | ASN  |
| 1   | C     | 137 | PHE  |
| 1   | C     | 296 | LEU  |
| 1   | C     | 375 | LYS  |
| 1   | C     | 378 | VAL  |
| 1   | C     | 379 | ILE  |
| 1   | C     | 449 | VAL  |
| 1   | C     | 469 | PRO  |
| 1   | C     | 492 | LEU  |
| 1   | C     | 506 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 54  | SER  |
| 1   | D     | 59  | GLU  |
| 1   | D     | 130 | ASN  |
| 1   | D     | 137 | PHE  |
| 1   | D     | 296 | LEU  |
| 1   | D     | 375 | LYS  |
| 1   | D     | 378 | VAL  |
| 1   | D     | 379 | ILE  |
| 1   | D     | 449 | VAL  |
| 1   | D     | 469 | PRO  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 506 | ALA  |
| 1   | E     | 54  | SER  |
| 1   | E     | 59  | GLU  |
| 1   | E     | 130 | ASN  |
| 1   | E     | 137 | PHE  |
| 1   | E     | 296 | LEU  |
| 1   | E     | 375 | LYS  |
| 1   | E     | 378 | VAL  |
| 1   | E     | 379 | ILE  |
| 1   | E     | 449 | VAL  |
| 1   | E     | 469 | PRO  |
| 1   | E     | 492 | LEU  |
| 1   | E     | 506 | ALA  |
| 1   | A     | 50  | GLY  |
| 1   | A     | 79  | VAL  |
| 1   | A     | 157 | LYS  |
| 1   | A     | 196 | GLY  |
| 1   | A     | 204 | SER  |
| 1   | A     | 212 | THR  |
| 1   | A     | 216 | ARG  |
| 1   | A     | 251 | THR  |
| 1   | A     | 267 | PHE  |
| 1   | A     | 280 | GLY  |
| 1   | A     | 386 | SER  |
| 1   | A     | 527 | GLY  |
| 1   | B     | 50  | GLY  |
| 1   | B     | 79  | VAL  |
| 1   | B     | 157 | LYS  |
| 1   | B     | 196 | GLY  |
| 1   | B     | 204 | SER  |
| 1   | B     | 212 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 216 | ARG  |
| 1   | B     | 251 | THR  |
| 1   | B     | 267 | PHE  |
| 1   | B     | 280 | GLY  |
| 1   | B     | 386 | SER  |
| 1   | B     | 527 | GLY  |
| 1   | C     | 50  | GLY  |
| 1   | C     | 79  | VAL  |
| 1   | C     | 157 | LYS  |
| 1   | C     | 196 | GLY  |
| 1   | C     | 204 | SER  |
| 1   | C     | 212 | THR  |
| 1   | C     | 216 | ARG  |
| 1   | C     | 251 | THR  |
| 1   | C     | 267 | PHE  |
| 1   | C     | 280 | GLY  |
| 1   | C     | 386 | SER  |
| 1   | C     | 527 | GLY  |
| 1   | D     | 50  | GLY  |
| 1   | D     | 79  | VAL  |
| 1   | D     | 157 | LYS  |
| 1   | D     | 196 | GLY  |
| 1   | D     | 204 | SER  |
| 1   | D     | 212 | THR  |
| 1   | D     | 216 | ARG  |
| 1   | D     | 251 | THR  |
| 1   | D     | 267 | PHE  |
| 1   | D     | 280 | GLY  |
| 1   | D     | 386 | SER  |
| 1   | D     | 527 | GLY  |
| 1   | E     | 50  | GLY  |
| 1   | E     | 79  | VAL  |
| 1   | E     | 157 | LYS  |
| 1   | E     | 196 | GLY  |
| 1   | E     | 204 | SER  |
| 1   | E     | 212 | THR  |
| 1   | E     | 216 | ARG  |
| 1   | E     | 251 | THR  |
| 1   | E     | 267 | PHE  |
| 1   | E     | 280 | GLY  |
| 1   | E     | 386 | SER  |
| 1   | E     | 527 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | THR  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 198 | GLN  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 215 | PHE  |
| 1   | A     | 233 | ASN  |
| 1   | A     | 392 | ASN  |
| 1   | A     | 414 | ASP  |
| 1   | A     | 428 | PRO  |
| 1   | A     | 431 | THR  |
| 1   | A     | 479 | GLN  |
| 1   | B     | 66  | THR  |
| 1   | B     | 74  | ASN  |
| 1   | B     | 198 | GLN  |
| 1   | B     | 199 | ASN  |
| 1   | B     | 215 | PHE  |
| 1   | B     | 233 | ASN  |
| 1   | B     | 392 | ASN  |
| 1   | B     | 414 | ASP  |
| 1   | B     | 428 | PRO  |
| 1   | B     | 431 | THR  |
| 1   | B     | 479 | GLN  |
| 1   | C     | 66  | THR  |
| 1   | C     | 74  | ASN  |
| 1   | C     | 198 | GLN  |
| 1   | C     | 199 | ASN  |
| 1   | C     | 215 | PHE  |
| 1   | C     | 233 | ASN  |
| 1   | C     | 392 | ASN  |
| 1   | C     | 414 | ASP  |
| 1   | C     | 428 | PRO  |
| 1   | C     | 431 | THR  |
| 1   | C     | 479 | GLN  |
| 1   | D     | 66  | THR  |
| 1   | D     | 74  | ASN  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 199 | ASN  |
| 1   | D     | 215 | PHE  |
| 1   | D     | 233 | ASN  |
| 1   | D     | 392 | ASN  |
| 1   | D     | 414 | ASP  |
| 1   | D     | 428 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 431 | THR  |
| 1   | D     | 479 | GLN  |
| 1   | E     | 66  | THR  |
| 1   | E     | 74  | ASN  |
| 1   | E     | 198 | GLN  |
| 1   | E     | 199 | ASN  |
| 1   | E     | 215 | PHE  |
| 1   | E     | 233 | ASN  |
| 1   | E     | 392 | ASN  |
| 1   | E     | 414 | ASP  |
| 1   | E     | 428 | PRO  |
| 1   | E     | 431 | THR  |
| 1   | E     | 479 | GLN  |
| 1   | A     | 388 | LYS  |
| 1   | B     | 388 | LYS  |
| 1   | C     | 388 | LYS  |
| 1   | D     | 388 | LYS  |
| 1   | E     | 388 | LYS  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 179 | MET  |
| 1   | A     | 232 | THR  |
| 1   | A     | 490 | THR  |
| 1   | A     | 513 | ILE  |
| 1   | B     | 155 | LYS  |
| 1   | B     | 179 | MET  |
| 1   | B     | 232 | THR  |
| 1   | B     | 490 | THR  |
| 1   | B     | 513 | ILE  |
| 1   | C     | 155 | LYS  |
| 1   | C     | 179 | MET  |
| 1   | C     | 266 | PRO  |
| 1   | C     | 490 | THR  |
| 1   | C     | 513 | ILE  |
| 1   | D     | 155 | LYS  |
| 1   | D     | 179 | MET  |
| 1   | D     | 490 | THR  |
| 1   | D     | 513 | ILE  |
| 1   | E     | 155 | LYS  |
| 1   | E     | 179 | MET  |
| 1   | E     | 490 | THR  |
| 1   | E     | 513 | ILE  |
| 1   | A     | 61  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 237 | HIS  |
| 1   | A     | 266 | PRO  |
| 1   | B     | 61  | ALA  |
| 1   | B     | 237 | HIS  |
| 1   | B     | 266 | PRO  |
| 1   | C     | 61  | ALA  |
| 1   | C     | 232 | THR  |
| 1   | C     | 237 | HIS  |
| 1   | D     | 61  | ALA  |
| 1   | D     | 232 | THR  |
| 1   | D     | 237 | HIS  |
| 1   | D     | 266 | PRO  |
| 1   | E     | 61  | ALA  |
| 1   | E     | 232 | THR  |
| 1   | E     | 237 | HIS  |
| 1   | E     | 266 | PRO  |
| 1   | A     | 486 | ILE  |
| 1   | B     | 486 | ILE  |
| 1   | C     | 486 | ILE  |
| 1   | D     | 486 | ILE  |
| 1   | E     | 486 | ILE  |
| 1   | B     | 195 | VAL  |
| 1   | C     | 195 | VAL  |
| 1   | D     | 195 | VAL  |
| 1   | A     | 195 | VAL  |
| 1   | E     | 195 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 404/451 (90%) | 369 (91%) | 35 (9%)  | 13          | 45 |
| 1   | B     | 404/451 (90%) | 369 (91%) | 35 (9%)  | 13          | 45 |
| 1   | C     | 404/451 (90%) | 369 (91%) | 35 (9%)  | 13          | 45 |
| 1   | D     | 404/451 (90%) | 369 (91%) | 35 (9%)  | 13          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | E     | 404/451 (90%)   | 369 (91%)  | 35 (9%)  | 13          | 45 |
| All | All   | 2020/2255 (90%) | 1845 (91%) | 175 (9%) | 17          | 45 |

All (175) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | SER  |
| 1   | A     | 76  | SER  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 102 | SER  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 153 | LEU  |
| 1   | A     | 166 | VAL  |
| 1   | A     | 214 | ASN  |
| 1   | A     | 223 | THR  |
| 1   | A     | 232 | THR  |
| 1   | A     | 233 | ASN  |
| 1   | A     | 238 | PRO  |
| 1   | A     | 249 | ASP  |
| 1   | A     | 256 | SER  |
| 1   | A     | 258 | LEU  |
| 1   | A     | 271 | PHE  |
| 1   | A     | 287 | LEU  |
| 1   | A     | 401 | THR  |
| 1   | A     | 420 | ARG  |
| 1   | A     | 429 | ASP  |
| 1   | A     | 440 | SER  |
| 1   | A     | 446 | GLN  |
| 1   | A     | 459 | ASN  |
| 1   | A     | 468 | LEU  |
| 1   | A     | 482 | TYR  |
| 1   | A     | 501 | GLU  |
| 1   | A     | 512 | THR  |
| 1   | A     | 525 | ASP  |
| 1   | A     | 528 | THR  |
| 1   | A     | 531 | LEU  |
| 1   | A     | 533 | ASN  |
| 1   | A     | 534 | SER  |
| 1   | A     | 562 | SER  |
| 1   | B     | 58  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 76  | SER  |
| 1   | B     | 83  | ASN  |
| 1   | B     | 98  | ASN  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 102 | SER  |
| 1   | B     | 146 | ARG  |
| 1   | B     | 153 | LEU  |
| 1   | B     | 166 | VAL  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 223 | THR  |
| 1   | B     | 232 | THR  |
| 1   | B     | 233 | ASN  |
| 1   | B     | 238 | PRO  |
| 1   | B     | 249 | ASP  |
| 1   | B     | 256 | SER  |
| 1   | B     | 258 | LEU  |
| 1   | B     | 271 | PHE  |
| 1   | B     | 287 | LEU  |
| 1   | B     | 401 | THR  |
| 1   | B     | 420 | ARG  |
| 1   | B     | 429 | ASP  |
| 1   | B     | 440 | SER  |
| 1   | B     | 446 | GLN  |
| 1   | B     | 459 | ASN  |
| 1   | B     | 468 | LEU  |
| 1   | B     | 482 | TYR  |
| 1   | B     | 501 | GLU  |
| 1   | B     | 512 | THR  |
| 1   | B     | 525 | ASP  |
| 1   | B     | 528 | THR  |
| 1   | B     | 531 | LEU  |
| 1   | B     | 533 | ASN  |
| 1   | B     | 534 | SER  |
| 1   | B     | 562 | SER  |
| 1   | C     | 58  | SER  |
| 1   | C     | 76  | SER  |
| 1   | C     | 83  | ASN  |
| 1   | C     | 98  | ASN  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 102 | SER  |
| 1   | C     | 146 | ARG  |
| 1   | C     | 153 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 166 | VAL  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 223 | THR  |
| 1   | C     | 232 | THR  |
| 1   | C     | 233 | ASN  |
| 1   | C     | 238 | PRO  |
| 1   | C     | 249 | ASP  |
| 1   | C     | 256 | SER  |
| 1   | C     | 258 | LEU  |
| 1   | C     | 271 | PHE  |
| 1   | C     | 287 | LEU  |
| 1   | C     | 401 | THR  |
| 1   | C     | 420 | ARG  |
| 1   | C     | 429 | ASP  |
| 1   | C     | 440 | SER  |
| 1   | C     | 446 | GLN  |
| 1   | C     | 459 | ASN  |
| 1   | C     | 468 | LEU  |
| 1   | C     | 482 | TYR  |
| 1   | C     | 501 | GLU  |
| 1   | C     | 512 | THR  |
| 1   | C     | 525 | ASP  |
| 1   | C     | 528 | THR  |
| 1   | C     | 531 | LEU  |
| 1   | C     | 533 | ASN  |
| 1   | C     | 534 | SER  |
| 1   | C     | 562 | SER  |
| 1   | D     | 58  | SER  |
| 1   | D     | 76  | SER  |
| 1   | D     | 83  | ASN  |
| 1   | D     | 98  | ASN  |
| 1   | D     | 100 | ASP  |
| 1   | D     | 102 | SER  |
| 1   | D     | 146 | ARG  |
| 1   | D     | 153 | LEU  |
| 1   | D     | 166 | VAL  |
| 1   | D     | 214 | ASN  |
| 1   | D     | 223 | THR  |
| 1   | D     | 232 | THR  |
| 1   | D     | 233 | ASN  |
| 1   | D     | 238 | PRO  |
| 1   | D     | 249 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 256 | SER  |
| 1   | D     | 258 | LEU  |
| 1   | D     | 271 | PHE  |
| 1   | D     | 287 | LEU  |
| 1   | D     | 401 | THR  |
| 1   | D     | 420 | ARG  |
| 1   | D     | 429 | ASP  |
| 1   | D     | 440 | SER  |
| 1   | D     | 446 | GLN  |
| 1   | D     | 459 | ASN  |
| 1   | D     | 468 | LEU  |
| 1   | D     | 482 | TYR  |
| 1   | D     | 501 | GLU  |
| 1   | D     | 512 | THR  |
| 1   | D     | 525 | ASP  |
| 1   | D     | 528 | THR  |
| 1   | D     | 531 | LEU  |
| 1   | D     | 533 | ASN  |
| 1   | D     | 534 | SER  |
| 1   | D     | 562 | SER  |
| 1   | E     | 58  | SER  |
| 1   | E     | 76  | SER  |
| 1   | E     | 83  | ASN  |
| 1   | E     | 98  | ASN  |
| 1   | E     | 100 | ASP  |
| 1   | E     | 102 | SER  |
| 1   | E     | 146 | ARG  |
| 1   | E     | 153 | LEU  |
| 1   | E     | 166 | VAL  |
| 1   | E     | 214 | ASN  |
| 1   | E     | 223 | THR  |
| 1   | E     | 232 | THR  |
| 1   | E     | 233 | ASN  |
| 1   | E     | 238 | PRO  |
| 1   | E     | 249 | ASP  |
| 1   | E     | 256 | SER  |
| 1   | E     | 258 | LEU  |
| 1   | E     | 271 | PHE  |
| 1   | E     | 287 | LEU  |
| 1   | E     | 401 | THR  |
| 1   | E     | 420 | ARG  |
| 1   | E     | 429 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 440 | SER  |
| 1   | E     | 446 | GLN  |
| 1   | E     | 459 | ASN  |
| 1   | E     | 468 | LEU  |
| 1   | E     | 482 | TYR  |
| 1   | E     | 501 | GLU  |
| 1   | E     | 512 | THR  |
| 1   | E     | 525 | ASP  |
| 1   | E     | 528 | THR  |
| 1   | E     | 531 | LEU  |
| 1   | E     | 533 | ASN  |
| 1   | E     | 534 | SER  |
| 1   | E     | 562 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | ASN  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 99  | ASN  |
| 1   | A     | 128 | HIS  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 214 | ASN  |
| 1   | A     | 265 | GLN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 402 | GLN  |
| 1   | A     | 459 | ASN  |
| 1   | A     | 471 | HIS  |
| 1   | B     | 74  | ASN  |
| 1   | B     | 86  | ASN  |
| 1   | B     | 98  | ASN  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 128 | HIS  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 265 | GLN  |
| 1   | B     | 282 | ASN  |
| 1   | B     | 402 | GLN  |
| 1   | B     | 459 | ASN  |
| 1   | B     | 471 | HIS  |
| 1   | C     | 74  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 86  | ASN  |
| 1   | C     | 98  | ASN  |
| 1   | C     | 99  | ASN  |
| 1   | C     | 128 | HIS  |
| 1   | C     | 130 | ASN  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 265 | GLN  |
| 1   | C     | 282 | ASN  |
| 1   | C     | 402 | GLN  |
| 1   | C     | 459 | ASN  |
| 1   | C     | 471 | HIS  |
| 1   | D     | 74  | ASN  |
| 1   | D     | 86  | ASN  |
| 1   | D     | 98  | ASN  |
| 1   | D     | 99  | ASN  |
| 1   | D     | 128 | HIS  |
| 1   | D     | 130 | ASN  |
| 1   | D     | 199 | ASN  |
| 1   | D     | 214 | ASN  |
| 1   | D     | 265 | GLN  |
| 1   | D     | 282 | ASN  |
| 1   | D     | 402 | GLN  |
| 1   | D     | 459 | ASN  |
| 1   | D     | 471 | HIS  |
| 1   | E     | 74  | ASN  |
| 1   | E     | 86  | ASN  |
| 1   | E     | 98  | ASN  |
| 1   | E     | 99  | ASN  |
| 1   | E     | 128 | HIS  |
| 1   | E     | 130 | ASN  |
| 1   | E     | 214 | ASN  |
| 1   | E     | 265 | GLN  |
| 1   | E     | 282 | ASN  |
| 1   | E     | 402 | GLN  |
| 1   | E     | 459 | ASN  |
| 1   | E     | 471 | HIS  |

### 5.3.3 RNA ⓘ

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.