



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:33 am GMT

PDB ID : 3J7V  
EMDB ID: : EMD-6034  
Title : Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions  
Authors : Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.  
Deposited on : 2014-08-12  
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

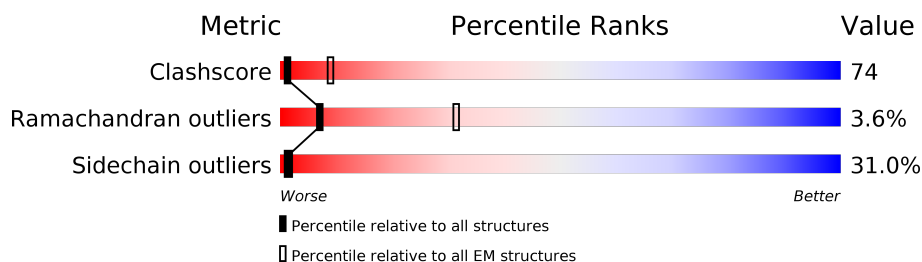
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |

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     | 345    | 30% 42% 13% • 13% |
| 1   | B     | 345    | 29% 40% 19% • 10% |
| 1   | C     | 345    | 23% 40% 21% • 14% |
| 1   | D     | 345    | 31% 37% 17% • 14% |
| 1   | E     | 345    | 28% 39% 16% • 15% |
| 1   | F     | 345    | 32% 39% 14% • 13% |
| 1   | G     | 345    | 31% 43% 17% • 8%  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15873 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.

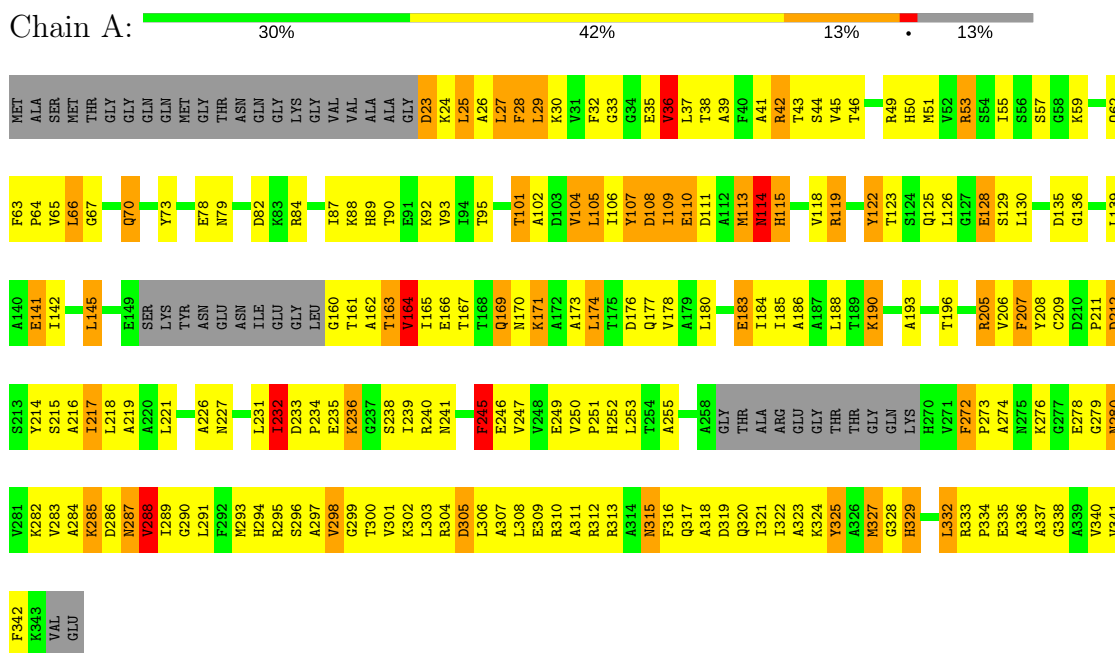
- Molecule 1 is a protein called Major capsid protein 10A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 300      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2250  | 1418 | 396 | 427 | 9 |         |       |
| 1   | B     | 309      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2321  | 1462 | 406 | 444 | 9 |         |       |
| 1   | C     | 296      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2234  | 1411 | 393 | 421 | 9 |         |       |
| 1   | D     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2241  | 1413 | 394 | 425 | 9 |         |       |
| 1   | E     | 293      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2208  | 1393 | 387 | 419 | 9 |         |       |
| 1   | F     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2245  | 1415 | 395 | 426 | 9 |         |       |
| 1   | G     | 317      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2374  | 1492 | 419 | 454 | 9 |         |       |

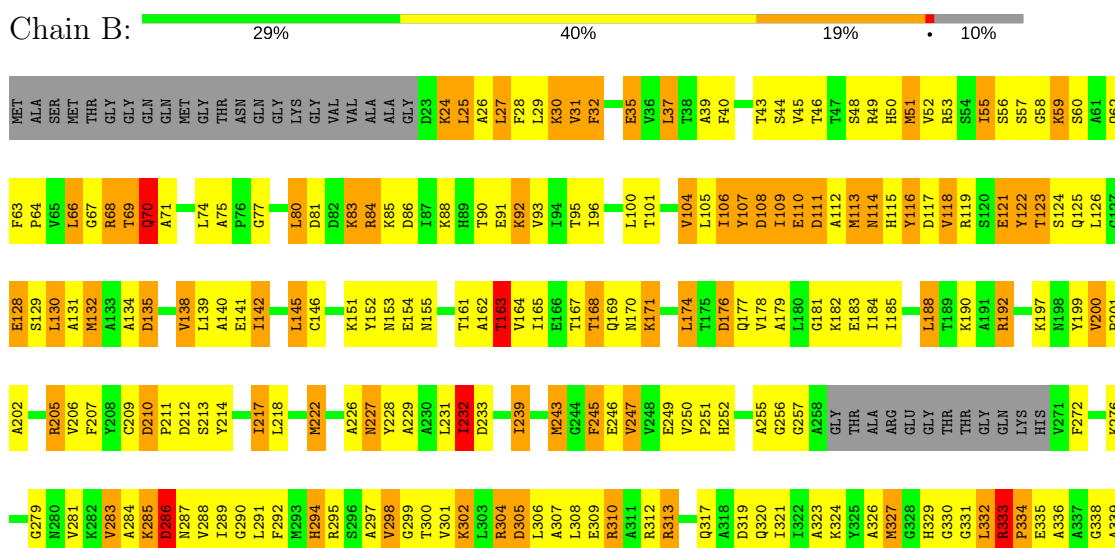
### 3 Residue-property plots

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

#### • Molecule 1: Major capsid protein 10A

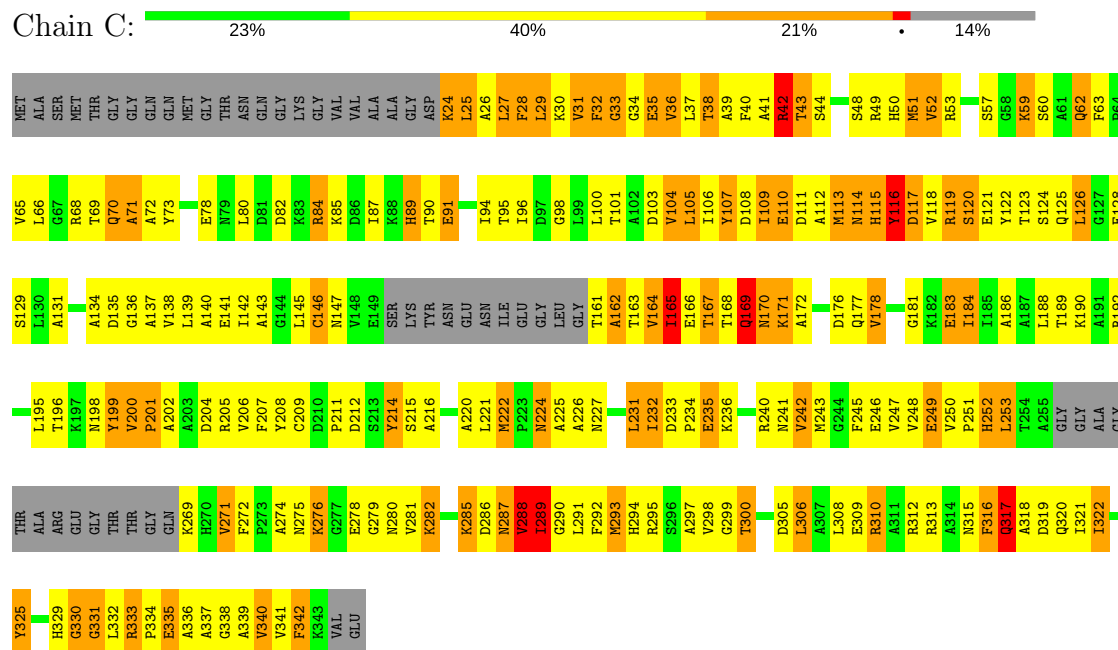


#### • Molecule 1: Major capsid protein 10A

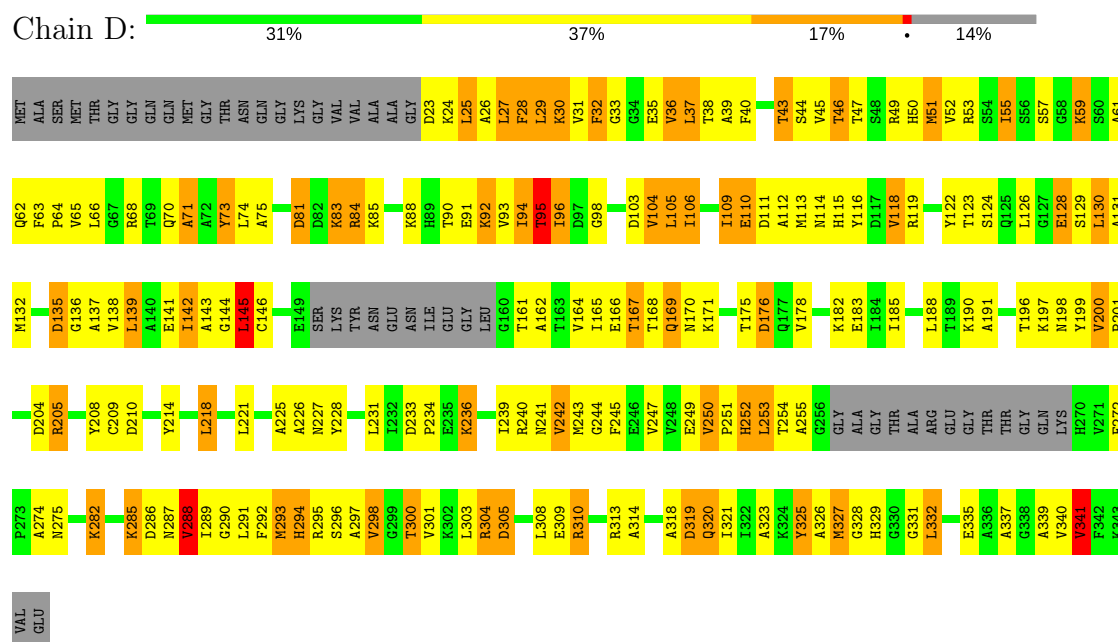


V340  
V341  
F342  
K343  
VAL  
GLU

• Molecule 1: Major capsid protein 10A

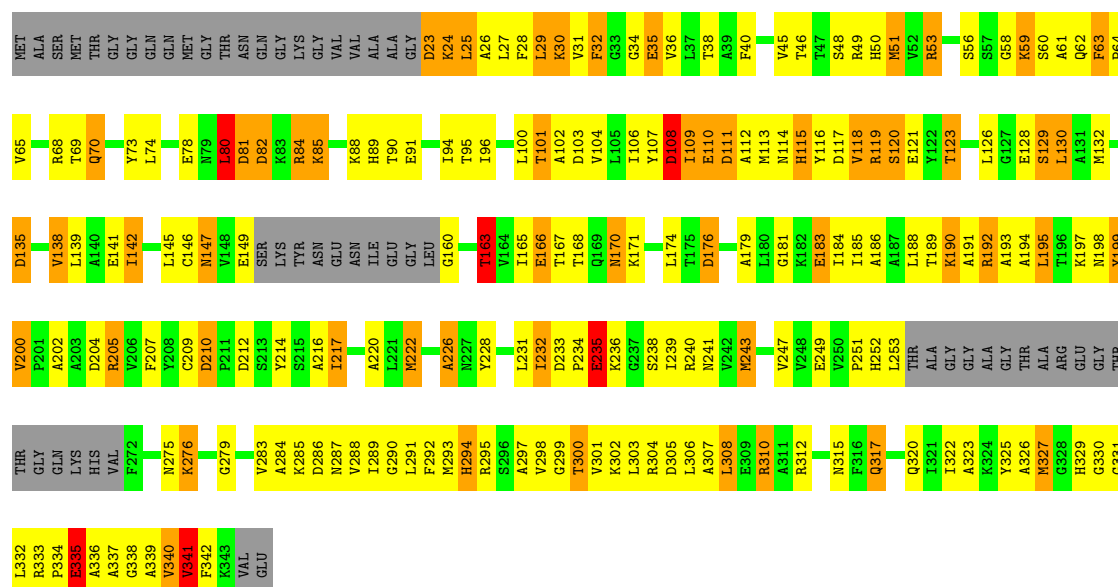


• Molecule 1: Major capsid protein 10A



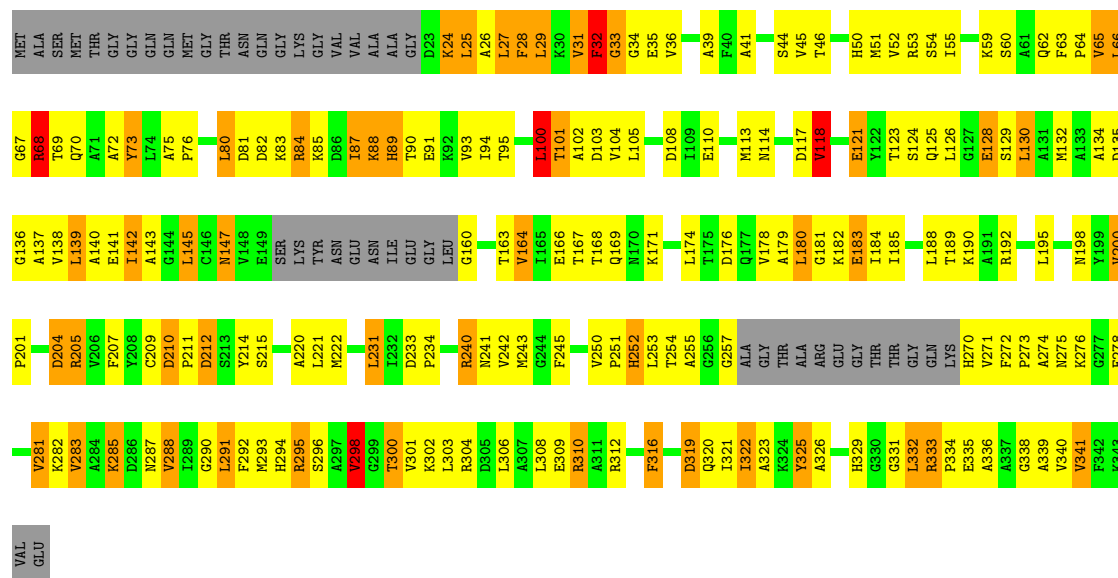
• Molecule 1: Major capsid protein 10A





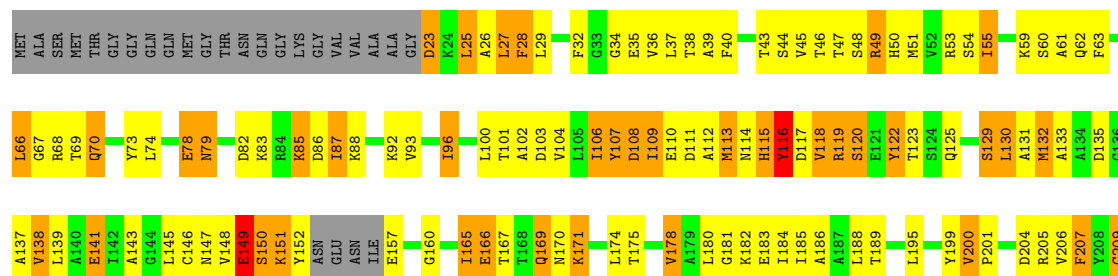
### • Molecule 1: Major capsid protein 10A

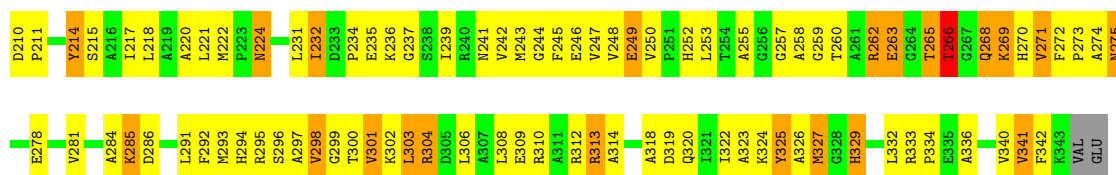
Chain F: 32% 39% 14% 13%



### • Molecule 1: Major capsid protein 10A

Chain G: 31% 43% 17% 8%





## 4 Experimental information

| Property                             | Value             | Source    |
|--------------------------------------|-------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE   | Depositor |
| Imposed symmetry                     | POINT, I          | Depositor |
| Number of particles used             | 27520             | Depositor |
| Resolution determination method      | FSC 0.143         | Depositor |
| CTF correction method                | Each particle     | Depositor |
| Microscope                           | FEI TITAN KRIOS   | Depositor |
| Voltage (kV)                         | 300               | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                | Depositor |
| Minimum defocus (nm)                 | 800               | Depositor |
| Maximum defocus (nm)                 | 4500              | Depositor |
| Magnification                        | 57727             | Depositor |
| Image detector                       | KODAK SO-163 FILM | Depositor |



## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 2$ | RMSZ        | $\# Z  > 2$     |
| 1   | A     | 0.35         | 0/2282      | 0.69        | 1/3087 (0.0%)   |
| 1   | B     | 0.40         | 0/2354      | 0.82        | 3/3185 (0.1%)   |
| 1   | C     | 0.45         | 0/2266      | 0.82        | 2/3065 (0.1%)   |
| 1   | D     | 0.38         | 0/2273      | 0.74        | 2/3075 (0.1%)   |
| 1   | E     | 0.38         | 0/2239      | 0.70        | 2/3028 (0.1%)   |
| 1   | F     | 0.37         | 0/2277      | 0.70        | 2/3080 (0.1%)   |
| 1   | G     | 0.30         | 0/2408      | 0.65        | 1/3256 (0.0%)   |
| All | All   | 0.38         | 0/16099     | 0.73        | 13/21776 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 5                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 6                   |
| 1   | D     | 0                   | 5                   |
| 1   | E     | 0                   | 7                   |
| 1   | F     | 0                   | 3                   |
| 1   | G     | 0                   | 1                   |
| All | All   | 0                   | 30                  |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | B     | 333 | ARG  | C-N-CD   | -20.55 | 75.40       | 120.60   |
| 1   | B     | 70  | GLN  | CB-CA-C  | -7.36  | 95.67       | 110.40   |
| 1   | C     | 200 | VAL  | C-N-CD   | 6.03   | 141.06      | 128.40   |
| 1   | E     | 80  | LEU  | CA-CB-CG | 5.80   | 128.65      | 115.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 331 | GLY  | N-CA-C    | 5.50  | 126.84      | 113.10   |
| 1   | B     | 70  | GLN  | C-N-CA    | 5.49  | 135.41      | 121.70   |
| 1   | F     | 69  | THR  | N-CA-C    | -5.43 | 96.33       | 111.00   |
| 1   | G     | 23  | ASP  | CB-CG-OD2 | 5.24  | 123.02      | 118.30   |
| 1   | D     | 23  | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | E     | 23  | ASP  | CB-CG-OD2 | 5.17  | 122.96      | 118.30   |
| 1   | A     | 305 | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | D     | 288 | VAL  | CB-CA-C   | -5.09 | 101.73      | 111.40   |
| 1   | F     | 100 | LEU  | CA-CB-CG  | 5.02  | 126.84      | 115.30   |

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 108 | ASP  | Peptide |
| 1   | A     | 114 | ASN  | Peptide |
| 1   | A     | 316 | PHE  | Peptide |
| 1   | A     | 329 | HIS  | Peptide |
| 1   | A     | 332 | LEU  | Peptide |
| 1   | B     | 106 | ILE  | Peptide |
| 1   | B     | 163 | THR  | Peptide |
| 1   | B     | 70  | GLN  | Peptide |
| 1   | C     | 164 | VAL  | Peptide |
| 1   | C     | 233 | ASP  | Peptide |
| 1   | C     | 287 | ASN  | Peptide |
| 1   | C     | 317 | GLN  | Peptide |
| 1   | C     | 330 | GLY  | Peptide |
| 1   | C     | 71  | ALA  | Peptide |
| 1   | D     | 250 | VAL  | Peptide |
| 1   | D     | 292 | PHE  | Peptide |
| 1   | D     | 331 | GLY  | Peptide |
| 1   | D     | 95  | THR  | Peptide |
| 1   | D     | 98  | GLY  | Peptide |
| 1   | E     | 107 | TYR  | Peptide |
| 1   | E     | 108 | ASP  | Peptide |
| 1   | E     | 146 | CYS  | Peptide |
| 1   | E     | 163 | THR  | Peptide |
| 1   | E     | 231 | LEU  | Peptide |
| 1   | E     | 232 | ILE  | Peptide |
| 1   | E     | 317 | GLN  | Peptide |
| 1   | F     | 316 | PHE  | Peptide |
| 1   | F     | 66  | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | F     | 68  | ARG  | Peptide |
| 1   | G     | 292 | PHE  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2250  | 0        | 2279     | 343     | 0            |
| 1   | B     | 2321  | 0        | 2348     | 415     | 0            |
| 1   | C     | 2234  | 0        | 2271     | 465     | 0            |
| 1   | D     | 2241  | 0        | 2272     | 281     | 0            |
| 1   | E     | 2208  | 0        | 2240     | 372     | 0            |
| 1   | F     | 2245  | 0        | 2275     | 229     | 0            |
| 1   | G     | 2374  | 0        | 2403     | 333     | 0            |
| All | All   | 15873 | 0        | 16088    | 2351    | 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 74.

All (2351) 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:28:PHE:CE1   | 1:B:112:ALA:HA   | 1.24                     | 1.71              |
| 1:B:251:PRO:HB2  | 1:C:199:TYR:CZ   | 1.09                     | 1.60              |
| 1:E:298:VAL:C    | 1:E:333:ARG:HH12 | 1.06                     | 1.57              |
| 1:E:189:THR:HG22 | 1:E:243:MET:SD   | 1.45                     | 1.55              |
| 1:E:25:LEU:HD21  | 1:E:310:ARG:CZ   | 1.08                     | 1.55              |
| 1:A:207:PHE:CZ   | 1:A:209:CYS:HB2  | 1.36                     | 1.54              |
| 1:A:309:GLU:CB   | 1:A:322:ILE:HG13 | 1.38                     | 1.53              |
| 1:D:142:ILE:CA   | 1:D:145:LEU:HD23 | 1.31                     | 1.53              |
| 1:B:251:PRO:CB   | 1:C:199:TYR:CE1  | 1.93                     | 1.52              |
| 1:B:251:PRO:CG   | 1:C:199:TYR:CE1  | 1.92                     | 1.52              |
| 1:E:25:LEU:CD2   | 1:E:310:ARG:NH2  | 1.70                     | 1.51              |
| 1:B:28:PHE:CZ    | 1:B:112:ALA:HA   | 1.44                     | 1.51              |
| 1:E:25:LEU:CD2   | 1:E:310:ARG:CZ   | 1.89                     | 1.50              |
| 1:B:251:PRO:CB   | 1:C:199:TYR:CZ   | 1.93                     | 1.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:142:ILE:HA   | 1:D:145:LEU:CD2  | 1.40                     | 1.49              |
| 1:E:189:THR:CG2  | 1:E:243:MET:CE   | 1.91                     | 1.49              |
| 1:G:110:GLU:HA   | 1:G:114:ASN:CG   | 1.35                     | 1.48              |
| 1:E:189:THR:CG2  | 1:E:243:MET:SD   | 2.04                     | 1.45              |
| 1:C:195:LEU:CD2  | 1:C:205:ARG:NH2  | 1.78                     | 1.44              |
| 1:B:141:GLU:OE1  | 1:B:330:GLY:CA   | 1.65                     | 1.43              |
| 1:E:145:LEU:CB   | 1:E:332:LEU:HD23 | 1.45                     | 1.43              |
| 1:C:161:THR:OG1  | 1:C:336:ALA:CB   | 1.64                     | 1.42              |
| 1:D:138:VAL:HG23 | 1:D:139:LEU:CD1  | 1.51                     | 1.40              |
| 1:E:25:LEU:HD21  | 1:E:310:ARG:NH2  | 1.10                     | 1.38              |
| 1:E:192:ARG:HA   | 1:E:195:LEU:CD1  | 1.53                     | 1.38              |
| 1:D:130:LEU:HD12 | 1:D:131:ALA:N    | 1.38                     | 1.36              |
| 1:B:145:LEU:HD21 | 1:B:332:LEU:CD1  | 1.53                     | 1.36              |
| 1:C:195:LEU:CD2  | 1:C:202:ALA:HB1  | 1.54                     | 1.36              |
| 1:F:25:LEU:HA    | 1:F:28:PHE:CD2   | 1.61                     | 1.36              |
| 1:B:145:LEU:CD2  | 1:B:332:LEU:HG   | 1.55                     | 1.35              |
| 1:E:192:ARG:CA   | 1:E:195:LEU:HD11 | 1.53                     | 1.35              |
| 1:D:29:LEU:HD13  | 1:D:30:LYS:N     | 1.36                     | 1.34              |
| 1:C:25:LEU:HD23  | 1:C:26:ALA:N     | 1.41                     | 1.33              |
| 1:A:289:ILE:HG13 | 1:A:340:VAL:CG2  | 1.57                     | 1.33              |
| 1:B:109:ILE:HD13 | 1:B:110:GLU:N    | 1.37                     | 1.33              |
| 1:E:25:LEU:CG    | 1:E:310:ARG:NH2  | 1.89                     | 1.33              |
| 1:B:40:PHE:HE1   | 1:B:130:LEU:CD1  | 1.11                     | 1.33              |
| 1:B:40:PHE:CE1   | 1:B:130:LEU:HD11 | 1.41                     | 1.33              |
| 1:A:27:LEU:HD12  | 1:A:28:PHE:N     | 1.41                     | 1.32              |
| 1:B:113:MET:HA   | 1:B:115:HIS:NE2  | 1.42                     | 1.32              |
| 1:A:309:GLU:CB   | 1:A:322:ILE:CG1  | 2.07                     | 1.31              |
| 1:E:145:LEU:HD22 | 1:E:332:LEU:CD2  | 1.58                     | 1.31              |
| 1:E:181:GLY:O    | 1:E:185:ILE:CD1  | 1.75                     | 1.31              |
| 1:E:40:PHE:HA    | 1:E:130:LEU:CD2  | 1.35                     | 1.31              |
| 1:B:28:PHE:CE1   | 1:B:112:ALA:CA   | 2.14                     | 1.30              |
| 1:E:25:LEU:CD2   | 1:E:310:ARG:NH1  | 1.91                     | 1.29              |
| 1:C:195:LEU:HD23 | 1:C:205:ARG:CZ   | 1.60                     | 1.29              |
| 1:A:309:GLU:CA   | 1:A:322:ILE:HG13 | 1.59                     | 1.29              |
| 1:B:251:PRO:HG3  | 1:C:199:TYR:CE1  | 1.59                     | 1.28              |
| 1:C:188:LEU:HD22 | 1:C:207:PHE:CE1  | 1.69                     | 1.28              |
| 1:A:119:ARG:CB   | 1:A:119:ARG:HH11 | 1.46                     | 1.28              |
| 1:G:149:GLU:CG   | 1:G:150:SER:H    | 1.45                     | 1.27              |
| 1:C:26:ALA:CA    | 1:C:29:LEU:HD13  | 1.62                     | 1.27              |
| 1:C:195:LEU:HD21 | 1:C:202:ALA:CB   | 1.63                     | 1.27              |
| 1:C:206:VAL:HA   | 1:C:246:GLU:O    | 1.20                     | 1.27              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:106:ILE:C    | 1:G:106:ILE:HD13 | 1.54                     | 1.27              |
| 1:E:189:THR:HG22 | 1:E:243:MET:CE   | 1.54                     | 1.26              |
| 1:A:26:ALA:O     | 1:A:29:LEU:HD12  | 1.36                     | 1.26              |
| 1:E:145:LEU:HD22 | 1:E:332:LEU:CG   | 1.66                     | 1.26              |
| 1:E:145:LEU:HB2  | 1:E:332:LEU:CD2  | 1.65                     | 1.26              |
| 1:A:309:GLU:HB3  | 1:A:322:ILE:CD1  | 1.66                     | 1.26              |
| 1:A:309:GLU:O    | 1:A:322:ILE:HG12 | 1.26                     | 1.26              |
| 1:E:25:LEU:HD22  | 1:E:310:ARG:NH1  | 1.45                     | 1.25              |
| 1:C:27:LEU:HD23  | 1:C:27:LEU:C     | 1.53                     | 1.25              |
| 1:C:26:ALA:HA    | 1:C:29:LEU:CD1   | 1.65                     | 1.25              |
| 1:E:298:VAL:C    | 1:E:333:ARG:NH1  | 1.86                     | 1.25              |
| 1:B:113:MET:SD   | 1:B:115:HIS:CE1  | 2.30                     | 1.25              |
| 1:D:36:VAL:O     | 1:D:39:ALA:N     | 1.69                     | 1.25              |
| 1:A:289:ILE:CG1  | 1:A:340:VAL:HG22 | 1.64                     | 1.24              |
| 1:E:181:GLY:O    | 1:E:185:ILE:HD12 | 1.10                     | 1.24              |
| 1:C:109:ILE:C    | 1:C:109:ILE:HD13 | 1.54                     | 1.24              |
| 1:A:207:PHE:CZ   | 1:A:209:CYS:CB   | 2.21                     | 1.23              |
| 1:B:130:LEU:HD12 | 1:B:130:LEU:C    | 1.53                     | 1.23              |
| 1:G:25:LEU:O     | 1:G:29:LEU:HG    | 1.39                     | 1.23              |
| 1:C:207:PHE:CD2  | 1:C:247:VAL:HG22 | 1.72                     | 1.23              |
| 1:C:195:LEU:HD23 | 1:C:205:ARG:NH2  | 0.90                     | 1.23              |
| 1:G:110:GLU:HA   | 1:G:114:ASN:CB   | 1.68                     | 1.23              |
| 1:D:144:GLY:O    | 1:D:146:CYS:N    | 1.69                     | 1.22              |
| 1:B:139:LEU:O    | 1:B:142:ILE:HG23 | 1.34                     | 1.22              |
| 1:D:142:ILE:O    | 1:D:145:LEU:HB2  | 1.36                     | 1.22              |
| 1:G:146:CYS:CB   | 1:G:336:ALA:HB3  | 1.69                     | 1.22              |
| 1:B:145:LEU:CD2  | 1:B:332:LEU:CD1  | 2.17                     | 1.21              |
| 1:B:31:VAL:CG1   | 1:B:35:GLU:OE2   | 1.87                     | 1.21              |
| 1:E:40:PHE:CA    | 1:E:130:LEU:HD22 | 1.52                     | 1.21              |
| 1:E:142:ILE:HD12 | 1:E:142:ILE:C    | 1.59                     | 1.21              |
| 1:C:116:TYR:O    | 1:C:118:VAL:N    | 1.73                     | 1.21              |
| 1:E:142:ILE:HD12 | 1:E:142:ILE:O    | 1.37                     | 1.21              |
| 1:G:25:LEU:HA    | 1:G:28:PHE:CD2   | 1.77                     | 1.20              |
| 1:A:27:LEU:C     | 1:A:27:LEU:HD12  | 1.58                     | 1.20              |
| 1:A:309:GLU:O    | 1:A:322:ILE:CG1  | 1.90                     | 1.20              |
| 1:G:109:ILE:CD1  | 1:G:109:ILE:H    | 1.51                     | 1.20              |
| 1:G:130:LEU:C    | 1:G:130:LEU:HD23 | 1.59                     | 1.20              |
| 1:G:110:GLU:OE2  | 1:G:118:VAL:CG1  | 1.90                     | 1.19              |
| 1:B:145:LEU:CD2  | 1:B:332:LEU:CG   | 2.19                     | 1.19              |
| 1:B:132:MET:HE2  | 1:B:132:MET:HA   | 1.21                     | 1.19              |
| 1:B:113:MET:HA   | 1:B:115:HIS:CD2  | 1.78                     | 1.19              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:40:PHE:CE1   | 1:B:130:LEU:CD1  | 1.86                     | 1.19              |
| 1:G:113:MET:CA   | 1:G:113:MET:HE3  | 1.72                     | 1.19              |
| 1:A:119:ARG:HB2  | 1:A:119:ARG:HH11 | 1.07                     | 1.18              |
| 1:A:114:ASN:N    | 1:A:115:HIS:CD2  | 2.09                     | 1.18              |
| 1:C:25:LEU:CD2   | 1:C:26:ALA:H     | 1.58                     | 1.17              |
| 1:B:132:MET:CE   | 1:B:132:MET:HA   | 1.64                     | 1.17              |
| 1:D:46:THR:HG23  | 1:D:135:ASP:OD1  | 1.41                     | 1.17              |
| 1:E:25:LEU:HD12  | 1:E:25:LEU:C     | 1.54                     | 1.17              |
| 1:A:25:LEU:O     | 1:A:25:LEU:HD13  | 1.39                     | 1.16              |
| 1:E:145:LEU:CD2  | 1:E:332:LEU:CD2  | 2.24                     | 1.16              |
| 1:F:25:LEU:HA    | 1:F:28:PHE:CE2   | 1.80                     | 1.16              |
| 1:G:106:ILE:HD13 | 1:G:107:TYR:N    | 1.59                     | 1.16              |
| 1:G:28:PHE:CE1   | 1:G:111:ASP:OD2  | 1.99                     | 1.16              |
| 1:G:110:GLU:O    | 1:G:114:ASN:HB3  | 1.41                     | 1.16              |
| 1:A:289:ILE:HG12 | 1:A:340:VAL:O    | 1.42                     | 1.16              |
| 1:A:309:GLU:CB   | 1:A:322:ILE:CD1  | 2.23                     | 1.16              |
| 1:A:309:GLU:O    | 1:A:322:ILE:N    | 1.78                     | 1.16              |
| 1:E:63:PHE:CE2   | 1:E:333:ARG:NH2  | 2.13                     | 1.16              |
| 1:B:24:LYS:HD2   | 1:B:24:LYS:C     | 1.64                     | 1.15              |
| 1:C:26:ALA:C     | 1:C:29:LEU:HD13  | 1.65                     | 1.15              |
| 1:A:294:HIS:CD2  | 1:A:337:ALA:HA   | 1.81                     | 1.15              |
| 1:B:138:VAL:O    | 1:B:142:ILE:HG22 | 1.43                     | 1.15              |
| 1:E:24:LYS:HZ1   | 1:E:112:ALA:HB1  | 1.01                     | 1.15              |
| 1:C:26:ALA:HA    | 1:C:29:LEU:HD13  | 1.15                     | 1.15              |
| 1:E:40:PHE:CA    | 1:E:130:LEU:CD2  | 2.03                     | 1.15              |
| 1:D:130:LEU:C    | 1:D:130:LEU:HD12 | 1.60                     | 1.14              |
| 1:A:109:ILE:N    | 1:A:109:ILE:HD13 | 1.55                     | 1.14              |
| 1:C:116:TYR:CD2  | 1:C:117:ASP:N    | 2.15                     | 1.14              |
| 1:C:25:LEU:N     | 1:C:25:LEU:HD22  | 1.58                     | 1.14              |
| 1:E:298:VAL:CA   | 1:E:333:ARG:HH12 | 1.59                     | 1.14              |
| 1:F:25:LEU:CA    | 1:F:28:PHE:CE2   | 2.30                     | 1.14              |
| 1:A:309:GLU:HB2  | 1:A:322:ILE:CG1  | 1.72                     | 1.14              |
| 1:E:25:LEU:CD1   | 1:E:310:ARG:NH2  | 2.10                     | 1.14              |
| 1:G:270:HIS:O    | 1:G:272:PHE:N    | 1.78                     | 1.14              |
| 1:E:119:ARG:HG2  | 1:E:119:ARG:HH11 | 1.03                     | 1.14              |
| 1:E:145:LEU:HD22 | 1:E:332:LEU:HG   | 1.30                     | 1.14              |
| 1:A:110:GLU:OE1  | 1:A:118:VAL:HG11 | 1.46                     | 1.14              |
| 1:B:251:PRO:HB2  | 1:C:199:TYR:CE2  | 1.83                     | 1.14              |
| 1:F:29:LEU:HD23  | 1:F:29:LEU:O     | 1.45                     | 1.13              |
| 1:E:40:PHE:CZ    | 1:E:130:LEU:CD1  | 2.24                     | 1.13              |
| 1:A:119:ARG:O    | 1:A:123:THR:HG23 | 1.46                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:GLU:OE2  | 1:F:201:PRO:HG3  | 1.45                     | 1.13              |
| 1:F:27:LEU:HD13  | 1:F:27:LEU:O     | 1.45                     | 1.13              |
| 1:B:334:PRO:HA   | 1:B:335:GLU:HB2  | 1.23                     | 1.13              |
| 1:C:205:ARG:O    | 1:C:246:GLU:HB3  | 1.49                     | 1.12              |
| 1:A:308:LEU:HA   | 1:A:323:ALA:HA   | 1.15                     | 1.12              |
| 1:D:27:LEU:C     | 1:D:27:LEU:HD12  | 1.69                     | 1.12              |
| 1:F:25:LEU:HD12  | 1:F:26:ALA:H     | 1.00                     | 1.12              |
| 1:E:109:ILE:N    | 1:E:109:ILE:HD12 | 1.55                     | 1.12              |
| 1:G:110:GLU:HA   | 1:G:114:ASN:ND2  | 1.62                     | 1.12              |
| 1:E:119:ARG:HH11 | 1:E:119:ARG:CG   | 1.63                     | 1.12              |
| 1:C:207:PHE:CZ   | 1:C:245:PHE:CD2  | 2.37                     | 1.12              |
| 1:E:189:THR:HG21 | 1:E:243:MET:CE   | 1.67                     | 1.12              |
| 1:G:257:GLY:HA3  | 1:G:268:GLN:OE1  | 1.47                     | 1.12              |
| 1:A:309:GLU:HB2  | 1:A:322:ILE:HG13 | 1.16                     | 1.12              |
| 1:B:113:MET:SD   | 1:B:115:HIS:NE2  | 2.22                     | 1.11              |
| 1:D:25:LEU:HD12  | 1:D:25:LEU:C     | 1.70                     | 1.11              |
| 1:C:208:TYR:HB2  | 1:C:291:LEU:HG   | 1.31                     | 1.11              |
| 1:B:141:GLU:OE1  | 1:B:330:GLY:HA2  | 0.95                     | 1.10              |
| 1:C:161:THR:OG1  | 1:C:336:ALA:HB2  | 1.38                     | 1.10              |
| 1:A:205:ARG:NH1  | 1:A:293:MET:SD   | 2.24                     | 1.10              |
| 1:G:25:LEU:N     | 1:G:25:LEU:HD23  | 1.56                     | 1.10              |
| 1:C:208:TYR:HB3  | 1:C:291:LEU:HD11 | 1.27                     | 1.10              |
| 1:G:132:MET:SD   | 1:G:132:MET:C    | 2.30                     | 1.10              |
| 1:G:113:MET:CE   | 1:G:113:MET:CA   | 2.30                     | 1.10              |
| 1:B:132:MET:CA   | 1:B:132:MET:CE   | 2.30                     | 1.10              |
| 1:C:204:ASP:O    | 1:C:205:ARG:HG3  | 1.50                     | 1.10              |
| 1:C:206:VAL:HG21 | 1:C:248:VAL:HG23 | 1.28                     | 1.10              |
| 1:D:138:VAL:HG23 | 1:D:139:LEU:HD13 | 1.20                     | 1.10              |
| 1:E:110:GLU:CG   | 1:E:118:VAL:HG21 | 1.78                     | 1.10              |
| 1:D:110:GLU:HB2  | 1:D:114:ASN:HB2  | 1.25                     | 1.10              |
| 1:B:132:MET:HA   | 1:B:135:ASP:OD2  | 1.52                     | 1.09              |
| 1:C:201:PRO:HA   | 1:C:202:ALA:HB3  | 1.34                     | 1.09              |
| 1:E:145:LEU:CD2  | 1:E:332:LEU:HD21 | 1.82                     | 1.09              |
| 1:G:109:ILE:N    | 1:G:109:ILE:HD13 | 1.54                     | 1.09              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:HG2  | 1.34                     | 1.09              |
| 1:E:109:ILE:H    | 1:E:109:ILE:CD1  | 1.51                     | 1.09              |
| 1:C:33:GLY:HA2   | 1:C:36:VAL:CG2   | 1.82                     | 1.09              |
| 1:E:110:GLU:HG3  | 1:E:118:VAL:CG1  | 1.83                     | 1.09              |
| 1:B:251:PRO:HB2  | 1:C:199:TYR:CE1  | 1.72                     | 1.08              |
| 1:G:110:GLU:CD   | 1:G:118:VAL:HB   | 1.74                     | 1.08              |
| 1:C:207:PHE:HD2  | 1:C:247:VAL:CG2  | 1.65                     | 1.08              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:110:GLU:HG2  | 1:E:118:VAL:HG21 | 1.34                     | 1.08              |
| 1:E:145:LEU:CB   | 1:E:332:LEU:CD2  | 2.28                     | 1.08              |
| 1:G:115:HIS:CD2  | 1:G:119:ARG:HH22 | 1.70                     | 1.08              |
| 1:E:25:LEU:HD11  | 1:E:310:ARG:NH2  | 1.64                     | 1.08              |
| 1:A:287:ASN:HD22 | 1:A:288:VAL:N    | 1.50                     | 1.08              |
| 1:A:309:GLU:HB3  | 1:A:322:ILE:HD11 | 1.20                     | 1.08              |
| 1:B:29:LEU:HD11  | 1:B:310:ARG:HD3  | 1.09                     | 1.08              |
| 1:D:142:ILE:HD13 | 1:D:145:LEU:CD2  | 1.82                     | 1.08              |
| 1:A:208:TYR:HE2  | 1:A:293:MET:HE3  | 1.17                     | 1.08              |
| 1:C:27:LEU:HD23  | 1:C:28:PHE:N     | 1.66                     | 1.08              |
| 1:B:128:GLU:OE1  | 1:C:68:ARG:HD3   | 1.54                     | 1.08              |
| 1:C:119:ARG:HH11 | 1:C:119:ARG:HG3  | 1.19                     | 1.08              |
| 1:B:114:ASN:OD1  | 1:C:53:ARG:NH2   | 1.86                     | 1.07              |
| 1:C:29:LEU:HD12  | 1:C:29:LEU:H     | 0.96                     | 1.07              |
| 1:A:109:ILE:HD13 | 1:A:109:ILE:H    | 1.09                     | 1.07              |
| 1:B:114:ASN:H    | 1:B:115:HIS:CD2  | 1.72                     | 1.07              |
| 1:A:55:ILE:CG2   | 1:A:301:VAL:HG23 | 1.83                     | 1.07              |
| 1:G:34:GLY:O     | 1:G:38:THR:HG23  | 1.51                     | 1.07              |
| 1:G:113:MET:CE   | 1:G:113:MET:HA   | 1.81                     | 1.07              |
| 1:G:113:MET:HA   | 1:G:113:MET:HE3  | 1.09                     | 1.07              |
| 1:B:28:PHE:CZ    | 1:B:112:ALA:CA   | 2.31                     | 1.06              |
| 1:B:114:ASN:N    | 1:B:115:HIS:HD2  | 1.54                     | 1.06              |
| 1:A:287:ASN:ND2  | 1:A:288:VAL:H    | 1.51                     | 1.06              |
| 1:C:110:GLU:OE2  | 1:C:118:VAL:HG21 | 1.52                     | 1.06              |
| 1:E:303:LEU:HB2  | 1:E:327:MET:HG2  | 1.32                     | 1.06              |
| 1:B:145:LEU:HD22 | 1:B:332:LEU:CG   | 1.82                     | 1.06              |
| 1:B:31:VAL:HG13  | 1:B:35:GLU:OE2   | 1.54                     | 1.06              |
| 1:A:302:LYS:HG2  | 1:A:327:MET:CB   | 1.84                     | 1.05              |
| 1:B:130:LEU:O    | 1:B:130:LEU:HD12 | 1.54                     | 1.05              |
| 1:G:25:LEU:H     | 1:G:25:LEU:HD23  | 0.90                     | 1.05              |
| 1:G:119:ARG:CG   | 1:G:119:ARG:HH11 | 1.69                     | 1.05              |
| 1:G:132:MET:HE3  | 1:G:252:HIS:NE2  | 1.71                     | 1.05              |
| 1:B:24:LYS:NZ    | 1:B:24:LYS:HB3   | 1.69                     | 1.05              |
| 1:G:132:MET:SD   | 1:G:133:ALA:N    | 2.30                     | 1.05              |
| 1:B:29:LEU:CD1   | 1:B:310:ARG:HD3  | 1.85                     | 1.05              |
| 1:C:161:THR:OG1  | 1:C:336:ALA:HB1  | 1.30                     | 1.05              |
| 1:G:149:GLU:HG2  | 1:G:150:SER:N    | 1.70                     | 1.05              |
| 1:C:28:PHE:C     | 1:C:28:PHE:CD2   | 2.30                     | 1.04              |
| 1:G:113:MET:HE1  | 1:G:115:HIS:HB2  | 1.36                     | 1.04              |
| 1:G:25:LEU:HA    | 1:G:28:PHE:CE2   | 1.92                     | 1.04              |
| 1:G:146:CYS:SG   | 1:G:336:ALA:N    | 2.30                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:33:GLY:CA    | 1:C:36:VAL:HG23  | 1.88                     | 1.04              |
| 1:A:208:TYR:CE2  | 1:A:293:MET:HE3  | 1.92                     | 1.04              |
| 1:E:298:VAL:CA   | 1:E:333:ARG:NH1  | 2.17                     | 1.04              |
| 1:G:113:MET:C    | 1:G:113:MET:HE2  | 1.78                     | 1.04              |
| 1:B:35:GLU:HB2   | 1:B:123:THR:HG23 | 1.36                     | 1.04              |
| 1:E:25:LEU:HD12  | 1:E:25:LEU:O     | 1.58                     | 1.04              |
| 1:D:141:GLU:O    | 1:D:145:LEU:HD22 | 1.56                     | 1.04              |
| 1:B:108:ASP:HA   | 1:B:111:ASP:OD2  | 1.57                     | 1.04              |
| 1:B:40:PHE:CE1   | 1:B:130:LEU:HD13 | 1.92                     | 1.04              |
| 1:D:139:LEU:N    | 1:D:139:LEU:HD13 | 1.73                     | 1.03              |
| 1:B:132:MET:CA   | 1:B:132:MET:HE2  | 1.84                     | 1.03              |
| 1:B:30:LYS:HD3   | 1:B:30:LYS:C     | 1.76                     | 1.03              |
| 1:G:146:CYS:CB   | 1:G:336:ALA:CB   | 2.35                     | 1.03              |
| 1:D:26:ALA:O     | 1:D:29:LEU:HD12  | 1.56                     | 1.03              |
| 1:D:142:ILE:HD13 | 1:D:145:LEU:HD21 | 1.35                     | 1.03              |
| 1:E:110:GLU:OE2  | 1:E:111:ASP:HA   | 1.56                     | 1.03              |
| 1:E:299:GLY:N    | 1:E:331:GLY:O    | 1.91                     | 1.03              |
| 1:G:110:GLU:OE2  | 1:G:118:VAL:HG12 | 1.59                     | 1.02              |
| 1:A:302:LYS:HG2  | 1:A:327:MET:HB3  | 1.39                     | 1.02              |
| 1:A:36:VAL:O     | 1:A:39:ALA:N     | 1.91                     | 1.02              |
| 1:G:119:ARG:HG3  | 1:G:119:ARG:HH11 | 0.86                     | 1.02              |
| 1:D:139:LEU:H    | 1:D:139:LEU:HD13 | 1.23                     | 1.02              |
| 1:A:207:PHE:HE1  | 1:A:290:GLY:HA3  | 1.23                     | 1.02              |
| 1:C:33:GLY:HA2   | 1:C:36:VAL:HG23  | 1.40                     | 1.01              |
| 1:A:309:GLU:C    | 1:A:322:ILE:HG12 | 1.81                     | 1.01              |
| 1:E:189:THR:HG21 | 1:E:243:MET:HE3  | 1.02                     | 1.01              |
| 1:G:141:GLU:N    | 1:G:270:HIS:ND1  | 2.06                     | 1.01              |
| 1:F:25:LEU:CA    | 1:F:28:PHE:CD2   | 2.41                     | 1.01              |
| 1:B:116:TYR:H    | 1:B:116:TYR:HD1  | 1.07                     | 1.01              |
| 1:F:25:LEU:HD12  | 1:F:26:ALA:N     | 1.76                     | 1.01              |
| 1:G:141:GLU:N    | 1:G:270:HIS:CE1  | 2.29                     | 1.01              |
| 1:A:309:GLU:C    | 1:A:322:ILE:CG1  | 2.27                     | 1.01              |
| 1:E:110:GLU:HG3  | 1:E:118:VAL:HG11 | 1.04                     | 1.00              |
| 1:G:113:MET:CE   | 1:G:115:HIS:HB2  | 1.91                     | 1.00              |
| 1:G:26:ALA:HA    | 1:G:29:LEU:HD12  | 1.37                     | 1.00              |
| 1:B:27:LEU:HD23  | 1:B:30:LYS:HB3   | 1.40                     | 1.00              |
| 1:G:110:GLU:CA   | 1:G:114:ASN:CG   | 2.30                     | 1.00              |
| 1:B:141:GLU:CD   | 1:B:330:GLY:HA2  | 1.82                     | 1.00              |
| 1:D:25:LEU:O     | 1:D:25:LEU:HD12  | 1.62                     | 1.00              |
| 1:G:149:GLU:HG2  | 1:G:150:SER:H    | 0.87                     | 1.00              |
| 1:A:27:LEU:C     | 1:A:27:LEU:CD1   | 2.30                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:24:LYS:NZ    | 1:E:112:ALA:HB1  | 1.76                     | 1.00              |
| 1:F:27:LEU:C     | 1:F:27:LEU:CD1   | 2.30                     | 1.00              |
| 1:A:302:LYS:HG2  | 1:A:327:MET:CG   | 1.90                     | 0.99              |
| 1:C:26:ALA:O     | 1:C:29:LEU:HD13  | 1.60                     | 0.99              |
| 1:E:189:THR:HG23 | 1:E:243:MET:SD   | 1.96                     | 0.99              |
| 1:C:29:LEU:O     | 1:C:32:PHE:HB3   | 1.61                     | 0.99              |
| 1:E:115:HIS:CE1  | 1:E:119:ARG:NH2  | 2.30                     | 0.99              |
| 1:G:25:LEU:H     | 1:G:25:LEU:CD2   | 1.71                     | 0.99              |
| 1:B:141:GLU:OE2  | 1:B:331:GLY:N    | 1.94                     | 0.99              |
| 1:F:28:PHE:CD1   | 1:F:29:LEU:N     | 2.30                     | 0.99              |
| 1:G:113:MET:CE   | 1:G:113:MET:C    | 2.30                     | 0.99              |
| 1:B:116:TYR:N    | 1:B:116:TYR:HD1  | 1.60                     | 0.99              |
| 1:C:29:LEU:CD1   | 1:C:29:LEU:H     | 1.76                     | 0.99              |
| 1:D:130:LEU:HD12 | 1:D:131:ALA:CA   | 1.93                     | 0.99              |
| 1:D:45:VAL:HG23  | 1:D:135:ASP:OD2  | 1.62                     | 0.99              |
| 1:F:25:LEU:CD1   | 1:F:26:ALA:H     | 1.75                     | 0.99              |
| 1:G:106:ILE:CD1  | 1:G:106:ILE:C    | 2.30                     | 0.99              |
| 1:A:25:LEU:C     | 1:A:25:LEU:HD13  | 1.84                     | 0.99              |
| 1:C:26:ALA:CA    | 1:C:29:LEU:CD1   | 2.30                     | 0.99              |
| 1:E:25:LEU:CD1   | 1:E:25:LEU:C     | 2.30                     | 0.99              |
| 1:A:287:ASN:OD1  | 1:A:341:VAL:HB   | 1.63                     | 0.98              |
| 1:E:115:HIS:CE1  | 1:E:119:ARG:HH22 | 1.81                     | 0.98              |
| 1:G:130:LEU:CD2  | 1:G:130:LEU:C    | 2.30                     | 0.98              |
| 1:C:27:LEU:CD2   | 1:C:27:LEU:C     | 2.30                     | 0.98              |
| 1:F:27:LEU:HD13  | 1:F:27:LEU:C     | 1.79                     | 0.98              |
| 1:C:28:PHE:HD2   | 1:C:29:LEU:N     | 1.61                     | 0.98              |
| 1:D:138:VAL:CG2  | 1:D:139:LEU:CD1  | 2.41                     | 0.98              |
| 1:G:148:VAL:HG23 | 1:G:148:VAL:O    | 1.59                     | 0.98              |
| 1:B:107:TYR:N    | 1:B:107:TYR:HD2  | 1.61                     | 0.98              |
| 1:G:147:ASN:ND2  | 1:G:273:PRO:HG3  | 1.78                     | 0.98              |
| 1:G:149:GLU:OE1  | 1:G:150:SER:N    | 1.96                     | 0.98              |
| 1:C:113:MET:HE1  | 1:C:119:ARG:NH2  | 1.79                     | 0.97              |
| 1:E:114:ASN:O    | 1:E:115:HIS:HB2  | 1.62                     | 0.97              |
| 1:G:146:CYS:HB2  | 1:G:336:ALA:CB   | 1.94                     | 0.97              |
| 1:G:27:LEU:C     | 1:G:27:LEU:HD12  | 1.84                     | 0.97              |
| 1:C:207:PHE:HD2  | 1:C:247:VAL:HG22 | 0.82                     | 0.97              |
| 1:G:146:CYS:SG   | 1:G:336:ALA:HB3  | 2.04                     | 0.97              |
| 1:C:109:ILE:O    | 1:C:109:ILE:HD13 | 1.65                     | 0.97              |
| 1:D:130:LEU:C    | 1:D:130:LEU:CD1  | 2.30                     | 0.97              |
| 1:D:138:VAL:CG2  | 1:D:139:LEU:HD13 | 1.95                     | 0.97              |
| 1:D:32:PHE:C     | 1:D:32:PHE:CD1   | 2.37                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:110:GLU:OE2  | 1:G:118:VAL:HG11 | 1.63                     | 0.97              |
| 1:B:24:LYS:CD    | 1:B:24:LYS:C     | 2.30                     | 0.97              |
| 1:B:145:LEU:HD21 | 1:B:332:LEU:HD12 | 1.00                     | 0.97              |
| 1:C:109:ILE:CD1  | 1:C:109:ILE:C    | 2.30                     | 0.97              |
| 1:C:28:PHE:HD2   | 1:C:28:PHE:C     | 1.67                     | 0.96              |
| 1:B:31:VAL:HG12  | 1:B:35:GLU:OE2   | 1.65                     | 0.96              |
| 1:G:146:CYS:SG   | 1:G:336:ALA:CB   | 2.53                     | 0.96              |
| 1:B:69:THR:HG22  | 1:B:70:GLN:H     | 1.30                     | 0.96              |
| 1:C:107:TYR:N    | 1:C:107:TYR:CD2  | 2.30                     | 0.96              |
| 1:C:119:ARG:HH11 | 1:C:119:ARG:CG   | 1.77                     | 0.96              |
| 1:B:24:LYS:O     | 1:B:24:LYS:HD2   | 1.63                     | 0.96              |
| 1:C:207:PHE:HZ   | 1:C:245:PHE:CD2  | 1.83                     | 0.96              |
| 1:A:55:ILE:CG2   | 1:A:301:VAL:CG2  | 2.44                     | 0.96              |
| 1:C:117:ASP:OD2  | 1:D:51:MET:CE    | 2.13                     | 0.96              |
| 1:G:110:GLU:HG2  | 1:G:118:VAL:HG21 | 1.43                     | 0.96              |
| 1:A:302:LYS:CE   | 1:A:327:MET:HG2  | 1.96                     | 0.95              |
| 1:B:30:LYS:HE2   | 1:B:30:LYS:O     | 1.66                     | 0.95              |
| 1:B:35:GLU:HB2   | 1:B:123:THR:CG2  | 1.95                     | 0.95              |
| 1:B:130:LEU:C    | 1:B:130:LEU:CD1  | 2.30                     | 0.95              |
| 1:E:189:THR:CG2  | 1:E:243:MET:HE3  | 1.67                     | 0.95              |
| 1:A:119:ARG:CB   | 1:A:119:ARG:NH1  | 2.30                     | 0.95              |
| 1:B:24:LYS:CE    | 1:B:25:LEU:N     | 2.30                     | 0.95              |
| 1:G:110:GLU:CA   | 1:G:114:ASN:ND2  | 2.30                     | 0.95              |
| 1:C:40:PHE:HE1   | 1:C:131:ALA:HA   | 1.32                     | 0.95              |
| 1:D:139:LEU:N    | 1:D:139:LEU:CD1  | 2.30                     | 0.95              |
| 1:D:28:PHE:CD2   | 1:D:29:LEU:N     | 2.34                     | 0.95              |
| 1:C:188:LEU:CD2  | 1:C:207:PHE:CE1  | 2.49                     | 0.95              |
| 1:C:29:LEU:N     | 1:C:29:LEU:HD12  | 1.78                     | 0.95              |
| 1:B:29:LEU:HD11  | 1:B:310:ARG:CD   | 1.98                     | 0.94              |
| 1:D:29:LEU:CD1   | 1:D:30:LYS:N     | 2.30                     | 0.94              |
| 1:G:141:GLU:OE1  | 1:G:141:GLU:HA   | 1.63                     | 0.94              |
| 1:A:109:ILE:N    | 1:A:109:ILE:CD1  | 2.30                     | 0.94              |
| 1:C:207:PHE:CD2  | 1:C:247:VAL:CG2  | 2.45                     | 0.94              |
| 1:G:109:ILE:O    | 1:G:114:ASN:HB2  | 1.67                     | 0.94              |
| 1:A:119:ARG:HB2  | 1:A:119:ARG:NH1  | 1.81                     | 0.94              |
| 1:B:24:LYS:HZ2   | 1:B:24:LYS:HB3   | 1.28                     | 0.94              |
| 1:G:110:GLU:CA   | 1:G:114:ASN:CB   | 2.45                     | 0.94              |
| 1:G:149:GLU:CG   | 1:G:150:SER:N    | 2.17                     | 0.94              |
| 1:C:195:LEU:HD21 | 1:C:202:ALA:HB1  | 0.95                     | 0.94              |
| 1:F:29:LEU:CD2   | 1:F:29:LEU:C     | 2.33                     | 0.94              |
| 1:E:40:PHE:HA    | 1:E:130:LEU:HD22 | 1.07                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:LEU:CD2  | 1:G:131:ALA:N    | 2.30                     | 0.94              |
| 1:D:46:THR:CG2   | 1:D:135:ASP:OD1  | 2.16                     | 0.94              |
| 1:A:205:ARG:HE   | 1:A:295:ARG:HA   | 1.31                     | 0.93              |
| 1:C:27:LEU:CD2   | 1:C:28:PHE:N     | 2.30                     | 0.93              |
| 1:G:106:ILE:CD1  | 1:G:107:TYR:N    | 2.30                     | 0.93              |
| 1:B:24:LYS:CB    | 1:B:24:LYS:NZ    | 2.30                     | 0.93              |
| 1:B:30:LYS:HD3   | 1:B:30:LYS:O     | 1.67                     | 0.93              |
| 1:B:114:ASN:H    | 1:B:115:HIS:HD2  | 0.97                     | 0.93              |
| 1:C:41:ALA:O     | 1:C:42:ARG:HB2   | 1.64                     | 0.93              |
| 1:B:132:MET:HE2  | 1:B:135:ASP:OD2  | 1.67                     | 0.93              |
| 1:F:29:LEU:HD23  | 1:F:29:LEU:C     | 1.84                     | 0.93              |
| 1:B:28:PHE:HZ    | 1:B:111:ASP:O    | 1.50                     | 0.93              |
| 1:A:107:TYR:OH   | 1:B:90:THR:HG21  | 1.68                     | 0.93              |
| 1:D:142:ILE:CD1  | 1:D:145:LEU:CD2  | 2.46                     | 0.93              |
| 1:F:25:LEU:HA    | 1:F:28:PHE:HD2   | 1.32                     | 0.93              |
| 1:C:25:LEU:N     | 1:C:25:LEU:CD2   | 2.30                     | 0.93              |
| 1:A:115:HIS:CD2  | 1:A:115:HIS:H    | 1.83                     | 0.93              |
| 1:A:57:SER:H     | 1:A:303:LEU:HD13 | 1.30                     | 0.93              |
| 1:B:113:MET:CA   | 1:B:115:HIS:NE2  | 2.30                     | 0.93              |
| 1:C:25:LEU:H     | 1:C:25:LEU:HD22  | 1.16                     | 0.93              |
| 1:E:25:LEU:HD22  | 1:E:310:ARG:HH12 | 0.99                     | 0.93              |
| 1:C:188:LEU:HD22 | 1:C:207:PHE:CZ   | 2.03                     | 0.92              |
| 1:G:113:MET:HE1  | 1:G:115:HIS:CB   | 2.00                     | 0.92              |
| 1:E:186:ALA:O    | 1:E:190:LYS:HD3  | 1.70                     | 0.92              |
| 1:D:252:HIS:HE1  | 1:E:192:ARG:HH21 | 1.16                     | 0.92              |
| 1:E:63:PHE:HE2   | 1:E:333:ARG:NH2  | 1.59                     | 0.92              |
| 1:D:40:PHE:CE1   | 1:D:131:ALA:HA   | 2.03                     | 0.92              |
| 1:G:119:ARG:HG3  | 1:G:119:ARG:NH1  | 1.69                     | 0.92              |
| 1:A:27:LEU:CD1   | 1:A:28:PHE:N     | 2.33                     | 0.92              |
| 1:C:162:ALA:HB3  | 1:C:337:ALA:O    | 1.70                     | 0.92              |
| 1:E:40:PHE:HA    | 1:E:130:LEU:HD23 | 1.50                     | 0.92              |
| 1:A:119:ARG:CG   | 1:A:119:ARG:HH11 | 1.81                     | 0.92              |
| 1:G:130:LEU:HD23 | 1:G:131:ALA:N    | 1.85                     | 0.92              |
| 1:E:24:LYS:HZ1   | 1:E:112:ALA:CB   | 1.81                     | 0.92              |
| 1:A:302:LYS:HG2  | 1:A:327:MET:HG2  | 1.48                     | 0.92              |
| 1:D:141:GLU:C    | 1:D:145:LEU:HD22 | 1.90                     | 0.92              |
| 1:E:145:LEU:CG   | 1:E:332:LEU:HD23 | 1.99                     | 0.92              |
| 1:B:109:ILE:CD1  | 1:B:110:GLU:N    | 2.30                     | 0.91              |
| 1:A:207:PHE:HZ   | 1:A:209:CYS:HB2  | 1.16                     | 0.91              |
| 1:C:113:MET:CE   | 1:C:119:ARG:CZ   | 2.48                     | 0.91              |
| 1:G:113:MET:HE2  | 1:G:114:ASN:N    | 1.83                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:109:ILE:H    | 1:E:109:ILE:HD12 | 0.75                     | 0.91              |
| 1:C:107:TYR:N    | 1:C:107:TYR:HD2  | 1.67                     | 0.91              |
| 1:C:208:TYR:HB3  | 1:C:291:LEU:CD1  | 2.00                     | 0.91              |
| 1:D:135:ASP:O    | 1:D:139:LEU:HD22 | 1.70                     | 0.91              |
| 1:A:106:ILE:C    | 1:A:107:TYR:HD2  | 1.72                     | 0.91              |
| 1:D:92:LYS:HD2   | 1:D:332:LEU:H    | 1.36                     | 0.91              |
| 1:E:142:ILE:HA   | 1:E:332:LEU:HD22 | 1.52                     | 0.91              |
| 1:E:28:PHE:CE1   | 1:E:111:ASP:O    | 2.24                     | 0.91              |
| 1:D:33:GLY:O     | 1:D:36:VAL:HG12  | 1.70                     | 0.91              |
| 1:A:106:ILE:HG22 | 1:A:122:TYR:CE2  | 2.06                     | 0.91              |
| 1:B:24:LYS:CA    | 1:B:24:LYS:HZ3   | 1.83                     | 0.91              |
| 1:D:32:PHE:O     | 1:D:32:PHE:HD1   | 1.53                     | 0.90              |
| 1:D:130:LEU:CD1  | 1:D:131:ALA:N    | 2.30                     | 0.90              |
| 1:E:299:GLY:CA   | 1:E:333:ARG:HH22 | 1.84                     | 0.90              |
| 1:A:107:TYR:HD2  | 1:A:107:TYR:N    | 1.69                     | 0.90              |
| 1:C:117:ASP:OD2  | 1:D:51:MET:HE3   | 1.69                     | 0.90              |
| 1:C:208:TYR:HB2  | 1:C:291:LEU:CG   | 2.01                     | 0.90              |
| 1:E:141:GLU:HG3  | 1:E:330:GLY:C    | 1.91                     | 0.90              |
| 1:G:114:ASN:O    | 1:G:116:TYR:N    | 2.04                     | 0.90              |
| 1:F:25:LEU:CB    | 1:F:28:PHE:CE2   | 2.54                     | 0.90              |
| 1:G:110:GLU:CD   | 1:G:118:VAL:CB   | 2.40                     | 0.90              |
| 1:D:135:ASP:O    | 1:D:139:LEU:HD13 | 1.72                     | 0.90              |
| 1:E:142:ILE:CD1  | 1:E:142:ILE:C    | 2.34                     | 0.90              |
| 1:B:251:PRO:HB2  | 1:C:199:TYR:OH   | 1.72                     | 0.90              |
| 1:B:251:PRO:HG3  | 1:C:199:TYR:HE1  | 1.02                     | 0.90              |
| 1:C:206:VAL:CG2  | 1:C:246:GLU:OE1  | 2.20                     | 0.90              |
| 1:B:63:PHE:O     | 1:B:333:ARG:NH2  | 2.04                     | 0.90              |
| 1:C:206:VAL:CA   | 1:C:246:GLU:O    | 2.16                     | 0.90              |
| 1:E:303:LEU:CB   | 1:E:327:MET:HG2  | 2.02                     | 0.90              |
| 1:B:145:LEU:HD22 | 1:B:332:LEU:HG   | 0.90                     | 0.90              |
| 1:D:110:GLU:CB   | 1:D:114:ASN:HB2  | 2.01                     | 0.90              |
| 1:D:201:PRO:O    | 1:D:205:ARG:NH2  | 2.05                     | 0.90              |
| 1:E:192:ARG:O    | 1:E:195:LEU:HD12 | 1.72                     | 0.90              |
| 1:A:27:LEU:HD12  | 1:A:28:PHE:CA    | 2.02                     | 0.89              |
| 1:B:28:PHE:HE1   | 1:B:112:ALA:HA   | 1.17                     | 0.89              |
| 1:C:113:MET:HE2  | 1:C:119:ARG:CZ   | 2.02                     | 0.89              |
| 1:E:192:ARG:HA   | 1:E:195:LEU:CG   | 2.02                     | 0.89              |
| 1:B:107:TYR:CD2  | 1:B:107:TYR:N    | 2.37                     | 0.89              |
| 1:E:119:ARG:HG2  | 1:E:119:ARG:NH1  | 1.84                     | 0.89              |
| 1:C:32:PHE:CE2   | 1:C:123:THR:HG22 | 2.07                     | 0.89              |
| 1:C:42:ARG:HH11  | 1:C:42:ARG:HG3   | 1.35                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:297:ALA:O    | 1:E:333:ARG:N    | 2.06                     | 0.89              |
| 1:E:110:GLU:C    | 1:E:110:GLU:CD   | 2.30                     | 0.89              |
| 1:F:25:LEU:CB    | 1:F:28:PHE:HE2   | 1.84                     | 0.89              |
| 1:E:145:LEU:HD22 | 1:E:332:LEU:HD21 | 1.42                     | 0.89              |
| 1:E:25:LEU:CD2   | 1:E:310:ARG:HH12 | 1.69                     | 0.88              |
| 1:C:119:ARG:O    | 1:C:123:THR:HG23 | 1.74                     | 0.88              |
| 1:D:128:GLU:C    | 1:D:128:GLU:CD   | 2.30                     | 0.88              |
| 1:F:25:LEU:CD1   | 1:F:26:ALA:N     | 2.35                     | 0.88              |
| 1:A:114:ASN:N    | 1:A:115:HIS:HD2  | 1.69                     | 0.88              |
| 1:C:35:GLU:HA    | 1:C:38:THR:OG1   | 1.72                     | 0.88              |
| 1:F:143:ALA:O    | 1:F:147:ASN:CG   | 2.11                     | 0.88              |
| 1:D:132:MET:HE1  | 1:D:251:PRO:CG   | 2.03                     | 0.88              |
| 1:G:146:CYS:HB3  | 1:G:336:ALA:HB3  | 1.52                     | 0.88              |
| 1:A:308:LEU:HA   | 1:A:323:ALA:CA   | 2.03                     | 0.88              |
| 1:E:110:GLU:CG   | 1:E:118:VAL:HG11 | 2.00                     | 0.88              |
| 1:B:116:TYR:CD1  | 1:B:116:TYR:N    | 2.35                     | 0.88              |
| 1:C:206:VAL:HB   | 1:C:246:GLU:OE1  | 1.74                     | 0.88              |
| 1:E:192:ARG:CA   | 1:E:195:LEU:CD1  | 2.30                     | 0.88              |
| 1:A:49:ARG:HD3   | 1:A:206:VAL:HG21 | 1.55                     | 0.88              |
| 1:B:251:PRO:CG   | 1:C:199:TYR:HE1  | 1.52                     | 0.88              |
| 1:A:294:HIS:HD2  | 1:A:337:ALA:HA   | 1.37                     | 0.87              |
| 1:B:251:PRO:HB3  | 1:C:199:TYR:CE1  | 2.06                     | 0.87              |
| 1:C:33:GLY:C     | 1:C:36:VAL:HG23  | 1.94                     | 0.87              |
| 1:G:110:GLU:CD   | 1:G:118:VAL:CG1  | 2.41                     | 0.87              |
| 1:B:145:LEU:O    | 1:B:145:LEU:HD12 | 1.72                     | 0.87              |
| 1:B:332:LEU:HD12 | 1:B:334:PRO:HD2  | 1.54                     | 0.87              |
| 1:A:207:PHE:CE2  | 1:A:247:VAL:HG23 | 2.09                     | 0.87              |
| 1:C:207:PHE:HE2  | 1:C:242:VAL:HG21 | 1.39                     | 0.87              |
| 1:E:110:GLU:CD   | 1:E:111:ASP:HA   | 1.93                     | 0.87              |
| 1:C:26:ALA:HA    | 1:C:29:LEU:HD11  | 1.56                     | 0.87              |
| 1:G:109:ILE:HD13 | 1:G:109:ILE:H    | 0.71                     | 0.87              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:CE   | 2.05                     | 0.87              |
| 1:C:161:THR:O    | 1:C:336:ALA:HB1  | 1.73                     | 0.87              |
| 1:G:25:LEU:N     | 1:G:25:LEU:CD2   | 2.30                     | 0.87              |
| 1:D:132:MET:HE1  | 1:D:251:PRO:CB   | 2.04                     | 0.87              |
| 1:G:135:ASP:O    | 1:G:138:VAL:HG23 | 1.74                     | 0.87              |
| 1:A:115:HIS:HD2  | 1:A:115:HIS:H    | 1.22                     | 0.87              |
| 1:A:115:HIS:CD2  | 1:A:115:HIS:N    | 2.42                     | 0.87              |
| 1:C:207:PHE:CZ   | 1:C:245:PHE:HD2  | 1.88                     | 0.87              |
| 1:G:165:ILE:HD13 | 1:G:166:GLU:N    | 1.90                     | 0.87              |
| 1:B:117:ASP:OD2  | 1:C:51:MET:CE    | 2.23                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:289:ILE:CG1  | 1:A:340:VAL:O    | 2.23                     | 0.86              |
| 1:C:26:ALA:C     | 1:C:29:LEU:CD1   | 2.42                     | 0.86              |
| 1:B:24:LYS:HE2   | 1:B:25:LEU:CA    | 2.04                     | 0.86              |
| 1:C:204:ASP:O    | 1:C:205:ARG:CG   | 2.23                     | 0.86              |
| 1:D:40:PHE:HE1   | 1:D:131:ALA:HA   | 1.36                     | 0.86              |
| 1:G:115:HIS:O    | 1:G:119:ARG:HB3  | 1.74                     | 0.86              |
| 1:A:207:PHE:HZ   | 1:A:209:CYS:CB   | 1.75                     | 0.86              |
| 1:A:207:PHE:CE1  | 1:A:209:CYS:HB2  | 2.08                     | 0.86              |
| 1:A:55:ILE:HG22  | 1:A:301:VAL:HG23 | 1.57                     | 0.86              |
| 1:C:114:ASN:O    | 1:C:115:HIS:CG   | 2.29                     | 0.86              |
| 1:G:28:PHE:CZ    | 1:G:111:ASP:OD1  | 2.27                     | 0.86              |
| 1:C:146:CYS:HG   | 1:C:161:THR:N    | 1.73                     | 0.86              |
| 1:C:195:LEU:CD2  | 1:C:202:ALA:CB   | 2.36                     | 0.86              |
| 1:G:150:SER:O    | 1:G:151:LYS:O    | 1.93                     | 0.86              |
| 1:D:128:GLU:OE2  | 1:D:129:SER:HA   | 1.76                     | 0.86              |
| 1:C:195:LEU:HD23 | 1:C:205:ARG:HH22 | 1.03                     | 0.85              |
| 1:C:206:VAL:CG2  | 1:C:248:VAL:N    | 2.39                     | 0.85              |
| 1:E:128:GLU:OE2  | 1:F:201:PRO:CG   | 2.23                     | 0.85              |
| 1:E:189:THR:HG22 | 1:E:243:MET:HE1  | 1.55                     | 0.85              |
| 1:G:149:GLU:CD   | 1:G:150:SER:N    | 2.29                     | 0.85              |
| 1:G:27:LEU:O     | 1:G:27:LEU:HD12  | 1.76                     | 0.85              |
| 1:B:106:ILE:HG22 | 1:B:122:TYR:OH   | 1.76                     | 0.85              |
| 1:D:29:LEU:HD13  | 1:D:30:LYS:H     | 1.39                     | 0.85              |
| 1:D:28:PHE:HD2   | 1:D:29:LEU:N     | 1.73                     | 0.85              |
| 1:E:121:GLU:OE1  | 1:F:51:MET:SD    | 2.34                     | 0.85              |
| 1:B:131:ALA:C    | 1:B:132:MET:HE2  | 1.96                     | 0.85              |
| 1:B:132:MET:HE2  | 1:B:132:MET:N    | 1.92                     | 0.85              |
| 1:D:142:ILE:N    | 1:D:145:LEU:HD23 | 1.90                     | 0.85              |
| 1:E:191:ALA:O    | 1:E:195:LEU:HG   | 1.76                     | 0.85              |
| 1:E:31:VAL:HG12  | 1:E:35:GLU:OE2   | 1.77                     | 0.85              |
| 1:B:109:ILE:HD13 | 1:B:110:GLU:H    | 1.42                     | 0.85              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CD2   | 2.30                     | 0.85              |
| 1:G:132:MET:CE   | 1:G:252:HIS:NE2  | 2.38                     | 0.85              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:CG   | 2.55                     | 0.85              |
| 1:E:189:THR:CG2  | 1:E:243:MET:HE1  | 2.07                     | 0.85              |
| 1:B:206:VAL:HG13 | 1:B:246:GLU:HB3  | 1.59                     | 0.84              |
| 1:B:28:PHE:CZ    | 1:B:111:ASP:O    | 2.30                     | 0.84              |
| 1:B:29:LEU:HD21  | 1:B:310:ARG:HG2  | 1.57                     | 0.84              |
| 1:E:24:LYS:NZ    | 1:E:112:ALA:CB   | 2.38                     | 0.84              |
| 1:E:298:VAL:O    | 1:E:333:ARG:NH1  | 2.08                     | 0.84              |
| 1:D:128:GLU:CD   | 1:D:129:SER:N    | 2.30                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:174:LEU:HB2  | 1:B:179:ALA:HB1  | 1.58                     | 0.84              |
| 1:G:147:ASN:HD21 | 1:G:273:PRO:HG3  | 1.41                     | 0.84              |
| 1:G:132:MET:HE2  | 1:G:132:MET:O    | 1.78                     | 0.84              |
| 1:A:302:LYS:CG   | 1:A:327:MET:HG2  | 2.07                     | 0.84              |
| 1:B:334:PRO:HA   | 1:B:335:GLU:CB   | 2.08                     | 0.84              |
| 1:C:116:TYR:O    | 1:C:118:VAL:HG12 | 1.76                     | 0.84              |
| 1:A:207:PHE:HE1  | 1:A:290:GLY:CA   | 1.90                     | 0.84              |
| 1:B:24:LYS:CB    | 1:B:24:LYS:HZ3   | 1.88                     | 0.84              |
| 1:C:114:ASN:O    | 1:C:115:HIS:CD2  | 2.30                     | 0.84              |
| 1:C:25:LEU:HD23  | 1:C:26:ALA:H     | 0.71                     | 0.84              |
| 1:A:288:VAL:O    | 1:A:289:ILE:HD13 | 1.78                     | 0.84              |
| 1:E:298:VAL:CG1  | 1:E:332:LEU:CD1  | 2.55                     | 0.84              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:CG   | 2.08                     | 0.84              |
| 1:C:33:GLY:HA2   | 1:C:36:VAL:HG21  | 1.58                     | 0.84              |
| 1:B:132:MET:CE   | 1:B:132:MET:N    | 2.41                     | 0.83              |
| 1:E:96:ILE:HD11  | 1:E:327:MET:O    | 1.78                     | 0.83              |
| 1:C:110:GLU:OE1  | 1:C:122:TYR:CD2  | 2.31                     | 0.83              |
| 1:C:42:ARG:HG3   | 1:C:42:ARG:NH1   | 1.90                     | 0.83              |
| 1:A:107:TYR:N    | 1:A:107:TYR:CD2  | 2.44                     | 0.83              |
| 1:A:309:GLU:HB2  | 1:A:322:ILE:CD1  | 1.99                     | 0.83              |
| 1:B:128:GLU:OE1  | 1:C:68:ARG:CD    | 2.26                     | 0.83              |
| 1:C:40:PHE:HE1   | 1:C:131:ALA:CA   | 1.91                     | 0.83              |
| 1:E:115:HIS:HE1  | 1:E:119:ARG:HH22 | 1.25                     | 0.83              |
| 1:D:110:GLU:O    | 1:D:113:MET:HG3  | 1.76                     | 0.83              |
| 1:D:45:VAL:CG2   | 1:D:135:ASP:OD2  | 2.26                     | 0.83              |
| 1:A:108:ASP:HB2  | 1:A:111:ASP:HB2  | 1.61                     | 0.83              |
| 1:B:139:LEU:C    | 1:B:142:ILE:HG23 | 1.98                     | 0.83              |
| 1:D:40:PHE:HE1   | 1:D:131:ALA:CA   | 1.92                     | 0.83              |
| 1:B:114:ASN:N    | 1:B:115:HIS:CD2  | 2.39                     | 0.83              |
| 1:D:29:LEU:C     | 1:D:29:LEU:HD13  | 1.98                     | 0.83              |
| 1:A:286:ASP:N    | 1:A:287:ASN:O    | 2.12                     | 0.83              |
| 1:B:117:ASP:OD1  | 1:C:53:ARG:HA    | 1.77                     | 0.83              |
| 1:E:114:ASN:O    | 1:E:115:HIS:CB   | 2.26                     | 0.83              |
| 1:E:333:ARG:HH11 | 1:E:333:ARG:HG3  | 1.43                     | 0.83              |
| 1:C:188:LEU:HD22 | 1:C:207:PHE:HE1  | 1.37                     | 0.83              |
| 1:G:146:CYS:HB2  | 1:G:336:ALA:HB2  | 1.60                     | 0.83              |
| 1:C:109:ILE:HD13 | 1:C:110:GLU:N    | 1.93                     | 0.82              |
| 1:C:202:ALA:HB1  | 1:C:205:ARG:NH2  | 1.94                     | 0.82              |
| 1:E:25:LEU:HG    | 1:E:310:ARG:NH2  | 1.94                     | 0.82              |
| 1:B:192:ARG:NE   | 1:B:243:MET:SD   | 2.52                     | 0.82              |
| 1:G:110:GLU:C    | 1:G:114:ASN:HB3  | 1.99                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:107:TYR:N    | 1:G:107:TYR:HD2  | 1.75                     | 0.82              |
| 1:A:308:LEU:CA   | 1:A:323:ALA:HA   | 2.06                     | 0.82              |
| 1:B:239:ILE:HB   | 1:B:247:VAL:HG23 | 1.60                     | 0.82              |
| 1:D:142:ILE:HD12 | 1:D:145:LEU:HG   | 1.62                     | 0.82              |
| 1:A:110:GLU:OE1  | 1:A:118:VAL:CG1  | 2.25                     | 0.82              |
| 1:E:119:ARG:NH1  | 1:E:119:ARG:CG   | 2.34                     | 0.82              |
| 1:A:287:ASN:ND2  | 1:A:288:VAL:N    | 2.16                     | 0.82              |
| 1:A:309:GLU:C    | 1:A:322:ILE:HG13 | 1.92                     | 0.82              |
| 1:B:106:ILE:C    | 1:B:107:TYR:HD2  | 1.81                     | 0.82              |
| 1:G:40:PHE:HD1   | 1:G:131:ALA:HB2  | 1.44                     | 0.82              |
| 1:C:206:VAL:CG2  | 1:C:248:VAL:H    | 1.92                     | 0.82              |
| 1:D:313:ARG:HB2  | 1:D:318:ALA:HB3  | 1.60                     | 0.82              |
| 1:E:24:LYS:C     | 1:E:24:LYS:CD    | 2.46                     | 0.82              |
| 1:G:107:TYR:N    | 1:G:107:TYR:CD2  | 2.45                     | 0.82              |
| 1:C:110:GLU:OE2  | 1:C:118:VAL:CG2  | 2.26                     | 0.82              |
| 1:D:36:VAL:CG1   | 1:D:37:LEU:N     | 2.43                     | 0.82              |
| 1:G:110:GLU:HG2  | 1:G:118:VAL:CG2  | 2.09                     | 0.82              |
| 1:G:110:GLU:CG   | 1:G:118:VAL:HB   | 2.10                     | 0.82              |
| 1:C:110:GLU:OE1  | 1:C:122:TYR:CE2  | 2.33                     | 0.81              |
| 1:G:28:PHE:CE2   | 1:G:111:ASP:OD1  | 2.32                     | 0.81              |
| 1:B:92:LYS:HZ1   | 1:B:333:ARG:HE   | 1.28                     | 0.81              |
| 1:C:106:ILE:C    | 1:C:107:TYR:CD2  | 2.54                     | 0.81              |
| 1:C:43:THR:HG21  | 1:C:128:GLU:HG3  | 1.62                     | 0.81              |
| 1:D:49:ARG:O     | 1:D:50:HIS:ND1   | 2.14                     | 0.81              |
| 1:B:332:LEU:HD12 | 1:B:334:PRO:CD   | 2.10                     | 0.81              |
| 1:C:119:ARG:NH1  | 1:C:119:ARG:HB2  | 1.95                     | 0.81              |
| 1:D:27:LEU:HD12  | 1:D:28:PHE:N     | 1.95                     | 0.81              |
| 1:G:113:MET:HG3  | 1:G:114:ASN:H    | 1.46                     | 0.81              |
| 1:G:79:ASN:HB2   | 1:G:82:ASP:HB2   | 1.62                     | 0.81              |
| 1:A:108:ASP:CB   | 1:A:111:ASP:HB2  | 2.11                     | 0.81              |
| 1:C:110:GLU:CD   | 1:C:118:VAL:CG2  | 2.48                     | 0.81              |
| 1:G:222:MET:SD   | 1:G:224:ASN:ND2  | 2.53                     | 0.81              |
| 1:A:26:ALA:HA    | 1:A:29:LEU:HD11  | 1.60                     | 0.81              |
| 1:B:141:GLU:OE1  | 1:B:330:GLY:C    | 2.17                     | 0.81              |
| 1:D:205:ARG:HG2  | 1:D:245:PHE:HA   | 1.62                     | 0.81              |
| 1:E:53:ARG:HH12  | 1:E:62:GLN:H     | 1.29                     | 0.81              |
| 1:A:302:LYS:CD   | 1:A:327:MET:HG2  | 2.09                     | 0.81              |
| 1:B:109:ILE:C    | 1:B:109:ILE:HD13 | 2.01                     | 0.81              |
| 1:B:134:ALA:O    | 1:B:138:VAL:HG22 | 1.81                     | 0.81              |
| 1:E:116:TYR:O    | 1:E:120:SER:HB3  | 1.80                     | 0.81              |
| 1:B:125:GLN:HG3  | 1:C:66:LEU:HD13  | 1.62                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:24:LYS:NZ    | 1:B:25:LEU:N     | 2.30                     | 0.80              |
| 1:E:298:VAL:CG1  | 1:E:332:LEU:HD13 | 2.12                     | 0.80              |
| 1:B:30:LYS:O     | 1:B:30:LYS:CE    | 2.30                     | 0.80              |
| 1:D:27:LEU:O     | 1:D:31:VAL:HG23  | 1.81                     | 0.80              |
| 1:B:332:LEU:CD1  | 1:B:334:PRO:HG2  | 2.11                     | 0.80              |
| 1:C:108:ASP:OD2  | 1:C:111:ASP:CB   | 2.30                     | 0.80              |
| 1:A:306:LEU:O    | 1:A:306:LEU:HD12 | 1.81                     | 0.80              |
| 1:E:24:LYS:O     | 1:E:24:LYS:CD    | 2.30                     | 0.80              |
| 1:B:28:PHE:HE1   | 1:B:112:ALA:CA   | 1.73                     | 0.80              |
| 1:E:110:GLU:CD   | 1:E:111:ASP:N    | 2.35                     | 0.80              |
| 1:D:141:GLU:C    | 1:D:145:LEU:CD2  | 2.49                     | 0.80              |
| 1:E:194:ALA:O    | 1:E:197:LYS:HB3  | 1.81                     | 0.80              |
| 1:A:289:ILE:HG13 | 1:A:340:VAL:HG22 | 0.81                     | 0.80              |
| 1:D:135:ASP:O    | 1:D:139:LEU:CD2  | 2.30                     | 0.80              |
| 1:D:252:HIS:CE1  | 1:E:192:ARG:NH2  | 2.49                     | 0.80              |
| 1:E:300:THR:OG1  | 1:E:301:VAL:N    | 2.13                     | 0.80              |
| 1:E:135:ASP:OD1  | 1:E:252:HIS:CE1  | 2.34                     | 0.80              |
| 1:E:25:LEU:CD1   | 1:E:25:LEU:O     | 2.30                     | 0.80              |
| 1:E:119:ARG:O    | 1:E:123:THR:HG22 | 1.83                     | 0.79              |
| 1:A:26:ALA:O     | 1:A:29:LEU:CD1   | 2.25                     | 0.79              |
| 1:D:141:GLU:O    | 1:D:145:LEU:CD2  | 2.30                     | 0.79              |
| 1:E:138:VAL:O    | 1:E:142:ILE:HG22 | 1.81                     | 0.79              |
| 1:G:132:MET:CE   | 1:G:132:MET:O    | 2.30                     | 0.79              |
| 1:G:148:VAL:CG2  | 1:G:148:VAL:O    | 2.30                     | 0.79              |
| 1:A:92:LYS:NZ    | 1:A:93:VAL:O     | 2.15                     | 0.79              |
| 1:B:132:MET:CE   | 1:B:135:ASP:OD2  | 2.30                     | 0.79              |
| 1:G:137:ALA:O    | 1:G:270:HIS:CE1  | 2.35                     | 0.79              |
| 1:A:185:ILE:HD13 | 1:A:188:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:207:PHE:CE1  | 1:A:209:CYS:CB   | 2.65                     | 0.79              |
| 1:A:274:ALA:HA   | 1:A:285:LYS:O    | 1.82                     | 0.79              |
| 1:B:40:PHE:HE1   | 1:B:130:LEU:HD11 | 0.64                     | 0.79              |
| 1:C:25:LEU:O     | 1:C:29:LEU:CD1   | 2.30                     | 0.79              |
| 1:G:148:VAL:O    | 1:G:149:GLU:HB3  | 1.79                     | 0.79              |
| 1:C:26:ALA:O     | 1:C:29:LEU:CD1   | 2.30                     | 0.79              |
| 1:D:135:ASP:O    | 1:D:139:LEU:CD1  | 2.30                     | 0.79              |
| 1:D:25:LEU:CD1   | 1:D:25:LEU:C     | 2.47                     | 0.79              |
| 1:G:115:HIS:O    | 1:G:119:ARG:CB   | 2.30                     | 0.79              |
| 1:G:141:GLU:OE1  | 1:G:141:GLU:CA   | 2.30                     | 0.79              |
| 1:C:116:TYR:CG   | 1:C:117:ASP:N    | 2.42                     | 0.79              |
| 1:D:32:PHE:C     | 1:D:32:PHE:HD1   | 1.85                     | 0.79              |
| 1:E:141:GLU:CD   | 1:E:330:GLY:O    | 2.20                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:40:PHE:CZ    | 1:E:130:LEU:HD12 | 2.18                     | 0.79              |
| 1:B:30:LYS:CD    | 1:B:30:LYS:O     | 2.30                     | 0.79              |
| 1:C:206:VAL:CB   | 1:C:246:GLU:OE1  | 2.31                     | 0.79              |
| 1:A:119:ARG:O    | 1:A:123:THR:CG2  | 2.30                     | 0.79              |
| 1:C:116:TYR:C    | 1:C:116:TYR:CD2  | 2.55                     | 0.79              |
| 1:E:60:SER:HA    | 1:E:95:THR:HA    | 1.65                     | 0.79              |
| 1:B:125:GLN:HG3  | 1:C:66:LEU:CD1   | 2.12                     | 0.79              |
| 1:A:205:ARG:NH1  | 1:A:293:MET:HG2  | 1.98                     | 0.78              |
| 1:B:132:MET:CA   | 1:B:135:ASP:OD2  | 2.30                     | 0.78              |
| 1:B:26:ALA:O     | 1:B:29:LEU:HB2   | 1.82                     | 0.78              |
| 1:E:192:ARG:O    | 1:E:195:LEU:CD1  | 2.30                     | 0.78              |
| 1:B:113:MET:CA   | 1:B:115:HIS:CD2  | 2.63                     | 0.78              |
| 1:B:125:GLN:CG   | 1:C:66:LEU:CD1   | 2.62                     | 0.78              |
| 1:B:109:ILE:HD13 | 1:B:110:GLU:CA   | 2.12                     | 0.78              |
| 1:C:299:GLY:O    | 1:C:330:GLY:HA2  | 1.82                     | 0.78              |
| 1:E:298:VAL:HG12 | 1:E:332:LEU:CD1  | 2.14                     | 0.78              |
| 1:G:87:ILE:HG22  | 1:G:88:LYS:HG2   | 1.65                     | 0.78              |
| 1:A:308:LEU:HD12 | 1:A:308:LEU:O    | 1.84                     | 0.78              |
| 1:C:112:ALA:HB3  | 1:C:115:HIS:CE1  | 2.18                     | 0.78              |
| 1:D:252:HIS:CE1  | 1:E:192:ARG:HH21 | 1.99                     | 0.78              |
| 1:A:208:TYR:OH   | 1:A:293:MET:CE   | 2.31                     | 0.78              |
| 1:C:206:VAL:HG22 | 1:C:248:VAL:H    | 1.47                     | 0.78              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:HD11 | 2.09                     | 0.78              |
| 1:G:130:LEU:O    | 1:G:130:LEU:HD23 | 1.84                     | 0.78              |
| 1:A:55:ILE:HG21  | 1:A:301:VAL:CG2  | 2.12                     | 0.78              |
| 1:B:138:VAL:O    | 1:B:142:ILE:CG2  | 2.30                     | 0.78              |
| 1:C:205:ARG:O    | 1:C:246:GLU:CB   | 2.30                     | 0.78              |
| 1:E:191:ALA:O    | 1:E:195:LEU:CD2  | 2.31                     | 0.78              |
| 1:D:36:VAL:O     | 1:D:37:LEU:C     | 2.22                     | 0.77              |
| 1:C:25:LEU:O     | 1:C:29:LEU:HD11  | 1.83                     | 0.77              |
| 1:C:25:LEU:CD2   | 1:C:26:ALA:N     | 2.30                     | 0.77              |
| 1:D:36:VAL:HG13  | 1:D:37:LEU:N     | 1.98                     | 0.77              |
| 1:E:110:GLU:OE2  | 1:E:111:ASP:CA   | 2.30                     | 0.77              |
| 1:G:106:ILE:HD13 | 1:G:107:TYR:CA   | 2.13                     | 0.77              |
| 1:B:30:LYS:C     | 1:B:30:LYS:CD    | 2.52                     | 0.77              |
| 1:E:145:LEU:HB2  | 1:E:332:LEU:HD23 | 0.78                     | 0.77              |
| 1:B:68:ARG:O     | 1:B:69:THR:OG1   | 2.02                     | 0.77              |
| 1:C:205:ARG:HE   | 1:C:294:HIS:HB3  | 1.50                     | 0.77              |
| 1:B:251:PRO:CB   | 1:C:199:TYR:CD1  | 2.65                     | 0.77              |
| 1:C:288:VAL:HG12 | 1:C:341:VAL:HA   | 1.66                     | 0.77              |
| 1:B:125:GLN:HG2  | 1:C:66:LEU:HD12  | 1.67                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:142:ILE:HG21 | 1:D:293:MET:HE3  | 1.67                     | 0.77              |
| 1:C:53:ARG:NH1   | 1:C:62:GLN:O     | 2.17                     | 0.77              |
| 1:D:138:VAL:HG23 | 1:D:139:LEU:HD12 | 1.64                     | 0.77              |
| 1:D:142:ILE:O    | 1:D:145:LEU:CB   | 2.28                     | 0.77              |
| 1:E:192:ARG:HA   | 1:E:195:LEU:HD11 | 0.79                     | 0.77              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:HG   | 2.13                     | 0.77              |
| 1:A:25:LEU:O     | 1:A:25:LEU:CD1   | 2.30                     | 0.77              |
| 1:E:65:VAL:HG12  | 1:E:333:ARG:HD3  | 1.67                     | 0.77              |
| 1:E:327:MET:SD   | 1:E:327:MET:N    | 2.57                     | 0.76              |
| 1:F:300:THR:OG1  | 1:F:301:VAL:N    | 2.16                     | 0.76              |
| 1:A:205:ARG:NH1  | 1:A:293:MET:CG   | 2.48                     | 0.76              |
| 1:F:29:LEU:O     | 1:F:29:LEU:CD2   | 2.30                     | 0.76              |
| 1:F:24:LYS:HD2   | 1:F:24:LYS:H     | 1.49                     | 0.76              |
| 1:C:36:VAL:HG11  | 1:C:126:LEU:HD21 | 1.66                     | 0.76              |
| 1:D:142:ILE:C    | 1:D:145:LEU:HB2  | 2.05                     | 0.76              |
| 1:F:141:GLU:HG2  | 1:F:329:HIS:NE2  | 2.01                     | 0.76              |
| 1:A:207:PHE:CE1  | 1:A:290:GLY:HA3  | 2.15                     | 0.76              |
| 1:B:68:ARG:N     | 1:B:68:ARG:HD2   | 2.00                     | 0.76              |
| 1:C:195:LEU:HD23 | 1:C:202:ALA:HB1  | 1.63                     | 0.76              |
| 1:D:27:LEU:C     | 1:D:27:LEU:CD1   | 2.46                     | 0.76              |
| 1:D:36:VAL:O     | 1:D:38:THR:N     | 2.18                     | 0.76              |
| 1:F:141:GLU:HG2  | 1:F:329:HIS:CD2  | 2.20                     | 0.76              |
| 1:C:195:LEU:HD23 | 1:C:205:ARG:HH21 | 1.43                     | 0.76              |
| 1:D:53:ARG:HB3   | 1:D:301:VAL:HG12 | 1.67                     | 0.76              |
| 1:E:119:ARG:O    | 1:E:123:THR:CG2  | 2.33                     | 0.76              |
| 1:E:145:LEU:HD23 | 1:E:332:LEU:HD21 | 1.68                     | 0.76              |
| 1:A:207:PHE:HZ   | 1:A:209:CYS:SG   | 2.08                     | 0.76              |
| 1:E:119:ARG:CB   | 1:E:119:ARG:NH1  | 2.49                     | 0.76              |
| 1:C:225:ALA:HA   | 1:C:226:ALA:HB3  | 1.66                     | 0.76              |
| 1:E:298:VAL:O    | 1:E:333:ARG:CZ   | 2.33                     | 0.76              |
| 1:C:288:VAL:HG22 | 1:C:289:ILE:HG13 | 1.66                     | 0.75              |
| 1:F:136:GLY:O    | 1:F:140:ALA:N    | 2.18                     | 0.75              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CE2   | 2.38                     | 0.75              |
| 1:D:40:PHE:CE1   | 1:D:131:ALA:CA   | 2.67                     | 0.75              |
| 1:E:192:ARG:CB   | 1:E:195:LEU:HD11 | 2.16                     | 0.75              |
| 1:E:68:ARG:HE    | 1:E:70:GLN:HE22  | 1.34                     | 0.75              |
| 1:G:110:GLU:CG   | 1:G:118:VAL:CB   | 2.64                     | 0.75              |
| 1:G:25:LEU:O     | 1:G:29:LEU:CG    | 2.29                     | 0.75              |
| 1:A:106:ILE:C    | 1:A:107:TYR:CD2  | 2.58                     | 0.75              |
| 1:B:145:LEU:HD21 | 1:B:332:LEU:CG   | 1.98                     | 0.75              |
| 1:B:334:PRO:CA   | 1:B:335:GLU:HB2  | 2.12                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:110:GLU:CD   | 1:C:118:VAL:HG21 | 2.07                     | 0.75              |
| 1:C:42:ARG:O     | 1:C:44:SER:OG    | 2.01                     | 0.75              |
| 1:D:138:VAL:HG23 | 1:D:139:LEU:HD11 | 1.67                     | 0.75              |
| 1:A:29:LEU:CD2   | 1:A:310:ARG:HD3  | 2.17                     | 0.75              |
| 1:D:252:HIS:HE1  | 1:E:192:ARG:NH2  | 1.84                     | 0.75              |
| 1:A:309:GLU:HB3  | 1:A:322:ILE:CG1  | 1.93                     | 0.75              |
| 1:E:135:ASP:OD1  | 1:E:252:HIS:NE2  | 2.19                     | 0.75              |
| 1:E:110:GLU:CG   | 1:E:118:VAL:CG2  | 2.62                     | 0.75              |
| 1:E:24:LYS:HD2   | 1:E:24:LYS:O     | 1.87                     | 0.75              |
| 1:E:29:LEU:O     | 1:E:32:PHE:N     | 2.20                     | 0.75              |
| 1:E:298:VAL:CG1  | 1:E:332:LEU:HD12 | 2.17                     | 0.75              |
| 1:C:43:THR:HG21  | 1:C:128:GLU:CG   | 2.17                     | 0.74              |
| 1:B:132:MET:SD   | 1:C:199:TYR:CE1  | 2.80                     | 0.74              |
| 1:B:251:PRO:HB3  | 1:C:199:TYR:CD1  | 2.21                     | 0.74              |
| 1:B:251:PRO:HG2  | 1:C:199:TYR:CE1  | 2.18                     | 0.74              |
| 1:D:29:LEU:HD13  | 1:D:30:LYS:CA    | 2.16                     | 0.74              |
| 1:E:135:ASP:CG   | 1:E:252:HIS:CE1  | 2.61                     | 0.74              |
| 1:G:130:LEU:HD22 | 1:G:131:ALA:N    | 2.00                     | 0.74              |
| 1:E:96:ILE:CD1   | 1:E:327:MET:O    | 2.35                     | 0.74              |
| 1:E:145:LEU:CD2  | 1:E:332:LEU:HG   | 2.15                     | 0.74              |
| 1:G:110:GLU:O    | 1:G:114:ASN:CB   | 2.30                     | 0.74              |
| 1:C:40:PHE:CE1   | 1:C:131:ALA:HA   | 2.18                     | 0.74              |
| 1:E:141:GLU:HG3  | 1:E:330:GLY:CA   | 2.18                     | 0.74              |
| 1:G:25:LEU:CA    | 1:G:28:PHE:CE2   | 2.69                     | 0.74              |
| 1:B:101:THR:HG21 | 1:B:323:ALA:H    | 1.53                     | 0.74              |
| 1:C:33:GLY:O     | 1:C:36:VAL:HG23  | 1.87                     | 0.74              |
| 1:E:186:ALA:HB1  | 1:E:190:LYS:HZ2  | 1.52                     | 0.74              |
| 1:A:205:ARG:HH21 | 1:A:296:SER:H    | 1.33                     | 0.74              |
| 1:D:227:ASN:O    | 1:D:231:LEU:N    | 2.19                     | 0.73              |
| 1:F:143:ALA:O    | 1:F:147:ASN:ND2  | 2.21                     | 0.73              |
| 1:F:24:LYS:HD2   | 1:F:24:LYS:N     | 2.02                     | 0.73              |
| 1:A:32:PHE:O     | 1:A:36:VAL:HG23  | 1.87                     | 0.73              |
| 1:B:288:VAL:HA   | 1:B:341:VAL:HG12 | 1.69                     | 0.73              |
| 1:B:69:THR:HG22  | 1:B:70:GLN:N     | 2.02                     | 0.73              |
| 1:D:142:ILE:CD1  | 1:D:145:LEU:HD23 | 2.16                     | 0.73              |
| 1:A:32:PHE:O     | 1:A:36:VAL:CG2   | 2.35                     | 0.73              |
| 1:C:206:VAL:HG23 | 1:C:247:VAL:CA   | 2.18                     | 0.73              |
| 1:C:89:HIS:ND1   | 1:C:89:HIS:O     | 2.21                     | 0.73              |
| 1:E:32:PHE:O     | 1:E:32:PHE:HD1   | 1.71                     | 0.73              |
| 1:G:165:ILE:HG12 | 1:G:341:VAL:HG12 | 1.70                     | 0.73              |
| 1:E:214:TYR:HA   | 1:E:217:ILE:HG23 | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:50:HIS:CE1   | 1:E:300:THR:HG22 | 2.23                     | 0.73              |
| 1:C:104:VAL:O    | 1:C:320:GLN:NE2  | 2.21                     | 0.73              |
| 1:E:110:GLU:CD   | 1:E:111:ASP:CA   | 2.56                     | 0.73              |
| 1:A:160:GLY:N    | 1:A:334:PRO:O    | 2.21                     | 0.73              |
| 1:C:117:ASP:OD2  | 1:D:51:MET:HE1   | 1.86                     | 0.73              |
| 1:E:117:ASP:HB3  | 1:F:53:ARG:HD2   | 1.68                     | 0.73              |
| 1:G:28:PHE:CZ    | 1:G:111:ASP:CG   | 2.62                     | 0.73              |
| 1:C:35:GLU:CA    | 1:C:38:THR:OG1   | 2.37                     | 0.73              |
| 1:E:298:VAL:O    | 1:E:333:ARG:NH2  | 2.22                     | 0.73              |
| 1:B:24:LYS:HZ3   | 1:B:25:LEU:N     | 1.86                     | 0.73              |
| 1:B:332:LEU:CD1  | 1:B:334:PRO:CD   | 2.66                     | 0.73              |
| 1:F:308:LEU:HB3  | 1:F:323:ALA:HA   | 1.69                     | 0.73              |
| 1:F:145:LEU:HD21 | 1:F:334:PRO:HB3  | 1.69                     | 0.73              |
| 1:B:70:GLN:HA    | 1:B:70:GLN:NE2   | 2.02                     | 0.73              |
| 1:C:142:ILE:HA   | 1:C:145:LEU:HD23 | 1.70                     | 0.73              |
| 1:C:28:PHE:CD2   | 1:C:29:LEU:N     | 2.51                     | 0.73              |
| 1:A:306:LEU:HB3  | 1:A:325:TYR:CZ   | 2.24                     | 0.72              |
| 1:B:209:CYS:SG   | 1:B:210:ASP:N    | 2.61                     | 0.72              |
| 1:B:24:LYS:HE2   | 1:B:25:LEU:N     | 2.01                     | 0.72              |
| 1:C:119:ARG:O    | 1:C:123:THR:CG2  | 2.37                     | 0.72              |
| 1:E:145:LEU:CG   | 1:E:332:LEU:CD2  | 2.64                     | 0.72              |
| 1:D:28:PHE:C     | 1:D:28:PHE:CD2   | 2.63                     | 0.72              |
| 1:E:235:GLU:HG2  | 1:E:236:LYS:HG2  | 1.70                     | 0.72              |
| 1:A:209:CYS:HA   | 1:A:290:GLY:CA   | 2.19                     | 0.72              |
| 1:B:115:HIS:CD2  | 1:B:115:HIS:N    | 2.55                     | 0.72              |
| 1:G:115:HIS:CD2  | 1:G:119:ARG:NH2  | 2.53                     | 0.72              |
| 1:B:60:SER:HA    | 1:B:95:THR:HA    | 1.70                     | 0.72              |
| 1:E:147:ASN:N    | 1:E:147:ASN:OD1  | 2.19                     | 0.72              |
| 1:A:114:ASN:H    | 1:A:115:HIS:CD2  | 2.08                     | 0.72              |
| 1:C:42:ARG:CG    | 1:C:42:ARG:HH11  | 2.02                     | 0.72              |
| 1:D:293:MET:N    | 1:D:293:MET:SD   | 2.60                     | 0.72              |
| 1:G:302:LYS:HA   | 1:G:327:MET:HA   | 1.71                     | 0.72              |
| 1:A:207:PHE:HE2  | 1:A:247:VAL:HG23 | 1.51                     | 0.72              |
| 1:D:26:ALA:O     | 1:D:29:LEU:CD1   | 2.36                     | 0.72              |
| 1:A:309:GLU:CA   | 1:A:322:ILE:CG1  | 2.46                     | 0.72              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:CD1  | 2.68                     | 0.72              |
| 1:D:113:MET:SD   | 1:D:114:ASN:ND2  | 2.63                     | 0.72              |
| 1:E:25:LEU:HD12  | 1:E:26:ALA:N     | 2.05                     | 0.72              |
| 1:E:333:ARG:NH1  | 1:E:333:ARG:HG3  | 2.03                     | 0.72              |
| 1:C:207:PHE:HZ   | 1:C:245:PHE:CE2  | 2.07                     | 0.71              |
| 1:G:115:HIS:NE2  | 1:G:119:ARG:NH2  | 2.38                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:119:ARG:CB   | 1:E:119:ARG:HH11 | 2.03                     | 0.71              |
| 1:E:28:PHE:CG    | 1:E:111:ASP:OD1  | 2.27                     | 0.71              |
| 1:A:289:ILE:HG22 | 1:A:290:GLY:N    | 2.06                     | 0.71              |
| 1:B:27:LEU:CD2   | 1:B:30:LYS:HB3   | 2.18                     | 0.71              |
| 1:F:25:LEU:C     | 1:F:28:PHE:CE2   | 2.63                     | 0.71              |
| 1:G:32:PHE:O     | 1:G:36:VAL:HG23  | 1.90                     | 0.71              |
| 1:B:300:THR:OG1  | 1:B:301:VAL:N    | 2.24                     | 0.71              |
| 1:C:310:ARG:NH2  | 1:C:319:ASP:OD2  | 2.23                     | 0.71              |
| 1:F:205:ARG:HG2  | 1:F:245:PHE:HA   | 1.73                     | 0.71              |
| 1:G:120:SER:O    | 1:G:123:THR:OG1  | 2.06                     | 0.71              |
| 1:A:287:ASN:HD21 | 1:A:341:VAL:CG1  | 2.04                     | 0.71              |
| 1:B:108:ASP:CA   | 1:B:111:ASP:OD2  | 2.37                     | 0.71              |
| 1:B:113:MET:SD   | 1:B:115:HIS:HE1  | 2.09                     | 0.71              |
| 1:B:49:ARG:NH2   | 1:B:246:GLU:OE2  | 2.23                     | 0.71              |
| 1:D:132:MET:HE1  | 1:D:251:PRO:HB2  | 1.72                     | 0.71              |
| 1:D:27:LEU:HD12  | 1:D:27:LEU:O     | 1.91                     | 0.71              |
| 1:G:40:PHE:CD1   | 1:G:131:ALA:HB2  | 2.26                     | 0.71              |
| 1:B:96:ILE:HG22  | 1:B:327:MET:HB3  | 1.73                     | 0.71              |
| 1:C:207:PHE:CZ   | 1:C:245:PHE:CE2  | 2.78                     | 0.71              |
| 1:E:115:HIS:ND1  | 1:E:119:ARG:NH2  | 2.38                     | 0.71              |
| 1:E:117:ASP:HB3  | 1:F:53:ARG:CD    | 2.20                     | 0.71              |
| 1:E:147:ASN:HB3  | 1:E:283:VAL:H    | 1.55                     | 0.71              |
| 1:E:335:GLU:O    | 1:E:336:ALA:C    | 2.28                     | 0.71              |
| 1:A:109:ILE:H    | 1:A:109:ILE:CD1  | 1.79                     | 0.71              |
| 1:C:36:VAL:CG1   | 1:C:126:LEU:HG   | 2.20                     | 0.71              |
| 1:E:170:ASN:HA   | 1:E:342:PHE:HB3  | 1.72                     | 0.71              |
| 1:A:240:ARG:NH1  | 1:A:246:GLU:OE2  | 2.24                     | 0.71              |
| 1:C:38:THR:O     | 1:C:41:ALA:HB3   | 1.90                     | 0.71              |
| 1:E:80:LEU:HD13  | 1:E:81:ASP:H     | 1.54                     | 0.71              |
| 1:D:32:PHE:O     | 1:D:32:PHE:CD1   | 2.37                     | 0.70              |
| 1:B:111:ASP:OD1  | 1:B:112:ALA:N    | 2.23                     | 0.70              |
| 1:E:202:ALA:HB1  | 1:E:205:ARG:CZ   | 2.20                     | 0.70              |
| 1:B:110:GLU:C    | 1:B:110:GLU:OE1  | 2.30                     | 0.70              |
| 1:C:29:LEU:O     | 1:C:32:PHE:CB    | 2.39                     | 0.70              |
| 1:C:42:ARG:N     | 1:C:44:SER:OG    | 2.24                     | 0.70              |
| 1:E:108:ASP:OD1  | 1:E:108:ASP:C    | 2.30                     | 0.70              |
| 1:G:150:SER:OG   | 1:G:334:PRO:O    | 2.09                     | 0.70              |
| 1:B:57:SER:O     | 1:B:59:LYS:NZ    | 2.23                     | 0.70              |
| 1:C:27:LEU:HD23  | 1:C:27:LEU:O     | 1.91                     | 0.70              |
| 1:D:142:ILE:N    | 1:D:145:LEU:CD2  | 2.53                     | 0.70              |
| 1:D:45:VAL:CB    | 1:D:135:ASP:OD2  | 2.40                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:106:ILE:CG1  | 1:G:107:TYR:N    | 2.54                     | 0.70              |
| 1:A:110:GLU:OE2  | 1:A:110:GLU:C    | 2.30                     | 0.70              |
| 1:B:130:LEU:HD12 | 1:B:131:ALA:N    | 2.05                     | 0.70              |
| 1:C:119:ARG:CG   | 1:C:119:ARG:NH1  | 2.46                     | 0.70              |
| 1:G:28:PHE:CZ    | 1:G:111:ASP:OD2  | 2.45                     | 0.70              |
| 1:B:113:MET:O    | 1:B:114:ASN:CG   | 2.30                     | 0.70              |
| 1:D:144:GLY:C    | 1:D:146:CYS:H    | 1.92                     | 0.70              |
| 1:D:294:HIS:HD2  | 1:D:297:ALA:HB2  | 1.56                     | 0.70              |
| 1:D:300:THR:OG1  | 1:D:301:VAL:N    | 2.18                     | 0.70              |
| 1:D:313:ARG:N    | 1:D:318:ALA:O    | 2.24                     | 0.70              |
| 1:G:108:ASP:C    | 1:G:108:ASP:OD2  | 2.30                     | 0.70              |
| 1:G:149:GLU:OE1  | 1:G:149:GLU:C    | 2.30                     | 0.70              |
| 1:B:181:GLY:HA2  | 1:B:184:ILE:HB   | 1.72                     | 0.70              |
| 1:C:195:LEU:HD21 | 1:C:202:ALA:HB3  | 1.72                     | 0.70              |
| 1:E:40:PHE:CA    | 1:E:130:LEU:HD21 | 1.92                     | 0.70              |
| 1:E:121:GLU:OE1  | 1:F:51:MET:HG2   | 1.92                     | 0.70              |
| 1:A:55:ILE:HG21  | 1:A:301:VAL:HG21 | 1.72                     | 0.70              |
| 1:F:143:ALA:O    | 1:F:147:ASN:OD1  | 2.09                     | 0.70              |
| 1:A:205:ARG:NE   | 1:A:295:ARG:HA   | 2.04                     | 0.70              |
| 1:B:125:GLN:CG   | 1:C:66:LEU:HD12  | 2.22                     | 0.70              |
| 1:E:111:ASP:OD1  | 1:E:111:ASP:C    | 2.30                     | 0.69              |
| 1:E:299:GLY:HA2  | 1:E:333:ARG:HH22 | 1.56                     | 0.69              |
| 1:C:201:PRO:CA   | 1:C:202:ALA:HB3  | 2.16                     | 0.69              |
| 1:A:240:ARG:HG3  | 1:A:241:ASN:H    | 1.56                     | 0.69              |
| 1:C:37:LEU:HD13  | 1:C:306:LEU:HD11 | 1.73                     | 0.69              |
| 1:D:132:MET:CE   | 1:D:251:PRO:CG   | 2.71                     | 0.69              |
| 1:D:142:ILE:CA   | 1:D:145:LEU:CD2  | 2.26                     | 0.69              |
| 1:G:132:MET:CE   | 1:G:132:MET:C    | 2.61                     | 0.69              |
| 1:A:23:ASP:C     | 1:A:23:ASP:OD1   | 2.30                     | 0.69              |
| 1:C:195:LEU:CD2  | 1:C:205:ARG:CZ   | 2.49                     | 0.69              |
| 1:C:206:VAL:HG23 | 1:C:246:GLU:OE1  | 1.91                     | 0.69              |
| 1:C:117:ASP:CG   | 1:D:51:MET:HE1   | 2.13                     | 0.69              |
| 1:F:32:PHE:O     | 1:F:35:GLU:N     | 2.25                     | 0.69              |
| 1:G:106:ILE:O    | 1:G:106:ILE:HD13 | 1.91                     | 0.69              |
| 1:B:114:ASN:O    | 1:B:118:VAL:HB   | 1.93                     | 0.69              |
| 1:B:141:GLU:OE1  | 1:B:329:HIS:O    | 2.09                     | 0.69              |
| 1:B:132:MET:SD   | 1:B:135:ASP:OD2  | 2.51                     | 0.69              |
| 1:C:108:ASP:OD1  | 1:C:111:ASP:CG   | 2.30                     | 0.69              |
| 1:C:162:ALA:CB   | 1:C:337:ALA:O    | 2.41                     | 0.69              |
| 1:D:165:ILE:HD11 | 1:D:190:LYS:HD2  | 1.73                     | 0.69              |
| 1:E:191:ALA:O    | 1:E:195:LEU:CG   | 2.39                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:141:GLU:HG3  | 1:E:330:GLY:HA3  | 1.75                     | 0.69              |
| 1:A:302:LYS:CG   | 1:A:327:MET:HB3  | 2.22                     | 0.69              |
| 1:A:59:LYS:O     | 1:A:95:THR:OG1   | 2.10                     | 0.69              |
| 1:B:110:GLU:OE1  | 1:B:111:ASP:HA   | 1.92                     | 0.69              |
| 1:A:311:ALA:O    | 1:A:319:ASP:OD1  | 2.11                     | 0.69              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CG    | 2.46                     | 0.69              |
| 1:A:29:LEU:HD22  | 1:A:310:ARG:HD3  | 1.75                     | 0.69              |
| 1:C:27:LEU:HD23  | 1:C:28:PHE:CA    | 2.23                     | 0.69              |
| 1:C:40:PHE:O     | 1:C:44:SER:HB3   | 1.93                     | 0.69              |
| 1:B:28:PHE:CE1   | 1:B:112:ALA:CB   | 2.76                     | 0.69              |
| 1:A:208:TYR:CE2  | 1:A:293:MET:CE   | 2.75                     | 0.68              |
| 1:C:168:THR:O    | 1:C:169:GLN:NE2  | 2.26                     | 0.68              |
| 1:D:142:ILE:HG21 | 1:D:293:MET:CE   | 2.23                     | 0.68              |
| 1:G:314:ALA:HA   | 1:G:318:ALA:H    | 1.57                     | 0.68              |
| 1:B:24:LYS:NZ    | 1:B:25:LEU:H     | 1.91                     | 0.68              |
| 1:C:207:PHE:CE2  | 1:C:242:VAL:HG21 | 2.27                     | 0.68              |
| 1:G:129:SER:O    | 1:G:132:MET:HG3  | 1.93                     | 0.68              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:HD21 | 2.16                     | 0.68              |
| 1:G:113:MET:CE   | 1:G:115:HIS:CB   | 2.66                     | 0.68              |
| 1:G:25:LEU:HA    | 1:G:28:PHE:HD2   | 1.56                     | 0.68              |
| 1:B:145:LEU:CD2  | 1:B:332:LEU:HD12 | 1.91                     | 0.68              |
| 1:C:200:VAL:O    | 1:C:202:ALA:HB3  | 1.93                     | 0.68              |
| 1:G:106:ILE:C    | 1:G:107:TYR:CD2  | 2.67                     | 0.68              |
| 1:A:101:THR:C    | 1:B:71:ALA:HB1   | 2.14                     | 0.68              |
| 1:B:312:ARG:NH1  | 1:B:317:GLN:O    | 2.17                     | 0.68              |
| 1:B:332:LEU:CD1  | 1:B:334:PRO:CG   | 2.72                     | 0.68              |
| 1:C:108:ASP:O    | 1:C:111:ASP:HB3  | 1.93                     | 0.68              |
| 1:F:68:ARG:O     | 1:F:68:ARG:NH1   | 2.23                     | 0.68              |
| 1:C:195:LEU:CD2  | 1:C:205:ARG:HH22 | 1.71                     | 0.68              |
| 1:C:206:VAL:CG2  | 1:C:248:VAL:HG23 | 2.16                     | 0.68              |
| 1:D:209:CYS:HB2  | 1:D:249:GLU:HG2  | 1.75                     | 0.68              |
| 1:E:135:ASP:OD1  | 1:E:135:ASP:C    | 2.30                     | 0.68              |
| 1:A:289:ILE:CB   | 1:A:340:VAL:HG22 | 2.23                     | 0.68              |
| 1:C:113:MET:SD   | 1:C:113:MET:O    | 2.51                     | 0.68              |
| 1:B:281:VAL:HB   | 1:B:283:VAL:HG23 | 1.76                     | 0.68              |
| 1:D:36:VAL:CG1   | 1:D:37:LEU:H     | 2.05                     | 0.68              |
| 1:E:103:ASP:HB2  | 1:E:322:ILE:HA   | 1.76                     | 0.68              |
| 1:F:163:THR:OG1  | 1:F:164:VAL:N    | 2.26                     | 0.68              |
| 1:B:214:TYR:HA   | 1:B:217:ILE:HG23 | 1.76                     | 0.67              |
| 1:A:309:GLU:O    | 1:A:322:ILE:CA   | 2.41                     | 0.67              |
| 1:C:186:ALA:O    | 1:C:189:THR:OG1  | 2.12                     | 0.67              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:37:LEU:CD1  | 1:C:306:LEU:HD21 | 2.23                     | 0.67              |
| 1:D:214:TYR:HD1 | 1:D:249:GLU:HB2  | 1.59                     | 0.67              |
| 1:F:59:LYS:O    | 1:F:95:THR:OG1   | 2.09                     | 0.67              |
| 1:G:149:GLU:CD  | 1:G:150:SER:H    | 1.91                     | 0.67              |
| 1:B:112:ALA:O   | 1:B:113:MET:SD   | 2.52                     | 0.67              |
| 1:C:124:SER:OG  | 1:C:125:GLN:N    | 2.24                     | 0.67              |
| 1:C:171:LYS:HE3 | 1:C:171:LYS:H    | 1.59                     | 0.67              |
| 1:E:298:VAL:HA  | 1:E:332:LEU:HA   | 1.77                     | 0.67              |
| 1:E:50:HIS:CD2  | 1:E:51:MET:H     | 2.12                     | 0.67              |
| 1:G:110:GLU:HG2 | 1:G:118:VAL:CB   | 2.24                     | 0.67              |
| 1:C:32:PHE:O    | 1:C:35:GLU:N     | 2.27                     | 0.67              |
| 1:G:132:MET:HE2 | 1:G:132:MET:C    | 2.15                     | 0.67              |
| 1:G:132:MET:SD  | 1:G:133:ALA:CA   | 2.83                     | 0.67              |
| 1:G:271:VAL:O   | 1:G:271:VAL:HG22 | 1.93                     | 0.67              |
| 1:B:327:MET:SD  | 1:B:327:MET:N    | 2.68                     | 0.67              |
| 1:D:136:GLY:HA2 | 1:D:139:LEU:HD22 | 1.76                     | 0.67              |
| 1:E:192:ARG:C   | 1:E:195:LEU:CD1  | 2.62                     | 0.67              |
| 1:A:211:PRO:HG3 | 1:A:251:PRO:HA   | 1.75                     | 0.67              |
| 1:A:25:LEU:CD1  | 1:A:25:LEU:C     | 2.57                     | 0.67              |
| 1:A:306:LEU:HB3 | 1:A:325:TYR:CE1  | 2.30                     | 0.67              |
| 1:D:29:LEU:O    | 1:D:29:LEU:HD22  | 1.94                     | 0.67              |
| 1:D:95:THR:HA   | 1:D:96:ILE:HG23  | 1.77                     | 0.67              |
| 1:E:110:GLU:OE1 | 1:E:111:ASP:CA   | 2.42                     | 0.67              |
| 1:A:287:ASN:ND2 | 1:A:341:VAL:HG12 | 2.10                     | 0.67              |
| 1:B:251:PRO:HG3 | 1:C:199:TYR:CD1  | 2.27                     | 0.67              |
| 1:C:109:ILE:CD1 | 1:C:110:GLU:N    | 2.56                     | 0.67              |
| 1:E:110:GLU:OE1 | 1:E:111:ASP:HA   | 1.94                     | 0.67              |
| 1:A:205:ARG:HG3 | 1:A:293:MET:O    | 1.95                     | 0.66              |
| 1:B:66:LEU:HD23 | 1:B:201:PRO:HD2  | 1.77                     | 0.66              |
| 1:E:119:ARG:HB3 | 1:E:119:ARG:NH1  | 2.08                     | 0.66              |
| 1:A:207:PHE:CZ  | 1:A:209:CYS:SG   | 2.87                     | 0.66              |
| 1:B:66:LEU:CD2  | 1:B:200:VAL:HB   | 2.26                     | 0.66              |
| 1:E:24:LYS:HD2  | 1:E:24:LYS:C     | 2.16                     | 0.66              |
| 1:E:298:VAL:N   | 1:E:333:ARG:NH1  | 2.41                     | 0.66              |
| 1:G:300:THR:OG1 | 1:G:301:VAL:N    | 2.27                     | 0.66              |
| 1:B:88:LYS:NZ   | 1:B:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:B:24:LYS:HE2  | 1:B:25:LEU:HA    | 1.77                     | 0.66              |
| 1:C:100:LEU:O   | 1:C:101:THR:OG1  | 2.12                     | 0.66              |
| 1:C:290:GLY:HA3 | 1:C:340:VAL:H    | 1.61                     | 0.66              |
| 1:F:25:LEU:C    | 1:F:28:PHE:CD2   | 2.68                     | 0.66              |
| 1:E:121:GLU:OE1 | 1:F:51:MET:CG    | 2.43                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:207:PHE:HB2  | 1:A:291:LEU:O    | 1.94                     | 0.66              |
| 1:B:115:HIS:CD2  | 1:B:115:HIS:H    | 2.14                     | 0.66              |
| 1:C:119:ARG:NH1  | 1:C:119:ARG:CB   | 2.57                     | 0.66              |
| 1:C:181:GLY:HA2  | 1:C:216:ALA:HB1  | 1.78                     | 0.66              |
| 1:B:145:LEU:CD2  | 1:B:332:LEU:HD11 | 2.21                     | 0.66              |
| 1:C:208:TYR:CB   | 1:C:291:LEU:CD2  | 2.73                     | 0.66              |
| 1:D:218:LEU:HD22 | 1:D:221:LEU:HD23 | 1.76                     | 0.66              |
| 1:G:110:GLU:CA   | 1:G:114:ASN:HB3  | 2.22                     | 0.66              |
| 1:G:217:ILE:HG12 | 1:G:221:LEU:HB2  | 1.76                     | 0.66              |
| 1:A:284:ALA:O    | 1:A:288:VAL:HB   | 1.94                     | 0.66              |
| 1:C:110:GLU:C    | 1:C:110:GLU:OE2  | 2.34                     | 0.66              |
| 1:E:299:GLY:N    | 1:E:333:ARG:HH12 | 1.86                     | 0.66              |
| 1:G:28:PHE:CD1   | 1:G:111:ASP:OD2  | 2.48                     | 0.66              |
| 1:A:36:VAL:CG1   | 1:A:126:LEU:HD11 | 2.26                     | 0.66              |
| 1:A:205:ARG:HH21 | 1:A:296:SER:N    | 1.94                     | 0.66              |
| 1:B:28:PHE:CZ    | 1:B:111:ASP:C    | 2.69                     | 0.66              |
| 1:C:107:TYR:HA   | 1:C:318:ALA:HB3  | 1.78                     | 0.66              |
| 1:E:24:LYS:O     | 1:E:24:LYS:HD3   | 1.95                     | 0.66              |
| 1:E:298:VAL:C    | 1:E:333:ARG:CZ   | 2.63                     | 0.66              |
| 1:E:34:GLY:O     | 1:E:38:THR:HG23  | 1.96                     | 0.66              |
| 1:F:254:THR:OG1  | 1:F:285:LYS:NZ   | 2.29                     | 0.66              |
| 1:F:28:PHE:C     | 1:F:28:PHE:CD1   | 2.69                     | 0.66              |
| 1:B:106:ILE:CG2  | 1:B:122:TYR:OH   | 2.44                     | 0.66              |
| 1:B:66:LEU:H     | 1:B:66:LEU:CD1   | 2.08                     | 0.66              |
| 1:G:241:ASN:ND2  | 1:G:245:PHE:O    | 2.28                     | 0.66              |
| 1:F:113:MET:SD   | 1:F:114:ASN:ND2  | 2.57                     | 0.66              |
| 1:E:298:VAL:HG13 | 1:E:332:LEU:HD12 | 1.78                     | 0.65              |
| 1:C:113:MET:CE   | 1:C:119:ARG:NH2  | 2.49                     | 0.65              |
| 1:C:195:LEU:CD2  | 1:C:205:ARG:HH21 | 2.03                     | 0.65              |
| 1:C:205:ARG:NE   | 1:C:294:HIS:HB3  | 2.10                     | 0.65              |
| 1:D:40:PHE:O     | 1:D:43:THR:OG1   | 2.13                     | 0.65              |
| 1:B:27:LEU:HD22  | 1:B:27:LEU:O     | 1.96                     | 0.65              |
| 1:C:108:ASP:O    | 1:C:111:ASP:CB   | 2.45                     | 0.65              |
| 1:E:142:ILE:CD1  | 1:E:142:ILE:O    | 2.30                     | 0.65              |
| 1:F:250:VAL:HG21 | 1:F:253:LEU:HG   | 1.77                     | 0.65              |
| 1:G:262:ARG:NH2  | 1:G:263:GLU:OE2  | 2.29                     | 0.65              |
| 1:B:113:MET:O    | 1:B:114:ASN:ND2  | 2.30                     | 0.65              |
| 1:D:36:VAL:HG12  | 1:D:37:LEU:H     | 1.61                     | 0.65              |
| 1:E:186:ALA:HB1  | 1:E:190:LYS:NZ   | 2.12                     | 0.65              |
| 1:E:195:LEU:O    | 1:E:199:TYR:N    | 2.30                     | 0.65              |
| 1:D:132:MET:HE1  | 1:D:251:PRO:HG2  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:110:GLU:OE1  | 1:E:111:ASP:N    | 2.30                     | 0.65              |
| 1:E:45:VAL:HG13  | 1:E:46:THR:HG23  | 1.78                     | 0.65              |
| 1:A:309:GLU:N    | 1:A:322:ILE:HG13 | 2.12                     | 0.65              |
| 1:A:41:ALA:HA    | 1:A:44:SER:HB3   | 1.78                     | 0.65              |
| 1:B:45:VAL:HG13  | 1:B:46:THR:HG23  | 1.77                     | 0.65              |
| 1:B:64:PRO:O     | 1:B:333:ARG:NH1  | 2.26                     | 0.65              |
| 1:E:298:VAL:HG13 | 1:E:332:LEU:CD1  | 2.25                     | 0.65              |
| 1:G:106:ILE:C    | 1:G:107:TYR:HD2  | 2.00                     | 0.65              |
| 1:A:297:ALA:HB1  | 1:A:334:PRO:HB3  | 1.79                     | 0.65              |
| 1:C:211:PRO:HG3  | 1:C:251:PRO:HA   | 1.79                     | 0.65              |
| 1:C:297:ALA:O    | 1:C:298:VAL:HG13 | 1.97                     | 0.65              |
| 1:D:288:VAL:HG11 | 1:D:340:VAL:HG13 | 1.79                     | 0.65              |
| 1:A:208:TYR:OH   | 1:A:293:MET:HE1  | 1.97                     | 0.65              |
| 1:E:291:LEU:HD13 | 1:E:339:ALA:HB2  | 1.79                     | 0.65              |
| 1:G:141:GLU:HB2  | 1:G:270:HIS:HE1  | 1.62                     | 0.65              |
| 1:A:285:LYS:HG2  | 1:A:286:ASP:N    | 2.11                     | 0.65              |
| 1:A:53:ARG:NH2   | 1:F:114:ASN:OD1  | 2.30                     | 0.65              |
| 1:B:110:GLU:OE1  | 1:B:111:ASP:N    | 2.30                     | 0.65              |
| 1:B:125:GLN:NE2  | 1:C:66:LEU:O     | 2.26                     | 0.65              |
| 1:F:25:LEU:HB2   | 1:F:28:PHE:CE2   | 2.30                     | 0.65              |
| 1:A:57:SER:N     | 1:A:303:LEU:HD13 | 2.09                     | 0.64              |
| 1:C:329:HIS:CD2  | 1:C:331:GLY:H    | 2.15                     | 0.64              |
| 1:E:195:LEU:O    | 1:E:199:TYR:O    | 2.15                     | 0.64              |
| 1:G:115:HIS:CE1  | 1:G:119:ARG:NH2  | 2.65                     | 0.64              |
| 1:G:141:GLU:H    | 1:G:270:HIS:CE1  | 2.14                     | 0.64              |
| 1:G:53:ARG:NH1   | 1:G:62:GLN:O     | 2.30                     | 0.64              |
| 1:A:70:GLN:NE2   | 1:F:129:SER:OG   | 2.30                     | 0.64              |
| 1:F:295:ARG:NH2  | 1:F:296:SER:OG   | 2.28                     | 0.64              |
| 1:B:24:LYS:HD2   | 1:B:25:LEU:N     | 2.11                     | 0.64              |
| 1:B:24:LYS:HZ3   | 1:B:24:LYS:N     | 1.94                     | 0.64              |
| 1:B:55:ILE:O     | 1:B:304:ARG:NH2  | 2.31                     | 0.64              |
| 1:C:35:GLU:O     | 1:C:39:ALA:N     | 2.30                     | 0.64              |
| 1:G:49:ARG:HH22  | 1:G:248:VAL:HG21 | 1.63                     | 0.64              |
| 1:C:248:VAL:HG12 | 1:C:249:GLU:H    | 1.63                     | 0.64              |
| 1:A:287:ASN:CG   | 1:A:341:VAL:HB   | 2.18                     | 0.64              |
| 1:C:110:GLU:OE1  | 1:C:122:TYR:HD2  | 1.81                     | 0.64              |
| 1:C:110:GLU:HG2  | 1:C:122:TYR:HE2  | 1.62                     | 0.64              |
| 1:C:43:THR:CG2   | 1:C:128:GLU:HG3  | 2.27                     | 0.64              |
| 1:D:200:VAL:HG22 | 1:D:201:PRO:HD2  | 1.79                     | 0.64              |
| 1:G:25:LEU:HB3   | 1:G:28:PHE:CE2   | 2.33                     | 0.64              |
| 1:G:28:PHE:C     | 1:G:28:PHE:CD1   | 2.70                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:50:HIS:NE2   | 1:B:298:VAL:HB   | 2.12                     | 0.64              |
| 1:G:110:GLU:N    | 1:G:114:ASN:ND2  | 2.45                     | 0.64              |
| 1:A:45:VAL:HG22  | 1:A:250:VAL:HG11 | 1.80                     | 0.64              |
| 1:A:300:THR:OG1  | 1:A:301:VAL:N    | 2.28                     | 0.64              |
| 1:B:106:ILE:C    | 1:B:107:TYR:CD2  | 2.67                     | 0.64              |
| 1:B:139:LEU:HA   | 1:B:142:ILE:CG2  | 2.28                     | 0.64              |
| 1:E:106:ILE:HD12 | 1:E:108:ASP:HA   | 1.80                     | 0.64              |
| 1:E:139:LEU:O    | 1:E:142:ILE:HG23 | 1.98                     | 0.64              |
| 1:F:332:LEU:HD13 | 1:F:333:ARG:H    | 1.62                     | 0.64              |
| 1:G:109:ILE:C    | 1:G:114:ASN:HD22 | 2.01                     | 0.64              |
| 1:A:302:LYS:CE   | 1:A:327:MET:CE   | 2.76                     | 0.64              |
| 1:G:303:LEU:HD22 | 1:G:304:ARG:HG3  | 1.80                     | 0.64              |
| 1:A:327:MET:SD   | 1:A:328:GLY:N    | 2.66                     | 0.63              |
| 1:A:161:THR:H    | 1:A:336:ALA:HA   | 1.62                     | 0.63              |
| 1:B:113:MET:CG   | 1:B:115:HIS:NE2  | 2.61                     | 0.63              |
| 1:B:24:LYS:CD    | 1:B:25:LEU:N     | 2.59                     | 0.63              |
| 1:C:129:SER:OG   | 1:D:70:GLN:O     | 2.15                     | 0.63              |
| 1:C:114:ASN:N    | 1:C:114:ASN:OD1  | 2.30                     | 0.63              |
| 1:A:294:HIS:NE2  | 1:A:337:ALA:HA   | 2.11                     | 0.63              |
| 1:C:49:ARG:NH2   | 1:C:246:GLU:OE2  | 2.30                     | 0.63              |
| 1:G:78:GLU:OE2   | 1:G:79:ASN:N     | 2.31                     | 0.63              |
| 1:B:27:LEU:HD23  | 1:B:30:LYS:CB    | 2.22                     | 0.63              |
| 1:B:53:ARG:NH1   | 1:B:62:GLN:O     | 2.23                     | 0.63              |
| 1:D:29:LEU:C     | 1:D:29:LEU:HD22  | 2.19                     | 0.63              |
| 1:G:25:LEU:CA    | 1:G:28:PHE:CD2   | 2.70                     | 0.63              |
| 1:B:92:LYS:HZ1   | 1:B:333:ARG:NE   | 1.96                     | 0.63              |
| 1:F:276:LYS:HZ2  | 1:F:278:GLU:H    | 1.46                     | 0.63              |
| 1:G:54:SER:OG    | 1:G:302:LYS:N    | 2.31                     | 0.63              |
| 1:A:208:TYR:OH   | 1:A:293:MET:SD   | 2.57                     | 0.63              |
| 1:C:205:ARG:HG2  | 1:C:294:HIS:HB3  | 1.80                     | 0.63              |
| 1:C:43:THR:CB    | 1:C:128:GLU:HG3  | 2.29                     | 0.63              |
| 1:D:128:GLU:OE1  | 1:D:129:SER:N    | 2.30                     | 0.63              |
| 1:C:36:VAL:CG1   | 1:C:126:LEU:HD21 | 2.28                     | 0.63              |
| 1:C:162:ALA:O    | 1:C:164:VAL:N    | 2.31                     | 0.63              |
| 1:F:167:THR:OG1  | 1:F:168:THR:N    | 2.32                     | 0.63              |
| 1:G:119:ARG:CG   | 1:G:119:ARG:NH1  | 2.39                     | 0.63              |
| 1:B:113:MET:O    | 1:B:114:ASN:CB   | 2.47                     | 0.63              |
| 1:B:161:THR:OG1  | 1:B:162:ALA:N    | 2.32                     | 0.63              |
| 1:G:165:ILE:HG12 | 1:G:341:VAL:CG1  | 2.28                     | 0.63              |
| 1:B:145:LEU:HD23 | 1:B:332:LEU:CD1  | 2.24                     | 0.63              |
| 1:E:138:VAL:O    | 1:E:142:ILE:CG2  | 2.45                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:36:VAL:HG13  | 1:C:126:LEU:HG   | 1.80                     | 0.62              |
| 1:E:50:HIS:CD2   | 1:E:298:VAL:HG23 | 2.34                     | 0.62              |
| 1:A:309:GLU:HB2  | 1:A:322:ILE:HD12 | 1.81                     | 0.62              |
| 1:B:332:LEU:HD12 | 1:B:334:PRO:HG2  | 1.80                     | 0.62              |
| 1:F:36:VAL:HG21  | 1:F:126:LEU:HD11 | 1.81                     | 0.62              |
| 1:F:145:LEU:CD2  | 1:F:334:PRO:HB3  | 2.29                     | 0.62              |
| 1:D:110:GLU:OE1  | 1:D:111:ASP:N    | 2.30                     | 0.62              |
| 1:D:142:ILE:HA   | 1:D:145:LEU:CG   | 2.25                     | 0.62              |
| 1:D:59:LYS:O     | 1:D:96:ILE:HG21  | 1.98                     | 0.62              |
| 1:A:207:PHE:CE1  | 1:A:209:CYS:CA   | 2.83                     | 0.62              |
| 1:A:57:SER:H     | 1:A:303:LEU:CD1  | 2.07                     | 0.62              |
| 1:C:40:PHE:CE1   | 1:C:131:ALA:CA   | 2.78                     | 0.62              |
| 1:C:170:ASN:HB3  | 1:C:172:ALA:H    | 1.64                     | 0.62              |
| 1:B:128:GLU:OE1  | 1:C:68:ARG:CG    | 2.47                     | 0.62              |
| 1:G:110:GLU:C    | 1:G:114:ASN:CB   | 2.65                     | 0.62              |
| 1:D:142:ILE:CD1  | 1:D:145:LEU:HD21 | 2.20                     | 0.62              |
| 1:G:27:LEU:C     | 1:G:27:LEU:CD1   | 2.58                     | 0.62              |
| 1:A:209:CYS:HA   | 1:A:290:GLY:HA3  | 1.82                     | 0.62              |
| 1:A:207:PHE:HE2  | 1:A:247:VAL:CG2  | 2.13                     | 0.62              |
| 1:D:128:GLU:OE2  | 1:D:129:SER:CA   | 2.47                     | 0.62              |
| 1:E:135:ASP:OD2  | 1:E:252:HIS:CE1  | 2.52                     | 0.62              |
| 1:E:192:ARG:CA   | 1:E:195:LEU:CG   | 2.74                     | 0.62              |
| 1:F:171:LYS:HD2  | 1:F:174:LEU:HD12 | 1.82                     | 0.62              |
| 1:G:209:CYS:SG   | 1:G:210:ASP:N    | 2.73                     | 0.62              |
| 1:A:110:GLU:HB2  | 1:A:114:ASN:ND2  | 2.15                     | 0.62              |
| 1:D:110:GLU:HG2  | 1:D:113:MET:O    | 2.00                     | 0.62              |
| 1:F:135:ASP:OD1  | 1:F:252:HIS:NE2  | 2.31                     | 0.62              |
| 1:F:51:MET:SD    | 1:F:295:ARG:NH2  | 2.72                     | 0.62              |
| 1:B:59:LYS:HB2   | 1:B:96:ILE:HD13  | 1.81                     | 0.62              |
| 1:D:142:ILE:HD12 | 1:D:145:LEU:CG   | 2.29                     | 0.62              |
| 1:A:27:LEU:HD12  | 1:A:28:PHE:HA    | 1.81                     | 0.62              |
| 1:A:315:ASN:OD1  | 1:A:315:ASN:N    | 2.31                     | 0.62              |
| 1:C:24:LYS:CG    | 1:C:25:LEU:N     | 2.63                     | 0.62              |
| 1:B:117:ASP:OD2  | 1:C:51:MET:HE1   | 1.98                     | 0.62              |
| 1:B:251:PRO:CG   | 1:C:199:TYR:CZ   | 2.53                     | 0.62              |
| 1:C:98:GLY:HA2   | 1:D:75:ALA:HB2   | 1.82                     | 0.62              |
| 1:E:192:ARG:HG2  | 1:E:193:ALA:N    | 2.14                     | 0.62              |
| 1:A:209:CYS:HA   | 1:A:290:GLY:HA2  | 1.82                     | 0.61              |
| 1:B:28:PHE:HZ    | 1:B:112:ALA:CA   | 2.07                     | 0.61              |
| 1:E:59:LYS:O     | 1:E:95:THR:OG1   | 2.12                     | 0.61              |
| 1:B:132:MET:HE3  | 1:B:132:MET:N    | 2.14                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:36:VAL:CG1   | 1:C:126:LEU:CG   | 2.78                     | 0.61              |
| 1:A:294:HIS:HD2  | 1:A:337:ALA:CA   | 2.11                     | 0.61              |
| 1:G:26:ALA:CA    | 1:G:29:LEU:HD12  | 2.23                     | 0.61              |
| 1:B:50:HIS:CD2   | 1:B:51:MET:H     | 2.18                     | 0.61              |
| 1:C:142:ILE:O    | 1:C:145:LEU:HB2  | 2.01                     | 0.61              |
| 1:F:288:VAL:HG21 | 1:F:340:VAL:O    | 1.99                     | 0.61              |
| 1:G:206:VAL:HA   | 1:G:246:GLU:HG2  | 1.81                     | 0.61              |
| 1:B:276:LYS:HD2  | 1:B:279:GLY:HA3  | 1.82                     | 0.61              |
| 1:C:108:ASP:CG   | 1:C:111:ASP:CG   | 2.59                     | 0.61              |
| 1:C:33:GLY:O     | 1:C:37:LEU:N     | 2.31                     | 0.61              |
| 1:D:104:VAL:HG22 | 1:D:321:ILE:HD11 | 1.81                     | 0.61              |
| 1:C:115:HIS:CD2  | 1:C:115:HIS:O    | 2.53                     | 0.61              |
| 1:E:299:GLY:HA3  | 1:E:333:ARG:HH22 | 1.65                     | 0.61              |
| 1:F:201:PRO:O    | 1:F:205:ARG:NH2  | 2.33                     | 0.61              |
| 1:A:287:ASN:O    | 1:A:288:VAL:HG12 | 2.00                     | 0.61              |
| 1:A:303:LEU:O    | 1:A:304:ARG:HB2  | 1.99                     | 0.61              |
| 1:B:110:GLU:OE1  | 1:B:111:ASP:CA   | 2.49                     | 0.61              |
| 1:C:294:HIS:CE1  | 1:C:335:GLU:HB2  | 2.35                     | 0.61              |
| 1:G:275:ASN:OD1  | 1:G:275:ASN:N    | 2.33                     | 0.61              |
| 1:B:109:ILE:C    | 1:B:109:ILE:CD1  | 2.66                     | 0.61              |
| 1:D:135:ASP:C    | 1:D:139:LEU:HD22 | 2.20                     | 0.61              |
| 1:G:178:VAL:O    | 1:G:182:LYS:NZ   | 2.28                     | 0.61              |
| 1:A:119:ARG:NH1  | 1:A:119:ARG:CG   | 2.47                     | 0.61              |
| 1:A:128:GLU:OE2  | 1:A:129:SER:N    | 2.34                     | 0.61              |
| 1:C:36:VAL:CG1   | 1:C:126:LEU:CD2  | 2.79                     | 0.61              |
| 1:A:102:ALA:HB2  | 1:B:71:ALA:HA    | 1.83                     | 0.60              |
| 1:B:125:GLN:HG2  | 1:C:66:LEU:CD1   | 2.28                     | 0.60              |
| 1:C:125:GLN:HG2  | 1:D:66:LEU:HB3   | 1.83                     | 0.60              |
| 1:C:298:VAL:HG12 | 1:C:331:GLY:C    | 2.20                     | 0.60              |
| 1:B:214:TYR:O    | 1:B:217:ILE:HG12 | 2.01                     | 0.60              |
| 1:F:166:GLU:HA   | 1:F:341:VAL:HG13 | 1.83                     | 0.60              |
| 1:B:118:VAL:CG1  | 1:B:119:ARG:N    | 2.64                     | 0.60              |
| 1:C:208:TYR:HB3  | 1:C:291:LEU:CG   | 2.25                     | 0.60              |
| 1:D:196:THR:O    | 1:D:199:TYR:N    | 2.34                     | 0.60              |
| 1:F:293:MET:HA   | 1:F:336:ALA:O    | 2.01                     | 0.60              |
| 1:G:180:LEU:O    | 1:G:184:ILE:N    | 2.35                     | 0.60              |
| 1:B:67:GLY:HA3   | 1:B:68:ARG:NH1   | 2.16                     | 0.60              |
| 1:E:299:GLY:O    | 1:E:331:GLY:N    | 2.33                     | 0.60              |
| 1:A:288:VAL:O    | 1:A:289:ILE:CD1  | 2.50                     | 0.60              |
| 1:B:131:ALA:O    | 1:B:135:ASP:CG   | 2.40                     | 0.60              |
| 1:B:139:LEU:HA   | 1:B:142:ILE:HG21 | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:286:ASP:OD2  | 1:B:286:ASP:N    | 2.33                     | 0.60              |
| 1:C:206:VAL:HG23 | 1:C:247:VAL:C    | 2.21                     | 0.60              |
| 1:G:167:THR:C    | 1:G:169:GLN:H    | 2.04                     | 0.60              |
| 1:B:108:ASP:O    | 1:B:111:ASP:CG   | 2.40                     | 0.60              |
| 1:D:45:VAL:HB    | 1:D:135:ASP:OD2  | 2.02                     | 0.60              |
| 1:F:303:LEU:HB2  | 1:F:326:ALA:HB2  | 1.82                     | 0.60              |
| 1:B:114:ASN:CB   | 1:B:118:VAL:HB   | 2.32                     | 0.60              |
| 1:F:253:LEU:O    | 1:F:285:LYS:NZ   | 2.27                     | 0.60              |
| 1:G:234:PRO:HD2  | 1:G:236:LYS:HE3  | 1.82                     | 0.60              |
| 1:B:332:LEU:HD12 | 1:B:334:PRO:CG   | 2.30                     | 0.60              |
| 1:G:167:THR:HG23 | 1:G:341:VAL:O    | 2.01                     | 0.60              |
| 1:A:29:LEU:HD21  | 1:A:310:ARG:HD3  | 1.84                     | 0.60              |
| 1:B:92:LYS:NZ    | 1:B:333:ARG:HE   | 1.98                     | 0.60              |
| 1:C:31:VAL:CG1   | 1:C:32:PHE:N     | 2.65                     | 0.60              |
| 1:E:109:ILE:N    | 1:E:109:ILE:CD1  | 2.30                     | 0.60              |
| 1:E:50:HIS:CD2   | 1:E:51:MET:N     | 2.70                     | 0.60              |
| 1:A:163:THR:HB   | 1:A:338:GLY:HA3  | 1.83                     | 0.60              |
| 1:A:287:ASN:ND2  | 1:A:341:VAL:CG1  | 2.64                     | 0.60              |
| 1:D:290:GLY:O    | 1:D:339:ALA:HA   | 2.02                     | 0.60              |
| 1:D:293:MET:HB3  | 1:D:337:ALA:HB2  | 1.82                     | 0.60              |
| 1:G:232:ILE:HG22 | 1:G:234:PRO:HD3  | 1.84                     | 0.60              |
| 1:B:24:LYS:HZ3   | 1:B:24:LYS:C     | 2.04                     | 0.59              |
| 1:D:81:ASP:N     | 1:D:81:ASP:OD1   | 2.33                     | 0.59              |
| 1:E:141:GLU:HG3  | 1:E:330:GLY:O    | 2.02                     | 0.59              |
| 1:F:174:LEU:HD22 | 1:F:180:LEU:HD21 | 1.84                     | 0.59              |
| 1:B:114:ASN:O    | 1:B:118:VAL:N    | 2.31                     | 0.59              |
| 1:B:92:LYS:HZ1   | 1:B:333:ARG:HH21 | 1.49                     | 0.59              |
| 1:C:202:ALA:HB1  | 1:C:205:ARG:HH21 | 1.63                     | 0.59              |
| 1:E:298:VAL:HG12 | 1:E:332:LEU:HD12 | 1.82                     | 0.59              |
| 1:G:119:ARG:O    | 1:G:123:THR:HG23 | 2.01                     | 0.59              |
| 1:C:275:ASN:HA   | 1:C:285:LYS:HE2  | 1.85                     | 0.59              |
| 1:D:310:ARG:HG2  | 1:D:321:ILE:HG22 | 1.85                     | 0.59              |
| 1:B:131:ALA:O    | 1:B:132:MET:HE2  | 2.02                     | 0.59              |
| 1:B:332:LEU:CD1  | 1:B:334:PRO:HD2  | 2.29                     | 0.59              |
| 1:E:61:ALA:N     | 1:E:94:ILE:O     | 2.33                     | 0.59              |
| 1:G:270:HIS:HE2  | 1:G:329:HIS:HE1  | 1.49                     | 0.59              |
| 1:A:294:HIS:CD2  | 1:A:337:ALA:CA   | 2.73                     | 0.59              |
| 1:B:62:GLN:HB3   | 1:B:93:VAL:HG12  | 1.84                     | 0.59              |
| 1:C:24:LYS:HG3   | 1:C:25:LEU:N     | 2.18                     | 0.59              |
| 1:F:27:LEU:C     | 1:F:27:LEU:HD12  | 2.20                     | 0.59              |
| 1:G:113:MET:C    | 1:G:113:MET:HE3  | 2.08                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:209:CYS:SG   | 1:E:210:ASP:N    | 2.75                     | 0.59              |
| 1:E:25:LEU:HD11  | 1:E:310:ARG:CZ   | 2.30                     | 0.59              |
| 1:G:28:PHE:CE1   | 1:G:29:LEU:HD23  | 2.37                     | 0.59              |
| 1:B:227:ASN:O    | 1:B:227:ASN:ND2  | 2.26                     | 0.59              |
| 1:E:239:ILE:HB   | 1:E:247:VAL:HB   | 1.84                     | 0.59              |
| 1:E:298:VAL:HA   | 1:E:333:ARG:NH1  | 2.11                     | 0.59              |
| 1:C:108:ASP:CG   | 1:C:111:ASP:HB3  | 2.23                     | 0.59              |
| 1:C:35:GLU:OE1   | 1:C:119:ARG:O    | 2.21                     | 0.59              |
| 1:E:56:SER:OG    | 1:E:304:ARG:NH2  | 2.29                     | 0.59              |
| 1:G:25:LEU:HB3   | 1:G:28:PHE:HE2   | 1.68                     | 0.59              |
| 1:B:307:ALA:HB3  | 1:B:324:LYS:HB3  | 1.85                     | 0.59              |
| 1:C:235:GLU:OE1  | 1:C:236:LYS:N    | 2.26                     | 0.59              |
| 1:E:110:GLU:HG3  | 1:E:118:VAL:CB   | 2.33                     | 0.59              |
| 1:E:284:ALA:H    | 1:E:288:VAL:HG21 | 1.68                     | 0.59              |
| 1:B:131:ALA:C    | 1:B:132:MET:CE   | 2.71                     | 0.58              |
| 1:C:201:PRO:HA   | 1:C:202:ALA:CB   | 2.13                     | 0.58              |
| 1:G:110:GLU:N    | 1:G:114:ASN:HD22 | 2.01                     | 0.58              |
| 1:B:134:ALA:O    | 1:B:138:VAL:CG2  | 2.50                     | 0.58              |
| 1:B:66:LEU:HD22  | 1:B:66:LEU:O     | 2.02                     | 0.58              |
| 1:C:188:LEU:HB3  | 1:C:245:PHE:HE2  | 1.67                     | 0.58              |
| 1:C:294:HIS:NE2  | 1:C:335:GLU:OE2  | 2.35                     | 0.58              |
| 1:D:142:ILE:HD12 | 1:D:145:LEU:CD2  | 2.32                     | 0.58              |
| 1:F:28:PHE:HD1   | 1:F:29:LEU:N     | 1.95                     | 0.58              |
| 1:C:135:ASP:OD1  | 1:C:135:ASP:N    | 2.34                     | 0.58              |
| 1:C:208:TYR:HB3  | 1:C:291:LEU:HD21 | 1.82                     | 0.58              |
| 1:C:32:PHE:CE1   | 1:C:36:VAL:CG2   | 2.87                     | 0.58              |
| 1:B:298:VAL:HA   | 1:B:332:LEU:HD22 | 1.86                     | 0.58              |
| 1:C:32:PHE:CZ    | 1:C:126:LEU:HD23 | 2.39                     | 0.58              |
| 1:D:161:THR:OG1  | 1:D:162:ALA:N    | 2.35                     | 0.58              |
| 1:G:113:MET:CG   | 1:G:114:ASN:H    | 2.09                     | 0.58              |
| 1:G:165:ILE:HD13 | 1:G:166:GLU:CA   | 2.32                     | 0.58              |
| 1:A:41:ALA:C     | 1:A:43:THR:H     | 2.07                     | 0.58              |
| 1:A:279:GLY:O    | 1:A:280:ASN:ND2  | 2.37                     | 0.58              |
| 1:B:117:ASP:OD2  | 1:C:51:MET:HE3   | 2.02                     | 0.58              |
| 1:B:63:PHE:CZ    | 1:B:299:GLY:HA3  | 2.38                     | 0.58              |
| 1:G:132:MET:SD   | 1:G:133:ALA:HA   | 2.43                     | 0.58              |
| 1:A:250:VAL:HB   | 1:A:251:PRO:HD2  | 1.86                     | 0.58              |
| 1:A:26:ALA:HA    | 1:A:29:LEU:CD1   | 2.31                     | 0.58              |
| 1:B:161:THR:HG22 | 1:B:335:GLU:N    | 2.18                     | 0.58              |
| 1:C:214:TYR:CD1  | 1:C:249:GLU:HG2  | 2.39                     | 0.58              |
| 1:D:57:SER:O     | 1:D:59:LYS:NZ    | 2.35                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:100:LEU:HA   | 1:F:72:ALA:O     | 2.03                     | 0.58              |
| 1:E:28:PHE:CD2   | 1:E:111:ASP:OD2  | 2.56                     | 0.58              |
| 1:G:101:THR:O    | 1:G:262:ARG:NH1  | 2.34                     | 0.58              |
| 1:G:146:CYS:SG   | 1:G:336:ALA:CA   | 2.92                     | 0.58              |
| 1:B:214:TYR:OH   | 1:C:192:ARG:NE   | 2.36                     | 0.57              |
| 1:C:116:TYR:C    | 1:C:116:TYR:HD2  | 2.03                     | 0.57              |
| 1:C:240:ARG:HG3  | 1:C:241:ASN:H    | 1.69                     | 0.57              |
| 1:D:295:ARG:NE   | 1:D:296:SER:OG   | 2.38                     | 0.57              |
| 1:F:310:ARG:HB3  | 1:F:321:ILE:HG22 | 1.86                     | 0.57              |
| 1:G:143:ALA:HB1  | 1:G:272:PHE:CB   | 2.34                     | 0.57              |
| 1:A:139:LEU:HD21 | 1:A:291:LEU:HD11 | 1.85                     | 0.57              |
| 1:C:32:PHE:CE1   | 1:C:36:VAL:HG22  | 2.39                     | 0.57              |
| 1:F:212:ASP:O    | 1:F:215:SER:OG   | 2.22                     | 0.57              |
| 1:F:141:GLU:CG   | 1:F:329:HIS:CD2  | 2.87                     | 0.57              |
| 1:G:45:VAL:HG22  | 1:G:46:THR:HG23  | 1.86                     | 0.57              |
| 1:C:206:VAL:HA   | 1:C:246:GLU:C    | 2.17                     | 0.57              |
| 1:C:271:VAL:H    | 1:C:274:ALA:HB2  | 1.69                     | 0.57              |
| 1:C:71:ALA:HB1   | 1:C:72:ALA:HA    | 1.85                     | 0.57              |
| 1:E:293:MET:HA   | 1:E:337:ALA:H    | 1.69                     | 0.57              |
| 1:A:141:GLU:OE1  | 1:A:142:ILE:HG12 | 2.05                     | 0.57              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:SD   | 2.45                     | 0.57              |
| 1:B:285:LYS:O    | 1:B:288:VAL:N    | 2.32                     | 0.57              |
| 1:C:171:LYS:HB3  | 1:C:342:PHE:CZ   | 2.39                     | 0.57              |
| 1:E:189:THR:HG23 | 1:E:243:MET:CG   | 2.35                     | 0.57              |
| 1:F:147:ASN:N    | 1:F:147:ASN:OD1  | 2.36                     | 0.57              |
| 1:A:287:ASN:HD22 | 1:A:287:ASN:C    | 2.04                     | 0.57              |
| 1:B:115:HIS:N    | 1:B:115:HIS:HD2  | 2.01                     | 0.57              |
| 1:C:108:ASP:CG   | 1:C:111:ASP:CB   | 2.73                     | 0.57              |
| 1:C:110:GLU:OE1  | 1:C:122:TYR:HE2  | 1.85                     | 0.57              |
| 1:B:28:PHE:HE1   | 1:B:112:ALA:CB   | 2.17                     | 0.57              |
| 1:E:29:LEU:O     | 1:E:30:LYS:C     | 2.42                     | 0.57              |
| 1:F:183:GLU:OE1  | 1:F:184:ILE:N    | 2.38                     | 0.57              |
| 1:G:171:LYS:H    | 1:G:342:PHE:HE2  | 1.50                     | 0.57              |
| 1:E:29:LEU:O     | 1:E:31:VAL:N     | 2.37                     | 0.57              |
| 1:G:115:HIS:HA   | 1:G:119:ARG:NH1  | 2.20                     | 0.57              |
| 1:B:24:LYS:HZ3   | 1:B:24:LYS:HB3   | 1.52                     | 0.57              |
| 1:C:188:LEU:HD13 | 1:C:207:PHE:CZ   | 2.40                     | 0.57              |
| 1:C:312:ARG:NH1  | 1:C:318:ALA:O    | 2.37                     | 0.57              |
| 1:D:290:GLY:HA3  | 1:D:340:VAL:H    | 1.70                     | 0.57              |
| 1:A:108:ASP:HB3  | 1:A:111:ASP:HB2  | 1.85                     | 0.57              |
| 1:A:207:PHE:CE1  | 1:A:290:GLY:CA   | 2.81                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:55:ILE:HG23  | 1:A:301:VAL:CG2  | 2.35                     | 0.57              |
| 1:B:206:VAL:HA   | 1:B:246:GLU:H    | 1.70                     | 0.57              |
| 1:B:141:GLU:CD   | 1:B:330:GLY:CA   | 2.58                     | 0.57              |
| 1:C:119:ARG:HH11 | 1:C:119:ARG:CB   | 2.15                     | 0.57              |
| 1:B:139:LEU:C    | 1:B:142:ILE:CG2  | 2.71                     | 0.56              |
| 1:C:119:ARG:NH1  | 1:C:119:ARG:HG3  | 2.01                     | 0.56              |
| 1:C:41:ALA:O     | 1:C:42:ARG:CB    | 2.41                     | 0.56              |
| 1:D:28:PHE:HD2   | 1:D:29:LEU:H     | 1.49                     | 0.56              |
| 1:E:110:GLU:CD   | 1:E:118:VAL:HG21 | 2.25                     | 0.56              |
| 1:F:242:VAL:HG22 | 1:F:243:MET:H    | 1.70                     | 0.56              |
| 1:B:319:ASP:OD2  | 1:B:320:GLN:N    | 2.38                     | 0.56              |
| 1:E:25:LEU:CD1   | 1:E:310:ARG:CZ   | 2.79                     | 0.56              |
| 1:E:294:HIS:NE2  | 1:E:295:ARG:O    | 2.37                     | 0.56              |
| 1:F:143:ALA:CB   | 1:F:272:PHE:CD2  | 2.89                     | 0.56              |
| 1:F:181:GLY:HA3  | 1:F:220:ALA:HB2  | 1.87                     | 0.56              |
| 1:F:272:PHE:O    | 1:F:274:ALA:N    | 2.37                     | 0.56              |
| 1:F:141:GLU:CG   | 1:F:329:HIS:NE2  | 2.69                     | 0.56              |
| 1:A:289:ILE:HG13 | 1:A:340:VAL:HG23 | 1.77                     | 0.56              |
| 1:C:271:VAL:HG23 | 1:C:274:ALA:HA   | 1.86                     | 0.56              |
| 1:E:141:GLU:CG   | 1:E:330:GLY:O    | 2.52                     | 0.56              |
| 1:A:212:ASP:N    | 1:A:212:ASP:OD2  | 2.30                     | 0.56              |
| 1:A:309:GLU:CB   | 1:A:322:ILE:HD12 | 2.27                     | 0.56              |
| 1:B:121:GLU:HA   | 1:B:121:GLU:OE1  | 2.05                     | 0.56              |
| 1:B:139:LEU:CA   | 1:B:142:ILE:CG2  | 2.84                     | 0.56              |
| 1:C:137:ALA:O    | 1:C:140:ALA:N    | 2.37                     | 0.56              |
| 1:C:207:PHE:O    | 1:C:248:VAL:O    | 2.23                     | 0.56              |
| 1:E:234:PRO:O    | 1:E:236:LYS:N    | 2.38                     | 0.56              |
| 1:F:308:LEU:CB   | 1:F:323:ALA:HA   | 2.34                     | 0.56              |
| 1:F:32:PHE:O     | 1:F:34:GLY:N     | 2.38                     | 0.56              |
| 1:A:276:LYS:HZ2  | 1:A:278:GLU:H    | 1.52                     | 0.56              |
| 1:G:44:SER:OG    | 1:G:135:ASP:HB2  | 2.05                     | 0.56              |
| 1:A:114:ASN:O    | 1:A:114:ASN:CG   | 2.43                     | 0.56              |
| 1:A:307:ALA:O    | 1:A:324:LYS:N    | 2.38                     | 0.56              |
| 1:B:210:ASP:OD2  | 1:B:213:SER:OG   | 2.23                     | 0.56              |
| 1:C:188:LEU:CD2  | 1:C:207:PHE:CZ   | 2.85                     | 0.56              |
| 1:D:164:VAL:HA   | 1:D:339:ALA:H    | 1.70                     | 0.56              |
| 1:D:205:ARG:CZ   | 1:D:205:ARG:HB3  | 2.35                     | 0.56              |
| 1:F:29:LEU:O     | 1:F:32:PHE:HB3   | 2.05                     | 0.56              |
| 1:G:110:GLU:OE1  | 1:G:118:VAL:HB   | 2.05                     | 0.56              |
| 1:A:320:GLN:NE2  | 1:A:321:ILE:O    | 2.32                     | 0.56              |
| 1:A:73:TYR:HE1   | 1:F:102:ALA:HB2  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:HIS:O    | 1:B:119:ARG:HB2  | 2.05                     | 0.56              |
| 1:B:121:GLU:O    | 1:B:121:GLU:CD   | 2.44                     | 0.56              |
| 1:E:299:GLY:CA   | 1:E:333:ARG:NH2  | 2.63                     | 0.56              |
| 1:D:136:GLY:CA   | 1:D:139:LEU:HD22 | 2.35                     | 0.56              |
| 1:E:233:ASP:OD2  | 1:E:238:SER:N    | 2.37                     | 0.56              |
| 1:F:130:LEU:HD11 | 1:F:325:TYR:HD2  | 1.71                     | 0.56              |
| 1:B:25:LEU:HD13  | 1:B:25:LEU:C     | 2.26                     | 0.56              |
| 1:G:113:MET:O    | 1:G:115:HIS:N    | 2.39                     | 0.56              |
| 1:B:28:PHE:CZ    | 1:B:112:ALA:N    | 2.74                     | 0.56              |
| 1:C:202:ALA:CB   | 1:C:205:ARG:HH21 | 2.19                     | 0.56              |
| 1:C:48:SER:OG    | 1:C:49:ARG:N     | 2.36                     | 0.56              |
| 1:E:53:ARG:HD3   | 1:E:63:PHE:CD1   | 2.41                     | 0.56              |
| 1:G:106:ILE:HD11 | 1:G:107:TYR:O    | 2.05                     | 0.56              |
| 1:A:66:LEU:HD23  | 1:A:89:HIS:HE1   | 1.69                     | 0.56              |
| 1:B:132:MET:HE2  | 1:B:135:ASP:CG   | 2.25                     | 0.56              |
| 1:C:290:GLY:HA2  | 1:C:340:VAL:HG22 | 1.87                     | 0.56              |
| 1:D:225:ALA:HB1  | 1:D:226:ALA:C    | 2.25                     | 0.56              |
| 1:F:147:ASN:HA   | 1:F:283:VAL:HG21 | 1.87                     | 0.56              |
| 1:G:110:GLU:CD   | 1:G:118:VAL:HG11 | 2.18                     | 0.56              |
| 1:G:130:LEU:HD23 | 1:G:131:ALA:CA   | 2.36                     | 0.56              |
| 1:C:29:LEU:O     | 1:C:32:PHE:N     | 2.39                     | 0.55              |
| 1:D:36:VAL:HG22  | 1:D:39:ALA:HB3   | 1.87                     | 0.55              |
| 1:E:50:HIS:HE2   | 1:E:299:GLY:HA2  | 1.71                     | 0.55              |
| 1:E:297:ALA:O    | 1:E:332:LEU:HD12 | 2.06                     | 0.55              |
| 1:C:162:ALA:C    | 1:C:164:VAL:H    | 2.09                     | 0.55              |
| 1:C:183:GLU:OE1  | 1:C:183:GLU:N    | 2.39                     | 0.55              |
| 1:E:167:THR:OG1  | 1:E:168:THR:N    | 2.39                     | 0.55              |
| 1:F:32:PHE:O     | 1:F:33:GLY:C     | 2.43                     | 0.55              |
| 1:C:299:GLY:H    | 1:C:330:GLY:C    | 2.09                     | 0.55              |
| 1:C:49:ARG:HH12  | 1:C:248:VAL:HG21 | 1.69                     | 0.55              |
| 1:E:110:GLU:OE2  | 1:E:110:GLU:C    | 2.43                     | 0.55              |
| 1:E:28:PHE:HE1   | 1:E:111:ASP:O    | 1.85                     | 0.55              |
| 1:E:232:ILE:HG22 | 1:E:240:ARG:HB2  | 1.88                     | 0.55              |
| 1:A:312:ARG:NH1  | 1:A:318:ALA:O    | 2.40                     | 0.55              |
| 1:F:164:VAL:HG12 | 1:F:339:ALA:H    | 1.72                     | 0.55              |
| 1:A:125:GLN:O    | 1:A:129:SER:OG   | 2.25                     | 0.55              |
| 1:B:66:LEU:HD12  | 1:B:66:LEU:H     | 1.72                     | 0.55              |
| 1:C:108:ASP:OD2  | 1:C:111:ASP:HB3  | 2.06                     | 0.55              |
| 1:C:108:ASP:O    | 1:C:111:ASP:CG   | 2.45                     | 0.55              |
| 1:D:128:GLU:OE2  | 1:D:128:GLU:C    | 2.44                     | 0.55              |
| 1:D:46:THR:CB    | 1:D:135:ASP:OD1  | 2.54                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:272:PHE:HE1  | 1:F:285:LYS:HB2  | 1.71                     | 0.55              |
| 1:D:300:THR:HG21 | 1:D:329:HIS:N    | 2.21                     | 0.55              |
| 1:E:226:ALA:O    | 1:E:228:TYR:N    | 2.40                     | 0.55              |
| 1:E:325:TYR:CG   | 1:E:326:ALA:N    | 2.75                     | 0.55              |
| 1:F:25:LEU:HD13  | 1:F:26:ALA:N     | 2.20                     | 0.55              |
| 1:E:298:VAL:HG12 | 1:E:332:LEU:HA   | 1.87                     | 0.55              |
| 1:F:32:PHE:CE1   | 1:F:123:THR:HG22 | 2.41                     | 0.55              |
| 1:G:102:ALA:HB2  | 1:G:262:ARG:CZ   | 2.37                     | 0.55              |
| 1:B:181:GLY:O    | 1:B:185:ILE:HG13 | 2.06                     | 0.55              |
| 1:B:39:ALA:O     | 1:B:43:THR:OG1   | 2.21                     | 0.55              |
| 1:C:103:ASP:HB3  | 1:C:321:ILE:HD12 | 1.87                     | 0.55              |
| 1:F:124:SER:OG   | 1:F:125:GLN:N    | 2.39                     | 0.55              |
| 1:F:200:VAL:HG22 | 1:F:201:PRO:HD2  | 1.87                     | 0.55              |
| 1:F:29:LEU:HD22  | 1:F:29:LEU:C     | 2.21                     | 0.55              |
| 1:F:36:VAL:HA    | 1:F:39:ALA:HB3   | 1.89                     | 0.55              |
| 1:G:92:LYS:HD3   | 1:G:332:LEU:N    | 2.22                     | 0.55              |
| 1:A:287:ASN:HD21 | 1:A:341:VAL:HG12 | 1.70                     | 0.55              |
| 1:C:206:VAL:HG23 | 1:C:248:VAL:N    | 2.19                     | 0.55              |
| 1:B:63:PHE:HZ    | 1:B:299:GLY:HA3  | 1.72                     | 0.55              |
| 1:B:141:GLU:CD   | 1:B:331:GLY:N    | 2.59                     | 0.55              |
| 1:D:254:THR:HG22 | 1:D:255:ALA:H    | 1.72                     | 0.55              |
| 1:F:291:LEU:HD13 | 1:F:291:LEU:H    | 1.71                     | 0.55              |
| 1:G:268:GLN:O    | 1:G:271:VAL:HG12 | 2.06                     | 0.55              |
| 1:A:119:ARG:NH1  | 1:A:119:ARG:HG3  | 2.22                     | 0.54              |
| 1:A:289:ILE:CG2  | 1:A:290:GLY:N    | 2.70                     | 0.54              |
| 1:A:36:VAL:O     | 1:A:37:LEU:C     | 2.45                     | 0.54              |
| 1:C:108:ASP:O    | 1:C:108:ASP:CG   | 2.45                     | 0.54              |
| 1:C:285:LYS:NZ   | 1:C:286:ASP:OD2  | 2.27                     | 0.54              |
| 1:A:113:MET:O    | 1:A:114:ASN:HB3  | 2.06                     | 0.54              |
| 1:A:285:LYS:HA   | 1:A:287:ASN:O    | 2.08                     | 0.54              |
| 1:A:303:LEU:HG   | 1:A:304:ARG:HG3  | 1.89                     | 0.54              |
| 1:A:90:THR:HG21  | 1:A:333:ARG:HH22 | 1.72                     | 0.54              |
| 1:B:32:PHE:O     | 1:B:35:GLU:HG2   | 2.07                     | 0.54              |
| 1:C:204:ASP:C    | 1:C:205:ARG:HG3  | 2.24                     | 0.54              |
| 1:D:112:ALA:O    | 1:D:115:HIS:NE2  | 2.40                     | 0.54              |
| 1:D:113:MET:HA   | 1:D:115:HIS:CE1  | 2.42                     | 0.54              |
| 1:F:24:LYS:CD    | 1:F:24:LYS:H     | 2.16                     | 0.54              |
| 1:G:171:LYS:HA   | 1:G:174:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:28:PHE:CD2   | 1:A:28:PHE:C     | 2.81                     | 0.54              |
| 1:A:289:ILE:HG22 | 1:A:290:GLY:H    | 1.73                     | 0.54              |
| 1:B:309:GLU:OE1  | 1:B:310:ARG:NE   | 2.35                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:235:GLU:HG2  | 1:C:236:LYS:HG3  | 1.89                     | 0.54              |
| 1:D:138:VAL:CG2  | 1:D:139:LEU:HD11 | 2.33                     | 0.54              |
| 1:A:235:GLU:O    | 1:A:236:LYS:NZ   | 2.32                     | 0.54              |
| 1:B:118:VAL:HG12 | 1:B:119:ARG:N    | 2.21                     | 0.54              |
| 1:B:25:LEU:O     | 1:B:25:LEU:HD22  | 2.08                     | 0.54              |
| 1:B:81:ASP:HA    | 1:B:84:ARG:HB2   | 1.88                     | 0.54              |
| 1:E:216:ALA:O    | 1:E:220:ALA:N    | 2.33                     | 0.54              |
| 1:G:137:ALA:HB2  | 1:G:258:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:207:PHE:CB   | 1:A:291:LEU:O    | 2.55                     | 0.54              |
| 1:A:328:GLY:O    | 1:A:329:HIS:HB3  | 2.08                     | 0.54              |
| 1:B:232:ILE:HA   | 1:B:239:ILE:HA   | 1.89                     | 0.54              |
| 1:C:25:LEU:O     | 1:C:29:LEU:HD12  | 2.07                     | 0.54              |
| 1:D:132:MET:CE   | 1:D:251:PRO:HG2  | 2.35                     | 0.54              |
| 1:E:24:LYS:NZ    | 1:E:112:ALA:HB2  | 2.22                     | 0.54              |
| 1:C:36:VAL:HG13  | 1:C:126:LEU:CD2  | 2.38                     | 0.54              |
| 1:E:307:ALA:H    | 1:E:325:TYR:HB2  | 1.73                     | 0.54              |
| 1:F:298:VAL:HA   | 1:F:332:LEU:HB2  | 1.89                     | 0.54              |
| 1:G:141:GLU:HG2  | 1:G:329:HIS:ND1  | 2.22                     | 0.54              |
| 1:B:28:PHE:CZ    | 1:B:111:ASP:OD1  | 2.60                     | 0.54              |
| 1:B:40:PHE:HE1   | 1:B:130:LEU:HD13 | 1.32                     | 0.54              |
| 1:D:298:VAL:HG12 | 1:D:332:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:HE2  | 1.86                     | 0.54              |
| 1:B:35:GLU:CB    | 1:B:123:THR:CG2  | 2.80                     | 0.54              |
| 1:C:110:GLU:CD   | 1:C:118:VAL:HG23 | 2.29                     | 0.54              |
| 1:C:206:VAL:HG23 | 1:C:247:VAL:HA   | 1.87                     | 0.54              |
| 1:D:196:THR:OG1  | 1:D:197:LYS:N    | 2.40                     | 0.54              |
| 1:C:28:PHE:CD2   | 1:C:28:PHE:O     | 2.61                     | 0.54              |
| 1:E:24:LYS:HZ3   | 1:E:112:ALA:HB2  | 1.71                     | 0.54              |
| 1:E:50:HIS:HE1   | 1:E:300:THR:HG22 | 1.73                     | 0.54              |
| 1:E:306:LEU:HA   | 1:E:325:TYR:CD1  | 2.43                     | 0.54              |
| 1:B:145:LEU:HD23 | 1:B:332:LEU:HD11 | 1.85                     | 0.54              |
| 1:C:113:MET:HE2  | 1:C:119:ARG:NE   | 2.23                     | 0.54              |
| 1:E:104:VAL:HG21 | 1:F:66:LEU:HD21  | 1.90                     | 0.54              |
| 1:E:50:HIS:HD2   | 1:E:51:MET:H     | 1.56                     | 0.54              |
| 1:G:303:LEU:HB2  | 1:G:326:ALA:HB3  | 1.89                     | 0.54              |
| 1:A:186:ALA:O    | 1:A:190:LYS:NZ   | 2.41                     | 0.53              |
| 1:A:208:TYR:CZ   | 1:A:293:MET:CE   | 2.91                     | 0.53              |
| 1:B:167:THR:OG1  | 1:B:168:THR:N    | 2.38                     | 0.53              |
| 1:C:205:ARG:CG   | 1:C:294:HIS:HB3  | 2.37                     | 0.53              |
| 1:C:162:ALA:HB3  | 1:C:338:GLY:HA3  | 1.90                     | 0.53              |
| 1:D:50:HIS:CD2   | 1:D:298:VAL:HG23 | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:VAL:O    | 1:A:320:GLN:NE2  | 2.41                     | 0.53              |
| 1:C:110:GLU:O    | 1:C:118:VAL:HG21 | 2.08                     | 0.53              |
| 1:D:110:GLU:CG   | 1:D:113:MET:O    | 2.57                     | 0.53              |
| 1:E:298:VAL:CA   | 1:E:331:GLY:O    | 2.56                     | 0.53              |
| 1:E:299:GLY:HA3  | 1:E:333:ARG:NH2  | 2.22                     | 0.53              |
| 1:E:81:ASP:OD2   | 1:E:81:ASP:N     | 2.40                     | 0.53              |
| 1:F:300:THR:HG1  | 1:F:301:VAL:H    | 1.52                     | 0.53              |
| 1:G:130:LEU:CD2  | 1:G:131:ALA:CA   | 2.86                     | 0.53              |
| 1:G:44:SER:HB2   | 1:G:131:ALA:HB1  | 1.90                     | 0.53              |
| 1:E:112:ALA:O    | 1:E:113:MET:HB2  | 2.09                     | 0.53              |
| 1:B:209:CYS:O    | 1:B:250:VAL:HG22 | 2.08                     | 0.53              |
| 1:B:24:LYS:CE    | 1:B:25:LEU:CA    | 2.78                     | 0.53              |
| 1:C:31:VAL:HG12  | 1:C:32:PHE:N     | 2.23                     | 0.53              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CZ    | 2.61                     | 0.53              |
| 1:G:92:LYS:HD3   | 1:G:332:LEU:H    | 1.74                     | 0.53              |
| 1:C:32:PHE:CD1   | 1:C:33:GLY:N     | 2.77                     | 0.53              |
| 1:E:115:HIS:HE1  | 1:E:119:ARG:NH2  | 1.90                     | 0.53              |
| 1:D:116:TYR:O    | 1:D:119:ARG:HB3  | 2.09                     | 0.53              |
| 1:A:66:LEU:HD23  | 1:A:89:HIS:CE1   | 2.44                     | 0.53              |
| 1:B:58:GLY:O     | 1:B:59:LYS:HG2   | 2.08                     | 0.53              |
| 1:C:32:PHE:HZ    | 1:C:126:LEU:HD23 | 1.74                     | 0.53              |
| 1:E:192:ARG:C    | 1:E:195:LEU:HG   | 2.29                     | 0.53              |
| 1:F:211:PRO:HD3  | 1:F:250:VAL:O    | 2.08                     | 0.53              |
| 1:F:312:ARG:NH1  | 1:F:319:ASP:OD2  | 2.41                     | 0.53              |
| 1:B:165:ILE:H    | 1:B:340:VAL:HG12 | 1.74                     | 0.53              |
| 1:C:37:LEU:HD13  | 1:C:306:LEU:HD21 | 1.89                     | 0.53              |
| 1:D:242:VAL:HG22 | 1:D:243:MET:H    | 1.72                     | 0.53              |
| 1:A:207:PHE:CE1  | 1:A:290:GLY:C    | 2.83                     | 0.53              |
| 1:B:50:HIS:CD2   | 1:B:51:MET:N     | 2.77                     | 0.53              |
| 1:D:167:THR:O    | 1:D:168:THR:OG1  | 2.27                     | 0.53              |
| 1:F:250:VAL:HG21 | 1:F:253:LEU:CG   | 2.39                     | 0.53              |
| 1:G:106:ILE:HD11 | 1:G:107:TYR:C    | 2.29                     | 0.53              |
| 1:A:73:TYR:CE1   | 1:F:102:ALA:HB2  | 2.44                     | 0.53              |
| 1:E:298:VAL:HG12 | 1:E:332:LEU:HD13 | 1.85                     | 0.53              |
| 1:A:115:HIS:HB2  | 1:A:119:ARG:CG   | 2.39                     | 0.52              |
| 1:D:253:LEU:O    | 1:D:254:THR:OG1  | 2.26                     | 0.52              |
| 1:D:53:ARG:HH12  | 1:D:61:ALA:HB1   | 1.73                     | 0.52              |
| 1:G:260:THR:CG2  | 1:G:269:LYS:NZ   | 2.73                     | 0.52              |
| 1:G:306:LEU:HD13 | 1:G:325:TYR:CE1  | 2.44                     | 0.52              |
| 1:A:110:GLU:OE1  | 1:A:118:VAL:CB   | 2.57                     | 0.52              |
| 1:B:151:LYS:HG2  | 1:B:152:TYR:H    | 1.73                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:84:ARG:O     | 1:F:84:ARG:HD2   | 2.08                     | 0.52              |
| 1:A:305:ASP:C    | 1:A:325:TYR:HE1  | 2.12                     | 0.52              |
| 1:E:65:VAL:CG1   | 1:E:333:ARG:HD3  | 2.37                     | 0.52              |
| 1:G:341:VAL:HG22 | 1:G:342:PHE:H    | 1.75                     | 0.52              |
| 1:C:184:ILE:HD11 | 1:C:289:ILE:HD13 | 1.92                     | 0.52              |
| 1:C:141:GLU:HG3  | 1:C:329:HIS:HE1  | 1.74                     | 0.52              |
| 1:D:166:GLU:HA   | 1:D:341:VAL:HG23 | 1.91                     | 0.52              |
| 1:D:272:PHE:HE1  | 1:D:285:LYS:HB2  | 1.74                     | 0.52              |
| 1:E:24:LYS:C     | 1:E:24:LYS:HD3   | 2.28                     | 0.52              |
| 1:F:204:ASP:N    | 1:F:205:ARG:HH21 | 2.07                     | 0.52              |
| 1:G:146:CYS:SG   | 1:G:336:ALA:HB2  | 2.49                     | 0.52              |
| 1:G:149:GLU:OE1  | 1:G:150:SER:CA   | 2.57                     | 0.52              |
| 1:G:304:ARG:O    | 1:G:304:ARG:NE   | 2.39                     | 0.52              |
| 1:A:273:PRO:HD2  | 1:A:284:ALA:HB2  | 1.92                     | 0.52              |
| 1:B:27:LEU:CD2   | 1:B:27:LEU:O     | 2.56                     | 0.52              |
| 1:C:134:ALA:O    | 1:C:138:VAL:HG13 | 2.09                     | 0.52              |
| 1:D:272:PHE:CE1  | 1:D:285:LYS:HB2  | 2.44                     | 0.52              |
| 1:F:241:ASN:N    | 1:F:241:ASN:OD1  | 2.43                     | 0.52              |
| 1:F:28:PHE:CE1   | 1:F:29:LEU:HB2   | 2.44                     | 0.52              |
| 1:G:100:LEU:O    | 1:G:325:TYR:N    | 2.39                     | 0.52              |
| 1:G:115:HIS:O    | 1:G:119:ARG:HB2  | 2.10                     | 0.52              |
| 1:F:143:ALA:CB   | 1:F:272:PHE:CE2  | 2.92                     | 0.52              |
| 1:G:270:HIS:HE2  | 1:G:329:HIS:CE1  | 2.27                     | 0.52              |
| 1:A:51:MET:HB2   | 1:A:299:GLY:HA3  | 1.92                     | 0.52              |
| 1:B:24:LYS:HZ3   | 1:B:25:LEU:H     | 1.55                     | 0.52              |
| 1:C:34:GLY:O     | 1:C:38:THR:N     | 2.30                     | 0.52              |
| 1:D:142:ILE:CD1  | 1:D:145:LEU:HG   | 2.38                     | 0.52              |
| 1:A:313:ARG:HH11 | 1:A:320:GLN:HG2  | 1.74                     | 0.52              |
| 1:B:113:MET:CB   | 1:B:115:HIS:NE2  | 2.73                     | 0.52              |
| 1:B:53:ARG:HH11  | 1:B:63:PHE:HB3   | 1.73                     | 0.52              |
| 1:C:208:TYR:HB3  | 1:C:291:LEU:CD2  | 2.39                     | 0.52              |
| 1:E:102:ALA:O    | 1:F:70:GLN:NE2   | 2.43                     | 0.52              |
| 1:E:36:VAL:HG22  | 1:E:126:LEU:HD12 | 1.91                     | 0.52              |
| 1:B:163:THR:HG23 | 1:B:164:VAL:HG12 | 1.92                     | 0.52              |
| 1:B:309:GLU:OE1  | 1:B:310:ARG:N    | 2.41                     | 0.52              |
| 1:C:299:GLY:O    | 1:C:300:THR:HB   | 2.10                     | 0.52              |
| 1:C:32:PHE:O     | 1:C:34:GLY:N     | 2.43                     | 0.52              |
| 1:F:31:VAL:HG12  | 1:F:32:PHE:N     | 2.24                     | 0.52              |
| 1:G:46:THR:HG23  | 1:G:135:ASP:OD1  | 2.10                     | 0.52              |
| 1:G:242:VAL:HG22 | 1:G:243:MET:H    | 1.75                     | 0.52              |
| 1:A:128:GLU:OE2  | 1:A:129:SER:OG   | 2.27                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:GLN:OE1   | 1:A:62:GLN:N     | 2.43                     | 0.52              |
| 1:B:92:LYS:NZ    | 1:B:333:ARG:HH21 | 2.08                     | 0.52              |
| 1:C:91:GLU:OE1   | 1:C:91:GLU:N     | 2.42                     | 0.52              |
| 1:C:117:ASP:CG   | 1:D:51:MET:CE    | 2.73                     | 0.52              |
| 1:E:181:GLY:N    | 1:E:183:GLU:OE1  | 2.43                     | 0.52              |
| 1:G:143:ALA:CB   | 1:G:272:PHE:HB3  | 2.39                     | 0.52              |
| 1:A:170:ASN:OD1  | 1:A:171:LYS:NZ   | 2.43                     | 0.51              |
| 1:C:27:LEU:HD22  | 1:C:28:PHE:N     | 2.20                     | 0.51              |
| 1:E:192:ARG:HA   | 1:E:195:LEU:CD2  | 2.40                     | 0.51              |
| 1:F:195:LEU:HD21 | 1:F:205:ARG:NH1  | 2.26                     | 0.51              |
| 1:F:294:HIS:CG   | 1:F:295:ARG:N    | 2.78                     | 0.51              |
| 1:B:68:ARG:N     | 1:B:68:ARG:CD    | 2.73                     | 0.51              |
| 1:C:178:VAL:HG13 | 1:C:220:ALA:HA   | 1.92                     | 0.51              |
| 1:C:192:ARG:O    | 1:C:195:LEU:HB3  | 2.10                     | 0.51              |
| 1:D:46:THR:HG23  | 1:D:135:ASP:CG   | 2.25                     | 0.51              |
| 1:E:40:PHE:C     | 1:E:130:LEU:HD21 | 2.29                     | 0.51              |
| 1:A:302:LYS:CE   | 1:A:327:MET:HE2  | 2.40                     | 0.51              |
| 1:B:139:LEU:HD21 | 1:B:255:ALA:HA   | 1.91                     | 0.51              |
| 1:C:162:ALA:C    | 1:C:164:VAL:N    | 2.63                     | 0.51              |
| 1:C:32:PHE:HD1   | 1:C:33:GLY:N     | 2.08                     | 0.51              |
| 1:D:204:ASP:N    | 1:D:205:ARG:HH21 | 2.08                     | 0.51              |
| 1:D:62:GLN:HB2   | 1:D:93:VAL:HG12  | 1.92                     | 0.51              |
| 1:G:100:LEU:HD13 | 1:G:259:GLY:N    | 2.25                     | 0.51              |
| 1:A:142:ILE:HA   | 1:A:145:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:32:PHE:O     | 1:A:36:VAL:HG22  | 2.10                     | 0.51              |
| 1:D:130:LEU:HD12 | 1:D:131:ALA:HA   | 1.76                     | 0.51              |
| 1:F:254:THR:HA   | 1:F:270:HIS:NE2  | 2.25                     | 0.51              |
| 1:F:25:LEU:HB3   | 1:F:28:PHE:HE2   | 1.70                     | 0.51              |
| 1:A:211:PRO:HA   | 1:A:214:TYR:HB2  | 1.93                     | 0.51              |
| 1:B:135:ASP:O    | 1:B:138:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:59:LYS:O     | 1:B:95:THR:OG1   | 2.27                     | 0.51              |
| 1:G:181:GLY:HA3  | 1:G:220:ALA:HB2  | 1.92                     | 0.51              |
| 1:A:166:GLU:OE1  | 1:A:166:GLU:N    | 2.43                     | 0.51              |
| 1:C:108:ASP:OD2  | 1:C:111:ASP:CG   | 2.48                     | 0.51              |
| 1:C:103:ASP:CG   | 1:C:322:ILE:HA   | 2.31                     | 0.51              |
| 1:D:51:MET:HB2   | 1:D:298:VAL:O    | 2.10                     | 0.51              |
| 1:E:333:ARG:CG   | 1:E:333:ARG:HH11 | 2.19                     | 0.51              |
| 1:G:50:HIS:HD2   | 1:G:298:VAL:HG23 | 1.76                     | 0.51              |
| 1:B:171:LYS:HG3  | 1:B:342:PHE:CZ   | 2.45                     | 0.51              |
| 1:B:64:PRO:HA    | 1:B:91:GLU:HB3   | 1.93                     | 0.51              |
| 1:C:162:ALA:HB3  | 1:C:337:ALA:C    | 2.29                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:285:LYS:NZ   | 1:C:285:LYS:O    | 2.40                     | 0.51              |
| 1:F:295:ARG:HE   | 1:F:296:SER:N    | 2.09                     | 0.51              |
| 1:F:306:LEU:HB2  | 1:F:325:TYR:CZ   | 2.45                     | 0.51              |
| 1:F:64:PRO:N     | 1:F:91:GLU:HG3   | 2.25                     | 0.51              |
| 1:G:106:ILE:HG12 | 1:G:107:TYR:N    | 2.26                     | 0.51              |
| 1:A:135:ASP:OD1  | 1:A:135:ASP:N    | 2.43                     | 0.51              |
| 1:B:121:GLU:CD   | 1:B:121:GLU:C    | 2.70                     | 0.51              |
| 1:B:132:MET:CA   | 1:B:132:MET:HE3  | 2.36                     | 0.51              |
| 1:B:294:HIS:CG   | 1:B:295:ARG:N    | 2.79                     | 0.51              |
| 1:D:83:LYS:HZ2   | 1:D:83:LYS:H     | 1.58                     | 0.51              |
| 1:E:181:GLY:O    | 1:E:185:ILE:HD11 | 1.93                     | 0.51              |
| 1:F:134:ALA:O    | 1:F:137:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:207:PHE:HD1  | 1:A:291:LEU:O    | 1.93                     | 0.51              |
| 1:B:298:VAL:HG12 | 1:B:299:GLY:H    | 1.76                     | 0.51              |
| 1:B:81:ASP:H     | 1:B:83:LYS:CE    | 2.24                     | 0.51              |
| 1:B:132:MET:SD   | 1:C:199:TYR:HE1  | 2.32                     | 0.51              |
| 1:F:251:PRO:HD2  | 1:F:252:HIS:CE1  | 2.46                     | 0.51              |
| 1:F:270:HIS:N    | 1:F:272:PHE:O    | 2.44                     | 0.51              |
| 1:G:200:VAL:HG22 | 1:G:201:PRO:HD2  | 1.92                     | 0.51              |
| 1:A:26:ALA:C     | 1:A:29:LEU:HD12  | 2.24                     | 0.51              |
| 1:B:130:LEU:O    | 1:B:130:LEU:CD1  | 2.41                     | 0.51              |
| 1:B:312:ARG:NH2  | 1:B:317:GLN:OE1  | 2.44                     | 0.51              |
| 1:B:70:GLN:CA    | 1:B:70:GLN:NE2   | 2.72                     | 0.51              |
| 1:F:103:ASP:CG   | 1:F:322:ILE:HA   | 2.31                     | 0.51              |
| 1:A:78:GLU:OE1   | 1:A:79:ASN:N     | 2.44                     | 0.50              |
| 1:B:100:LEU:HB3  | 1:B:326:ALA:HB3  | 1.92                     | 0.50              |
| 1:B:92:LYS:HZ1   | 1:B:333:ARG:NH2  | 2.09                     | 0.50              |
| 1:B:292:PHE:N    | 1:B:338:GLY:O    | 2.31                     | 0.50              |
| 1:C:192:ARG:HH21 | 1:C:243:MET:HG3  | 1.75                     | 0.50              |
| 1:C:207:PHE:CE2  | 1:C:245:PHE:HD2  | 2.28                     | 0.50              |
| 1:C:36:VAL:HG11  | 1:C:126:LEU:CD2  | 2.37                     | 0.50              |
| 1:D:142:ILE:CD1  | 1:D:145:LEU:CG   | 2.89                     | 0.50              |
| 1:D:214:TYR:N    | 1:D:249:GLU:OE1  | 2.45                     | 0.50              |
| 1:D:305:ASP:N    | 1:D:305:ASP:OD2  | 2.44                     | 0.50              |
| 1:F:63:PHE:C     | 1:F:91:GLU:HG3   | 2.31                     | 0.50              |
| 1:G:106:ILE:CD1  | 1:G:107:TYR:CA   | 2.87                     | 0.50              |
| 1:B:332:LEU:HD13 | 1:B:334:PRO:CD   | 2.41                     | 0.50              |
| 1:D:135:ASP:O    | 1:D:138:VAL:HG22 | 2.11                     | 0.50              |
| 1:D:204:ASP:O    | 1:D:295:ARG:HB3  | 2.11                     | 0.50              |
| 1:D:310:ARG:HG2  | 1:D:321:ILE:HA   | 1.93                     | 0.50              |
| 1:F:138:VAL:HG12 | 1:F:329:HIS:HE1  | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:312:ARG:HA   | 1:F:319:ASP:HA   | 1.92                     | 0.50              |
| 1:G:239:ILE:HB   | 1:G:247:VAL:HB   | 1.93                     | 0.50              |
| 1:B:112:ALA:C    | 1:B:113:MET:SD   | 2.89                     | 0.50              |
| 1:B:28:PHE:HZ    | 1:B:111:ASP:C    | 2.09                     | 0.50              |
| 1:E:119:ARG:O    | 1:E:123:THR:HG23 | 2.11                     | 0.50              |
| 1:F:135:ASP:HB3  | 1:F:252:HIS:CE1  | 2.46                     | 0.50              |
| 1:G:110:GLU:CG   | 1:G:118:VAL:CG2  | 2.84                     | 0.50              |
| 1:A:114:ASN:O    | 1:A:114:ASN:OD1  | 2.30                     | 0.50              |
| 1:A:302:LYS:HE2  | 1:A:327:MET:HE3  | 1.90                     | 0.50              |
| 1:A:226:ALA:HB3  | 1:C:232:ILE:HB   | 1.92                     | 0.50              |
| 1:E:110:GLU:OE2  | 1:E:110:GLU:O    | 2.30                     | 0.50              |
| 1:G:110:GLU:CG   | 1:G:118:VAL:HG11 | 2.42                     | 0.50              |
| 1:G:115:HIS:O    | 1:G:116:TYR:O    | 2.30                     | 0.50              |
| 1:G:205:ARG:HE   | 1:G:294:HIS:HB2  | 1.76                     | 0.50              |
| 1:A:115:HIS:O    | 1:A:119:ARG:HG3  | 2.11                     | 0.50              |
| 1:A:233:ASP:HA   | 1:A:236:LYS:HZ1  | 1.76                     | 0.50              |
| 1:A:232:ILE:HB   | 1:A:240:ARG:HB2  | 1.93                     | 0.50              |
| 1:B:132:MET:O    | 1:B:135:ASP:OD2  | 2.30                     | 0.50              |
| 1:C:108:ASP:O    | 1:C:108:ASP:OD1  | 2.30                     | 0.50              |
| 1:C:121:GLU:O    | 1:C:124:SER:OG   | 2.25                     | 0.50              |
| 1:C:63:PHE:HE1   | 1:C:94:ILE:HD11  | 1.76                     | 0.50              |
| 1:D:253:LEU:O    | 1:D:285:LYS:NZ   | 2.44                     | 0.50              |
| 1:A:183:GLU:OE1  | 1:A:184:ILE:N    | 2.34                     | 0.50              |
| 1:C:108:ASP:OD2  | 1:C:111:ASP:OD1  | 2.30                     | 0.50              |
| 1:C:147:ASN:HB3  | 1:C:281:VAL:HG11 | 1.93                     | 0.50              |
| 1:C:57:SER:O     | 1:C:59:LYS:NZ    | 2.43                     | 0.50              |
| 1:D:123:THR:OG1  | 1:D:124:SER:N    | 2.45                     | 0.50              |
| 1:D:240:ARG:NE   | 1:D:241:ASN:H    | 2.10                     | 0.50              |
| 1:D:24:LYS:O     | 1:D:27:LEU:HG    | 2.11                     | 0.50              |
| 1:F:174:LEU:HD13 | 1:F:180:LEU:HD11 | 1.94                     | 0.50              |
| 1:F:41:ALA:O     | 1:F:44:SER:OG    | 2.26                     | 0.50              |
| 1:G:265:THR:C    | 1:G:266:THR:OG1  | 2.49                     | 0.50              |
| 1:C:143:ALA:HB3  | 1:C:271:VAL:HG13 | 1.94                     | 0.50              |
| 1:D:176:ASP:OD2  | 1:D:178:VAL:N    | 2.34                     | 0.50              |
| 1:F:143:ALA:HB3  | 1:F:272:PHE:CD2  | 2.47                     | 0.50              |
| 1:G:109:ILE:O    | 1:G:112:ALA:O    | 2.30                     | 0.50              |
| 1:G:291:LEU:HD12 | 1:G:291:LEU:H    | 1.77                     | 0.50              |
| 1:B:170:ASN:O    | 1:B:171:LYS:NZ   | 2.36                     | 0.50              |
| 1:E:110:GLU:HG3  | 1:E:118:VAL:CG2  | 2.37                     | 0.50              |
| 1:B:108:ASP:O    | 1:B:111:ASP:OD2  | 2.30                     | 0.50              |
| 1:B:300:THR:HB   | 1:B:329:HIS:HA   | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:66:LEU:HD21  | 1:B:200:VAL:HB   | 1.93                     | 0.50              |
| 1:F:129:SER:HA   | 1:F:132:MET:HB2  | 1.93                     | 0.50              |
| 1:F:253:LEU:O    | 1:F:270:HIS:NE2  | 2.42                     | 0.50              |
| 1:G:106:ILE:CD1  | 1:G:107:TYR:C    | 2.80                     | 0.50              |
| 1:G:141:GLU:O    | 1:G:141:GLU:OE1  | 2.30                     | 0.50              |
| 1:G:295:ARG:CZ   | 1:G:296:SER:HB2  | 2.41                     | 0.50              |
| 1:A:64:PRO:HG2   | 1:F:121:GLU:HG2  | 1.94                     | 0.49              |
| 1:F:50:HIS:CD2   | 1:F:51:MET:H     | 2.30                     | 0.49              |
| 1:G:104:VAL:HG21 | 1:G:122:TYR:HE1  | 1.77                     | 0.49              |
| 1:A:171:LYS:HE3  | 1:A:342:PHE:HD2  | 1.76                     | 0.49              |
| 1:B:332:LEU:HD11 | 1:B:334:PRO:HG2  | 1.94                     | 0.49              |
| 1:C:166:GLU:HA   | 1:C:341:VAL:O    | 2.12                     | 0.49              |
| 1:C:35:GLU:O     | 1:C:38:THR:OG1   | 2.30                     | 0.49              |
| 1:C:82:ASP:HA    | 1:C:85:LYS:HB3   | 1.93                     | 0.49              |
| 1:E:212:ASP:C    | 1:E:214:TYR:H    | 2.16                     | 0.49              |
| 1:F:251:PRO:HB2  | 1:F:252:HIS:CD2  | 2.47                     | 0.49              |
| 1:G:110:GLU:O    | 1:G:113:MET:O    | 2.30                     | 0.49              |
| 1:A:55:ILE:HG21  | 1:A:301:VAL:HG23 | 1.77                     | 0.49              |
| 1:B:111:ASP:C    | 1:B:111:ASP:OD1  | 2.50                     | 0.49              |
| 1:B:255:ALA:HB3  | 1:B:272:PHE:CZ   | 2.47                     | 0.49              |
| 1:B:285:LYS:O    | 1:B:287:ASN:N    | 2.45                     | 0.49              |
| 1:B:46:THR:C     | 1:B:48:SER:H     | 2.14                     | 0.49              |
| 1:F:221:LEU:HG   | 1:F:222:MET:HG3  | 1.94                     | 0.49              |
| 1:G:113:MET:CG   | 1:G:114:ASN:N    | 2.74                     | 0.49              |
| 1:G:114:ASN:O    | 1:G:116:TYR:HB2  | 2.11                     | 0.49              |
| 1:A:207:PHE:CE1  | 1:A:209:CYS:HA   | 2.47                     | 0.49              |
| 1:A:236:LYS:HE2  | 1:A:238:SER:HB2  | 1.94                     | 0.49              |
| 1:B:252:HIS:N    | 1:C:199:TYR:OH   | 2.45                     | 0.49              |
| 1:C:292:PHE:O    | 1:C:337:ALA:HB1  | 2.11                     | 0.49              |
| 1:D:128:GLU:OE2  | 1:D:128:GLU:O    | 2.30                     | 0.49              |
| 1:D:303:LEU:H    | 1:D:326:ALA:HB3  | 1.76                     | 0.49              |
| 1:D:45:VAL:N     | 1:D:135:ASP:OD2  | 2.45                     | 0.49              |
| 1:G:116:TYR:O    | 1:G:120:SER:OG   | 2.30                     | 0.49              |
| 1:A:105:LEU:O    | 1:A:107:TYR:HE2  | 1.95                     | 0.49              |
| 1:B:119:ARG:O    | 1:B:123:THR:OG1  | 2.30                     | 0.49              |
| 1:B:131:ALA:O    | 1:B:135:ASP:OD2  | 2.30                     | 0.49              |
| 1:D:340:VAL:HG22 | 1:D:341:VAL:H    | 1.77                     | 0.49              |
| 1:D:83:LYS:CE    | 1:D:83:LYS:H     | 2.25                     | 0.49              |
| 1:F:301:VAL:HG12 | 1:F:302:LYS:H    | 1.76                     | 0.49              |
| 1:G:137:ALA:HB2  | 1:G:258:ALA:CB   | 2.42                     | 0.49              |
| 1:G:25:LEU:CB    | 1:G:28:PHE:CE2   | 2.94                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:108:ASP:HB3 | 1:A:111:ASP:N    | 2.27                     | 0.49              |
| 1:E:294:HIS:CG  | 1:E:295:ARG:N    | 2.80                     | 0.49              |
| 1:F:205:ARG:HE  | 1:F:205:ARG:N    | 2.09                     | 0.49              |
| 1:G:45:VAL:HG22 | 1:G:135:ASP:CG   | 2.32                     | 0.49              |
| 1:B:114:ASN:HB3 | 1:B:118:VAL:HB   | 1.93                     | 0.49              |
| 1:C:116:TYR:O   | 1:C:118:VAL:CG1  | 2.56                     | 0.49              |
| 1:E:192:ARG:O   | 1:E:195:LEU:CG   | 2.60                     | 0.49              |
| 1:B:131:ALA:O   | 1:B:135:ASP:OD1  | 2.30                     | 0.49              |
| 1:C:195:LEU:HB2 | 1:C:205:ARG:HH12 | 1.77                     | 0.49              |
| 1:D:228:TYR:HA  | 1:D:231:LEU:HB3  | 1.94                     | 0.49              |
| 1:F:27:LEU:CD1  | 1:F:27:LEU:O     | 2.32                     | 0.49              |
| 1:F:62:GLN:HB2  | 1:F:91:GLU:HB3   | 1.93                     | 0.49              |
| 1:F:83:LYS:O    | 1:F:83:LYS:NZ    | 2.34                     | 0.49              |
| 1:G:143:ALA:HB1 | 1:G:272:PHE:HB3  | 1.94                     | 0.49              |
| 1:A:62:GLN:HA   | 1:A:93:VAL:HA    | 1.94                     | 0.49              |
| 1:B:308:LEU:HA  | 1:B:323:ALA:HA   | 1.94                     | 0.49              |
| 1:C:110:GLU:O   | 1:C:110:GLU:OE2  | 2.30                     | 0.49              |
| 1:D:327:MET:SD  | 1:D:328:GLY:N    | 2.86                     | 0.49              |
| 1:E:32:PHE:C    | 1:E:32:PHE:HD1   | 2.16                     | 0.49              |
| 1:G:108:ASP:OD2 | 1:G:109:ILE:N    | 2.45                     | 0.49              |
| 1:A:306:LEU:C   | 1:A:306:LEU:HD12 | 2.34                     | 0.49              |
| 1:C:165:ILE:CG2 | 1:C:340:VAL:HB   | 2.43                     | 0.49              |
| 1:C:192:ARG:NH2 | 1:C:243:MET:HG3  | 2.28                     | 0.49              |
| 1:C:294:HIS:HE1 | 1:C:335:GLU:HB2  | 1.74                     | 0.49              |
| 1:D:204:ASP:H   | 1:D:205:ARG:HH21 | 1.60                     | 0.49              |
| 1:D:94:ILE:HD13 | 1:D:94:ILE:H     | 1.78                     | 0.49              |
| 1:E:240:ARG:HG3 | 1:E:241:ASN:ND2  | 2.28                     | 0.49              |
| 1:E:285:LYS:O   | 1:E:287:ASN:N    | 2.46                     | 0.49              |
| 1:E:101:THR:OG1 | 1:E:323:ALA:O    | 2.28                     | 0.49              |
| 1:F:278:GLU:OE2 | 1:F:287:ASN:ND2  | 2.46                     | 0.49              |
| 1:C:108:ASP:OD1 | 1:C:111:ASP:OD1  | 2.30                     | 0.48              |
| 1:D:272:PHE:O   | 1:D:274:ALA:N    | 2.46                     | 0.48              |
| 1:F:189:THR:OG1 | 1:F:190:LYS:N    | 2.45                     | 0.48              |
| 1:F:209:CYS:O   | 1:F:250:VAL:HG22 | 2.13                     | 0.48              |
| 1:G:132:MET:O   | 1:G:132:MET:SD   | 2.66                     | 0.48              |
| 1:G:204:ASP:O   | 1:G:205:ARG:NH1  | 2.36                     | 0.48              |
| 1:A:234:PRO:HD2 | 1:A:236:LYS:HE3  | 1.95                     | 0.48              |
| 1:A:33:GLY:HA2  | 1:A:36:VAL:HG23  | 1.95                     | 0.48              |
| 1:B:140:ALA:HB2 | 1:B:256:GLY:HA3  | 1.95                     | 0.48              |
| 1:C:108:ASP:O   | 1:C:111:ASP:OD2  | 2.30                     | 0.48              |
| 1:E:106:ILE:CD1 | 1:E:108:ASP:HA   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:145:LEU:HD21 | 1:E:334:PRO:HA   | 1.95                     | 0.48              |
| 1:G:53:ARG:O     | 1:G:301:VAL:HA   | 2.13                     | 0.48              |
| 1:B:104:VAL:HG23 | 1:B:321:ILE:HD11 | 1.94                     | 0.48              |
| 1:C:298:VAL:HB   | 1:C:330:GLY:HA3  | 1.94                     | 0.48              |
| 1:C:32:PHE:CD1   | 1:C:36:VAL:CG2   | 2.97                     | 0.48              |
| 1:D:241:ASN:ND2  | 1:D:242:VAL:O    | 2.46                     | 0.48              |
| 1:E:276:LYS:HD2  | 1:E:279:GLY:HA3  | 1.95                     | 0.48              |
| 1:E:160:GLY:N    | 1:E:336:ALA:O    | 2.46                     | 0.48              |
| 1:E:65:VAL:HG12  | 1:E:333:ARG:CD   | 2.40                     | 0.48              |
| 1:C:108:ASP:OD2  | 1:C:111:ASP:HB2  | 2.12                     | 0.48              |
| 1:E:183:GLU:OE1  | 1:E:183:GLU:N    | 2.47                     | 0.48              |
| 1:B:284:ALA:O    | 1:B:288:VAL:HB   | 2.12                     | 0.48              |
| 1:B:29:LEU:HD21  | 1:B:310:ARG:CG   | 2.35                     | 0.48              |
| 1:C:299:GLY:O    | 1:C:330:GLY:CA   | 2.59                     | 0.48              |
| 1:C:334:PRO:C    | 1:C:336:ALA:H    | 2.16                     | 0.48              |
| 1:F:207:PHE:HE2  | 1:F:209:CYS:HB3  | 1.77                     | 0.48              |
| 1:F:28:PHE:CD1   | 1:F:29:LEU:CA    | 2.96                     | 0.48              |
| 1:F:55:ILE:HD13  | 1:F:301:VAL:HG11 | 1.95                     | 0.48              |
| 1:G:115:HIS:CG   | 1:G:119:ARG:HH22 | 2.25                     | 0.48              |
| 1:A:29:LEU:HD21  | 1:A:310:ARG:CD   | 2.43                     | 0.48              |
| 1:C:282:LYS:HE2  | 1:C:282:LYS:H    | 1.78                     | 0.48              |
| 1:D:319:ASP:OD1  | 1:D:319:ASP:N    | 2.47                     | 0.48              |
| 1:F:145:LEU:HD21 | 1:F:334:PRO:CB   | 2.42                     | 0.48              |
| 1:G:110:GLU:CG   | 1:G:114:ASN:ND2  | 2.76                     | 0.48              |
| 1:G:201:PRO:HG2  | 1:G:205:ARG:HH22 | 1.78                     | 0.48              |
| 1:G:265:THR:O    | 1:G:266:THR:OG1  | 2.30                     | 0.48              |
| 1:G:146:CYS:CB   | 1:G:336:ALA:HB2  | 2.25                     | 0.48              |
| 1:G:37:LEU:HD12  | 1:G:40:PHE:HD2   | 1.78                     | 0.48              |
| 1:A:29:LEU:CD2   | 1:A:310:ARG:CD   | 2.88                     | 0.48              |
| 1:A:308:LEU:C    | 1:A:308:LEU:HD12 | 2.33                     | 0.48              |
| 1:B:121:GLU:OE1  | 1:B:121:GLU:CA   | 2.61                     | 0.48              |
| 1:C:240:ARG:HH21 | 1:C:240:ARG:HG3  | 1.79                     | 0.48              |
| 1:C:32:PHE:CE1   | 1:C:36:VAL:HG21  | 2.49                     | 0.48              |
| 1:C:36:VAL:HG13  | 1:C:126:LEU:CG   | 2.43                     | 0.48              |
| 1:D:122:TYR:CE1  | 1:E:64:PRO:HG3   | 2.49                     | 0.48              |
| 1:D:65:VAL:HG11  | 1:D:90:THR:HG23  | 1.95                     | 0.48              |
| 1:F:89:HIS:O     | 1:F:89:HIS:CG    | 2.67                     | 0.48              |
| 1:G:25:LEU:C     | 1:G:29:LEU:HG    | 2.27                     | 0.48              |
| 1:A:110:GLU:OE2  | 1:A:110:GLU:O    | 2.30                     | 0.48              |
| 1:A:113:MET:HG2  | 1:A:114:ASN:H    | 1.78                     | 0.48              |
| 1:A:110:GLU:HB2  | 1:A:114:ASN:HD22 | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:211:PRO:HA   | 1:B:249:GLU:HB3  | 1.95                     | 0.48              |
| 1:D:106:ILE:HG13 | 1:D:122:TYR:CZ   | 2.49                     | 0.48              |
| 1:D:53:ARG:HD3   | 1:D:63:PHE:CZ    | 2.49                     | 0.48              |
| 1:E:28:PHE:CE1   | 1:E:111:ASP:C    | 2.87                     | 0.48              |
| 1:E:68:ARG:HG2   | 1:E:69:THR:H     | 1.78                     | 0.48              |
| 1:F:204:ASP:C    | 1:F:205:ARG:HE   | 2.17                     | 0.48              |
| 1:G:215:SER:HA   | 1:G:218:LEU:HD23 | 1.96                     | 0.48              |
| 1:C:207:PHE:CE2  | 1:C:247:VAL:CG2  | 2.95                     | 0.48              |
| 1:C:287:ASN:O    | 1:C:288:VAL:HB   | 2.14                     | 0.48              |
| 1:E:191:ALA:C    | 1:E:195:LEU:HD21 | 2.34                     | 0.48              |
| 1:E:234:PRO:C    | 1:E:236:LYS:H    | 2.17                     | 0.48              |
| 1:E:289:ILE:O    | 1:E:339:ALA:HB1  | 2.14                     | 0.48              |
| 1:E:289:ILE:HG22 | 1:E:290:GLY:H    | 1.79                     | 0.48              |
| 1:E:117:ASP:OD1  | 1:F:52:VAL:O     | 2.31                     | 0.48              |
| 1:G:122:TYR:O    | 1:G:125:GLN:HB3  | 2.13                     | 0.48              |
| 1:G:260:THR:CG2  | 1:G:269:LYS:HZ1  | 2.27                     | 0.48              |
| 1:C:269:LYS:HD2  | 1:C:289:ILE:N    | 2.29                     | 0.48              |
| 1:D:287:ASN:HB3  | 1:D:341:VAL:HG12 | 1.96                     | 0.48              |
| 1:G:151:LYS:NZ   | 1:G:160:GLY:O    | 2.35                     | 0.48              |
| 1:G:49:ARG:O     | 1:G:50:HIS:ND1   | 2.47                     | 0.48              |
| 1:B:67:GLY:HA3   | 1:B:68:ARG:CZ    | 2.44                     | 0.47              |
| 1:C:329:HIS:CG   | 1:C:330:GLY:N    | 2.83                     | 0.47              |
| 1:D:40:PHE:CD1   | 1:D:131:ALA:HB2  | 2.49                     | 0.47              |
| 1:E:32:PHE:C     | 1:E:32:PHE:CD1   | 2.87                     | 0.47              |
| 1:E:80:LEU:HD22  | 1:E:82:ASP:H     | 1.79                     | 0.47              |
| 1:A:73:TYR:HB2   | 1:F:100:LEU:HD22 | 1.95                     | 0.47              |
| 1:D:106:ILE:HG13 | 1:D:122:TYR:CE2  | 2.49                     | 0.47              |
| 1:D:128:GLU:CD   | 1:D:129:SER:CA   | 2.81                     | 0.47              |
| 1:C:100:LEU:HA   | 1:D:73:TYR:HB3   | 1.95                     | 0.47              |
| 1:D:84:ARG:HB3   | 1:D:84:ARG:NH1   | 2.29                     | 0.47              |
| 1:E:284:ALA:N    | 1:E:288:VAL:HG21 | 2.29                     | 0.47              |
| 1:E:60:SER:HA    | 1:E:95:THR:CA    | 2.40                     | 0.47              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CD1   | 2.67                     | 0.47              |
| 1:G:38:THR:OG1   | 1:G:39:ALA:N     | 2.47                     | 0.47              |
| 1:E:222:MET:N    | 1:E:222:MET:SD   | 2.87                     | 0.47              |
| 1:E:46:THR:C     | 1:E:48:SER:H     | 2.17                     | 0.47              |
| 1:F:27:LEU:HD12  | 1:F:28:PHE:N     | 2.28                     | 0.47              |
| 1:F:290:GLY:HA3  | 1:F:340:VAL:H    | 1.79                     | 0.47              |
| 1:A:162:ALA:O    | 1:A:163:THR:OG1  | 2.32                     | 0.47              |
| 1:E:189:THR:HG23 | 1:E:243:MET:HG3  | 1.97                     | 0.47              |
| 1:E:96:ILE:HD13  | 1:E:327:MET:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:291:LEU:HA   | 1:F:338:GLY:O    | 2.14                     | 0.47              |
| 1:B:66:LEU:N     | 1:B:66:LEU:CD1   | 2.73                     | 0.47              |
| 1:B:67:GLY:C     | 1:B:68:ARG:HD2   | 2.35                     | 0.47              |
| 1:C:165:ILE:HA   | 1:C:165:ILE:HD12 | 1.60                     | 0.47              |
| 1:B:251:PRO:HG2  | 1:C:199:TYR:HE1  | 1.61                     | 0.47              |
| 1:D:55:ILE:HG23  | 1:D:303:LEU:HD23 | 1.96                     | 0.47              |
| 1:D:288:VAL:HG21 | 1:D:340:VAL:O    | 2.15                     | 0.47              |
| 1:A:309:GLU:O    | 1:A:322:ILE:CB   | 2.59                     | 0.47              |
| 1:A:310:ARG:HA   | 1:A:321:ILE:HA   | 1.97                     | 0.47              |
| 1:A:65:VAL:HB    | 1:A:90:THR:HB    | 1.95                     | 0.47              |
| 1:C:251:PRO:O    | 1:C:252:HIS:ND1  | 2.48                     | 0.47              |
| 1:C:32:PHE:O     | 1:C:33:GLY:C     | 2.51                     | 0.47              |
| 1:D:103:ASP:CG   | 1:D:323:ALA:H    | 2.18                     | 0.47              |
| 1:E:101:THR:N    | 1:F:72:ALA:HB1   | 2.29                     | 0.47              |
| 1:E:288:VAL:HA   | 1:E:341:VAL:HG12 | 1.96                     | 0.47              |
| 1:E:53:ARG:HD3   | 1:E:63:PHE:CE1   | 2.50                     | 0.47              |
| 1:B:24:LYS:HE2   | 1:B:25:LEU:CB    | 2.44                     | 0.47              |
| 1:C:25:LEU:C     | 1:C:29:LEU:HD11  | 2.35                     | 0.47              |
| 1:C:26:ALA:CA    | 1:C:29:LEU:HD11  | 2.25                     | 0.47              |
| 1:C:27:LEU:HA    | 1:C:30:LYS:HD2   | 1.96                     | 0.47              |
| 1:F:129:SER:O    | 1:F:132:MET:N    | 2.48                     | 0.47              |
| 1:B:251:PRO:CB   | 1:C:199:TYR:CE2  | 2.66                     | 0.47              |
| 1:B:207:PHE:HE1  | 1:B:290:GLY:HA2  | 1.79                     | 0.47              |
| 1:E:204:ASP:OD2  | 1:E:204:ASP:N    | 2.48                     | 0.47              |
| 1:G:188:LEU:HD23 | 1:G:245:PHE:CD1  | 2.50                     | 0.47              |
| 1:A:23:ASP:O     | 1:A:26:ALA:HB3   | 2.14                     | 0.47              |
| 1:B:117:ASP:OD1  | 1:C:53:ARG:CA    | 2.56                     | 0.47              |
| 1:B:176:ASP:OD1  | 1:B:178:VAL:N    | 2.47                     | 0.47              |
| 1:B:70:GLN:HA    | 1:B:70:GLN:HE21  | 1.78                     | 0.47              |
| 1:C:141:GLU:HG3  | 1:C:329:HIS:CE1  | 2.49                     | 0.47              |
| 1:E:110:GLU:HG3  | 1:E:118:VAL:HG21 | 1.83                     | 0.47              |
| 1:E:325:TYR:HA   | 1:E:327:MET:CE   | 2.45                     | 0.47              |
| 1:F:128:GLU:OE2  | 1:F:129:SER:N    | 2.47                     | 0.47              |
| 1:F:136:GLY:HA2  | 1:F:139:LEU:HB2  | 1.97                     | 0.47              |
| 1:G:113:MET:HE1  | 1:G:115:HIS:HB3  | 1.93                     | 0.47              |
| 1:A:174:LEU:HD13 | 1:A:183:GLU:HG2  | 1.97                     | 0.47              |
| 1:A:289:ILE:CG2  | 1:A:290:GLY:H    | 2.28                     | 0.47              |
| 1:B:297:ALA:O    | 1:B:332:LEU:HD13 | 2.15                     | 0.47              |
| 1:D:165:ILE:HA   | 1:D:165:ILE:HD12 | 1.77                     | 0.47              |
| 1:A:205:ARG:CZ   | 1:A:293:MET:HG2  | 2.45                     | 0.47              |
| 1:B:332:LEU:HD13 | 1:B:333:ARG:H    | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:218:LEU:HA   | 1:D:221:LEU:HB3  | 1.97                     | 0.47              |
| 1:E:117:ASP:CG   | 1:F:53:ARG:HA    | 2.23                     | 0.47              |
| 1:E:207:PHE:CZ   | 1:E:209:CYS:HB2  | 2.49                     | 0.47              |
| 1:G:205:ARG:HD2  | 1:G:294:HIS:HA   | 1.97                     | 0.47              |
| 1:A:207:PHE:CD1  | 1:A:291:LEU:O    | 2.68                     | 0.46              |
| 1:A:33:GLY:CA    | 1:A:36:VAL:HG23  | 2.45                     | 0.46              |
| 1:B:37:LEU:O     | 1:B:40:PHE:HB3   | 2.16                     | 0.46              |
| 1:B:59:LYS:O     | 1:B:96:ILE:HG12  | 2.15                     | 0.46              |
| 1:C:34:GLY:O     | 1:C:38:THR:OG1   | 2.30                     | 0.46              |
| 1:D:25:LEU:O     | 1:D:28:PHE:HD2   | 1.98                     | 0.46              |
| 1:D:288:VAL:HG23 | 1:D:290:GLY:H    | 1.80                     | 0.46              |
| 1:E:35:GLU:HG2   | 1:E:35:GLU:H     | 1.39                     | 0.46              |
| 1:F:65:VAL:HG23  | 1:F:333:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:136:GLY:HA3  | 1:A:255:ALA:HB3  | 1.97                     | 0.46              |
| 1:B:212:ASP:C    | 1:B:214:TYR:H    | 2.19                     | 0.46              |
| 1:C:177:GLN:HE21 | 1:C:215:SER:HG   | 1.57                     | 0.46              |
| 1:D:314:ALA:HA   | 1:D:318:ALA:H    | 1.80                     | 0.46              |
| 1:F:160:GLY:HA2  | 1:F:198:ASN:HD21 | 1.80                     | 0.46              |
| 1:G:28:PHE:CD1   | 1:G:29:LEU:N     | 2.83                     | 0.46              |
| 1:A:115:HIS:HD2  | 1:A:115:HIS:N    | 1.93                     | 0.46              |
| 1:A:142:ILE:O    | 1:A:145:LEU:HB2  | 2.15                     | 0.46              |
| 1:C:27:LEU:HD23  | 1:C:28:PHE:HA    | 1.97                     | 0.46              |
| 1:D:214:TYR:OH   | 1:D:239:ILE:HG12 | 2.15                     | 0.46              |
| 1:D:27:LEU:CD1   | 1:D:28:PHE:N     | 2.74                     | 0.46              |
| 1:D:208:TYR:HD1  | 1:D:293:MET:HE2  | 1.80                     | 0.46              |
| 1:D:294:HIS:CE1  | 1:D:295:ARG:O    | 2.68                     | 0.46              |
| 1:E:240:ARG:HA   | 1:E:240:ARG:HH11 | 1.80                     | 0.46              |
| 1:G:104:VAL:HG21 | 1:G:122:TYR:CE1  | 2.50                     | 0.46              |
| 1:G:211:PRO:O    | 1:G:214:TYR:HB2  | 2.15                     | 0.46              |
| 1:G:248:VAL:HG12 | 1:G:249:GLU:H    | 1.81                     | 0.46              |
| 1:G:272:PHE:O    | 1:G:274:ALA:N    | 2.44                     | 0.46              |
| 1:G:294:HIS:CE1  | 1:G:297:ALA:HB2  | 2.50                     | 0.46              |
| 1:G:66:LEU:HB2   | 1:G:67:GLY:H     | 1.52                     | 0.46              |
| 1:A:136:GLY:HA2  | 1:A:139:LEU:HB3  | 1.97                     | 0.46              |
| 1:B:50:HIS:CE1   | 1:B:298:VAL:HB   | 2.51                     | 0.46              |
| 1:B:62:GLN:OE1   | 1:B:62:GLN:N     | 2.48                     | 0.46              |
| 1:C:111:ASP:OD2  | 1:C:112:ALA:N    | 2.48                     | 0.46              |
| 1:D:314:ALA:H    | 1:D:318:ALA:H    | 1.62                     | 0.46              |
| 1:G:109:ILE:CD1  | 1:G:109:ILE:N    | 2.30                     | 0.46              |
| 1:G:110:GLU:HG2  | 1:G:118:VAL:HG11 | 1.95                     | 0.46              |
| 1:A:209:CYS:SG   | 1:A:290:GLY:HA3  | 2.56                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:GLY:O    | 1:C:139:LEU:HB3  | 2.15                     | 0.46              |
| 1:E:232:ILE:HG12 | 1:E:233:ASP:N    | 2.31                     | 0.46              |
| 1:G:108:ASP:OD2  | 1:G:109:ILE:HA   | 2.15                     | 0.46              |
| 1:G:141:GLU:CA   | 1:G:270:HIS:CE1  | 2.96                     | 0.46              |
| 1:B:114:ASN:O    | 1:B:118:VAL:CB   | 2.61                     | 0.46              |
| 1:B:165:ILE:HG21 | 1:B:190:LYS:HD3  | 1.98                     | 0.46              |
| 1:B:301:VAL:HG22 | 1:B:302:LYS:H    | 1.79                     | 0.46              |
| 1:B:81:ASP:H     | 1:B:83:LYS:HE2   | 1.78                     | 0.46              |
| 1:C:278:GLU:OE1  | 1:C:287:ASN:ND2  | 2.41                     | 0.46              |
| 1:F:121:GLU:O    | 1:F:124:SER:OG   | 2.26                     | 0.46              |
| 1:G:106:ILE:HG12 | 1:G:107:TYR:H    | 1.81                     | 0.46              |
| 1:B:132:MET:C    | 1:B:135:ASP:OD2  | 2.53                     | 0.46              |
| 1:D:46:THR:H     | 1:D:135:ASP:CG   | 2.19                     | 0.46              |
| 1:E:28:PHE:CE2   | 1:E:111:ASP:OD2  | 2.40                     | 0.46              |
| 1:F:210:ASP:HA   | 1:F:250:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:207:PHE:CE2  | 1:A:247:VAL:CG2  | 2.88                     | 0.46              |
| 1:E:192:ARG:O    | 1:E:195:LEU:HG   | 2.15                     | 0.46              |
| 1:E:232:ILE:O    | 1:E:233:ASP:HB2  | 2.16                     | 0.46              |
| 1:G:96:ILE:HG13  | 1:G:96:ILE:H     | 1.47                     | 0.46              |
| 1:B:141:GLU:CD   | 1:B:330:GLY:C    | 2.72                     | 0.46              |
| 1:B:291:LEU:H    | 1:B:339:ALA:HA   | 1.81                     | 0.46              |
| 1:D:109:ILE:HG13 | 1:D:110:GLU:H    | 1.80                     | 0.46              |
| 1:E:298:VAL:HA   | 1:E:331:GLY:O    | 2.15                     | 0.46              |
| 1:C:109:ILE:HD13 | 1:C:110:GLU:CA   | 2.46                     | 0.46              |
| 1:D:209:CYS:O    | 1:D:249:GLU:HA   | 2.15                     | 0.46              |
| 1:D:36:VAL:C     | 1:D:38:THR:N     | 2.67                     | 0.46              |
| 1:A:36:VAL:HG13  | 1:A:126:LEU:HD11 | 1.98                     | 0.45              |
| 1:B:141:GLU:OE1  | 1:B:329:HIS:C    | 2.54                     | 0.45              |
| 1:B:294:HIS:NE2  | 1:B:295:ARG:O    | 2.49                     | 0.45              |
| 1:C:40:PHE:CE1   | 1:C:131:ALA:HB2  | 2.51                     | 0.45              |
| 1:E:176:ASP:OD2  | 1:E:179:ALA:N    | 2.47                     | 0.45              |
| 1:F:209:CYS:O    | 1:F:250:VAL:N    | 2.28                     | 0.45              |
| 1:F:91:GLU:N     | 1:F:91:GLU:OE1   | 2.49                     | 0.45              |
| 1:G:235:GLU:HG2  | 1:G:237:GLY:H    | 1.81                     | 0.45              |
| 1:A:302:LYS:CE   | 1:A:327:MET:HE3  | 2.45                     | 0.45              |
| 1:C:105:LEU:HD21 | 1:D:84:ARG:CZ    | 2.47                     | 0.45              |
| 1:D:137:ALA:O    | 1:D:141:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:308:LEU:HB3  | 1:E:323:ALA:HA   | 1.97                     | 0.45              |
| 1:E:31:VAL:O     | 1:E:35:GLU:CD    | 2.55                     | 0.45              |
| 1:F:83:LYS:HA    | 1:F:83:LYS:HD2   | 1.76                     | 0.45              |
| 1:G:285:LYS:HD2  | 1:G:286:ASP:N    | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:239:ILE:HB   | 1:D:247:VAL:HB   | 1.98                     | 0.45              |
| 1:D:250:VAL:HB   | 1:D:251:PRO:HD3  | 1.98                     | 0.45              |
| 1:D:29:LEU:CD1   | 1:D:30:LYS:H     | 2.17                     | 0.45              |
| 1:E:192:ARG:HB2  | 1:E:195:LEU:HD11 | 1.95                     | 0.45              |
| 1:F:66:LEU:HB3   | 1:F:67:GLY:H     | 1.49                     | 0.45              |
| 1:B:132:MET:CE   | 1:B:135:ASP:CG   | 2.84                     | 0.45              |
| 1:B:341:VAL:HG23 | 1:B:342:PHE:H    | 1.81                     | 0.45              |
| 1:C:107:TYR:HA   | 1:C:318:ALA:CB   | 2.43                     | 0.45              |
| 1:D:138:VAL:HG23 | 1:D:139:LEU:N    | 2.32                     | 0.45              |
| 1:F:231:LEU:HB3  | 1:F:233:ASP:OD2  | 2.17                     | 0.45              |
| 1:G:141:GLU:CB   | 1:G:270:HIS:HE1  | 2.27                     | 0.45              |
| 1:G:272:PHE:HE1  | 1:G:285:LYS:HB2  | 1.81                     | 0.45              |
| 1:G:53:ARG:NH1   | 1:G:62:GLN:H     | 2.14                     | 0.45              |
| 1:A:231:LEU:HD13 | 1:A:231:LEU:HA   | 1.84                     | 0.45              |
| 1:A:27:LEU:CD1   | 1:A:28:PHE:HA    | 2.47                     | 0.45              |
| 1:B:255:ALA:HB3  | 1:B:272:PHE:CE2  | 2.51                     | 0.45              |
| 1:D:169:GLN:NE2  | 1:D:170:ASN:O    | 2.50                     | 0.45              |
| 1:G:32:PHE:HA    | 1:G:35:GLU:OE2   | 2.15                     | 0.45              |
| 1:B:250:VAL:HG23 | 1:B:251:PRO:O    | 2.16                     | 0.45              |
| 1:C:29:LEU:C     | 1:C:32:PHE:HB3   | 2.33                     | 0.45              |
| 1:C:70:GLN:OE1   | 1:C:71:ALA:N     | 2.49                     | 0.45              |
| 1:E:28:PHE:CD2   | 1:E:111:ASP:CG   | 2.49                     | 0.45              |
| 1:F:240:ARG:NE   | 1:F:241:ASN:OD1  | 2.46                     | 0.45              |
| 1:F:25:LEU:HD12  | 1:F:25:LEU:N     | 2.31                     | 0.45              |
| 1:A:113:MET:O    | 1:A:114:ASN:CB   | 2.65                     | 0.45              |
| 1:A:142:ILE:O    | 1:A:145:LEU:N    | 2.50                     | 0.45              |
| 1:C:293:MET:SD   | 1:C:294:HIS:N    | 2.90                     | 0.45              |
| 1:C:35:GLU:C     | 1:C:38:THR:OG1   | 2.55                     | 0.45              |
| 1:E:88:LYS:HE3   | 1:E:88:LYS:HB2   | 1.75                     | 0.45              |
| 1:B:59:LYS:HE3   | 1:B:59:LYS:HB3   | 1.82                     | 0.45              |
| 1:B:66:LEU:H     | 1:B:66:LEU:HD13  | 1.81                     | 0.45              |
| 1:C:290:GLY:O    | 1:C:339:ALA:HA   | 2.16                     | 0.45              |
| 1:D:288:VAL:HB   | 1:D:289:ILE:H    | 1.61                     | 0.45              |
| 1:E:82:ASP:O     | 1:E:85:LYS:N     | 2.43                     | 0.45              |
| 1:G:217:ILE:O    | 1:G:221:LEU:N    | 2.26                     | 0.45              |
| 1:G:301:VAL:HG12 | 1:G:302:LYS:H    | 1.82                     | 0.45              |
| 1:G:270:HIS:NE2  | 1:G:329:HIS:HE1  | 2.15                     | 0.45              |
| 1:G:62:GLN:HB3   | 1:G:93:VAL:HG13  | 1.99                     | 0.45              |
| 1:B:313:ARG:O    | 1:B:317:GLN:N    | 2.50                     | 0.45              |
| 1:C:252:HIS:HB2  | 1:C:253:LEU:H    | 1.55                     | 0.45              |
| 1:D:40:PHE:CE1   | 1:D:131:ALA:CB   | 2.99                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:50:HIS:NE2  | 1:E:298:VAL:O    | 2.48                     | 0.45              |
| 1:A:251:PRO:HB2 | 1:A:252:HIS:CD2  | 2.52                     | 0.45              |
| 1:A:35:GLU:O    | 1:A:38:THR:OG1   | 2.32                     | 0.45              |
| 1:B:117:ASP:OD2 | 1:C:51:MET:SD    | 2.74                     | 0.45              |
| 1:C:222:MET:HA  | 1:C:224:ASN:HD21 | 1.82                     | 0.45              |
| 1:D:126:LEU:O   | 1:D:129:SER:OG   | 2.28                     | 0.45              |
| 1:E:108:ASP:OD1 | 1:E:109:ILE:HA   | 2.17                     | 0.45              |
| 1:E:32:PHE:O    | 1:E:32:PHE:CD1   | 2.62                     | 0.45              |
| 1:A:227:ASN:N   | 1:A:227:ASN:OD1  | 2.48                     | 0.44              |
| 1:B:257:GLY:N   | 1:B:272:PHE:HB3  | 2.32                     | 0.44              |
| 1:B:285:LYS:HE3 | 1:B:286:ASP:H    | 1.82                     | 0.44              |
| 1:C:62:GLN:HB2  | 1:C:91:GLU:HB2   | 1.99                     | 0.44              |
| 1:D:233:ASP:OD1 | 1:D:240:ARG:N    | 2.49                     | 0.44              |
| 1:F:167:THR:HB  | 1:F:169:GLN:O    | 2.17                     | 0.44              |
| 1:F:45:VAL:HG23 | 1:F:46:THR:HG22  | 1.97                     | 0.44              |
| 1:B:199:TYR:O   | 1:B:200:VAL:HG22 | 2.18                     | 0.44              |
| 1:B:27:LEU:O    | 1:B:30:LYS:N     | 2.49                     | 0.44              |
| 1:B:56:SER:OG   | 1:B:304:ARG:NH2  | 2.49                     | 0.44              |
| 1:B:86:ASP:O    | 1:B:155:ASN:ND2  | 2.48                     | 0.44              |
| 1:D:196:THR:O   | 1:D:198:ASN:N    | 2.51                     | 0.44              |
| 1:E:305:ASP:OD2 | 1:E:306:LEU:N    | 2.44                     | 0.44              |
| 1:E:103:ASP:CG  | 1:E:323:ALA:H    | 2.17                     | 0.44              |
| 1:F:294:HIS:NE2 | 1:F:295:ARG:O    | 2.50                     | 0.44              |
| 1:C:117:ASP:OD1 | 1:C:117:ASP:O    | 2.36                     | 0.44              |
| 1:C:110:GLU:CG  | 1:C:122:TYR:HE2  | 2.29                     | 0.44              |
| 1:D:40:PHE:CE1  | 1:D:131:ALA:HB2  | 2.52                     | 0.44              |
| 1:E:31:VAL:O    | 1:E:35:GLU:OE2   | 2.36                     | 0.44              |
| 1:G:60:SER:OG   | 1:G:61:ALA:N     | 2.51                     | 0.44              |
| 1:A:36:VAL:HG11 | 1:A:126:LEU:HD11 | 1.98                     | 0.44              |
| 1:B:44:SER:OG   | 1:B:46:THR:N     | 2.36                     | 0.44              |
| 1:C:231:LEU:HB2 | 1:C:234:PRO:CG   | 2.47                     | 0.44              |
| 1:C:306:LEU:HB3 | 1:C:325:TYR:CZ   | 2.52                     | 0.44              |
| 1:E:119:ARG:CB  | 1:E:119:ARG:CZ   | 2.95                     | 0.44              |
| 1:E:198:ASN:ND2 | 1:E:198:ASN:O    | 2.51                     | 0.44              |
| 1:F:128:GLU:O   | 1:F:132:MET:HB2  | 2.17                     | 0.44              |
| 1:F:84:ARG:HH11 | 1:F:84:ARG:C     | 2.20                     | 0.44              |
| 1:G:151:LYS:HG2 | 1:G:152:TYR:H    | 1.82                     | 0.44              |
| 1:G:170:ASN:OD1 | 1:G:171:LYS:N    | 2.51                     | 0.44              |
| 1:G:241:ASN:ND2 | 1:G:244:GLY:O    | 2.47                     | 0.44              |
| 1:B:305:ASP:OD2 | 1:B:305:ASP:N    | 2.49                     | 0.44              |
| 1:C:288:VAL:N   | 1:C:341:VAL:HG12 | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:207:PHE:HB2  | 1:E:292:PHE:HB3  | 1.99                     | 0.44              |
| 1:E:84:ARG:HB3   | 1:E:84:ARG:NH1   | 2.33                     | 0.44              |
| 1:G:49:ARG:NH2   | 1:G:248:VAL:HG21 | 2.31                     | 0.44              |
| 1:C:24:LYS:HE3   | 1:C:24:LYS:HB2   | 1.46                     | 0.44              |
| 1:E:108:ASP:O    | 1:E:108:ASP:OD1  | 2.35                     | 0.44              |
| 1:G:274:ALA:HA   | 1:G:284:ALA:HB1  | 2.00                     | 0.44              |
| 1:A:102:ALA:HB2  | 1:B:71:ALA:CA    | 2.46                     | 0.44              |
| 1:B:95:THR:OG1   | 1:B:96:ILE:N     | 2.51                     | 0.44              |
| 1:C:251:PRO:C    | 1:C:252:HIS:CG   | 2.91                     | 0.44              |
| 1:D:25:LEU:O     | 1:D:28:PHE:CD2   | 2.70                     | 0.44              |
| 1:D:46:THR:OG1   | 1:D:46:THR:O     | 2.35                     | 0.44              |
| 1:A:160:GLY:N    | 1:A:334:PRO:HG2  | 2.33                     | 0.44              |
| 1:B:171:LYS:HE3  | 1:B:171:LYS:HB3  | 1.79                     | 0.44              |
| 1:B:188:LEU:HG   | 1:B:188:LEU:H    | 1.38                     | 0.44              |
| 1:C:120:SER:O    | 1:C:124:SER:HB3  | 2.18                     | 0.44              |
| 1:E:100:LEU:HD21 | 1:F:73:TYR:CE1   | 2.53                     | 0.44              |
| 1:A:66:LEU:HD22  | 1:F:125:GLN:HG2  | 2.00                     | 0.44              |
| 1:F:136:GLY:HA3  | 1:F:255:ALA:HB3  | 1.99                     | 0.44              |
| 1:G:265:THR:O    | 1:G:266:THR:HG23 | 2.18                     | 0.44              |
| 1:B:176:ASP:OD2  | 1:B:179:ALA:HB2  | 2.18                     | 0.44              |
| 1:E:239:ILE:HG22 | 1:E:240:ARG:N    | 2.33                     | 0.44              |
| 1:G:110:GLU:CA   | 1:G:114:ASN:HB2  | 2.44                     | 0.44              |
| 1:G:116:TYR:HB3  | 1:G:117:ASP:H    | 1.29                     | 0.44              |
| 1:G:132:MET:CG   | 1:G:133:ALA:N    | 2.81                     | 0.44              |
| 1:A:45:VAL:HG12  | 1:A:46:THR:HG23  | 2.00                     | 0.43              |
| 1:D:239:ILE:HD13 | 1:D:239:ILE:HA   | 1.85                     | 0.43              |
| 1:F:101:THR:OG1  | 1:F:325:TYR:N    | 2.38                     | 0.43              |
| 1:F:31:VAL:O     | 1:F:32:PHE:C     | 2.55                     | 0.43              |
| 1:B:145:LEU:HA   | 1:B:145:LEU:HD13 | 1.76                     | 0.43              |
| 1:C:110:GLU:HB2  | 1:C:118:VAL:CG2  | 2.49                     | 0.43              |
| 1:C:115:HIS:HD2  | 1:C:115:HIS:O    | 2.00                     | 0.43              |
| 1:C:125:GLN:HE22 | 1:D:68:ARG:HG3   | 1.82                     | 0.43              |
| 1:C:68:ARG:H     | 1:C:68:ARG:HG3   | 1.65                     | 0.43              |
| 1:D:25:LEU:O     | 1:D:25:LEU:CD1   | 2.49                     | 0.43              |
| 1:D:290:GLY:CA   | 1:D:340:VAL:HG12 | 2.47                     | 0.43              |
| 1:A:67:GLY:O     | 1:F:125:GLN:NE2  | 2.51                     | 0.43              |
| 1:G:47:THR:OG1   | 1:G:48:SER:N     | 2.51                     | 0.43              |
| 1:A:193:ALA:O    | 1:A:196:THR:OG1  | 2.30                     | 0.43              |
| 1:B:24:LYS:HE2   | 1:B:25:LEU:HB2   | 2.00                     | 0.43              |
| 1:C:113:MET:C    | 1:C:113:MET:SD   | 2.95                     | 0.43              |
| 1:C:119:ARG:CZ   | 1:C:119:ARG:HB2  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:40:PHE:CD1   | 1:C:131:ALA:HB2  | 2.52                     | 0.43              |
| 1:F:142:ILE:HD12 | 1:F:142:ILE:HA   | 1.73                     | 0.43              |
| 1:F:240:ARG:HA   | 1:F:240:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:167:THR:HG21 | 1:A:183:GLU:HB3  | 2.01                     | 0.43              |
| 1:A:245:PHE:HB2  | 1:A:246:GLU:H    | 1.52                     | 0.43              |
| 1:B:50:HIS:CG    | 1:B:51:MET:N     | 2.86                     | 0.43              |
| 1:C:119:ARG:CZ   | 1:C:119:ARG:CB   | 2.96                     | 0.43              |
| 1:C:162:ALA:CB   | 1:C:337:ALA:C    | 2.86                     | 0.43              |
| 1:C:202:ALA:HB1  | 1:C:205:ARG:CZ   | 2.46                     | 0.43              |
| 1:D:122:TYR:HE1  | 1:E:64:PRO:HG3   | 1.84                     | 0.43              |
| 1:E:329:HIS:HE1  | 1:F:73:TYR:OH    | 2.01                     | 0.43              |
| 1:A:160:GLY:HA2  | 1:A:336:ALA:HA   | 2.01                     | 0.43              |
| 1:B:153:ASN:N    | 1:B:153:ASN:OD1  | 2.51                     | 0.43              |
| 1:B:183:GLU:CD   | 1:B:183:GLU:H    | 2.21                     | 0.43              |
| 1:D:63:PHE:HA    | 1:D:64:PRO:HD2   | 1.76                     | 0.43              |
| 1:E:181:GLY:H    | 1:E:184:ILE:HG12 | 1.83                     | 0.43              |
| 1:E:212:ASP:O    | 1:E:214:TYR:N    | 2.50                     | 0.43              |
| 1:F:132:MET:HA   | 1:F:135:ASP:OD1  | 2.19                     | 0.43              |
| 1:A:276:LYS:NZ   | 1:A:278:GLU:H    | 2.16                     | 0.43              |
| 1:B:130:LEU:HD12 | 1:B:131:ALA:CA   | 2.48                     | 0.43              |
| 1:C:135:ASP:OD1  | 1:C:136:GLY:N    | 2.50                     | 0.43              |
| 1:C:206:VAL:HG21 | 1:C:248:VAL:CG2  | 2.21                     | 0.43              |
| 1:C:297:ALA:O    | 1:C:298:VAL:CG1  | 2.66                     | 0.43              |
| 1:D:325:TYR:HA   | 1:D:325:TYR:HD1  | 1.69                     | 0.43              |
| 1:E:31:VAL:O     | 1:E:35:GLU:HG2   | 2.18                     | 0.43              |
| 1:F:179:ALA:HA   | 1:F:182:LYS:HZ1  | 1.83                     | 0.43              |
| 1:F:143:ALA:HB3  | 1:F:272:PHE:CE2  | 2.52                     | 0.43              |
| 1:F:28:PHE:CG    | 1:F:29:LEU:N     | 2.84                     | 0.43              |
| 1:G:110:GLU:HG2  | 1:G:118:VAL:CG1  | 2.48                     | 0.43              |
| 1:G:167:THR:C    | 1:G:169:GLN:N    | 2.71                     | 0.43              |
| 1:A:107:TYR:HA   | 1:A:318:ALA:HB1  | 2.01                     | 0.43              |
| 1:A:302:LYS:CG   | 1:A:327:MET:CB   | 2.76                     | 0.43              |
| 1:B:335:GLU:O    | 1:B:336:ALA:C    | 2.57                     | 0.43              |
| 1:B:57:SER:O     | 1:B:57:SER:OG    | 2.35                     | 0.43              |
| 1:C:313:ARG:O    | 1:C:317:GLN:HB3  | 2.18                     | 0.43              |
| 1:D:241:ASN:HB2  | 1:D:244:GLY:O    | 2.19                     | 0.43              |
| 1:F:32:PHE:HB3   | 1:F:33:GLY:H     | 1.69                     | 0.43              |
| 1:G:270:HIS:O    | 1:G:271:VAL:C    | 2.48                     | 0.43              |
| 1:A:185:ILE:O    | 1:A:188:LEU:N    | 2.51                     | 0.43              |
| 1:B:40:PHE:HB2   | 1:B:130:LEU:HD23 | 1.63                     | 0.43              |
| 1:C:28:PHE:HD2   | 1:C:29:LEU:CA    | 2.30                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:321:ILE:HG13 | 1:C:321:ILE:H    | 1.59                     | 0.43              |
| 1:C:329:HIS:CG   | 1:C:330:GLY:H    | 2.36                     | 0.43              |
| 1:D:104:VAL:H    | 1:D:321:ILE:HD12 | 1.83                     | 0.43              |
| 1:E:301:VAL:HG22 | 1:E:302:LYS:H    | 1.84                     | 0.43              |
| 1:G:250:VAL:HG22 | 1:G:252:HIS:O    | 2.18                     | 0.43              |
| 1:A:55:ILE:CG2   | 1:A:301:VAL:HG21 | 2.31                     | 0.43              |
| 1:C:288:VAL:H    | 1:C:341:VAL:HG12 | 1.84                     | 0.43              |
| 1:D:185:ILE:O    | 1:D:188:LEU:N    | 2.51                     | 0.43              |
| 1:E:192:ARG:CA   | 1:E:195:LEU:HG   | 2.47                     | 0.43              |
| 1:F:211:PRO:HA   | 1:F:214:TYR:HB3  | 2.00                     | 0.43              |
| 1:F:28:PHE:HD1   | 1:F:28:PHE:C     | 2.16                     | 0.43              |
| 1:G:252:HIS:CE1  | 1:G:255:ALA:HB3  | 2.54                     | 0.43              |
| 1:C:107:TYR:H    | 1:C:107:TYR:HD2  | 1.58                     | 0.43              |
| 1:E:253:LEU:O    | 1:E:285:LYS:NZ   | 2.41                     | 0.43              |
| 1:F:298:VAL:HG12 | 1:F:331:GLY:HA2  | 2.01                     | 0.43              |
| 1:G:132:MET:HE2  | 1:G:132:MET:CA   | 2.49                     | 0.43              |
| 1:A:305:ASP:C    | 1:A:325:TYR:CE1  | 2.91                     | 0.42              |
| 1:B:176:ASP:OD1  | 1:B:177:GLN:N    | 2.52                     | 0.42              |
| 1:C:227:ASN:OD1  | 1:C:227:ASN:N    | 2.46                     | 0.42              |
| 1:B:110:GLU:HG2  | 1:C:53:ARG:HH22  | 1.84                     | 0.42              |
| 1:E:145:LEU:HB3  | 1:E:332:LEU:CD2  | 2.40                     | 0.42              |
| 1:F:62:GLN:HB3   | 1:F:93:VAL:HG12  | 2.01                     | 0.42              |
| 1:G:185:ILE:O    | 1:G:189:THR:HG23 | 2.18                     | 0.42              |
| 1:G:195:LEU:HD11 | 1:G:205:ARG:HG3  | 2.01                     | 0.42              |
| 1:G:23:ASP:HB3   | 1:G:26:ALA:HB3   | 2.01                     | 0.42              |
| 1:D:83:LYS:NZ    | 1:D:83:LYS:H     | 2.17                     | 0.42              |
| 1:E:192:ARG:HA   | 1:E:195:LEU:HD21 | 2.01                     | 0.42              |
| 1:F:183:GLU:OE1  | 1:F:184:ILE:HG13 | 2.19                     | 0.42              |
| 1:G:207:PHE:CE2  | 1:G:247:VAL:HG22 | 2.54                     | 0.42              |
| 1:B:334:PRO:HB3  | 1:B:335:GLU:O    | 2.19                     | 0.42              |
| 1:B:80:LEU:H     | 1:B:80:LEU:HD12  | 1.84                     | 0.42              |
| 1:E:126:LEU:O    | 1:E:129:SER:OG   | 2.31                     | 0.42              |
| 1:F:55:ILE:HA    | 1:F:55:ILE:HD12  | 1.77                     | 0.42              |
| 1:G:115:HIS:HA   | 1:G:119:ARG:HH12 | 1.85                     | 0.42              |
| 1:G:294:HIS:NE2  | 1:G:297:ALA:HB2  | 2.34                     | 0.42              |
| 1:G:270:HIS:NE2  | 1:G:329:HIS:CE1  | 2.87                     | 0.42              |
| 1:A:101:THR:HG21 | 1:A:323:ALA:O    | 2.20                     | 0.42              |
| 1:A:115:HIS:HB2  | 1:A:119:ARG:HG3  | 2.01                     | 0.42              |
| 1:A:92:LYS:HD2   | 1:A:92:LYS:HA    | 1.68                     | 0.42              |
| 1:B:114:ASN:HB2  | 1:B:118:VAL:HB   | 1.99                     | 0.42              |
| 1:E:166:GLU:HA   | 1:E:340:VAL:HG23 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:239:ILE:HG22 | 1:E:240:ARG:H    | 1.83                     | 0.42              |
| 1:E:207:PHE:HA   | 1:E:292:PHE:HA   | 2.00                     | 0.42              |
| 1:E:103:ASP:CB   | 1:E:322:ILE:HA   | 2.48                     | 0.42              |
| 1:E:163:THR:HB   | 1:E:338:GLY:HA2  | 2.01                     | 0.42              |
| 1:G:147:ASN:ND2  | 1:G:273:PRO:CG   | 2.66                     | 0.42              |
| 1:A:287:ASN:CG   | 1:A:288:VAL:H    | 2.08                     | 0.42              |
| 1:B:202:ALA:HB1  | 1:B:205:ARG:CZ   | 2.49                     | 0.42              |
| 1:C:27:LEU:CD2   | 1:C:28:PHE:CA    | 2.92                     | 0.42              |
| 1:E:320:GLN:HE21 | 1:E:322:ILE:HG23 | 1.83                     | 0.42              |
| 1:F:233:ASP:N    | 1:F:234:PRO:HD3  | 2.34                     | 0.42              |
| 1:F:94:ILE:HA    | 1:F:94:ILE:HD12  | 1.67                     | 0.42              |
| 1:G:186:ALA:O    | 1:G:189:THR:OG1  | 2.33                     | 0.42              |
| 1:G:217:ILE:HA   | 1:G:220:ALA:HB3  | 2.02                     | 0.42              |
| 1:A:106:ILE:HG22 | 1:A:122:TYR:HE2  | 1.73                     | 0.42              |
| 1:A:274:ALA:CB   | 1:A:285:LYS:HD2  | 2.49                     | 0.42              |
| 1:B:222:MET:H    | 1:B:222:MET:HG3  | 1.76                     | 0.42              |
| 1:B:218:LEU:HD23 | 1:B:228:TYR:CD1  | 2.54                     | 0.42              |
| 1:C:167:THR:OG1  | 1:C:168:THR:N    | 2.52                     | 0.42              |
| 1:C:29:LEU:O     | 1:C:32:PHE:CA    | 2.67                     | 0.42              |
| 1:C:332:LEU:HB3  | 1:C:333:ARG:H    | 1.42                     | 0.42              |
| 1:D:166:GLU:HB3  | 1:D:167:THR:HG22 | 2.01                     | 0.42              |
| 1:G:130:LEU:HD23 | 1:G:131:ALA:HA   | 2.01                     | 0.42              |
| 1:B:139:LEU:CA   | 1:B:142:ILE:HG23 | 2.49                     | 0.42              |
| 1:C:32:PHE:CZ    | 1:C:126:LEU:CD2  | 3.02                     | 0.42              |
| 1:D:27:LEU:HD12  | 1:D:28:PHE:CA    | 2.49                     | 0.42              |
| 1:E:202:ALA:HB1  | 1:E:205:ARG:NH1  | 2.34                     | 0.42              |
| 1:E:58:GLY:C     | 1:E:59:LYS:HD2   | 2.40                     | 0.42              |
| 1:G:130:LEU:CD2  | 1:G:131:ALA:HA   | 2.50                     | 0.42              |
| 1:C:280:ASN:O    | 1:C:280:ASN:ND2  | 2.52                     | 0.42              |
| 1:C:299:GLY:C    | 1:C:330:GLY:HA2  | 2.40                     | 0.42              |
| 1:D:43:THR:HG21  | 1:D:128:GLU:HA   | 2.02                     | 0.42              |
| 1:E:48:SER:OG    | 1:E:49:ARG:N     | 2.52                     | 0.42              |
| 1:F:275:ASN:OD1  | 1:F:275:ASN:N    | 2.52                     | 0.42              |
| 1:F:29:LEU:O     | 1:F:32:PHE:CB    | 2.67                     | 0.42              |
| 1:F:80:LEU:HG    | 1:F:80:LEU:H     | 1.46                     | 0.42              |
| 1:A:206:VAL:HG12 | 1:A:246:GLU:HB3  | 2.02                     | 0.42              |
| 1:A:161:THR:N    | 1:A:336:ALA:HA   | 2.31                     | 0.42              |
| 1:C:115:HIS:O    | 1:C:118:VAL:HG12 | 2.20                     | 0.42              |
| 1:C:171:LYS:H    | 1:C:171:LYS:CE   | 2.31                     | 0.42              |
| 1:D:46:THR:OG1   | 1:D:135:ASP:OD1  | 2.36                     | 0.42              |
| 1:D:171:LYS:HE3  | 1:D:171:LYS:HB2  | 1.90                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:285:LYS:HD3  | 1:D:286:ASP:H    | 1.85                     | 0.42              |
| 1:E:298:VAL:HG12 | 1:E:332:LEU:CB   | 2.50                     | 0.42              |
| 1:E:53:ARG:HD3   | 1:E:63:PHE:HD1   | 1.83                     | 0.42              |
| 1:C:37:LEU:HD12  | 1:C:37:LEU:HA    | 1.77                     | 0.42              |
| 1:D:142:ILE:HG22 | 1:D:143:ALA:N    | 2.35                     | 0.42              |
| 1:D:95:THR:OG1   | 1:D:96:ILE:HG12  | 2.20                     | 0.42              |
| 1:E:298:VAL:C    | 1:E:333:ARG:NH2  | 2.72                     | 0.42              |
| 1:F:276:LYS:NZ   | 1:F:278:GLU:H    | 2.17                     | 0.42              |
| 1:G:106:ILE:CD1  | 1:G:107:TYR:O    | 2.67                     | 0.42              |
| 1:G:313:ARG:N    | 1:G:318:ALA:O    | 2.42                     | 0.42              |
| 1:G:32:PHE:CE1   | 1:G:36:VAL:HG21  | 2.55                     | 0.42              |
| 1:B:125:GLN:HG2  | 1:C:66:LEU:HB2   | 1.56                     | 0.41              |
| 1:C:49:ARG:O     | 1:C:50:HIS:HB3   | 2.20                     | 0.41              |
| 1:D:135:ASP:C    | 1:D:139:LEU:CD2  | 2.86                     | 0.41              |
| 1:E:168:THR:HG22 | 1:E:183:GLU:HB2  | 2.02                     | 0.41              |
| 1:F:233:ASP:OD2  | 1:F:233:ASP:N    | 2.49                     | 0.41              |
| 1:F:257:GLY:HA3  | 1:F:271:VAL:HB   | 2.01                     | 0.41              |
| 1:A:122:TYR:HA   | 1:A:122:TYR:HD1  | 1.65                     | 0.41              |
| 1:A:272:PHE:O    | 1:A:274:ALA:N    | 2.53                     | 0.41              |
| 1:C:177:GLN:NE2  | 1:C:215:SER:OG   | 2.27                     | 0.41              |
| 1:D:142:ILE:HD13 | 1:D:145:LEU:HD23 | 1.71                     | 0.41              |
| 1:D:282:LYS:H    | 1:D:282:LYS:NZ   | 2.18                     | 0.41              |
| 1:E:292:PHE:O    | 1:E:337:ALA:N    | 2.53                     | 0.41              |
| 1:F:123:THR:OG1  | 1:F:124:SER:N    | 2.53                     | 0.41              |
| 1:F:240:ARG:NE   | 1:F:241:ASN:H    | 2.19                     | 0.41              |
| 1:F:81:ASP:OD2   | 1:F:81:ASP:N     | 2.51                     | 0.41              |
| 1:F:82:ASP:HA    | 1:F:85:LYS:HB2   | 2.01                     | 0.41              |
| 1:A:108:ASP:HB3  | 1:A:111:ASP:H    | 1.85                     | 0.41              |
| 1:A:215:SER:OG   | 1:A:218:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:218:LEU:HD12 | 1:A:221:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:42:ARG:HB3   | 1:A:42:ARG:NH2   | 2.35                     | 0.41              |
| 1:B:125:GLN:OE1  | 1:B:125:GLN:HA   | 2.20                     | 0.41              |
| 1:B:161:THR:CG2  | 1:B:335:GLU:H    | 2.32                     | 0.41              |
| 1:C:161:THR:OG1  | 1:C:161:THR:O    | 2.37                     | 0.41              |
| 1:D:128:GLU:OE2  | 1:D:129:SER:N    | 2.52                     | 0.41              |
| 1:D:175:THR:OG1  | 1:D:176:ASP:N    | 2.52                     | 0.41              |
| 1:D:188:LEU:HA   | 1:D:191:ALA:HB3  | 2.02                     | 0.41              |
| 1:D:105:LEU:HA   | 1:D:320:GLN:CB   | 2.50                     | 0.41              |
| 1:F:182:LYS:O    | 1:F:185:ILE:N    | 2.53                     | 0.41              |
| 1:F:205:ARG:CG   | 1:F:245:PHE:HA   | 2.47                     | 0.41              |
| 1:F:287:ASN:HB3  | 1:F:288:VAL:HG22 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:88:LYS:HG3   | 1:F:90:THR:H     | 1.84                     | 0.41              |
| 1:G:188:LEU:HB3  | 1:G:245:PHE:CE1  | 2.55                     | 0.41              |
| 1:G:51:MET:N     | 1:G:299:GLY:HA3  | 2.36                     | 0.41              |
| 1:A:63:PHE:N     | 1:A:92:LYS:O     | 2.49                     | 0.41              |
| 1:B:228:TYR:O    | 1:B:232:ILE:HG12 | 2.19                     | 0.41              |
| 1:C:242:VAL:HG23 | 1:C:243:MET:O    | 2.21                     | 0.41              |
| 1:C:308:LEU:HD23 | 1:C:308:LEU:H    | 1.85                     | 0.41              |
| 1:C:33:GLY:O     | 1:C:36:VAL:CG2   | 2.64                     | 0.41              |
| 1:C:60:SER:OG    | 1:C:94:ILE:O     | 2.27                     | 0.41              |
| 1:D:53:ARG:HD3   | 1:D:63:PHE:HZ    | 1.84                     | 0.41              |
| 1:F:128:GLU:OE2  | 1:F:128:GLU:N    | 2.53                     | 0.41              |
| 1:F:273:PRO:HG3  | 1:F:281:VAL:HG21 | 2.01                     | 0.41              |
| 1:G:115:HIS:CG   | 1:G:119:ARG:NH2  | 2.86                     | 0.41              |
| 1:A:126:LEU:O    | 1:A:130:LEU:HG   | 2.20                     | 0.41              |
| 1:A:207:PHE:HD1  | 1:A:291:LEU:N    | 2.18                     | 0.41              |
| 1:A:36:VAL:O     | 1:A:38:THR:N     | 2.54                     | 0.41              |
| 1:B:181:GLY:O    | 1:B:185:ILE:N    | 2.48                     | 0.41              |
| 1:B:92:LYS:HZ1   | 1:B:333:ARG:CZ   | 2.33                     | 0.41              |
| 1:C:104:VAL:H    | 1:C:321:ILE:HD11 | 1.86                     | 0.41              |
| 1:C:209:CYS:HB3  | 1:C:249:GLU:HB3  | 2.01                     | 0.41              |
| 1:E:301:VAL:HG22 | 1:E:302:LYS:N    | 2.36                     | 0.41              |
| 1:G:265:THR:O    | 1:G:266:THR:CB   | 2.69                     | 0.41              |
| 1:B:28:PHE:CE2   | 1:B:111:ASP:OD1  | 2.73                     | 0.41              |
| 1:B:130:LEU:CD1  | 1:B:131:ALA:N    | 2.75                     | 0.41              |
| 1:B:130:LEU:CG   | 1:B:131:ALA:N    | 2.81                     | 0.41              |
| 1:B:141:GLU:OE1  | 1:B:330:GLY:N    | 2.41                     | 0.41              |
| 1:E:110:GLU:CG   | 1:E:118:VAL:CB   | 2.96                     | 0.41              |
| 1:E:53:ARG:NH1   | 1:E:62:GLN:H     | 2.09                     | 0.41              |
| 1:F:117:ASP:O    | 1:F:118:VAL:HG12 | 2.21                     | 0.41              |
| 1:G:110:GLU:HG2  | 1:G:114:ASN:ND2  | 2.35                     | 0.41              |
| 1:G:137:ALA:CB   | 1:G:258:ALA:HB3  | 2.50                     | 0.41              |
| 1:G:312:ARG:HD3  | 1:G:319:ASP:OD1  | 2.20                     | 0.41              |
| 1:A:115:HIS:O    | 1:A:119:ARG:CG   | 2.69                     | 0.41              |
| 1:A:239:ILE:HB   | 1:A:247:VAL:O    | 2.21                     | 0.41              |
| 1:A:30:LYS:HB3   | 1:A:30:LYS:HE3   | 1.84                     | 0.41              |
| 1:A:41:ALA:C     | 1:A:43:THR:N     | 2.72                     | 0.41              |
| 1:B:178:VAL:O    | 1:B:182:LYS:HB2  | 2.20                     | 0.41              |
| 1:C:95:THR:OG1   | 1:C:96:ILE:N     | 2.53                     | 0.41              |
| 1:D:231:LEU:O    | 1:D:234:PRO:HD3  | 2.21                     | 0.41              |
| 1:D:236:LYS:HD3  | 1:D:236:LYS:HA   | 1.96                     | 0.41              |
| 1:D:286:ASP:OD2  | 1:D:286:ASP:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:29:LEU:C     | 1:D:29:LEU:CD2   | 2.85                     | 0.41              |
| 1:F:143:ALA:HB1  | 1:F:272:PHE:CD2  | 2.56                     | 0.41              |
| 1:F:310:ARG:HB3  | 1:F:321:ILE:HA   | 2.02                     | 0.41              |
| 1:F:63:PHE:HA    | 1:F:64:PRO:HD2   | 1.85                     | 0.41              |
| 1:A:207:PHE:CD1  | 1:A:290:GLY:C    | 2.93                     | 0.41              |
| 1:A:215:SER:O    | 1:A:216:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:232:ILE:HB   | 1:A:240:ARG:CB   | 2.51                     | 0.41              |
| 1:B:205:ARG:O    | 1:B:245:PHE:HA   | 2.20                     | 0.41              |
| 1:E:199:TYR:HB3  | 1:E:200:VAL:H    | 1.37                     | 0.41              |
| 1:G:298:VAL:HB   | 1:G:299:GLY:H    | 1.71                     | 0.41              |
| 1:G:101:THR:HG23 | 1:G:323:ALA:O    | 2.21                     | 0.41              |
| 1:A:110:GLU:OE2  | 1:A:111:ASP:HA   | 2.19                     | 0.41              |
| 1:A:163:THR:O    | 1:A:164:VAL:HG13 | 2.21                     | 0.41              |
| 1:A:217:ILE:O    | 1:A:219:ALA:N    | 2.54                     | 0.41              |
| 1:C:325:TYR:HD1  | 1:C:325:TYR:HA   | 1.75                     | 0.41              |
| 1:D:164:VAL:HG12 | 1:D:339:ALA:N    | 2.36                     | 0.41              |
| 1:D:73:TYR:N     | 1:D:73:TYR:CD2   | 2.88                     | 0.41              |
| 1:F:25:LEU:O     | 1:F:28:PHE:CE1   | 2.74                     | 0.41              |
| 1:G:113:MET:CE   | 1:G:114:ASN:N    | 2.65                     | 0.41              |
| 1:G:69:THR:H     | 1:G:70:GLN:NE2   | 2.19                     | 0.41              |
| 1:B:145:LEU:HD12 | 1:B:145:LEU:C    | 2.32                     | 0.41              |
| 1:B:227:ASN:O    | 1:B:229:ALA:N    | 2.54                     | 0.41              |
| 1:B:75:ALA:C     | 1:B:77:GLY:H     | 2.24                     | 0.41              |
| 1:C:236:LYS:HB2  | 1:C:236:LYS:NZ   | 2.36                     | 0.41              |
| 1:D:113:MET:SD   | 1:D:114:ASN:N    | 2.94                     | 0.41              |
| 1:E:195:LEU:H    | 1:E:195:LEU:HG   | 1.42                     | 0.41              |
| 1:E:315:ASN:ND2  | 1:E:315:ASN:H    | 2.19                     | 0.41              |
| 1:E:288:VAL:HG22 | 1:E:341:VAL:CG1  | 2.50                     | 0.41              |
| 1:E:100:LEU:HG   | 1:F:72:ALA:O     | 2.21                     | 0.41              |
| 1:G:37:LEU:HD12  | 1:G:40:PHE:CD2   | 2.56                     | 0.41              |
| 1:G:39:ALA:O     | 1:G:43:THR:OG1   | 2.38                     | 0.41              |
| 1:A:29:LEU:H     | 1:A:29:LEU:HG    | 1.72                     | 0.41              |
| 1:C:141:GLU:N    | 1:C:141:GLU:OE1  | 2.53                     | 0.41              |
| 1:C:146:CYS:SG   | 1:C:161:THR:N    | 2.87                     | 0.41              |
| 1:C:196:THR:C    | 1:C:198:ASN:H    | 2.24                     | 0.41              |
| 1:C:299:GLY:N    | 1:C:330:GLY:O    | 2.44                     | 0.41              |
| 1:C:43:THR:HG21  | 1:C:128:GLU:OE2  | 2.21                     | 0.41              |
| 1:D:303:LEU:HB3  | 1:D:304:ARG:HD3  | 2.03                     | 0.41              |
| 1:E:23:ASP:O     | 1:E:26:ALA:HB3   | 2.20                     | 0.41              |
| 1:E:73:TYR:O     | 1:E:74:LEU:HD23  | 2.21                     | 0.41              |
| 1:F:178:VAL:O    | 1:F:182:LYS:HG3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:54:SER:OG    | 1:F:302:LYS:NZ   | 2.54                     | 0.41              |
| 1:G:285:LYS:HD2  | 1:G:286:ASP:H    | 1.86                     | 0.41              |
| 1:B:27:LEU:CD2   | 1:B:27:LEU:C     | 2.90                     | 0.40              |
| 1:C:40:PHE:CE1   | 1:C:131:ALA:CB   | 3.04                     | 0.40              |
| 1:D:209:CYS:CB   | 1:D:249:GLU:HG2  | 2.48                     | 0.40              |
| 1:G:210:ASP:OD1  | 1:G:253:LEU:HD11 | 2.21                     | 0.40              |
| 1:A:233:ASP:O    | 1:A:235:GLU:N    | 2.55                     | 0.40              |
| 1:A:287:ASN:HD21 | 1:A:341:VAL:HG11 | 1.83                     | 0.40              |
| 1:B:24:LYS:CE    | 1:B:24:LYS:C     | 2.74                     | 0.40              |
| 1:E:126:LEU:HA   | 1:E:126:LEU:HD23 | 1.92                     | 0.40              |
| 1:E:68:ARG:HE    | 1:E:70:GLN:NE2   | 2.09                     | 0.40              |
| 1:G:150:SER:C    | 1:G:151:LYS:O    | 2.59                     | 0.40              |
| 1:G:205:ARG:HA   | 1:G:205:ARG:HD3  | 1.89                     | 0.40              |
| 1:G:252:HIS:O    | 1:G:253:LEU:HD23 | 2.21                     | 0.40              |
| 1:A:114:ASN:H    | 1:A:115:HIS:HD2  | 1.54                     | 0.40              |
| 1:B:68:ARG:C     | 1:B:69:THR:OG1   | 2.56                     | 0.40              |
| 1:C:315:ASN:CG   | 1:C:316:PHE:H    | 2.23                     | 0.40              |
| 1:C:292:PHE:N    | 1:C:338:GLY:O    | 2.48                     | 0.40              |
| 1:E:126:LEU:HA   | 1:E:129:SER:OG   | 2.22                     | 0.40              |
| 1:E:166:GLU:CD   | 1:E:167:THR:H    | 2.25                     | 0.40              |
| 1:F:75:ALA:HA    | 1:F:76:PRO:HD3   | 1.95                     | 0.40              |
| 1:G:110:GLU:CG   | 1:G:118:VAL:HG21 | 2.30                     | 0.40              |
| 1:G:271:VAL:O    | 1:G:271:VAL:HG13 | 2.21                     | 0.40              |
| 1:A:251:PRO:O    | 1:A:252:HIS:ND1  | 2.54                     | 0.40              |
| 1:C:141:GLU:OE2  | 1:C:142:ILE:HG12 | 2.20                     | 0.40              |
| 1:C:231:LEU:HA   | 1:C:231:LEU:HD22 | 1.90                     | 0.40              |
| 1:C:84:ARG:HH12  | 1:C:89:HIS:CE1   | 2.40                     | 0.40              |
| 1:D:226:ALA:HA   | 1:D:228:TYR:CD2  | 2.57                     | 0.40              |
| 1:E:192:ARG:C    | 1:E:195:LEU:CG   | 2.89                     | 0.40              |
| 1:E:61:ALA:O     | 1:E:94:ILE:N     | 2.45                     | 0.40              |
| 1:A:169:GLN:HE22 | 1:A:173:ALA:HB3  | 1.87                     | 0.40              |
| 1:A:295:ARG:NE   | 1:A:296:SER:H    | 2.20                     | 0.40              |
| 1:A:78:GLU:HB2   | 1:A:79:ASN:H     | 1.61                     | 0.40              |
| 1:B:67:GLY:C     | 1:B:68:ARG:CD    | 2.90                     | 0.40              |
| 1:C:112:ALA:O    | 1:C:115:HIS:NE2  | 2.55                     | 0.40              |
| 1:C:276:LYS:HD3  | 1:C:279:GLY:HA3  | 2.02                     | 0.40              |
| 1:D:70:GLN:HB2   | 1:D:71:ALA:H     | 1.70                     | 0.40              |
| 1:E:233:ASP:OD2  | 1:E:236:LYS:HG3  | 2.22                     | 0.40              |
| 1:E:25:LEU:HD12  | 1:E:26:ALA:CA    | 2.51                     | 0.40              |
| 1:F:303:LEU:H    | 1:F:326:ALA:HB3  | 1.87                     | 0.40              |
| 1:F:60:SER:HB3   | 1:F:94:ILE:O     | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 294/345 (85%)   | 224 (76%)  | 61 (21%)  | 9 (3%)   | 5           | 39 |
| 1   | B     | 305/345 (88%)   | 229 (75%)  | 67 (22%)  | 9 (3%)   | 5           | 39 |
| 1   | C     | 290/345 (84%)   | 206 (71%)  | 65 (22%)  | 19 (7%)  | 1           | 22 |
| 1   | D     | 292/345 (85%)   | 213 (73%)  | 70 (24%)  | 9 (3%)   | 5           | 39 |
| 1   | E     | 287/345 (83%)   | 214 (75%)  | 65 (23%)  | 8 (3%)   | 6           | 41 |
| 1   | F     | 293/345 (85%)   | 225 (77%)  | 61 (21%)  | 7 (2%)   | 7           | 44 |
| 1   | G     | 313/345 (91%)   | 240 (77%)  | 60 (19%)  | 13 (4%)  | 3           | 32 |
| All | All   | 2074/2415 (86%) | 1551 (75%) | 449 (22%) | 74 (4%)  | 7           | 35 |

All (74) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 178 | VAL  |
| 1   | A     | 288 | VAL  |
| 1   | B     | 70  | GLN  |
| 1   | B     | 114 | ASN  |
| 1   | B     | 232 | ILE  |
| 1   | B     | 334 | PRO  |
| 1   | C     | 42  | ARG  |
| 1   | C     | 43  | THR  |
| 1   | C     | 117 | ASP  |
| 1   | C     | 163 | THR  |
| 1   | C     | 178 | VAL  |
| 1   | C     | 300 | THR  |
| 1   | D     | 37  | LEU  |
| 1   | D     | 96  | ILE  |
| 1   | D     | 118 | VAL  |
| 1   | D     | 145 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 115 | HIS  |
| 1   | E     | 335 | GLU  |
| 1   | F     | 32  | PHE  |
| 1   | F     | 118 | VAL  |
| 1   | G     | 116 | TYR  |
| 1   | G     | 150 | SER  |
| 1   | G     | 151 | LYS  |
| 1   | G     | 271 | VAL  |
| 1   | B     | 245 | PHE  |
| 1   | B     | 286 | ASP  |
| 1   | C     | 32  | PHE  |
| 1   | C     | 289 | ILE  |
| 1   | D     | 341 | VAL  |
| 1   | F     | 87  | ILE  |
| 1   | F     | 298 | VAL  |
| 1   | G     | 85  | LYS  |
| 1   | G     | 166 | GLU  |
| 1   | G     | 266 | THR  |
| 1   | B     | 69  | THR  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 162 | ALA  |
| 1   | C     | 201 | PRO  |
| 1   | E     | 286 | ASP  |
| 1   | G     | 115 | HIS  |
| 1   | G     | 149 | GLU  |
| 1   | G     | 232 | ILE  |
| 1   | C     | 116 | TYR  |
| 1   | D     | 71  | ALA  |
| 1   | E     | 30  | LYS  |
| 1   | A     | 36  | VAL  |
| 1   | A     | 245 | PHE  |
| 1   | C     | 52  | VAL  |
| 1   | C     | 288 | VAL  |
| 1   | E     | 226 | ALA  |
| 1   | E     | 235 | GLU  |
| 1   | A     | 298 | VAL  |
| 1   | B     | 226 | ALA  |
| 1   | C     | 33  | GLY  |
| 1   | C     | 169 | GLN  |
| 1   | E     | 251 | PRO  |
| 1   | F     | 33  | GLY  |
| 1   | G     | 55  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 87  | ILE  |
| 1   | A     | 217 | ILE  |
| 1   | C     | 232 | ILE  |
| 1   | C     | 242 | VAL  |
| 1   | D     | 288 | VAL  |
| 1   | D     | 298 | VAL  |
| 1   | F     | 281 | VAL  |
| 1   | A     | 232 | ILE  |
| 1   | B     | 55  | ILE  |
| 1   | C     | 165 | ILE  |
| 1   | D     | 242 | VAL  |
| 1   | E     | 341 | VAL  |
| 1   | F     | 164 | VAL  |
| 1   | A     | 164 | VAL  |
| 1   | A     | 165 | ILE  |
| 1   | G     | 281 | 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     | 230/261 (88%)   | 168 (73%)  | 62 (27%)  | 0           | 4 |
| 1   | B     | 238/261 (91%)   | 157 (66%)  | 81 (34%)  | 0           | 2 |
| 1   | C     | 230/261 (88%)   | 151 (66%)  | 79 (34%)  | 0           | 2 |
| 1   | D     | 230/261 (88%)   | 160 (70%)  | 70 (30%)  | 0           | 3 |
| 1   | E     | 227/261 (87%)   | 157 (69%)  | 70 (31%)  | 0           | 2 |
| 1   | F     | 230/261 (88%)   | 167 (73%)  | 63 (27%)  | 0           | 4 |
| 1   | G     | 242/261 (93%)   | 163 (67%)  | 79 (33%)  | 0           | 2 |
| All | All   | 1627/1827 (89%) | 1123 (69%) | 504 (31%) | 1           | 2 |

All (504) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | LYS  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 27  | LEU  |
| 1   | A     | 28  | PHE  |
| 1   | A     | 29  | LEU  |
| 1   | A     | 36  | VAL  |
| 1   | A     | 42  | ARG  |
| 1   | A     | 50  | HIS  |
| 1   | A     | 53  | ARG  |
| 1   | A     | 66  | LEU  |
| 1   | A     | 70  | GLN  |
| 1   | A     | 82  | ASP  |
| 1   | A     | 84  | ARG  |
| 1   | A     | 87  | ILE  |
| 1   | A     | 88  | LYS  |
| 1   | A     | 101 | THR  |
| 1   | A     | 104 | VAL  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 107 | TYR  |
| 1   | A     | 109 | ILE  |
| 1   | A     | 110 | GLU  |
| 1   | A     | 113 | MET  |
| 1   | A     | 114 | ASN  |
| 1   | A     | 115 | HIS  |
| 1   | A     | 119 | ARG  |
| 1   | A     | 122 | TYR  |
| 1   | A     | 128 | GLU  |
| 1   | A     | 141 | GLU  |
| 1   | A     | 145 | LEU  |
| 1   | A     | 163 | THR  |
| 1   | A     | 164 | VAL  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 176 | ASP  |
| 1   | A     | 177 | GLN  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 190 | LYS  |
| 1   | A     | 205 | ARG  |
| 1   | A     | 207 | PHE  |
| 1   | A     | 212 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 232 | ILE  |
| 1   | A     | 236 | LYS  |
| 1   | A     | 245 | PHE  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 253 | LEU  |
| 1   | A     | 272 | PHE  |
| 1   | A     | 280 | ASN  |
| 1   | A     | 282 | LYS  |
| 1   | A     | 283 | VAL  |
| 1   | A     | 285 | LYS  |
| 1   | A     | 287 | ASN  |
| 1   | A     | 288 | VAL  |
| 1   | A     | 298 | VAL  |
| 1   | A     | 315 | ASN  |
| 1   | A     | 317 | GLN  |
| 1   | A     | 325 | TYR  |
| 1   | A     | 327 | MET  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 335 | GLU  |
| 1   | B     | 24  | LYS  |
| 1   | B     | 25  | LEU  |
| 1   | B     | 27  | LEU  |
| 1   | B     | 30  | LYS  |
| 1   | B     | 31  | VAL  |
| 1   | B     | 32  | PHE  |
| 1   | B     | 35  | GLU  |
| 1   | B     | 37  | LEU  |
| 1   | B     | 51  | MET  |
| 1   | B     | 52  | VAL  |
| 1   | B     | 59  | LYS  |
| 1   | B     | 66  | LEU  |
| 1   | B     | 68  | ARG  |
| 1   | B     | 70  | GLN  |
| 1   | B     | 74  | LEU  |
| 1   | B     | 80  | LEU  |
| 1   | B     | 83  | LYS  |
| 1   | B     | 84  | ARG  |
| 1   | B     | 85  | LYS  |
| 1   | B     | 92  | LYS  |
| 1   | B     | 104 | VAL  |
| 1   | B     | 105 | LEU  |
| 1   | B     | 107 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 108 | ASP  |
| 1   | B     | 109 | ILE  |
| 1   | B     | 110 | GLU  |
| 1   | B     | 111 | ASP  |
| 1   | B     | 113 | MET  |
| 1   | B     | 116 | TYR  |
| 1   | B     | 118 | VAL  |
| 1   | B     | 121 | GLU  |
| 1   | B     | 122 | TYR  |
| 1   | B     | 123 | THR  |
| 1   | B     | 124 | SER  |
| 1   | B     | 126 | LEU  |
| 1   | B     | 128 | GLU  |
| 1   | B     | 129 | SER  |
| 1   | B     | 130 | LEU  |
| 1   | B     | 132 | MET  |
| 1   | B     | 135 | ASP  |
| 1   | B     | 138 | VAL  |
| 1   | B     | 142 | ILE  |
| 1   | B     | 145 | LEU  |
| 1   | B     | 146 | CYS  |
| 1   | B     | 163 | THR  |
| 1   | B     | 168 | THR  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 171 | LYS  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 176 | ASP  |
| 1   | B     | 188 | LEU  |
| 1   | B     | 192 | ARG  |
| 1   | B     | 197 | LYS  |
| 1   | B     | 200 | VAL  |
| 1   | B     | 205 | ARG  |
| 1   | B     | 210 | ASP  |
| 1   | B     | 217 | ILE  |
| 1   | B     | 222 | MET  |
| 1   | B     | 227 | ASN  |
| 1   | B     | 231 | LEU  |
| 1   | B     | 232 | ILE  |
| 1   | B     | 233 | ASP  |
| 1   | B     | 239 | ILE  |
| 1   | B     | 243 | MET  |
| 1   | B     | 247 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 283 | VAL  |
| 1   | B     | 285 | LYS  |
| 1   | B     | 286 | ASP  |
| 1   | B     | 289 | ILE  |
| 1   | B     | 294 | HIS  |
| 1   | B     | 298 | VAL  |
| 1   | B     | 302 | LYS  |
| 1   | B     | 304 | ARG  |
| 1   | B     | 305 | ASP  |
| 1   | B     | 306 | LEU  |
| 1   | B     | 310 | ARG  |
| 1   | B     | 313 | ARG  |
| 1   | B     | 327 | MET  |
| 1   | B     | 332 | LEU  |
| 1   | B     | 333 | ARG  |
| 1   | B     | 343 | LYS  |
| 1   | C     | 24  | LYS  |
| 1   | C     | 25  | LEU  |
| 1   | C     | 27  | LEU  |
| 1   | C     | 28  | PHE  |
| 1   | C     | 29  | LEU  |
| 1   | C     | 31  | VAL  |
| 1   | C     | 35  | GLU  |
| 1   | C     | 36  | VAL  |
| 1   | C     | 38  | THR  |
| 1   | C     | 42  | ARG  |
| 1   | C     | 51  | MET  |
| 1   | C     | 52  | VAL  |
| 1   | C     | 59  | LYS  |
| 1   | C     | 62  | GLN  |
| 1   | C     | 65  | VAL  |
| 1   | C     | 69  | THR  |
| 1   | C     | 70  | GLN  |
| 1   | C     | 73  | TYR  |
| 1   | C     | 78  | GLU  |
| 1   | C     | 80  | LEU  |
| 1   | C     | 84  | ARG  |
| 1   | C     | 87  | ILE  |
| 1   | C     | 89  | HIS  |
| 1   | C     | 90  | THR  |
| 1   | C     | 91  | GLU  |
| 1   | C     | 104 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 105 | LEU  |
| 1   | C     | 107 | TYR  |
| 1   | C     | 109 | ILE  |
| 1   | C     | 110 | GLU  |
| 1   | C     | 113 | MET  |
| 1   | C     | 114 | ASN  |
| 1   | C     | 116 | TYR  |
| 1   | C     | 119 | ARG  |
| 1   | C     | 120 | SER  |
| 1   | C     | 126 | LEU  |
| 1   | C     | 146 | CYS  |
| 1   | C     | 165 | ILE  |
| 1   | C     | 167 | THR  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 171 | LYS  |
| 1   | C     | 176 | ASP  |
| 1   | C     | 183 | GLU  |
| 1   | C     | 184 | ILE  |
| 1   | C     | 190 | LYS  |
| 1   | C     | 199 | TYR  |
| 1   | C     | 212 | ASP  |
| 1   | C     | 214 | TYR  |
| 1   | C     | 221 | LEU  |
| 1   | C     | 222 | MET  |
| 1   | C     | 224 | ASN  |
| 1   | C     | 231 | LEU  |
| 1   | C     | 235 | GLU  |
| 1   | C     | 249 | GLU  |
| 1   | C     | 250 | VAL  |
| 1   | C     | 252 | HIS  |
| 1   | C     | 253 | LEU  |
| 1   | C     | 271 | VAL  |
| 1   | C     | 272 | PHE  |
| 1   | C     | 276 | LYS  |
| 1   | C     | 282 | LYS  |
| 1   | C     | 285 | LYS  |
| 1   | C     | 288 | VAL  |
| 1   | C     | 289 | ILE  |
| 1   | C     | 293 | MET  |
| 1   | C     | 295 | ARG  |
| 1   | C     | 305 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 306 | LEU  |
| 1   | C     | 309 | GLU  |
| 1   | C     | 310 | ARG  |
| 1   | C     | 316 | PHE  |
| 1   | C     | 317 | GLN  |
| 1   | C     | 322 | ILE  |
| 1   | C     | 325 | TYR  |
| 1   | C     | 333 | ARG  |
| 1   | C     | 335 | GLU  |
| 1   | C     | 340 | VAL  |
| 1   | C     | 342 | PHE  |
| 1   | D     | 25  | LEU  |
| 1   | D     | 27  | LEU  |
| 1   | D     | 28  | PHE  |
| 1   | D     | 29  | LEU  |
| 1   | D     | 30  | LYS  |
| 1   | D     | 32  | PHE  |
| 1   | D     | 35  | GLU  |
| 1   | D     | 36  | VAL  |
| 1   | D     | 43  | THR  |
| 1   | D     | 44  | SER  |
| 1   | D     | 46  | THR  |
| 1   | D     | 47  | THR  |
| 1   | D     | 51  | MET  |
| 1   | D     | 52  | VAL  |
| 1   | D     | 55  | ILE  |
| 1   | D     | 59  | LYS  |
| 1   | D     | 73  | TYR  |
| 1   | D     | 74  | LEU  |
| 1   | D     | 81  | ASP  |
| 1   | D     | 83  | LYS  |
| 1   | D     | 84  | ARG  |
| 1   | D     | 85  | LYS  |
| 1   | D     | 88  | LYS  |
| 1   | D     | 91  | GLU  |
| 1   | D     | 92  | LYS  |
| 1   | D     | 94  | ILE  |
| 1   | D     | 95  | THR  |
| 1   | D     | 104 | VAL  |
| 1   | D     | 105 | LEU  |
| 1   | D     | 106 | ILE  |
| 1   | D     | 109 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 110 | GLU  |
| 1   | D     | 118 | VAL  |
| 1   | D     | 128 | GLU  |
| 1   | D     | 130 | LEU  |
| 1   | D     | 135 | ASP  |
| 1   | D     | 139 | LEU  |
| 1   | D     | 142 | ILE  |
| 1   | D     | 145 | LEU  |
| 1   | D     | 167 | THR  |
| 1   | D     | 169 | GLN  |
| 1   | D     | 176 | ASP  |
| 1   | D     | 182 | LYS  |
| 1   | D     | 183 | GLU  |
| 1   | D     | 200 | VAL  |
| 1   | D     | 205 | ARG  |
| 1   | D     | 210 | ASP  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 236 | LYS  |
| 1   | D     | 252 | HIS  |
| 1   | D     | 253 | LEU  |
| 1   | D     | 275 | ASN  |
| 1   | D     | 282 | LYS  |
| 1   | D     | 285 | LYS  |
| 1   | D     | 291 | LEU  |
| 1   | D     | 293 | MET  |
| 1   | D     | 294 | HIS  |
| 1   | D     | 300 | THR  |
| 1   | D     | 304 | ARG  |
| 1   | D     | 305 | ASP  |
| 1   | D     | 308 | LEU  |
| 1   | D     | 309 | GLU  |
| 1   | D     | 310 | ARG  |
| 1   | D     | 319 | ASP  |
| 1   | D     | 320 | GLN  |
| 1   | D     | 325 | TYR  |
| 1   | D     | 327 | MET  |
| 1   | D     | 332 | LEU  |
| 1   | D     | 335 | GLU  |
| 1   | D     | 341 | VAL  |
| 1   | E     | 24  | LYS  |
| 1   | E     | 25  | LEU  |
| 1   | E     | 27  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 29  | LEU  |
| 1   | E     | 32  | PHE  |
| 1   | E     | 35  | GLU  |
| 1   | E     | 51  | MET  |
| 1   | E     | 53  | ARG  |
| 1   | E     | 59  | LYS  |
| 1   | E     | 63  | PHE  |
| 1   | E     | 70  | GLN  |
| 1   | E     | 78  | GLU  |
| 1   | E     | 80  | LEU  |
| 1   | E     | 81  | ASP  |
| 1   | E     | 82  | ASP  |
| 1   | E     | 84  | ARG  |
| 1   | E     | 85  | LYS  |
| 1   | E     | 89  | HIS  |
| 1   | E     | 90  | THR  |
| 1   | E     | 91  | GLU  |
| 1   | E     | 101 | THR  |
| 1   | E     | 108 | ASP  |
| 1   | E     | 109 | ILE  |
| 1   | E     | 110 | GLU  |
| 1   | E     | 111 | ASP  |
| 1   | E     | 118 | VAL  |
| 1   | E     | 119 | ARG  |
| 1   | E     | 120 | SER  |
| 1   | E     | 123 | THR  |
| 1   | E     | 129 | SER  |
| 1   | E     | 130 | LEU  |
| 1   | E     | 132 | MET  |
| 1   | E     | 135 | ASP  |
| 1   | E     | 138 | VAL  |
| 1   | E     | 142 | ILE  |
| 1   | E     | 147 | ASN  |
| 1   | E     | 149 | GLU  |
| 1   | E     | 163 | THR  |
| 1   | E     | 165 | ILE  |
| 1   | E     | 166 | GLU  |
| 1   | E     | 170 | ASN  |
| 1   | E     | 171 | LYS  |
| 1   | E     | 174 | LEU  |
| 1   | E     | 176 | ASP  |
| 1   | E     | 183 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 188 | LEU  |
| 1   | E     | 190 | LYS  |
| 1   | E     | 192 | ARG  |
| 1   | E     | 195 | LEU  |
| 1   | E     | 199 | TYR  |
| 1   | E     | 200 | VAL  |
| 1   | E     | 205 | ARG  |
| 1   | E     | 210 | ASP  |
| 1   | E     | 217 | ILE  |
| 1   | E     | 222 | MET  |
| 1   | E     | 235 | GLU  |
| 1   | E     | 243 | MET  |
| 1   | E     | 249 | GLU  |
| 1   | E     | 275 | ASN  |
| 1   | E     | 276 | LYS  |
| 1   | E     | 294 | HIS  |
| 1   | E     | 300 | THR  |
| 1   | E     | 308 | LEU  |
| 1   | E     | 310 | ARG  |
| 1   | E     | 312 | ARG  |
| 1   | E     | 317 | GLN  |
| 1   | E     | 327 | MET  |
| 1   | E     | 335 | GLU  |
| 1   | E     | 340 | VAL  |
| 1   | E     | 341 | VAL  |
| 1   | F     | 24  | LYS  |
| 1   | F     | 25  | LEU  |
| 1   | F     | 27  | LEU  |
| 1   | F     | 28  | PHE  |
| 1   | F     | 29  | LEU  |
| 1   | F     | 31  | VAL  |
| 1   | F     | 32  | PHE  |
| 1   | F     | 65  | VAL  |
| 1   | F     | 68  | ARG  |
| 1   | F     | 73  | TYR  |
| 1   | F     | 80  | LEU  |
| 1   | F     | 84  | ARG  |
| 1   | F     | 87  | ILE  |
| 1   | F     | 88  | LYS  |
| 1   | F     | 89  | HIS  |
| 1   | F     | 100 | LEU  |
| 1   | F     | 101 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 104 | VAL  |
| 1   | F     | 105 | LEU  |
| 1   | F     | 108 | ASP  |
| 1   | F     | 110 | GLU  |
| 1   | F     | 118 | VAL  |
| 1   | F     | 121 | GLU  |
| 1   | F     | 128 | GLU  |
| 1   | F     | 130 | LEU  |
| 1   | F     | 139 | LEU  |
| 1   | F     | 142 | ILE  |
| 1   | F     | 145 | LEU  |
| 1   | F     | 147 | ASN  |
| 1   | F     | 176 | ASP  |
| 1   | F     | 180 | LEU  |
| 1   | F     | 183 | GLU  |
| 1   | F     | 188 | LEU  |
| 1   | F     | 192 | ARG  |
| 1   | F     | 200 | VAL  |
| 1   | F     | 204 | ASP  |
| 1   | F     | 205 | ARG  |
| 1   | F     | 210 | ASP  |
| 1   | F     | 212 | ASP  |
| 1   | F     | 231 | LEU  |
| 1   | F     | 240 | ARG  |
| 1   | F     | 252 | HIS  |
| 1   | F     | 282 | LYS  |
| 1   | F     | 283 | VAL  |
| 1   | F     | 285 | LYS  |
| 1   | F     | 288 | VAL  |
| 1   | F     | 291 | LEU  |
| 1   | F     | 292 | PHE  |
| 1   | F     | 295 | ARG  |
| 1   | F     | 298 | VAL  |
| 1   | F     | 300 | THR  |
| 1   | F     | 304 | ARG  |
| 1   | F     | 309 | GLU  |
| 1   | F     | 310 | ARG  |
| 1   | F     | 316 | PHE  |
| 1   | F     | 319 | ASP  |
| 1   | F     | 320 | GLN  |
| 1   | F     | 322 | ILE  |
| 1   | F     | 325 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 332 | LEU  |
| 1   | F     | 333 | ARG  |
| 1   | F     | 335 | GLU  |
| 1   | F     | 341 | VAL  |
| 1   | G     | 25  | LEU  |
| 1   | G     | 27  | LEU  |
| 1   | G     | 28  | PHE  |
| 1   | G     | 49  | ARG  |
| 1   | G     | 55  | ILE  |
| 1   | G     | 59  | LYS  |
| 1   | G     | 63  | PHE  |
| 1   | G     | 66  | LEU  |
| 1   | G     | 68  | ARG  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 73  | TYR  |
| 1   | G     | 74  | LEU  |
| 1   | G     | 78  | GLU  |
| 1   | G     | 79  | ASN  |
| 1   | G     | 83  | LYS  |
| 1   | G     | 85  | LYS  |
| 1   | G     | 86  | ASP  |
| 1   | G     | 96  | ILE  |
| 1   | G     | 103 | ASP  |
| 1   | G     | 106 | ILE  |
| 1   | G     | 107 | TYR  |
| 1   | G     | 108 | ASP  |
| 1   | G     | 109 | ILE  |
| 1   | G     | 113 | MET  |
| 1   | G     | 116 | TYR  |
| 1   | G     | 118 | VAL  |
| 1   | G     | 119 | ARG  |
| 1   | G     | 120 | SER  |
| 1   | G     | 122 | TYR  |
| 1   | G     | 129 | SER  |
| 1   | G     | 130 | LEU  |
| 1   | G     | 132 | MET  |
| 1   | G     | 138 | VAL  |
| 1   | G     | 139 | LEU  |
| 1   | G     | 141 | GLU  |
| 1   | G     | 145 | LEU  |
| 1   | G     | 149 | GLU  |
| 1   | G     | 157 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 165 | ILE  |
| 1   | G     | 169 | GLN  |
| 1   | G     | 171 | LYS  |
| 1   | G     | 175 | THR  |
| 1   | G     | 178 | VAL  |
| 1   | G     | 183 | GLU  |
| 1   | G     | 199 | TYR  |
| 1   | G     | 200 | VAL  |
| 1   | G     | 207 | PHE  |
| 1   | G     | 209 | CYS  |
| 1   | G     | 214 | TYR  |
| 1   | G     | 224 | ASN  |
| 1   | G     | 231 | LEU  |
| 1   | G     | 249 | GLU  |
| 1   | G     | 262 | ARG  |
| 1   | G     | 263 | GLU  |
| 1   | G     | 265 | THR  |
| 1   | G     | 266 | THR  |
| 1   | G     | 268 | GLN  |
| 1   | G     | 269 | LYS  |
| 1   | G     | 275 | ASN  |
| 1   | G     | 278 | GLU  |
| 1   | G     | 285 | LYS  |
| 1   | G     | 293 | MET  |
| 1   | G     | 298 | VAL  |
| 1   | G     | 301 | VAL  |
| 1   | G     | 303 | LEU  |
| 1   | G     | 304 | ARG  |
| 1   | G     | 308 | LEU  |
| 1   | G     | 309 | GLU  |
| 1   | G     | 310 | ARG  |
| 1   | G     | 313 | ARG  |
| 1   | G     | 320 | GLN  |
| 1   | G     | 322 | ILE  |
| 1   | G     | 324 | LYS  |
| 1   | G     | 325 | TYR  |
| 1   | G     | 327 | MET  |
| 1   | G     | 329 | HIS  |
| 1   | G     | 333 | ARG  |
| 1   | G     | 340 | VAL  |
| 1   | G     | 341 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | GLN  |
| 1   | A     | 89  | HIS  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 287 | ASN  |
| 1   | B     | 70  | GLN  |
| 1   | B     | 115 | HIS  |
| 1   | B     | 287 | ASN  |
| 1   | B     | 315 | ASN  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 280 | ASN  |
| 1   | C     | 329 | HIS  |
| 1   | D     | 125 | GLN  |
| 1   | D     | 252 | HIS  |
| 1   | D     | 294 | HIS  |
| 1   | D     | 320 | GLN  |
| 1   | E     | 70  | GLN  |
| 1   | E     | 115 | HIS  |
| 1   | E     | 177 | GLN  |
| 1   | E     | 315 | ASN  |
| 1   | E     | 320 | GLN  |
| 1   | E     | 329 | HIS  |
| 1   | F     | 79  | ASN  |
| 1   | F     | 169 | GLN  |
| 1   | F     | 198 | ASN  |
| 1   | F     | 224 | ASN  |
| 1   | F     | 317 | GLN  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 79  | ASN  |
| 1   | G     | 114 | ASN  |
| 1   | G     | 115 | HIS  |
| 1   | G     | 241 | ASN  |
| 1   | G     | 329 | 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.