



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:41 AM UTC

PDB ID : 8SYF / pdb\_00008syf  
EMDB ID : EMD-29646  
Title : Homology model of Acto-HMM complex in ADP-state. Chicken smooth muscle HMM and chicken pectoralis actin  
Authors : Hojjatian, A.; Taylor, D.W.; Daneshparvar, N.; Trybus, K.M.; Taylor, K.A.  
Deposited on : 2023-05-25  
Resolution : 19.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

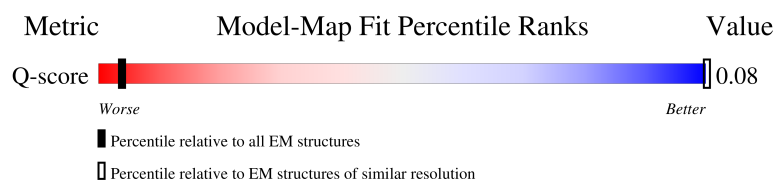
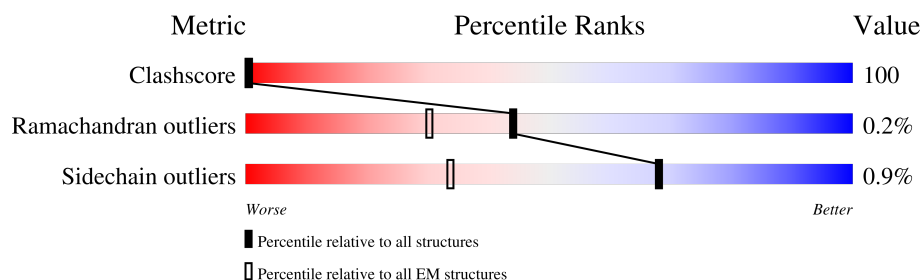
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 19.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 17 ( 18.70 - 19.50 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 843    |                  |
| 1   | B     | 843    |                  |
| 2   | C     | 375    |                  |
| 2   | D     | 375    |                  |

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| Mol | Chain | Length | Quality of chain                                      |
|-----|-------|--------|-------------------------------------------------------|
| 3   | E     | 148    | <div><div></div><div>15%84%</div><div></div></div>    |
| 3   | H     | 148    | <div><div></div><div>20%79%</div><div></div></div>    |
| 4   | F     | 143    | <div><div></div><div>6%40%60%</div><div></div></div>  |
| 4   | G     | 143    | <div><div></div><div>52%61%38%</div><div></div></div> |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23456 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 Myosin, heavy chain 11, smooth muscle.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 800      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6474  | 4129 | 1118 | 1195 | 32 |         |       |
| 1   | B     | 800      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6474  | 4129 | 1118 | 1195 | 32 |         |       |

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | C     | 375      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2933  | 1854 | 493 | 565 | 21 |         |       |
| 2   | D     | 375      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2933  | 1854 | 493 | 565 | 21 |         |       |

- Molecule 3 is a protein called Myosin light polypeptide 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | E     | 148      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1160  | 720 | 193 | 236 | 11 |         |       |
| 3   | H     | 148      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1160  | 720 | 193 | 236 | 11 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 65      | ASN      | LYS    | conflict | UNP P02607 |
| H     | 65      | ASN      | LYS    | conflict | UNP P02607 |

- Molecule 4 is a protein called Myosin regulatory light chain 2, smooth muscle major isoform.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | F     | 143      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1161  | 727 | 189 | 235 | 10 |         |       |

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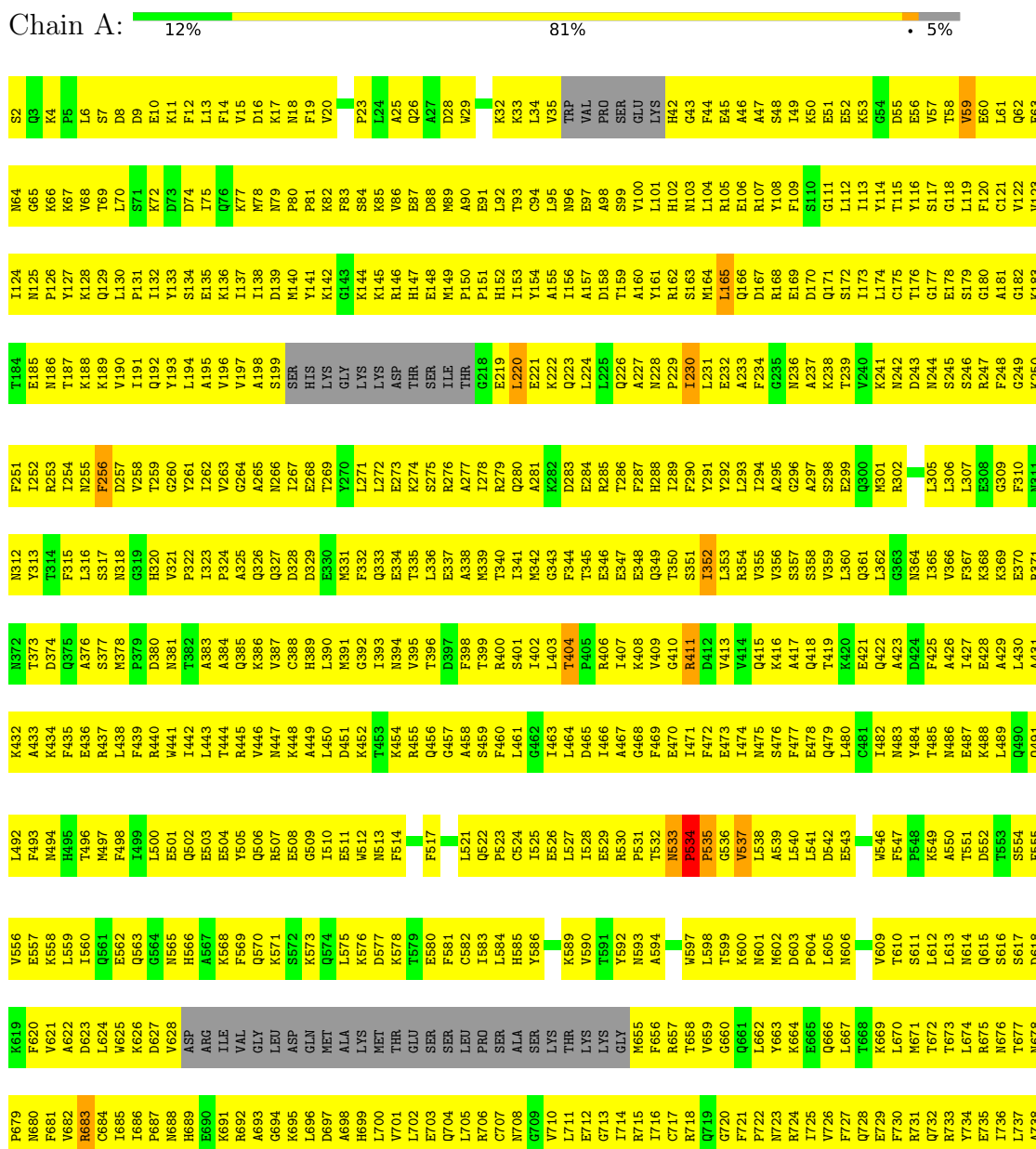
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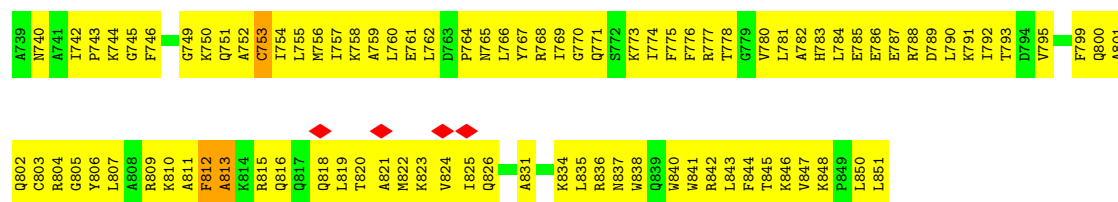
| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | G     | 143      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1161  | 727 | 189 | 235 | 10 |         |       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

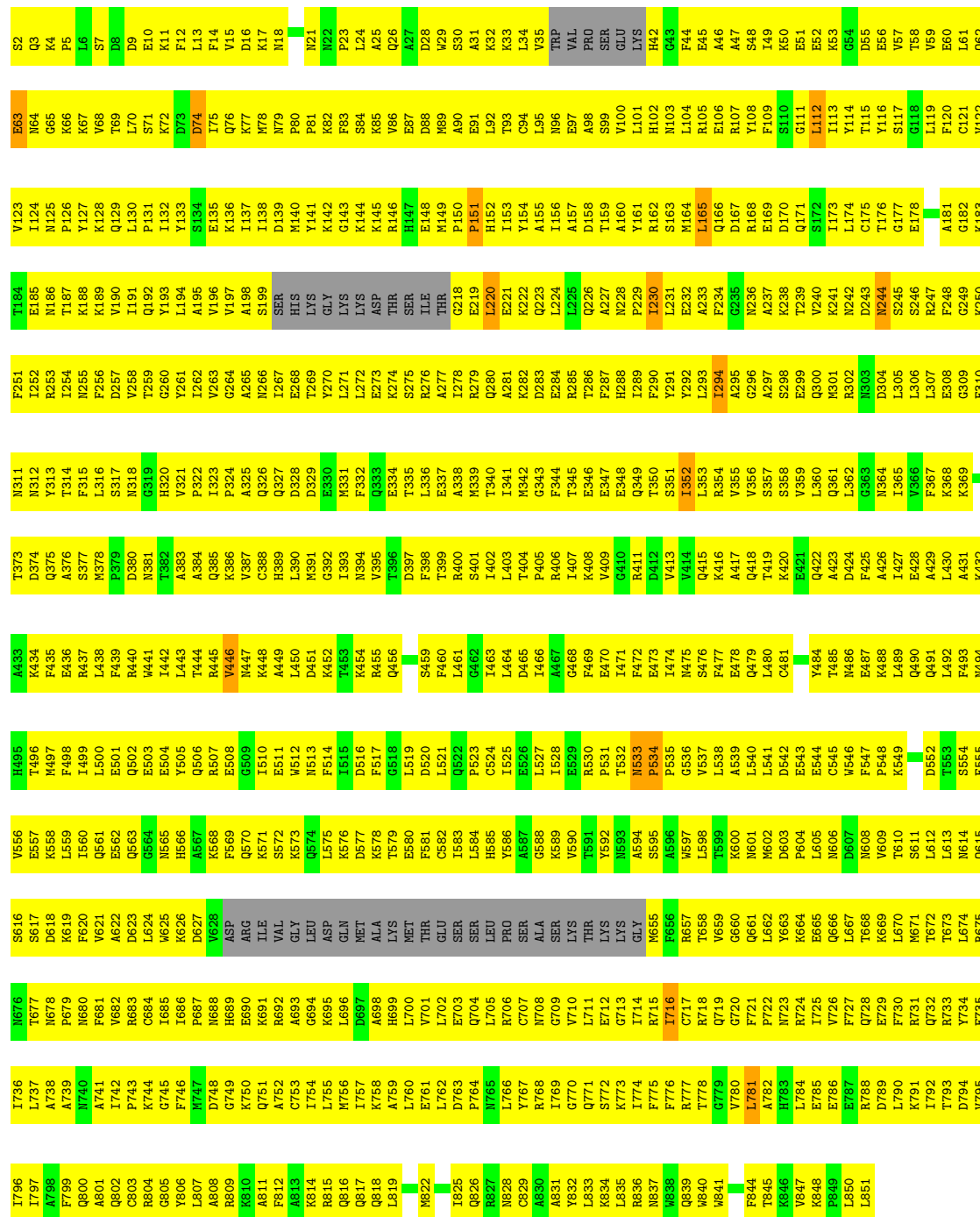
- Molecule 1: Myosin, heavy chain 11, smooth muscle



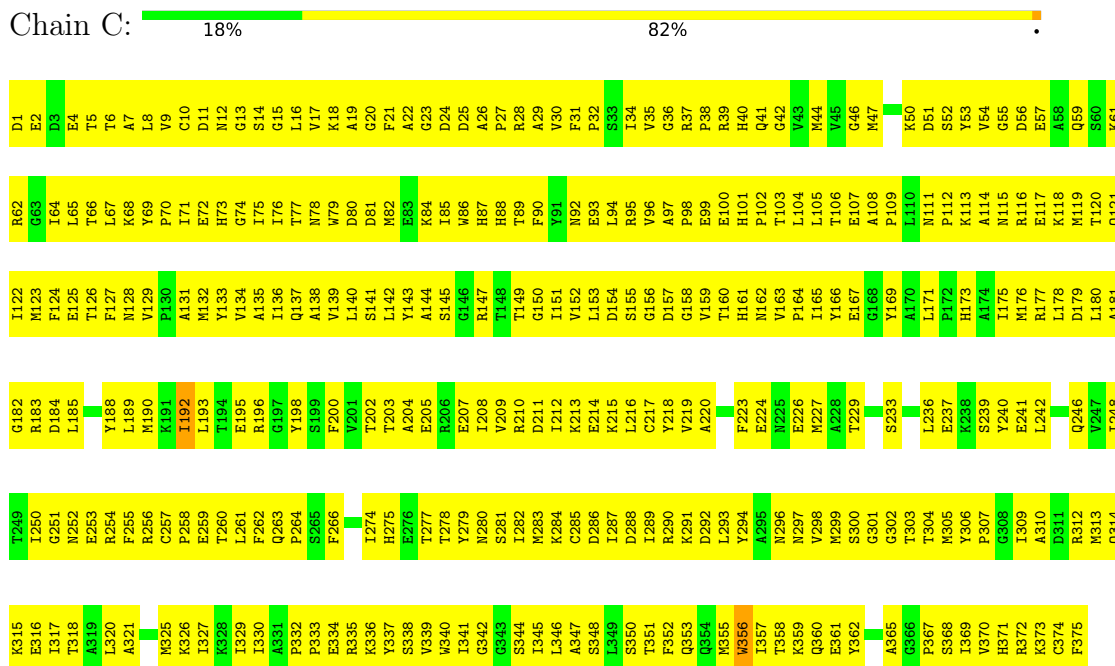


• Molecule 1: Myosin, heavy chain 11, smooth muscle

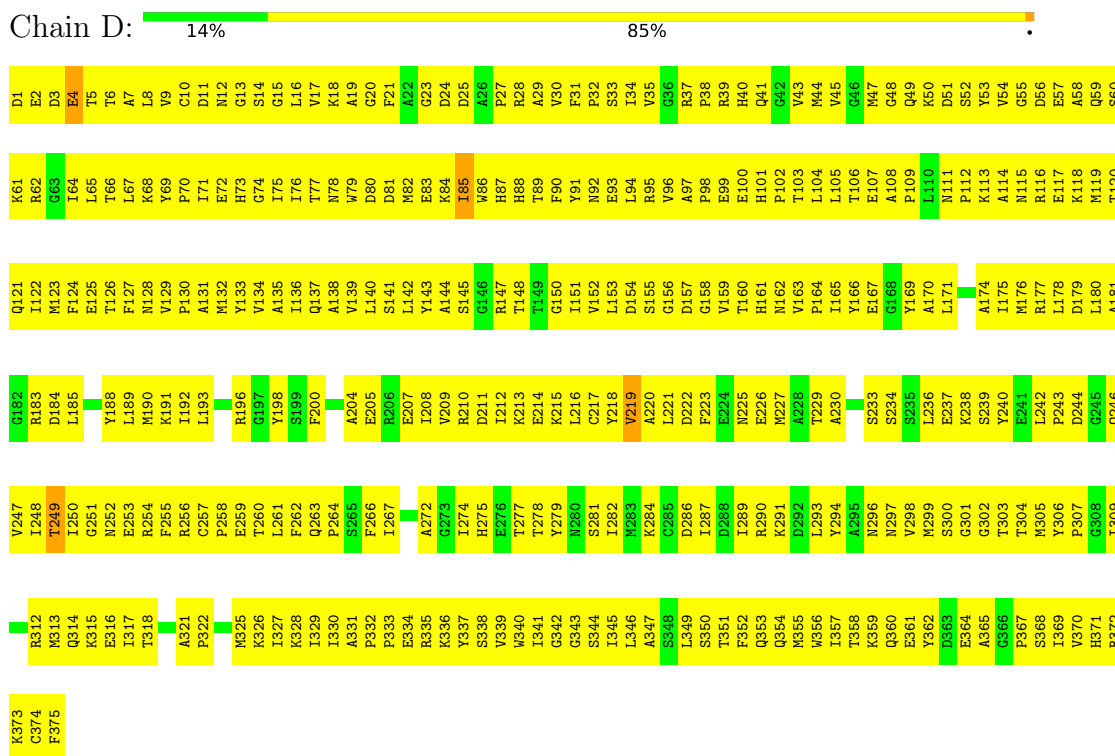
Chain B: 10% 83% 5%



- Molecule 2: Actin, alpha skeletal muscle

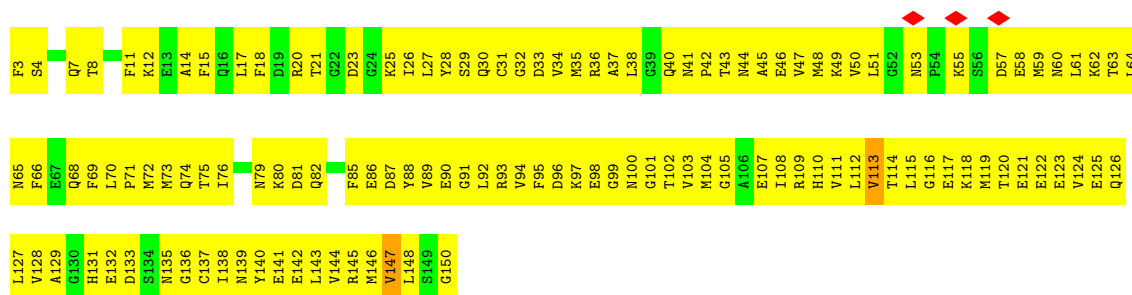


- Molecule 2: Actin, alpha skeletal muscle



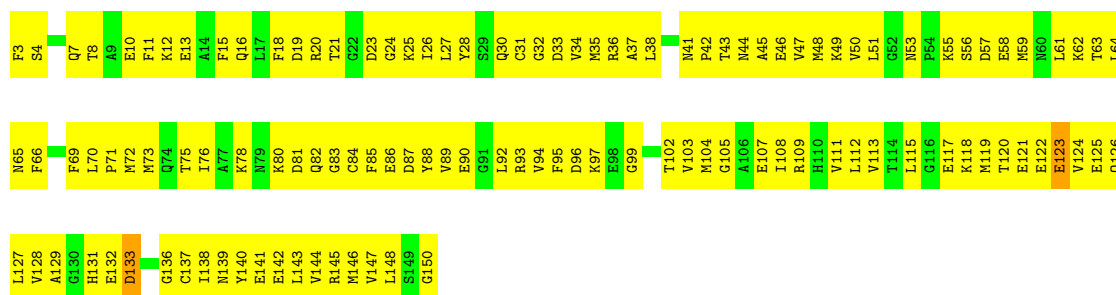
- Molecule 3: Myosin light polypeptide 6





• Molecule 3: Myosin light polypeptide 6

Chain H: 20% 79%



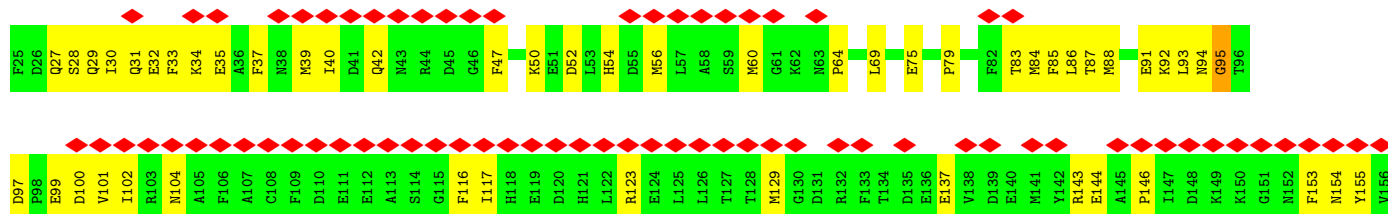
• Molecule 4: Myosin regulatory light chain 2, smooth muscle major isoform

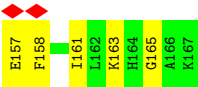
Chain F: 6% 40% 60%



• Molecule 4: Myosin regulatory light chain 2, smooth muscle major isoform

Chain G: 52% 61% 38%





## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 17394                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 29.6                            | Depositor |
| Minimum defocus (nm)                 | 200                             | Depositor |
| Maximum defocus (nm)                 | 2000                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | DIRECT ELECTRON DE-64 (8k x 8k) | Depositor |
| Maximum map value                    | 0.261                           | Depositor |
| Minimum map value                    | -0.127                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.026                           | Depositor |
| Recommended contour level            | 0.0472                          | Depositor |
| Map size ( $\text{\AA}$ )            | 537.6, 537.6, 537.6             | wwPDB     |
| Map dimensions                       | 210, 210, 210                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.56, 2.56, 2.56                | 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         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.42         | 0/6595         | 0.71        | 2/8886 (0.0%)   |
| 1   | B     | 0.42         | 0/6595         | 0.71        | 8/8886 (0.1%)   |
| 2   | C     | 0.38         | 0/2996         | 0.64        | 0/4058          |
| 2   | D     | 0.40         | 1/2996 (0.0%)  | 0.65        | 1/4058 (0.0%)   |
| 3   | E     | 0.32         | 0/1175         | 0.68        | 1/1575 (0.1%)   |
| 3   | H     | 0.29         | 0/1175         | 0.57        | 0/1575          |
| 4   | F     | 0.19         | 0/1185         | 0.50        | 0/1589          |
| 4   | G     | 0.17         | 0/1185         | 0.47        | 1/1589 (0.1%)   |
| All | All   | 0.38         | 1/23902 (0.0%) | 0.67        | 13/32216 (0.0%) |

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                   | 3                   |
| 1   | B     | 0                   | 1                   |
| 2   | C     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | D     | 170 | ALA  | C-N   | 5.63 | 1.42        | 1.33     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 63  | GLU  | N-CA-C | -7.08 | 105.83      | 114.75   |
| 4   | G     | 95  | GLY  | N-CA-C | -5.97 | 107.98      | 115.08   |
| 1   | B     | 244 | ASN  | N-CA-C | -5.95 | 105.84      | 112.57   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 126 | THR  | N-CA-C   | -5.92 | 106.68      | 114.31   |
| 1   | A     | 220 | LEU  | CA-CB-CG | -5.89 | 95.68       | 116.30   |
| 1   | B     | 741 | ALA  | N-CA-C   | -5.66 | 105.31      | 114.09   |
| 1   | B     | 151 | PRO  | CA-C-N   | -5.56 | 112.16      | 121.94   |
| 1   | B     | 151 | PRO  | C-N-CA   | -5.56 | 112.16      | 121.94   |
| 1   | B     | 220 | LEU  | CA-CB-CG | -5.37 | 97.50       | 116.30   |
| 1   | B     | 781 | LEU  | N-CA-C   | 5.37  | 116.82      | 110.97   |
| 3   | E     | 113 | VAL  | CB-CA-C  | -5.32 | 104.61      | 111.20   |
| 1   | B     | 588 | GLY  | N-CA-C   | -5.19 | 106.14      | 112.68   |
| 1   | A     | 411 | ARG  | N-CA-C   | -5.01 | 108.19      | 114.56   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 533 | ASN  | Peptide |
| 1   | A     | 534 | PRO  | Peptide |
| 1   | A     | 683 | ARG  | Peptide |
| 1   | B     | 533 | ASN  | Peptide |
| 2   | C     | 356 | TRP  | Peptide |
| 2   | D     | 4   | GLU  | 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     | 6474  | 0        | 6518     | 1468    | 0            |
| 1   | B     | 6474  | 0        | 6518     | 1506    | 0            |
| 2   | C     | 2933  | 0        | 2894     | 655     | 0            |
| 2   | D     | 2933  | 0        | 2894     | 642     | 0            |
| 3   | E     | 1160  | 0        | 1119     | 284     | 0            |
| 3   | H     | 1160  | 0        | 1119     | 203     | 0            |
| 4   | F     | 1161  | 0        | 1076     | 104     | 0            |
| 4   | G     | 1161  | 0        | 1076     | 62      | 0            |
| All | All   | 23456 | 0        | 23214    | 4678    | 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 100.

All (4678) 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:2:SER:N      | 1:B:141:TYR:HH   | 1.38                     | 1.22              |
| 1:B:446:VAL:O    | 1:B:450:LEU:HB2  | 1.45                     | 1.16              |
| 2:C:154:ASP:O    | 2:C:160:THR:HA   | 1.46                     | 1.14              |
| 3:E:32:GLY:HA2   | 3:E:72:MET:HE1   | 1.39                     | 1.05              |
| 1:A:61:LEU:O     | 1:A:65:GLY:N     | 1.91                     | 1.03              |
| 1:A:488:LYS:HB3  | 1:A:667:LEU:HD11 | 1.41                     | 1.02              |
| 2:D:156:GLY:HA2  | 2:D:302:GLY:H    | 1.26                     | 1.01              |
| 1:B:194:LEU:HD11 | 1:B:461:LEU:HD23 | 1.43                     | 1.00              |
| 1:B:540:LEU:HD22 | 1:B:558:LYS:HB3  | 1.40                     | 1.00              |
| 1:A:768:ARG:O    | 1:A:774:ILE:HA   | 1.60                     | 1.00              |
| 1:A:510:ILE:HG12 | 1:A:768:ARG:HG2  | 1.44                     | 0.99              |
| 3:E:104:MET:HA   | 3:E:137:CYS:HA   | 1.41                     | 0.99              |
| 2:D:237:GLU:HA   | 2:D:251:GLY:HA2  | 1.45                     | 0.97              |
| 1:A:233:ALA:HA   | 1:A:288:HIS:HB2  | 1.47                     | 0.96              |
| 1:A:221:GLU:O    | 1:A:224:LEU:HB3  | 1.65                     | 0.96              |
| 1:B:16:ASP:H     | 1:B:112:LEU:HD11 | 1.28                     | 0.96              |
| 1:B:138:ILE:HG12 | 1:B:193:TYR:HA   | 1.45                     | 0.95              |
| 1:B:299:GLU:HA   | 1:B:302:ARG:HB2  | 1.47                     | 0.95              |
| 2:C:79:TRP:HA    | 2:C:82:MET:HB2   | 1.47                     | 0.95              |
| 1:B:512:TRP:NE1  | 1:B:764:PRO:O    | 1.99                     | 0.95              |
| 2:D:10:CYS:SG    | 2:D:86:TRP:NE1   | 2.40                     | 0.94              |
| 1:A:97:GLU:O     | 1:A:101:LEU:HB2  | 1.68                     | 0.94              |
| 1:A:101:LEU:HD11 | 1:A:702:LEU:HB2  | 1.47                     | 0.94              |
| 1:B:411:ARG:H    | 2:C:28:ARG:HG3   | 1.32                     | 0.94              |
| 1:A:274:LYS:O    | 1:A:277:ALA:HB3  | 1.67                     | 0.94              |
| 1:B:375:GLN:HB2  | 1:B:417:ALA:HB3  | 1.49                     | 0.94              |
| 1:A:122:VAL:HG13 | 1:A:685:ILE:HD12 | 1.49                     | 0.94              |
| 1:B:739:ALA:HB1  | 1:B:742:ILE:HB   | 1.51                     | 0.94              |
| 1:B:293:LEU:HD11 | 1:B:353:LEU:HB3  | 1.49                     | 0.93              |
| 1:B:289:ILE:HA   | 1:B:292:TYR:HB2  | 1.50                     | 0.93              |
| 2:D:361:GLU:HB3  | 2:D:369:ILE:HG12 | 1.48                     | 0.93              |
| 2:C:218:TYR:HB3  | 2:C:255:PHE:HB3  | 1.50                     | 0.93              |
| 2:C:156:GLY:HA3  | 2:C:303:THR:H    | 1.34                     | 0.93              |
| 2:C:218:TYR:HA   | 2:C:307:PRO:HD2  | 1.48                     | 0.92              |
| 1:B:294:ILE:HG12 | 1:B:307:LEU:HD22 | 1.51                     | 0.92              |
| 2:C:237:GLU:HA   | 2:C:250:ILE:O    | 1.69                     | 0.92              |
| 2:D:162:ASN:HB2  | 2:D:176:MET:HE2  | 1.52                     | 0.92              |
| 1:B:492:LEU:HD11 | 1:B:671:MET:HG2  | 1.50                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:61:LEU:HD21  | 1:A:70:LEU:HD22  | 1.52                     | 0.91              |
| 1:A:293:LEU:HG   | 1:A:307:LEU:HD11 | 1.53                     | 0.91              |
| 1:A:294:ILE:HG12 | 1:A:307:LEU:HD22 | 1.49                     | 0.91              |
| 1:B:221:GLU:O    | 1:B:224:LEU:HB3  | 1.71                     | 0.90              |
| 2:D:242:LEU:HB3  | 2:D:246:GLN:HB3  | 1.52                     | 0.90              |
| 1:A:299:GLU:HA   | 1:A:302:ARG:HB2  | 1.53                     | 0.90              |
| 1:B:130:LEU:O    | 1:B:189:LYS:NZ   | 2.04                     | 0.90              |
| 1:B:29:TRP:HZ2   | 1:B:34:LEU:H     | 1.16                     | 0.90              |
| 1:B:430:LEU:O    | 1:B:434:LYS:HB2  | 1.69                     | 0.90              |
| 1:B:545:CYS:SG   | 1:B:601:ASN:ND2  | 2.44                     | 0.90              |
| 2:D:219:VAL:HG23 | 2:D:306:TYR:HB2  | 1.54                     | 0.90              |
| 2:D:11:ASP:O     | 2:D:17:VAL:HA    | 1.72                     | 0.90              |
| 2:D:81:ASP:HA    | 2:D:84:LYS:HD2   | 1.53                     | 0.89              |
| 1:A:610:THR:HA   | 1:A:613:LEU:HD12 | 1.53                     | 0.89              |
| 2:C:185:LEU:HB3  | 2:C:213:LYS:HD2  | 1.54                     | 0.89              |
| 1:A:238:LYS:HG3  | 1:A:324:PRO:HD2  | 1.54                     | 0.88              |
| 1:B:335:THR:HG22 | 1:B:339:MET:HE2  | 1.53                     | 0.88              |
| 1:A:10:GLU:O     | 1:A:14:PHE:N     | 2.06                     | 0.88              |
| 1:A:416:LYS:HD2  | 2:D:25:ASP:HB3   | 1.55                     | 0.88              |
| 3:E:43:THR:HG22  | 3:E:45:ALA:H     | 1.38                     | 0.88              |
| 1:B:488:LYS:HG3  | 1:B:671:MET:HG3  | 1.54                     | 0.88              |
| 2:C:321:ALA:HB2  | 2:C:327:ILE:HD11 | 1.56                     | 0.88              |
| 1:B:686:ILE:HG22 | 1:B:700:LEU:HB3  | 1.55                     | 0.88              |
| 2:C:76:ILE:HG23  | 2:C:82:MET:HG3   | 1.54                     | 0.88              |
| 2:D:299:MET:HE3  | 2:D:313:MET:HB3  | 1.56                     | 0.88              |
| 1:B:239:THR:HA   | 1:B:284:GLU:HG2  | 1.53                     | 0.88              |
| 1:B:558:LYS:O    | 1:B:562:GLU:HB2  | 1.74                     | 0.88              |
| 3:H:33:ASP:HA    | 3:H:36:ARG:HD2   | 1.55                     | 0.88              |
| 1:A:116:TYR:HA   | 1:A:120:PHE:O    | 1.73                     | 0.88              |
| 1:B:232:GLU:HA   | 1:B:236:ASN:HB2  | 1.56                     | 0.88              |
| 1:B:132:ILE:O    | 1:B:152:HIS:NE2  | 2.06                     | 0.88              |
| 2:C:88:HIS:O     | 2:C:93:GLU:N     | 2.07                     | 0.87              |
| 1:A:806:TYR:OH   | 3:H:144:VAL:O    | 1.91                     | 0.87              |
| 1:A:138:ILE:HD11 | 1:A:192:GLN:HG3  | 1.56                     | 0.87              |
| 1:B:488:LYS:HB3  | 1:B:667:LEU:HD11 | 1.54                     | 0.87              |
| 1:A:34:LEU:HD23  | 1:A:78:MET:HG3   | 1.56                     | 0.87              |
| 1:B:173:ILE:HG12 | 1:B:461:LEU:HD11 | 1.57                     | 0.87              |
| 2:C:6:THR:HA     | 2:C:22:ALA:HB3   | 1.56                     | 0.87              |
| 3:E:35:MET:O     | 3:E:40:GLN:NE2   | 2.06                     | 0.87              |
| 2:D:212:ILE:HG23 | 2:D:216:LEU:HB2  | 1.54                     | 0.87              |
| 1:A:193:TYR:HD2  | 1:A:194:LEU:HD23 | 1.40                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:238:LYS:HB3  | 1:B:285:ARG:H    | 1.39                     | 0.87              |
| 1:B:50:LYS:HG3   | 1:B:60:GLU:H     | 1.37                     | 0.86              |
| 1:B:285:ARG:NH2  | 1:B:328:ASP:OD1  | 2.07                     | 0.86              |
| 1:B:753:CYS:HB3  | 1:B:774:ILE:HD11 | 1.53                     | 0.86              |
| 2:C:347:ALA:HA   | 2:C:352:PHE:HB2  | 1.55                     | 0.86              |
| 2:D:78:ASN:HB3   | 2:D:81:ASP:HB2   | 1.56                     | 0.86              |
| 1:B:173:ILE:HA   | 1:B:680:ASN:HB2  | 1.55                     | 0.86              |
| 1:B:570:GLN:HB3  | 1:B:582:CYS:HB2  | 1.56                     | 0.86              |
| 2:D:153:LEU:HD11 | 2:D:274:ILE:HG12 | 1.57                     | 0.86              |
| 3:H:32:GLY:HA3   | 3:H:47:VAL:HG13  | 1.58                     | 0.86              |
| 1:B:79:ASN:HB2   | 1:B:83:PHE:HB2   | 1.55                     | 0.86              |
| 2:C:346:LEU:HB3  | 2:C:355:MET:HE1  | 1.56                     | 0.86              |
| 2:C:193:LEU:HD21 | 2:C:250:ILE:HG13 | 1.58                     | 0.86              |
| 1:A:228:ASN:O    | 1:A:232:GLU:N    | 2.09                     | 0.85              |
| 1:B:293:LEU:HG   | 1:B:307:LEU:HD11 | 1.57                     | 0.85              |
| 3:H:125:GLU:O    | 3:H:129:ALA:N    | 2.10                     | 0.85              |
| 1:A:512:TRP:HE1  | 1:A:721:PHE:HZ   | 1.24                     | 0.85              |
| 3:E:28:TYR:HB2   | 3:E:59:MET:HA    | 1.58                     | 0.85              |
| 1:A:352:ILE:HG13 | 1:A:620:PHE:CE2  | 2.12                     | 0.85              |
| 1:A:570:GLN:HB2  | 1:A:582:CYS:HB2  | 1.59                     | 0.85              |
| 1:A:848:LYS:HA   | 1:A:851:LEU:HB2  | 1.58                     | 0.85              |
| 2:C:11:ASP:HB3   | 2:C:18:LYS:HB2   | 1.58                     | 0.85              |
| 1:B:107:ARG:HG2  | 1:B:112:LEU:HD12 | 1.59                     | 0.85              |
| 1:A:505:TYR:HA   | 1:A:510:ILE:HD12 | 1.58                     | 0.84              |
| 1:A:249:GLY:H    | 1:A:271:LEU:HB2  | 1.38                     | 0.84              |
| 3:H:113:VAL:HG11 | 3:H:121:GLU:HA   | 1.59                     | 0.84              |
| 1:A:285:ARG:HH21 | 1:A:291:TYR:HB2  | 1.41                     | 0.84              |
| 1:B:293:LEU:HD22 | 1:B:356:VAL:HB   | 1.58                     | 0.84              |
| 1:B:340:THR:OG1  | 1:B:349:GLN:NE2  | 2.10                     | 0.84              |
| 1:B:722:PRO:HG2  | 1:B:778:THR:H    | 1.40                     | 0.84              |
| 2:C:361:GLU:HB3  | 2:C:369:ILE:HG12 | 1.59                     | 0.84              |
| 1:A:114:TYR:HA   | 1:A:122:VAL:O    | 1.78                     | 0.84              |
| 2:C:219:VAL:HG23 | 2:C:306:TYR:HB2  | 1.59                     | 0.84              |
| 1:A:163:SER:O    | 1:A:169:GLU:N    | 2.09                     | 0.84              |
| 1:B:138:ILE:HG23 | 1:B:197:VAL:HG23 | 1.60                     | 0.84              |
| 1:A:597:TRP:O    | 1:A:601:ASN:N    | 2.10                     | 0.84              |
| 2:C:151:ILE:HB   | 2:C:297:ASN:HA   | 1.59                     | 0.84              |
| 2:D:90:PHE:HA    | 2:D:94:LEU:HB2   | 1.60                     | 0.84              |
| 2:C:155:SER:N    | 2:C:300:SER:O    | 2.09                     | 0.83              |
| 2:C:286:ASP:OD2  | 2:D:39:ARG:NH1   | 2.10                     | 0.83              |
| 1:A:290:PHE:HB3  | 1:A:316:LEU:HD21 | 1.60                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:304:THR:HB   | 2:C:335:ARG:HE   | 1.41                     | 0.83              |
| 1:A:385:GLN:HG3  | 1:A:395:VAL:HG21 | 1.61                     | 0.83              |
| 1:B:704:GLN:HA   | 1:B:707:CYS:HB3  | 1.59                     | 0.83              |
| 3:H:35:MET:HB3   | 3:H:76:ILE:HG21  | 1.58                     | 0.83              |
| 1:B:601:ASN:OD1  | 1:B:660:GLY:N    | 2.09                     | 0.83              |
| 1:B:61:LEU:O     | 1:B:65:GLY:N     | 2.12                     | 0.83              |
| 1:B:220:LEU:HD21 | 1:B:452:LYS:HG3  | 1.60                     | 0.83              |
| 1:A:336:LEU:O    | 1:A:349:GLN:NE2  | 2.12                     | 0.82              |
| 1:B:171:GLN:HE22 | 1:B:678:ASN:HB3  | 1.43                     | 0.82              |
| 3:E:32:GLY:HA3   | 3:E:47:VAL:HG13  | 1.58                     | 0.82              |
| 1:B:120:PHE:HZ   | 1:B:497:MET:HB2  | 1.43                     | 0.82              |
| 2:D:136:ILE:HB   | 2:D:139:VAL:HB   | 1.62                     | 0.82              |
| 1:A:48:SER:O     | 1:A:60:GLU:N     | 2.11                     | 0.82              |
| 1:A:355:VAL:HG21 | 1:A:624:LEU:HD13 | 1.60                     | 0.82              |
| 3:E:104:MET:O    | 3:E:108:ILE:N    | 2.12                     | 0.82              |
| 1:B:138:ILE:HD11 | 1:B:192:GLN:HG3  | 1.59                     | 0.82              |
| 2:C:177:ARG:NH1  | 2:C:179:ASP:OD1  | 2.13                     | 0.82              |
| 2:C:236:LEU:HB3  | 2:C:255:PHE:HE1  | 1.44                     | 0.82              |
| 1:A:187:THR:OG1  | 1:A:465:ASP:OD1  | 1.97                     | 0.82              |
| 1:A:540:LEU:HD22 | 1:A:558:LYS:HB3  | 1.58                     | 0.82              |
| 1:B:802:GLN:HG3  | 3:E:147:VAL:HG12 | 1.61                     | 0.82              |
| 3:E:40:GLN:HG3   | 3:E:80:LYS:HA    | 1.62                     | 0.82              |
| 1:A:224:LEU:HD13 | 1:A:267:ILE:HG21 | 1.62                     | 0.81              |
| 2:C:8:LEU:HG     | 2:C:101:HIS:HB2  | 1.62                     | 0.81              |
| 2:C:239:SER:HA   | 2:C:248:ILE:O    | 1.80                     | 0.81              |
| 2:D:317:ILE:HG22 | 2:D:327:ILE:HD13 | 1.60                     | 0.81              |
| 1:A:53:LYS:HE2   | 1:A:56:GLU:HB3   | 1.60                     | 0.81              |
| 1:A:686:ILE:HB   | 1:A:704:GLN:HG3  | 1.62                     | 0.81              |
| 2:C:111:ASN:OD1  | 2:C:177:ARG:NH2  | 2.12                     | 0.81              |
| 1:A:162:ARG:O    | 1:A:166:GLN:N    | 2.13                     | 0.81              |
| 1:A:223:GLN:HB3  | 1:A:342:MET:HE1  | 1.60                     | 0.81              |
| 1:B:152:HIS:CD2  | 1:B:154:TYR:HB2  | 2.15                     | 0.81              |
| 1:B:480:LEU:HD11 | 1:B:528:ILE:HD12 | 1.62                     | 0.81              |
| 2:D:98:PRO:HB2   | 2:D:127:PHE:HB3  | 1.61                     | 0.81              |
| 1:A:32:LYS:HB3   | 1:A:49:ILE:HB    | 1.63                     | 0.81              |
| 1:B:803:CYS:SG   | 3:E:127:LEU:HB2  | 2.20                     | 0.81              |
| 3:E:46:GLU:HA    | 3:E:49:LYS:HG3   | 1.63                     | 0.81              |
| 1:A:179:SER:O    | 1:A:242:ASN:ND2  | 2.12                     | 0.81              |
| 1:B:826:GLN:HG2  | 4:F:129:MET:HB3  | 1.61                     | 0.81              |
| 1:A:174:LEU:HA   | 1:A:464:LEU:HB3  | 1.63                     | 0.81              |
| 2:C:279:TYR:HA   | 2:C:282:ILE:HD12 | 1.63                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:762:LEU:HD11 | 1:A:784:LEU:HD21 | 1.62                     | 0.81              |
| 2:D:166:TYR:HD1  | 2:D:293:LEU:HD21 | 1.44                     | 0.81              |
| 2:C:90:PHE:HA    | 2:C:94:LEU:HB2   | 1.62                     | 0.80              |
| 1:A:115:THR:HB   | 1:A:122:VAL:HB   | 1.63                     | 0.80              |
| 1:B:233:ALA:HB1  | 1:B:289:ILE:HB   | 1.63                     | 0.80              |
| 1:B:242:ASN:HB3  | 1:B:245:SER:HB3  | 1.64                     | 0.80              |
| 1:B:271:LEU:H    | 1:B:666:GLN:HB3  | 1.45                     | 0.80              |
| 2:D:79:TRP:HE3   | 2:D:122:ILE:HG12 | 1.44                     | 0.80              |
| 2:C:123:MET:O    | 2:C:129:VAL:N    | 2.12                     | 0.80              |
| 1:B:347:GLU:OE1  | 1:B:354:ARG:NH2  | 2.13                     | 0.80              |
| 1:A:107:ARG:HB3  | 1:A:112:LEU:HB2  | 1.63                     | 0.80              |
| 1:A:292:TYR:HB3  | 1:A:332:PHE:HB2  | 1.63                     | 0.80              |
| 1:B:105:ARG:HB2  | 1:B:698:ALA:HB2  | 1.62                     | 0.80              |
| 1:B:294:ILE:HD12 | 1:B:310:PHE:HA   | 1.64                     | 0.80              |
| 2:C:241:GLU:HA   | 2:C:246:GLN:O    | 1.82                     | 0.80              |
| 2:D:24:ASP:HB2   | 2:D:340:TRP:HH2  | 1.43                     | 0.80              |
| 1:B:29:TRP:HE1   | 1:B:34:LEU:HB2   | 1.47                     | 0.80              |
| 2:D:11:ASP:HB3   | 2:D:18:LYS:HB2   | 1.61                     | 0.80              |
| 2:D:102:PRO:HB3  | 2:D:131:ALA:HB3  | 1.60                     | 0.80              |
| 2:D:190:MET:HG3  | 2:D:200:PHE:HB2  | 1.62                     | 0.80              |
| 1:A:313:TYR:CG   | 1:A:360:LEU:HB3  | 2.17                     | 0.80              |
| 1:B:187:THR:HG21 | 1:B:252:ILE:HD13 | 1.62                     | 0.80              |
| 1:B:527:LEU:HD11 | 1:B:583:ILE:HG12 | 1.63                     | 0.80              |
| 1:A:530:ARG:O    | 1:A:536:GLY:N    | 2.14                     | 0.80              |
| 1:B:726:VAL:HA   | 1:B:773:LYS:HG2  | 1.63                     | 0.80              |
| 1:A:809:ARG:HB2  | 3:H:41:ASN:HB3   | 1.63                     | 0.80              |
| 1:B:451:ASP:OD2  | 1:B:455:ARG:NH1  | 2.15                     | 0.80              |
| 2:C:356:TRP:O    | 2:C:373:LYS:NZ   | 2.14                     | 0.80              |
| 2:D:365:ALA:O    | 2:D:372:ARG:NH1  | 2.15                     | 0.80              |
| 1:B:163:SER:HA   | 1:B:167:ASP:HB2  | 1.62                     | 0.79              |
| 1:B:336:LEU:HD21 | 1:B:353:LEU:HD11 | 1.64                     | 0.79              |
| 3:H:42:PRO:HG3   | 3:H:76:ILE:HD12  | 1.61                     | 0.79              |
| 3:H:141:GLU:HB3  | 3:H:145:ARG:HH21 | 1.47                     | 0.79              |
| 1:A:733:ARG:NH2  | 1:A:734:TYR:OH   | 2.15                     | 0.79              |
| 1:B:80:PRO:HG2   | 1:B:785:GLU:HB2  | 1.64                     | 0.79              |
| 1:A:194:LEU:HD12 | 1:A:254:ILE:HD12 | 1.65                     | 0.79              |
| 1:B:586:TYR:OH   | 1:B:715:ARG:NH2  | 2.15                     | 0.79              |
| 1:B:579:THR:HG1  | 1:B:595:SER:HG   | 1.22                     | 0.79              |
| 2:C:105:LEU:HD12 | 2:C:119:MET:HB3  | 1.64                     | 0.79              |
| 1:B:610:THR:HA   | 1:B:613:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:220:LEU:HD11 | 1:A:452:LYS:HE3  | 1.64                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:198:ALA:HB1  | 1:B:261:TYR:HA   | 1.62                     | 0.79              |
| 1:B:153:ILE:O    | 1:B:157:ALA:HB2  | 1.82                     | 0.79              |
| 2:C:105:LEU:HD11 | 2:C:123:MET:HG2  | 1.65                     | 0.79              |
| 2:D:262:PHE:HB3  | 2:D:275:HIS:HE1  | 1.45                     | 0.79              |
| 1:B:291:TYR:OH   | 1:B:318:ASN:O    | 2.00                     | 0.79              |
| 1:B:532:THR:HA   | 1:B:535:PRO:HG3  | 1.62                     | 0.79              |
| 1:A:186:ASN:ND2  | 1:A:684:CYS:SG   | 2.55                     | 0.79              |
| 1:B:101:LEU:HD11 | 1:B:702:LEU:HB2  | 1.63                     | 0.79              |
| 3:E:35:MET:HB3   | 3:E:76:ILE:HG21  | 1.65                     | 0.79              |
| 1:B:57:VAL:HB    | 1:B:75:ILE:HD13  | 1.65                     | 0.79              |
| 1:B:807:LEU:HD12 | 3:E:123:GLU:HG3  | 1.64                     | 0.79              |
| 1:A:445:ARG:HD3  | 1:A:448:LYS:HD2  | 1.65                     | 0.78              |
| 1:B:79:ASN:HD21  | 1:B:94:CYS:HB2   | 1.48                     | 0.78              |
| 1:B:469:PHE:HB2  | 1:B:707:CYS:HA   | 1.63                     | 0.78              |
| 1:B:613:LEU:HB3  | 1:B:625:TRP:HE3  | 1.48                     | 0.78              |
| 1:B:757:ILE:HD11 | 1:B:774:ILE:HD13 | 1.64                     | 0.78              |
| 1:B:702:LEU:HD12 | 1:B:705:LEU:HD12 | 1.63                     | 0.78              |
| 2:C:212:ILE:O    | 2:C:216:LEU:N    | 2.12                     | 0.78              |
| 1:B:416:LYS:HG2  | 2:C:333:PRO:HB2  | 1.65                     | 0.78              |
| 2:D:121:GLN:O    | 2:D:125:GLU:N    | 2.16                     | 0.78              |
| 1:A:135:GLU:HA   | 1:A:138:ILE:HD12 | 1.65                     | 0.78              |
| 1:A:293:LEU:HD13 | 1:A:353:LEU:HD22 | 1.66                     | 0.78              |
| 1:A:470:GLU:HB3  | 1:A:472:PHE:CZ   | 2.19                     | 0.78              |
| 1:A:527:LEU:HD23 | 1:A:583:ILE:HG23 | 1.65                     | 0.78              |
| 2:D:151:ILE:HA   | 2:D:164:PRO:HA   | 1.65                     | 0.78              |
| 1:B:191:ILE:HG12 | 1:B:254:ILE:HD11 | 1.64                     | 0.78              |
| 1:A:402:ILE:HG12 | 1:A:606:ASN:HD22 | 1.49                     | 0.78              |
| 1:B:406:ARG:H    | 1:B:608:ASN:HD21 | 1.30                     | 0.78              |
| 1:A:141:TYR:CE1  | 1:A:149:MET:HB2  | 2.19                     | 0.78              |
| 1:A:171:GLN:HA   | 1:A:677:THR:HB   | 1.64                     | 0.78              |
| 1:A:186:ASN:ND2  | 1:A:683:ARG:O    | 2.17                     | 0.78              |
| 1:A:315:PHE:HB2  | 1:A:360:LEU:HD23 | 1.66                     | 0.78              |
| 1:A:813:ALA:HB3  | 1:A:815:ARG:HG2  | 1.66                     | 0.78              |
| 1:B:26:GLN:H     | 1:B:789:ASP:HB3  | 1.49                     | 0.78              |
| 3:H:50:VAL:HB    | 3:H:75:THR:HG23  | 1.65                     | 0.78              |
| 1:A:285:ARG:NH2  | 1:A:291:TYR:HB2  | 1.97                     | 0.78              |
| 1:A:446:VAL:O    | 1:A:450:LEU:CB   | 2.32                     | 0.78              |
| 1:B:29:TRP:NE1   | 1:B:34:LEU:HB2   | 1.98                     | 0.78              |
| 1:B:173:ILE:HG13 | 1:B:190:VAL:HG11 | 1.65                     | 0.78              |
| 1:B:293:LEU:HD23 | 1:B:307:LEU:HD21 | 1.64                     | 0.78              |
| 2:C:123:MET:HG3  | 2:C:132:MET:HG3  | 1.66                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:ILE:HD11 | 1:A:224:LEU:HD23 | 1.66                     | 0.77              |
| 1:B:716:ILE:HA   | 1:B:719:GLN:HB2  | 1.65                     | 0.77              |
| 2:D:150:GLY:H    | 2:D:165:ILE:HB   | 1.49                     | 0.77              |
| 1:B:70:LEU:HB3   | 1:B:75:ILE:HD11  | 1.66                     | 0.77              |
| 2:D:188:TYR:HE2  | 2:D:256:ARG:HB3  | 1.49                     | 0.77              |
| 4:F:80:ILE:HA    | 4:F:84:MET:HE2   | 1.66                     | 0.77              |
| 1:A:816:GLN:NE2  | 3:H:37:ALA:O     | 2.17                     | 0.77              |
| 1:B:352:ILE:HG13 | 1:B:620:PHE:CE2  | 2.19                     | 0.77              |
| 2:D:176:MET:SD   | 2:D:277:THR:OG1  | 2.42                     | 0.77              |
| 1:A:621:VAL:HG13 | 1:A:625:TRP:CZ3  | 2.19                     | 0.77              |
| 1:B:359:VAL:HG21 | 1:B:435:PHE:HB2  | 1.66                     | 0.77              |
| 1:A:156:ILE:HG22 | 1:A:173:ILE:HD12 | 1.67                     | 0.77              |
| 1:A:288:HIS:HB3  | 1:A:292:TYR:CZ   | 2.20                     | 0.77              |
| 1:B:313:TYR:CG   | 1:B:360:LEU:HB3  | 2.20                     | 0.77              |
| 1:B:349:GLN:O    | 1:B:353:LEU:HG   | 1.85                     | 0.77              |
| 2:D:8:LEU:HD22   | 2:D:94:LEU:HD22  | 1.66                     | 0.77              |
| 2:D:90:PHE:HB2   | 2:D:98:PRO:HG3   | 1.66                     | 0.77              |
| 2:D:274:ILE:HD13 | 2:D:313:MET:HE1  | 1.66                     | 0.77              |
| 1:A:705:LEU:HB3  | 1:A:711:LEU:HB2  | 1.66                     | 0.77              |
| 1:B:2:SER:N      | 1:B:141:TYR:OH   | 2.16                     | 0.77              |
| 1:B:392:GLY:HA3  | 1:B:618:ASP:H    | 1.50                     | 0.77              |
| 1:B:437:ARG:HH21 | 1:B:605:LEU:HD21 | 1.49                     | 0.77              |
| 1:A:340:THR:OG1  | 1:A:349:GLN:NE2  | 2.17                     | 0.77              |
| 1:B:705:LEU:O    | 1:B:710:VAL:N    | 2.17                     | 0.77              |
| 1:B:13:LEU:HD11  | 1:B:152:HIS:HB2  | 1.64                     | 0.77              |
| 1:B:418:GLN:HB2  | 1:B:422:GLN:HB2  | 1.65                     | 0.77              |
| 2:C:185:LEU:HD11 | 2:C:261:LEU:HB2  | 1.67                     | 0.77              |
| 2:C:166:TYR:HA   | 2:D:44:MET:HG3   | 1.65                     | 0.77              |
| 1:A:194:LEU:HD11 | 1:A:461:LEU:HD13 | 1.65                     | 0.77              |
| 1:B:186:ASN:ND2  | 1:B:684:CYS:SG   | 2.57                     | 0.77              |
| 1:B:220:LEU:HB2  | 1:B:265:ALA:HB3  | 1.65                     | 0.77              |
| 1:B:402:ILE:HG13 | 1:B:609:VAL:HG21 | 1.66                     | 0.77              |
| 1:B:731:ARG:NH1  | 1:B:753:CYS:SG   | 2.58                     | 0.77              |
| 1:A:132:ILE:O    | 1:A:152:HIS:NE2  | 2.18                     | 0.76              |
| 1:A:346:GLU:HA   | 1:A:349:GLN:HB2  | 1.66                     | 0.76              |
| 1:A:532:THR:HG22 | 1:A:533:ASN:H    | 1.51                     | 0.76              |
| 2:C:107:GLU:HB2  | 2:C:119:MET:HE1  | 1.65                     | 0.76              |
| 2:D:35:VAL:HG11  | 2:D:84:LYS:HD3   | 1.65                     | 0.76              |
| 1:A:255:ASN:HB3  | 1:A:457:GLY:HA2  | 1.67                     | 0.76              |
| 1:A:810:LYS:HB2  | 3:H:147:VAL:HG13 | 1.67                     | 0.76              |
| 2:D:252:ASN:HA   | 2:D:255:PHE:CZ   | 2.20                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:368:LYS:HB2  | 1:A:376:ALA:HA   | 1.67                     | 0.76              |
| 1:B:148:GLU:OE2  | 1:B:162:ARG:NH2  | 2.18                     | 0.76              |
| 1:B:344:PHE:O    | 1:B:349:GLN:NE2  | 2.19                     | 0.76              |
| 2:C:188:TYR:HE2  | 2:C:256:ARG:HB3  | 1.49                     | 0.76              |
| 1:B:621:VAL:HA   | 1:B:624:LEU:HD12 | 1.66                     | 0.76              |
| 3:H:28:TYR:HB2   | 3:H:59:MET:HA    | 1.66                     | 0.76              |
| 1:A:237:ALA:HB3  | 1:A:247:ARG:HG3  | 1.66                     | 0.76              |
| 1:B:289:ILE:HD13 | 1:B:335:THR:HG21 | 1.67                     | 0.76              |
| 1:B:406:ARG:HB3  | 1:B:413:VAL:HG12 | 1.68                     | 0.76              |
| 2:C:153:LEU:HD21 | 2:C:274:ILE:HD11 | 1.68                     | 0.76              |
| 1:A:107:ARG:NH2  | 1:A:114:TYR:O    | 2.14                     | 0.76              |
| 1:B:107:ARG:HE   | 1:B:115:THR:HG22 | 1.50                     | 0.76              |
| 1:B:165:LEU:HB2  | 1:B:260:GLY:HA3  | 1.68                     | 0.76              |
| 1:A:101:LEU:HA   | 1:A:104:LEU:HD12 | 1.66                     | 0.76              |
| 1:A:335:THR:HG22 | 1:A:339:MET:HE2  | 1.65                     | 0.76              |
| 1:B:164:MET:O    | 1:B:168:ARG:NH1  | 2.19                     | 0.76              |
| 1:B:799:PHE:CE1  | 3:E:127:LEU:HD11 | 2.21                     | 0.76              |
| 4:F:142:TYR:HA   | 4:F:147:ILE:HD11 | 1.68                     | 0.76              |
| 1:A:49:ILE:HG23  | 1:A:57:VAL:HG13  | 1.67                     | 0.75              |
| 1:A:349:GLN:O    | 1:A:353:LEU:HG   | 1.85                     | 0.75              |
| 1:A:121:CYS:H    | 1:A:146:ARG:HH22 | 1.33                     | 0.75              |
| 1:B:289:ILE:O    | 1:B:293:LEU:N    | 2.17                     | 0.75              |
| 2:D:12:ASN:HA    | 2:D:17:VAL:HG22  | 1.68                     | 0.75              |
| 2:D:20:GLY:HA3   | 2:D:340:TRP:CZ2  | 2.21                     | 0.75              |
| 1:A:88:ASP:OD1   | 1:A:118:GLY:N    | 2.17                     | 0.75              |
| 1:A:302:ARG:O    | 1:A:307:LEU:N    | 2.13                     | 0.75              |
| 1:B:45:GLU:OE2   | 1:B:64:ASN:ND2   | 2.19                     | 0.75              |
| 1:B:484:TYR:HE1  | 1:B:525:ILE:HG23 | 1.51                     | 0.75              |
| 2:D:226:GLU:HB3  | 2:D:236:LEU:HD12 | 1.68                     | 0.75              |
| 1:A:359:VAL:HG13 | 1:A:431:ALA:HB1  | 1.69                     | 0.75              |
| 1:B:276:ARG:HH21 | 1:B:478:GLU:HG3  | 1.52                     | 0.75              |
| 1:B:803:CYS:HB2  | 3:E:127:LEU:HD13 | 1.67                     | 0.75              |
| 1:A:179:SER:HB2  | 1:A:246:SER:HB2  | 1.68                     | 0.75              |
| 1:A:713:GLY:HA2  | 1:A:716:ILE:HD12 | 1.68                     | 0.75              |
| 1:B:715:ARG:O    | 1:B:719:GLN:N    | 2.18                     | 0.75              |
| 2:D:62:ARG:NH2   | 2:D:211:ASP:OD2  | 2.20                     | 0.75              |
| 2:D:111:ASN:OD1  | 2:D:177:ARG:NH2  | 2.19                     | 0.75              |
| 1:A:345:THR:HG23 | 1:A:348:GLU:H    | 1.52                     | 0.75              |
| 1:B:295:ALA:HB3  | 1:B:328:ASP:HB2  | 1.68                     | 0.75              |
| 1:B:381:ASN:HB2  | 1:B:384:ALA:HB3  | 1.67                     | 0.75              |
| 1:B:485:THR:HA   | 1:B:667:LEU:HD13 | 1.67                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:180:LEU:HD21 | 2:D:261:LEU:HA   | 1.67                     | 0.75              |
| 2:D:260:THR:HG22 | 2:D:266:PHE:HB2  | 1.69                     | 0.75              |
| 3:H:104:MET:HB2  | 3:H:107:GLU:HB3  | 1.68                     | 0.75              |
| 3:H:131:HIS:HB2  | 3:H:138:ILE:HG23 | 1.68                     | 0.75              |
| 1:B:34:LEU:O     | 1:B:78:MET:N     | 2.19                     | 0.75              |
| 1:A:339:MET:SD   | 1:A:352:ILE:HD13 | 2.26                     | 0.74              |
| 1:B:438:LEU:HA   | 1:B:624:LEU:HD22 | 1.68                     | 0.74              |
| 1:B:490:GLN:HA   | 1:B:493:PHE:HB3  | 1.68                     | 0.74              |
| 1:B:732:GLN:HG2  | 1:B:744:LYS:HE3  | 1.68                     | 0.74              |
| 2:D:117:GLU:HA   | 2:D:367:PRO:HB2  | 1.68                     | 0.74              |
| 3:E:128:VAL:HG13 | 3:E:138:ILE:HG21 | 1.66                     | 0.74              |
| 1:A:123:VAL:H    | 1:A:683:ARG:HB2  | 1.53                     | 0.74              |
| 1:A:802:GLN:O    | 1:A:806:TYR:HB2  | 1.86                     | 0.74              |
| 1:B:306:LEU:HB2  | 1:B:390:LEU:HD21 | 1.69                     | 0.74              |
| 1:A:12:PHE:HD1   | 1:A:111:GLY:HA3  | 1.50                     | 0.74              |
| 1:B:161:TYR:O    | 1:B:164:MET:N    | 2.20                     | 0.74              |
| 2:C:302:GLY:HA2  | 2:C:336:LYS:HD3  | 1.69                     | 0.74              |
| 4:F:58:ALA:HA    | 4:F:62:LYS:HA    | 1.69                     | 0.74              |
| 1:A:229:PRO:HA   | 1:A:232:GLU:HB2  | 1.69                     | 0.74              |
| 1:A:602:MET:HG3  | 1:A:604:PRO:HD3  | 1.69                     | 0.74              |
| 1:B:355:VAL:HG21 | 1:B:624:LEU:HD13 | 1.69                     | 0.74              |
| 1:B:527:LEU:HD21 | 1:B:583:ILE:HG23 | 1.67                     | 0.74              |
| 1:B:804:ARG:NH1  | 3:E:43:THR:OG1   | 2.19                     | 0.74              |
| 1:B:807:LEU:HD11 | 3:E:126:GLN:HB2  | 1.69                     | 0.74              |
| 1:B:809:ARG:NH2  | 3:E:41:ASN:OD1   | 2.21                     | 0.74              |
| 3:E:127:LEU:O    | 3:E:131:HIS:ND1  | 2.20                     | 0.74              |
| 4:F:29:GLN:HE22  | 4:F:94:ASN:HD21  | 1.35                     | 0.74              |
| 1:B:292:TYR:HB3  | 1:B:332:PHE:HB2  | 1.69                     | 0.74              |
| 1:B:756:MET:O    | 1:B:760:LEU:HB2  | 1.88                     | 0.74              |
| 3:H:92:LEU:HA    | 3:H:95:PHE:HB2   | 1.69                     | 0.74              |
| 1:A:79:ASN:ND2   | 1:A:99:SER:OG    | 2.19                     | 0.74              |
| 1:A:446:VAL:O    | 1:A:450:LEU:HB2  | 1.88                     | 0.74              |
| 1:A:269:THR:HG23 | 1:A:443:LEU:HD13 | 1.68                     | 0.74              |
| 2:C:297:ASN:HB3  | 2:C:329:ILE:HA   | 1.70                     | 0.74              |
| 2:C:300:SER:HA   | 2:C:335:ARG:HB3  | 1.69                     | 0.74              |
| 1:A:323:ILE:HB   | 1:A:326:GLN:HB2  | 1.69                     | 0.74              |
| 1:A:799:PHE:O    | 1:A:803:CYS:HB2  | 1.88                     | 0.74              |
| 1:B:94:CYS:HA    | 1:B:778:THR:HB   | 1.67                     | 0.74              |
| 1:A:116:TYR:CZ   | 1:A:151:PRO:HA   | 2.23                     | 0.74              |
| 1:A:122:VAL:HG22 | 1:A:710:VAL:HG11 | 1.70                     | 0.74              |
| 1:A:294:ILE:HD12 | 1:A:316:LEU:HD12 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:72:LYS:HA    | 1:B:75:ILE:HB    | 1.69                     | 0.74              |
| 2:C:35:VAL:HG22  | 2:C:54:VAL:HA    | 1.70                     | 0.74              |
| 1:A:79:ASN:ND2   | 1:A:94:CYS:O     | 2.19                     | 0.73              |
| 1:A:158:ASP:OD1  | 1:A:193:TYR:OH   | 2.06                     | 0.73              |
| 2:D:87:HIS:HA    | 2:D:91:TYR:HB2   | 1.69                     | 0.73              |
| 3:H:25:LYS:HE2   | 3:H:63:THR:HG23  | 1.70                     | 0.73              |
| 1:A:138:ILE:HG12 | 1:A:193:TYR:HA   | 1.69                     | 0.73              |
| 1:B:612:LEU:HA   | 1:B:615:GLN:HB2  | 1.70                     | 0.73              |
| 2:C:152:VAL:O    | 2:C:162:ASN:HA   | 1.87                     | 0.73              |
| 2:C:332:PRO:HD2  | 2:C:335:ARG:HG2  | 1.70                     | 0.73              |
| 1:A:127:TYR:HE1  | 1:A:181:ALA:HB1  | 1.53                     | 0.73              |
| 2:C:19:ALA:HA    | 2:C:89:THR:HG23  | 1.68                     | 0.73              |
| 2:C:369:ILE:HA   | 2:C:372:ARG:HB2  | 1.70                     | 0.73              |
| 2:D:105:LEU:HD11 | 2:D:123:MET:HG3  | 1.70                     | 0.73              |
| 2:D:251:GLY:N    | 2:D:253:GLU:OE1  | 2.19                     | 0.73              |
| 1:B:585:HIS:HD2  | 1:B:590:VAL:HB   | 1.52                     | 0.73              |
| 1:B:731:ARG:HA   | 1:B:756:MET:SD   | 2.28                     | 0.73              |
| 2:D:297:ASN:HD22 | 2:D:317:ILE:HG13 | 1.51                     | 0.73              |
| 3:E:89:VAL:HA    | 3:E:140:TYR:HE2  | 1.53                     | 0.73              |
| 1:B:294:ILE:O    | 1:B:302:ARG:NE   | 2.20                     | 0.73              |
| 1:B:496:THR:OG1  | 1:B:675:ARG:NH1  | 2.22                     | 0.73              |
| 2:C:8:LEU:HB2    | 2:C:103:THR:HG22 | 1.68                     | 0.73              |
| 2:C:129:VAL:O    | 2:C:359:LYS:HB2  | 1.89                     | 0.73              |
| 2:C:138:ALA:HB2  | 2:C:161:HIS:HB2  | 1.71                     | 0.73              |
| 2:C:292:ASP:HB3  | 2:D:45:VAL:HB    | 1.70                     | 0.73              |
| 2:D:132:MET:O    | 2:D:357:ILE:N    | 2.20                     | 0.73              |
| 1:A:271:LEU:H    | 1:A:666:GLN:HB3  | 1.54                     | 0.73              |
| 1:A:393:ILE:HB   | 1:A:612:LEU:HG   | 1.69                     | 0.73              |
| 1:B:452:LYS:HD3  | 1:B:454:LYS:HE3  | 1.69                     | 0.73              |
| 1:B:508:GLU:HG3  | 1:B:773:LYS:HB2  | 1.71                     | 0.73              |
| 2:D:8:LEU:O      | 2:D:104:LEU:N    | 2.21                     | 0.73              |
| 2:D:104:LEU:HD12 | 2:D:352:PHE:HD1  | 1.53                     | 0.73              |
| 2:D:181:ALA:HB3  | 2:D:183:ARG:HG2  | 1.70                     | 0.73              |
| 3:H:27:LEU:O     | 3:H:31:CYS:N     | 2.20                     | 0.73              |
| 1:A:17:LYS:HE2   | 1:A:86:VAL:HG12  | 1.70                     | 0.73              |
| 1:A:173:ILE:HG12 | 1:A:461:LEU:HD21 | 1.71                     | 0.73              |
| 1:A:160:ALA:HA   | 1:A:171:GLN:HG3  | 1.71                     | 0.73              |
| 1:A:355:VAL:HG11 | 1:A:438:LEU:HB2  | 1.71                     | 0.73              |
| 1:A:438:LEU:HA   | 1:A:624:LEU:HD11 | 1.69                     | 0.73              |
| 1:A:659:VAL:HG12 | 1:A:662:LEU:HD12 | 1.69                     | 0.73              |
| 1:B:107:ARG:NH2  | 1:B:114:TYR:O    | 2.22                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:543:GLU:HA   | 1:B:546:TRP:CE3  | 2.24                     | 0.73              |
| 3:H:46:GLU:HA    | 3:H:49:LYS:HB3   | 1.70                     | 0.73              |
| 1:B:117:SER:HB3  | 1:B:714:ILE:HD11 | 1.69                     | 0.73              |
| 2:C:226:GLU:HB2  | 2:C:236:LEU:HD13 | 1.71                     | 0.73              |
| 1:A:138:ILE:O    | 1:A:142:LYS:N    | 2.20                     | 0.72              |
| 1:B:785:GLU:HA   | 1:B:788:ARG:CZ   | 2.20                     | 0.72              |
| 2:D:370:VAL:O    | 2:D:374:CYS:N    | 2.20                     | 0.72              |
| 1:B:15:VAL:HG22  | 1:B:107:ARG:HH12 | 1.54                     | 0.72              |
| 1:B:143:GLY:HA2  | 1:B:162:ARG:HD3  | 1.69                     | 0.72              |
| 2:D:104:LEU:HG   | 2:D:133:TYR:HB3  | 1.71                     | 0.72              |
| 1:B:57:VAL:HG12  | 1:B:59:VAL:HG13  | 1.70                     | 0.72              |
| 1:B:165:LEU:HG   | 1:B:166:GLN:HG2  | 1.71                     | 0.72              |
| 1:B:736:ILE:HB   | 3:E:94:VAL:HG21  | 1.71                     | 0.72              |
| 2:C:10:CYS:N     | 2:C:104:LEU:O    | 2.21                     | 0.72              |
| 2:C:121:GLN:O    | 2:C:125:GLU:N    | 2.22                     | 0.72              |
| 1:A:44:PHE:HD1   | 1:A:98:ALA:HA    | 1.54                     | 0.72              |
| 1:A:254:ILE:HD11 | 1:A:463:ILE:HD11 | 1.72                     | 0.72              |
| 1:A:285:ARG:HH12 | 1:A:288:HIS:HA   | 1.54                     | 0.72              |
| 1:B:114:TYR:HE1  | 1:B:153:ILE:HG13 | 1.55                     | 0.72              |
| 1:B:154:TYR:HA   | 1:B:157:ALA:HB3  | 1.71                     | 0.72              |
| 2:C:1:ASP:HB2    | 2:C:6:THR:HG21   | 1.71                     | 0.72              |
| 2:C:18:LYS:HA    | 2:C:29:ALA:O     | 1.90                     | 0.72              |
| 2:D:185:LEU:HB3  | 2:D:257:CYS:HB3  | 1.70                     | 0.72              |
| 2:D:233:SER:HA   | 2:D:237:GLU:HB3  | 1.70                     | 0.72              |
| 3:H:89:VAL:O     | 3:H:93:ARG:HB2   | 1.89                     | 0.72              |
| 1:A:180:GLY:H    | 1:A:183:LYS:HB3  | 1.53                     | 0.72              |
| 1:B:171:GLN:N    | 1:B:460:PHE:O    | 2.17                     | 0.72              |
| 1:B:256:PHE:HB3  | 1:B:260:GLY:HA2  | 1.71                     | 0.72              |
| 2:C:358:THR:HB   | 2:C:361:GLU:H    | 1.55                     | 0.72              |
| 2:D:79:TRP:O     | 2:D:83:GLU:N     | 2.23                     | 0.72              |
| 1:A:190:VAL:HG11 | 1:A:463:ILE:HG12 | 1.71                     | 0.72              |
| 1:A:194:LEU:HD22 | 1:A:256:PHE:HZ   | 1.54                     | 0.72              |
| 1:A:712:GLU:OE1  | 1:A:715:ARG:NH2  | 2.21                     | 0.72              |
| 1:B:808:ALA:CB   | 3:E:36:ARG:HD2   | 2.20                     | 0.72              |
| 2:D:20:GLY:HA3   | 2:D:340:TRP:HZ2  | 1.55                     | 0.72              |
| 1:A:436:GLU:OE1  | 1:A:437:ARG:NH1  | 2.21                     | 0.72              |
| 1:B:275:SER:HB2  | 1:B:600:LYS:HD2  | 1.72                     | 0.72              |
| 1:B:531:PRO:HA   | 1:B:539:ALA:HB1  | 1.71                     | 0.72              |
| 3:E:85:PHE:HA    | 3:E:88:TYR:HB2   | 1.71                     | 0.72              |
| 2:C:16:LEU:HA    | 2:C:32:PRO:HA    | 1.70                     | 0.72              |
| 3:E:131:HIS:HB3  | 3:E:143:LEU:HA   | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:381:ASN:O    | 1:A:385:GLN:N    | 2.22                     | 0.72              |
| 1:B:238:LYS:HE2  | 1:B:324:PRO:HG2  | 1.72                     | 0.72              |
| 1:A:267:ILE:H    | 1:A:450:LEU:HD21 | 1.54                     | 0.72              |
| 1:A:280:GLN:NE2  | 1:A:317:SER:O    | 2.23                     | 0.72              |
| 1:B:35:VAL:HG23  | 1:B:47:ALA:H     | 1.53                     | 0.72              |
| 2:D:248:ILE:HG22 | 2:D:250:ILE:HG13 | 1.72                     | 0.72              |
| 3:E:11:PHE:HD1   | 3:E:38:LEU:HD13  | 1.52                     | 0.72              |
| 1:A:435:PHE:CD1  | 1:A:438:LEU:HD23 | 2.25                     | 0.71              |
| 1:A:688:ASN:HA   | 1:A:700:LEU:HD13 | 1.70                     | 0.71              |
| 1:B:3:GLN:HA     | 1:B:14:PHE:HA    | 1.72                     | 0.71              |
| 1:B:145:LYS:HG3  | 1:B:162:ARG:HH21 | 1.55                     | 0.71              |
| 1:B:234:PHE:CD1  | 1:B:289:ILE:HG21 | 2.25                     | 0.71              |
| 1:B:389:HIS:HD2  | 1:B:390:LEU:HD23 | 1.55                     | 0.71              |
| 1:B:804:ARG:O    | 3:E:36:ARG:NH1   | 2.23                     | 0.71              |
| 2:C:162:ASN:ND2  | 2:C:281:SER:OG   | 2.22                     | 0.71              |
| 1:A:160:ALA:O    | 1:A:164:MET:HG3  | 1.89                     | 0.71              |
| 1:A:357:SER:HA   | 1:A:360:LEU:HD12 | 1.71                     | 0.71              |
| 1:A:393:ILE:HG21 | 1:A:613:LEU:HA   | 1.72                     | 0.71              |
| 1:A:530:ARG:NH1  | 1:A:565:ASN:O    | 2.22                     | 0.71              |
| 1:B:26:GLN:NE2   | 1:B:786:GLU:O    | 2.23                     | 0.71              |
| 1:B:231:LEU:O    | 1:B:236:ASN:N    | 2.16                     | 0.71              |
| 1:B:339:MET:HB3  | 1:B:344:PHE:HB2  | 1.70                     | 0.71              |
| 2:C:8:LEU:N      | 2:C:102:PRO:O    | 2.23                     | 0.71              |
| 2:C:117:GLU:HA   | 2:C:367:PRO:HB2  | 1.71                     | 0.71              |
| 3:E:20:ARG:HG2   | 3:E:30:GLN:HE22  | 1.55                     | 0.71              |
| 1:A:11:LYS:HA    | 1:A:14:PHE:HB3   | 1.72                     | 0.71              |
| 1:B:35:VAL:HG21  | 1:B:75:ILE:HA    | 1.71                     | 0.71              |
| 1:B:393:ILE:HB   | 1:B:612:LEU:HG   | 1.71                     | 0.71              |
| 2:D:105:LEU:N    | 2:D:133:TYR:O    | 2.22                     | 0.71              |
| 1:A:306:LEU:HD13 | 1:A:386:LYS:HG2  | 1.70                     | 0.71              |
| 2:D:82:MET:HA    | 2:D:85:ILE:HB    | 1.72                     | 0.71              |
| 2:D:242:LEU:HD12 | 2:D:243:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:35:VAL:HG12  | 1:A:45:GLU:H     | 1.55                     | 0.71              |
| 1:A:297:ALA:HB1  | 1:A:301:MET:HB2  | 1.73                     | 0.71              |
| 1:B:120:PHE:CZ   | 1:B:497:MET:HB2  | 2.24                     | 0.71              |
| 1:B:224:LEU:HD22 | 1:B:252:ILE:HG12 | 1.72                     | 0.71              |
| 1:A:13:LEU:HG    | 1:A:150:PRO:HB2  | 1.73                     | 0.71              |
| 1:A:289:ILE:HA   | 1:A:292:TYR:HB2  | 1.73                     | 0.71              |
| 1:A:401:SER:OG   | 1:A:606:ASN:ND2  | 2.20                     | 0.71              |
| 1:B:281:ALA:HB1  | 1:B:474:ILE:HG21 | 1.72                     | 0.71              |
| 1:B:804:ARG:HG3  | 3:E:119:MET:HE3  | 1.70                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:62:ARG:HA    | 2:D:65:LEU:HB2   | 1.71                     | 0.71              |
| 3:E:12:LYS:HZ3   | 3:E:66:PHE:HB2   | 1.55                     | 0.71              |
| 4:G:50:LYS:HG2   | 4:G:69:LEU:HD22  | 1.71                     | 0.71              |
| 1:A:232:GLU:O    | 1:A:288:HIS:ND1  | 2.24                     | 0.71              |
| 1:B:177:GLY:O    | 1:B:468:GLY:N    | 2.16                     | 0.71              |
| 1:B:223:GLN:HB2  | 1:B:450:LEU:HA   | 1.73                     | 0.71              |
| 3:E:89:VAL:HA    | 3:E:140:TYR:CE2  | 2.26                     | 0.71              |
| 1:B:355:VAL:HG11 | 1:B:438:LEU:HB2  | 1.73                     | 0.71              |
| 1:B:415:GLN:HE21 | 1:B:417:ALA:HB2  | 1.56                     | 0.71              |
| 2:C:202:THR:HG23 | 2:C:205:GLU:H    | 1.55                     | 0.71              |
| 2:C:297:ASN:HD21 | 2:C:317:ILE:HG13 | 1.55                     | 0.71              |
| 2:D:8:LEU:HB3    | 2:D:94:LEU:HD13  | 1.73                     | 0.71              |
| 2:D:47:MET:SD    | 2:D:49:GLN:NE2   | 2.64                     | 0.71              |
| 1:A:711:LEU:HD12 | 1:A:714:ILE:HD12 | 1.72                     | 0.71              |
| 1:B:492:LEU:HD13 | 1:B:675:ARG:HB2  | 1.72                     | 0.71              |
| 2:C:67:LEU:HD13  | 2:C:204:ALA:HA   | 1.72                     | 0.71              |
| 2:D:31:PHE:HB2   | 2:D:55:GLY:HA3   | 1.71                     | 0.71              |
| 2:D:88:HIS:HA    | 2:D:92:ASN:HB2   | 1.71                     | 0.71              |
| 3:H:105:GLY:N    | 3:H:136:GLY:O    | 2.23                     | 0.71              |
| 1:B:443:LEU:HA   | 1:B:446:VAL:HB   | 1.73                     | 0.71              |
| 1:B:621:VAL:HG13 | 1:B:625:TRP:CZ3  | 2.26                     | 0.71              |
| 2:C:14:SER:HG    | 2:C:74:GLY:H     | 1.39                     | 0.71              |
| 2:C:304:THR:HA   | 2:C:309:ILE:HG12 | 1.72                     | 0.71              |
| 1:B:221:GLU:OE1  | 1:B:221:GLU:N    | 2.21                     | 0.70              |
| 2:C:62:ARG:HD2   | 2:C:208:ILE:HG13 | 1.72                     | 0.70              |
| 2:C:73:HIS:O     | 2:C:177:ARG:NH2  | 2.24                     | 0.70              |
| 2:D:153:LEU:HD21 | 2:D:274:ILE:HD11 | 1.72                     | 0.70              |
| 1:B:108:TYR:CD1  | 1:B:113:ILE:HG13 | 2.26                     | 0.70              |
| 1:B:542:ASP:OD2  | 1:B:664:LYS:NZ   | 2.24                     | 0.70              |
| 2:D:300:SER:HA   | 2:D:335:ARG:HG3  | 1.72                     | 0.70              |
| 3:E:11:PHE:CD1   | 3:E:38:LEU:HD13  | 2.26                     | 0.70              |
| 3:E:36:ARG:HE    | 3:E:47:VAL:HG21  | 1.55                     | 0.70              |
| 1:A:80:PRO:HB2   | 1:A:82:LYS:HG2   | 1.72                     | 0.70              |
| 1:B:133:TYR:HB3  | 1:B:189:LYS:HD3  | 1.73                     | 0.70              |
| 2:C:156:GLY:HA2  | 2:C:182:GLY:H    | 1.56                     | 0.70              |
| 1:A:13:LEU:HD21  | 1:A:152:HIS:HB2  | 1.72                     | 0.70              |
| 1:A:13:LEU:HD22  | 1:A:152:HIS:HD2  | 1.57                     | 0.70              |
| 2:C:79:TRP:CE3   | 2:C:122:ILE:HD11 | 2.27                     | 0.70              |
| 3:E:105:GLY:HA2  | 3:E:108:ILE:HG22 | 1.73                     | 0.70              |
| 1:A:125:ASN:N    | 1:A:685:ILE:O    | 2.19                     | 0.70              |
| 1:A:806:TYR:HA   | 3:H:41:ASN:HD22  | 1.55                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:466:ILE:HD12 | 1:B:670:LEU:HD23 | 1.72                     | 0.70              |
| 1:B:730:PHE:CE2  | 1:B:756:MET:HB2  | 2.27                     | 0.70              |
| 2:C:212:ILE:HG21 | 2:C:250:ILE:HG12 | 1.73                     | 0.70              |
| 3:E:124:VAL:HA   | 3:E:127:LEU:HD23 | 1.73                     | 0.70              |
| 1:B:228:ASN:O    | 1:B:232:GLU:N    | 2.24                     | 0.70              |
| 1:A:49:ILE:HA    | 1:A:59:VAL:HA    | 1.74                     | 0.70              |
| 1:A:307:LEU:HD23 | 1:A:313:TYR:HE2  | 1.57                     | 0.70              |
| 1:A:492:LEU:HD22 | 1:A:675:ARG:HB2  | 1.73                     | 0.70              |
| 1:B:16:ASP:H     | 1:B:112:LEU:CD1  | 2.04                     | 0.70              |
| 1:B:737:LEU:HB3  | 1:B:760:LEU:HD21 | 1.73                     | 0.70              |
| 2:C:10:CYS:HB2   | 2:C:90:PHE:CZ    | 2.26                     | 0.70              |
| 2:C:236:LEU:HB3  | 2:C:255:PHE:CE1  | 2.26                     | 0.70              |
| 2:D:229:THR:O    | 2:D:234:SER:OG   | 2.10                     | 0.70              |
| 1:A:226:GLN:HG3  | 1:A:341:ILE:HG21 | 1.73                     | 0.70              |
| 1:B:398:PHE:HA   | 1:B:609:VAL:HG22 | 1.73                     | 0.70              |
| 2:C:94:LEU:HB3   | 2:C:96:VAL:HG22  | 1.74                     | 0.70              |
| 2:D:360:GLN:O    | 2:D:364:GLU:HG3  | 1.90                     | 0.70              |
| 1:B:50:LYS:H     | 1:B:59:VAL:HG12  | 1.57                     | 0.70              |
| 2:C:233:SER:HA   | 2:C:237:GLU:HB3  | 1.73                     | 0.70              |
| 1:A:128:LYS:HE3  | 1:A:130:LEU:HD11 | 1.72                     | 0.70              |
| 1:B:26:GLN:HG3   | 1:B:789:ASP:HB2  | 1.74                     | 0.70              |
| 3:H:103:VAL:O    | 3:H:138:ILE:N    | 2.25                     | 0.70              |
| 1:A:123:VAL:O    | 1:A:685:ILE:N    | 2.24                     | 0.69              |
| 1:A:220:LEU:HD13 | 1:A:264:GLY:HA2  | 1.74                     | 0.69              |
| 1:B:302:ARG:O    | 1:B:307:LEU:N    | 2.25                     | 0.69              |
| 1:B:812:PHE:CZ   | 3:E:34:VAL:HA    | 2.27                     | 0.69              |
| 2:C:151:ILE:HG12 | 2:C:282:ILE:HG12 | 1.74                     | 0.69              |
| 2:D:16:LEU:HA    | 2:D:32:PRO:HA    | 1.73                     | 0.69              |
| 1:A:276:ARG:NH2  | 1:A:479:GLN:OE1  | 2.25                     | 0.69              |
| 1:A:346:GLU:O    | 1:A:350:THR:OG1  | 2.08                     | 0.69              |
| 2:C:10:CYS:HG    | 2:C:86:TRP:CD1   | 2.09                     | 0.69              |
| 1:A:534:PRO:HB2  | 1:A:562:GLU:HG2  | 1.75                     | 0.69              |
| 2:C:20:GLY:HA3   | 2:C:340:TRP:CZ2  | 2.28                     | 0.69              |
| 2:C:59:GLN:HB3   | 2:C:62:ARG:HH21  | 1.54                     | 0.69              |
| 2:C:74:GLY:HA3   | 2:C:108:ALA:HB2  | 1.73                     | 0.69              |
| 2:D:189:LEU:HA   | 2:D:192:ILE:HD11 | 1.74                     | 0.69              |
| 3:H:48:MET:HG2   | 3:H:59:MET:HG2   | 1.74                     | 0.69              |
| 1:B:292:TYR:HA   | 1:B:328:ASP:HB3  | 1.73                     | 0.69              |
| 2:C:115:ASN:HA   | 2:C:118:LYS:HD2  | 1.73                     | 0.69              |
| 2:D:259:GLU:HB3  | 2:D:266:PHE:HE2  | 1.57                     | 0.69              |
| 3:H:75:THR:HA    | 3:H:78:LYS:HD2   | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:LEU:HD11  | 1:A:103:ASN:HD21 | 1.55                     | 0.69              |
| 1:A:301:MET:O    | 1:A:305:LEU:HG   | 1.92                     | 0.69              |
| 1:B:58:THR:O     | 1:B:67:LYS:NZ    | 2.26                     | 0.69              |
| 2:D:123:MET:HG3  | 2:D:132:MET:HG3  | 1.72                     | 0.69              |
| 4:F:123:ARG:NH1  | 4:F:133:PHE:O    | 2.26                     | 0.69              |
| 1:A:72:LYS:HA    | 1:A:75:ILE:HB    | 1.74                     | 0.69              |
| 1:A:223:GLN:O    | 1:A:227:ALA:N    | 2.24                     | 0.69              |
| 1:A:492:LEU:HD13 | 1:A:674:LEU:HB2  | 1.74                     | 0.69              |
| 1:A:508:GLU:HG2  | 1:A:770:GLY:HA3  | 1.73                     | 0.69              |
| 1:A:731:ARG:O    | 1:A:735:GLU:N    | 2.25                     | 0.69              |
| 1:B:31:ALA:HA    | 1:B:786:GLU:HB3  | 1.74                     | 0.69              |
| 1:B:411:ARG:N    | 2:C:28:ARG:HG3   | 2.07                     | 0.69              |
| 3:E:140:TYR:HA   | 3:E:143:LEU:HB3  | 1.72                     | 0.69              |
| 1:A:78:MET:SD    | 1:A:102:HIS:ND1  | 2.65                     | 0.69              |
| 1:B:47:ALA:HB2   | 1:B:61:LEU:HA    | 1.73                     | 0.69              |
| 1:B:730:PHE:HE2  | 1:B:756:MET:HB2  | 1.56                     | 0.69              |
| 2:C:18:LYS:HG3   | 2:C:30:VAL:HG22  | 1.75                     | 0.69              |
| 2:D:87:HIS:O     | 2:D:92:ASN:N     | 2.24                     | 0.69              |
| 1:A:386:LYS:O    | 1:A:390:LEU:HG   | 1.92                     | 0.69              |
| 1:A:485:THR:HA   | 1:A:667:LEU:HD13 | 1.73                     | 0.69              |
| 1:B:173:ILE:HG21 | 1:B:190:VAL:HG21 | 1.75                     | 0.69              |
| 1:B:234:PHE:HB2  | 1:B:439:PHE:CD1  | 2.28                     | 0.69              |
| 1:B:437:ARG:HH22 | 1:B:610:THR:HG21 | 1.58                     | 0.69              |
| 1:B:491:GLN:HA   | 1:B:521:LEU:HD13 | 1.75                     | 0.69              |
| 1:B:793:THR:HA   | 3:E:115:LEU:HD13 | 1.74                     | 0.69              |
| 2:D:47:MET:HE2   | 2:D:49:GLN:H     | 1.57                     | 0.69              |
| 2:D:79:TRP:HA    | 2:D:82:MET:HB2   | 1.74                     | 0.69              |
| 2:D:162:ASN:ND2  | 2:D:278:THR:OG1  | 2.26                     | 0.69              |
| 1:A:367:PHE:HA   | 1:A:378:MET:HA   | 1.75                     | 0.69              |
| 2:C:259:GLU:O    | 2:C:263:GLN:N    | 2.26                     | 0.69              |
| 2:C:262:PHE:HA   | 2:C:274:ILE:HG22 | 1.74                     | 0.69              |
| 2:D:54:VAL:HG22  | 2:D:84:LYS:HB3   | 1.74                     | 0.69              |
| 1:A:672:THR:O    | 1:A:676:ASN:N    | 2.25                     | 0.69              |
| 1:B:138:ILE:HG21 | 1:B:196:VAL:HB   | 1.75                     | 0.69              |
| 2:C:78:ASN:O     | 2:C:82:MET:N     | 2.24                     | 0.69              |
| 2:C:86:TRP:CE2   | 2:C:105:LEU:HD13 | 2.28                     | 0.69              |
| 4:F:99:GLU:HB2   | 4:F:159:THR:HB   | 1.74                     | 0.69              |
| 1:A:89:MET:HB3   | 1:A:100:VAL:HG22 | 1.75                     | 0.68              |
| 1:A:146:ARG:NH2  | 1:A:681:PHE:O    | 2.26                     | 0.68              |
| 1:A:394:ASN:H    | 1:A:612:LEU:HD11 | 1.58                     | 0.68              |
| 1:B:280:GLN:OE1  | 1:B:317:SER:OG   | 2.11                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:365:ILE:HG21 | 1:B:398:PHE:HE2  | 1.57                     | 0.68              |
| 1:B:376:ALA:HB1  | 1:B:403:LEU:HB3  | 1.74                     | 0.68              |
| 2:C:285:CYS:HB3  | 2:C:289:ILE:HG22 | 1.75                     | 0.68              |
| 1:A:15:VAL:HG11  | 1:A:87:GLU:N     | 2.08                     | 0.68              |
| 1:A:25:ALA:HB3   | 1:A:786:GLU:HA   | 1.74                     | 0.68              |
| 1:A:336:LEU:HD21 | 1:A:353:LEU:HD11 | 1.76                     | 0.68              |
| 1:B:161:TYR:HA   | 1:B:164:MET:HE3  | 1.75                     | 0.68              |
| 1:B:346:GLU:HA   | 1:B:349:GLN:HB2  | 1.75                     | 0.68              |
| 1:B:105:ARG:NH2  | 1:B:106:GLU:OE2  | 2.26                     | 0.68              |
| 1:B:101:LEU:HB3  | 1:B:698:ALA:HB1  | 1.73                     | 0.68              |
| 1:B:125:ASN:N    | 1:B:685:ILE:O    | 2.25                     | 0.68              |
| 1:B:469:PHE:CZ   | 1:B:586:TYR:HB3  | 2.28                     | 0.68              |
| 1:B:487:GLU:OE2  | 1:B:585:HIS:ND1  | 2.26                     | 0.68              |
| 1:B:568:LYS:HB3  | 1:B:584:LEU:HB2  | 1.75                     | 0.68              |
| 1:A:263:VAL:HB   | 1:A:455:ARG:HA   | 1.76                     | 0.68              |
| 1:B:107:ARG:HB3  | 1:B:112:LEU:HB2  | 1.74                     | 0.68              |
| 1:B:114:TYR:HB3  | 1:B:151:PRO:O    | 1.93                     | 0.68              |
| 1:B:173:ILE:HB   | 1:B:463:ILE:HG23 | 1.75                     | 0.68              |
| 1:B:276:ARG:NH2  | 1:B:284:GLU:OE2  | 2.27                     | 0.68              |
| 2:D:198:TYR:HB3  | 2:D:248:ILE:HD12 | 1.75                     | 0.68              |
| 3:H:92:LEU:O     | 3:H:96:ASP:N     | 2.26                     | 0.68              |
| 1:A:441:TRP:HE1  | 1:A:445:ARG:HH21 | 1.42                     | 0.68              |
| 1:B:736:ILE:HG21 | 1:B:792:ILE:HD11 | 1.76                     | 0.68              |
| 2:C:182:GLY:HA2  | 2:C:185:LEU:HB2  | 1.76                     | 0.68              |
| 2:C:213:LYS:O    | 2:C:217:CYS:HB2  | 1.94                     | 0.68              |
| 2:D:188:TYR:CE2  | 2:D:256:ARG:HB3  | 2.28                     | 0.68              |
| 1:B:123:VAL:HG21 | 1:B:153:ILE:HD11 | 1.75                     | 0.68              |
| 1:B:586:TYR:O    | 1:B:706:ARG:NE   | 2.24                     | 0.68              |
| 2:C:289:ILE:HD13 | 2:D:44:MET:HG2   | 1.75                     | 0.68              |
| 2:D:313:MET:O    | 2:D:317:ILE:HG12 | 1.93                     | 0.68              |
| 3:H:15:PHE:HE2   | 3:H:31:CYS:HB2   | 1.59                     | 0.68              |
| 3:H:44:ASN:HA    | 3:H:47:VAL:HB    | 1.75                     | 0.68              |
| 1:B:243:ASP:OD1  | 1:B:691:LYS:NZ   | 2.22                     | 0.68              |
| 2:C:188:TYR:CE2  | 2:C:256:ARG:HB3  | 2.29                     | 0.68              |
| 2:D:189:LEU:HB2  | 2:D:257:CYS:SG   | 2.34                     | 0.68              |
| 1:B:141:TYR:HA   | 1:B:144:LYS:HB2  | 1.76                     | 0.68              |
| 1:B:535:PRO:HG2  | 1:B:543:GLU:CD   | 2.17                     | 0.68              |
| 1:B:708:ASN:HB2  | 1:B:710:VAL:HG23 | 1.76                     | 0.68              |
| 2:D:37:ARG:NE    | 2:D:51:ASP:O     | 2.21                     | 0.68              |
| 2:D:141:SER:OG   | 2:D:154:ASP:OD1  | 2.12                     | 0.68              |
| 2:D:208:ILE:HD11 | 2:D:242:LEU:HD13 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:834:LYS:HZ1  | 4:G:161:ILE:HD12 | 1.59                     | 0.68              |
| 1:B:219:GLU:OE1  | 1:B:452:LYS:NZ   | 2.27                     | 0.68              |
| 1:B:537:VAL:HG21 | 1:B:583:ILE:HD11 | 1.76                     | 0.68              |
| 1:B:757:ILE:HD11 | 1:B:774:ILE:HG21 | 1.76                     | 0.68              |
| 1:B:805:GLY:HA3  | 3:E:41:ASN:HA    | 1.75                     | 0.68              |
| 2:C:62:ARG:NH2   | 2:C:211:ASP:OD1  | 2.27                     | 0.68              |
| 3:E:125:GLU:O    | 3:E:129:ALA:N    | 2.27                     | 0.68              |
| 1:A:244:ASN:HA   | 1:A:288:HIS:HE1  | 1.58                     | 0.67              |
| 1:A:807:LEU:HD13 | 3:H:124:VAL:HA   | 1.75                     | 0.67              |
| 1:B:722:PRO:HD2  | 1:B:777:ARG:HA   | 1.76                     | 0.67              |
| 2:C:51:ASP:OD2   | 2:C:52:SER:N     | 2.27                     | 0.67              |
| 3:H:4:SER:H      | 3:H:7:GLN:HE22   | 1.41                     | 0.67              |
| 1:A:316:LEU:HG   | 1:A:360:LEU:HD21 | 1.75                     | 0.67              |
| 1:A:418:GLN:HA   | 2:D:333:PRO:HB3  | 1.76                     | 0.67              |
| 1:B:138:ILE:HD13 | 1:B:196:VAL:HB   | 1.74                     | 0.67              |
| 1:B:357:SER:HA   | 1:B:360:LEU:HD12 | 1.75                     | 0.67              |
| 1:B:533:ASN:H    | 2:C:353:GLN:HE22 | 1.42                     | 0.67              |
| 1:B:709:GLY:O    | 1:B:713:GLY:N    | 2.27                     | 0.67              |
| 1:B:815:ARG:O    | 3:E:20:ARG:NH1   | 2.27                     | 0.67              |
| 2:C:282:ILE:HG23 | 2:C:293:LEU:HB2  | 1.75                     | 0.67              |
| 1:A:145:LYS:HA   | 1:A:162:ARG:HH22 | 1.59                     | 0.67              |
| 1:A:164:MET:HE1  | 1:A:461:LEU:HB2  | 1.76                     | 0.67              |
| 1:A:359:VAL:HG21 | 1:A:435:PHE:HB2  | 1.75                     | 0.67              |
| 1:B:769:ILE:HD13 | 1:B:774:ILE:HG12 | 1.76                     | 0.67              |
| 2:C:252:ASN:HA   | 2:C:255:PHE:CZ   | 2.29                     | 0.67              |
| 2:D:10:CYS:HB2   | 2:D:89:THR:HG21  | 1.76                     | 0.67              |
| 1:B:793:THR:HG23 | 3:E:115:LEU:HD22 | 1.75                     | 0.67              |
| 3:H:127:LEU:HD12 | 3:H:143:LEU:HD11 | 1.76                     | 0.67              |
| 1:A:785:GLU:HB3  | 1:A:788:ARG:HH21 | 1.59                     | 0.67              |
| 1:A:804:ARG:HH12 | 3:H:113:VAL:HA   | 1.58                     | 0.67              |
| 1:B:50:LYS:HZ2   | 1:B:60:GLU:HB2   | 1.60                     | 0.67              |
| 1:B:194:LEU:HD13 | 1:B:256:PHE:HZ   | 1.58                     | 0.67              |
| 1:B:568:LYS:HD2  | 1:B:584:LEU:HB2  | 1.76                     | 0.67              |
| 1:B:604:PRO:HA   | 1:B:655:MET:HA   | 1.75                     | 0.67              |
| 2:D:216:LEU:HD23 | 2:D:238:LYS:HG2  | 1.77                     | 0.67              |
| 3:E:28:TYR:CD1   | 3:E:51:LEU:HD22  | 2.29                     | 0.67              |
| 1:A:127:TYR:CE1  | 1:A:181:ALA:HB1  | 2.29                     | 0.67              |
| 1:A:48:SER:OG    | 1:A:62:GLN:NE2   | 2.27                     | 0.67              |
| 1:A:401:SER:OG   | 1:A:609:VAL:HG23 | 1.95                     | 0.67              |
| 1:A:506:GLN:OE1  | 1:A:513:ASN:ND2  | 2.28                     | 0.67              |
| 1:A:834:LYS:HG2  | 1:A:835:LEU:HG   | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:89:MET:HE3   | 1:B:104:LEU:HG   | 1.76                     | 0.67              |
| 1:B:501:GLU:OE2  | 1:B:724:ARG:NH2  | 2.28                     | 0.67              |
| 1:B:757:ILE:O    | 1:B:761:GLU:N    | 2.27                     | 0.67              |
| 2:C:70:PRO:HB2   | 2:C:82:MET:HG2   | 1.77                     | 0.67              |
| 2:C:73:HIS:HA    | 2:C:159:VAL:HB   | 1.76                     | 0.67              |
| 2:D:99:GLU:HG2   | 2:D:128:ASN:HB2  | 1.77                     | 0.67              |
| 2:D:156:GLY:HA2  | 2:D:302:GLY:N    | 2.05                     | 0.67              |
| 4:F:148:ASP:OD2  | 4:F:150:LYS:NZ   | 2.27                     | 0.67              |
| 1:B:714:ILE:HG22 | 1:B:718:ARG:HH21 | 1.60                     | 0.67              |
| 2:C:131:ALA:HB1  | 2:C:356:TRP:CG   | 2.29                     | 0.67              |
| 2:D:140:LEU:O    | 2:D:342:GLY:HA3  | 1.94                     | 0.67              |
| 2:D:356:TRP:NE1  | 2:D:358:THR:OG1  | 2.27                     | 0.67              |
| 3:H:82:GLN:O     | 3:H:88:TYR:OH    | 2.13                     | 0.67              |
| 1:A:464:LEU:HD13 | 1:A:674:LEU:HD21 | 1.75                     | 0.67              |
| 1:B:23:PRO:HB2   | 3:E:94:VAL:HB    | 1.77                     | 0.67              |
| 1:B:226:GLN:O    | 1:B:338:ALA:HB1  | 1.93                     | 0.67              |
| 3:E:112:LEU:HD22 | 3:E:127:LEU:HD21 | 1.76                     | 0.67              |
| 1:A:492:LEU:HD21 | 1:A:671:MET:HG2  | 1.77                     | 0.67              |
| 1:B:162:ARG:HA   | 1:B:166:GLN:HG3  | 1.76                     | 0.67              |
| 2:D:151:ILE:HD13 | 2:D:278:THR:HG23 | 1.76                     | 0.67              |
| 2:D:239:SER:HB2  | 2:D:249:THR:HG23 | 1.77                     | 0.67              |
| 2:D:368:SER:HA   | 2:D:371:HIS:CD2  | 2.30                     | 0.67              |
| 1:A:35:VAL:H     | 1:A:46:ALA:HA    | 1.60                     | 0.66              |
| 1:A:274:LYS:HG2  | 1:A:436:GLU:HB2  | 1.77                     | 0.66              |
| 1:B:298:SER:O    | 1:B:302:ARG:N    | 2.22                     | 0.66              |
| 1:B:302:ARG:HA   | 1:B:307:LEU:HD12 | 1.77                     | 0.66              |
| 2:C:88:HIS:HA    | 2:C:92:ASN:HB2   | 1.75                     | 0.66              |
| 2:D:164:PRO:HB2  | 2:D:293:LEU:HD22 | 1.76                     | 0.66              |
| 1:A:139:ASP:HA   | 1:A:142:LYS:HB3  | 1.75                     | 0.66              |
| 1:A:234:PHE:HB3  | 1:A:439:PHE:HB2  | 1.76                     | 0.66              |
| 1:B:85:LYS:HA    | 1:B:103:ASN:HA   | 1.76                     | 0.66              |
| 1:B:114:TYR:HE2  | 1:B:130:LEU:HD12 | 1.59                     | 0.66              |
| 2:D:212:ILE:O    | 2:D:216:LEU:N    | 2.27                     | 0.66              |
| 1:A:58:THR:HA    | 1:A:68:VAL:O     | 1.95                     | 0.66              |
| 1:A:108:TYR:HB3  | 1:A:696:LEU:HD12 | 1.77                     | 0.66              |
| 1:A:160:ALA:HB2  | 1:A:173:ILE:HD11 | 1.75                     | 0.66              |
| 1:A:267:ILE:HG23 | 1:A:450:LEU:HD21 | 1.76                     | 0.66              |
| 1:A:295:ALA:HB2  | 1:A:310:PHE:HZ   | 1.59                     | 0.66              |
| 1:A:389:HIS:HD2  | 1:A:390:LEU:HD23 | 1.60                     | 0.66              |
| 1:B:276:ARG:HG3  | 1:B:286:THR:HA   | 1.77                     | 0.66              |
| 1:B:536:GLY:HA2  | 1:B:566:HIS:NE2  | 2.09                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:802:GLN:NE2  | 3:E:41:ASN:OD1   | 2.22                     | 0.66              |
| 1:B:819:LEU:HA   | 1:B:822:MET:HE2  | 1.77                     | 0.66              |
| 1:B:850:LEU:HD22 | 4:F:40:ILE:HG12  | 1.77                     | 0.66              |
| 2:C:317:ILE:HA   | 2:C:320:LEU:HB2  | 1.77                     | 0.66              |
| 3:H:16:GLN:HA    | 3:H:19:ASP:HB2   | 1.76                     | 0.66              |
| 1:A:326:GLN:HG2  | 1:A:331:MET:HE2  | 1.76                     | 0.66              |
| 1:A:583:ILE:HG22 | 1:A:585:HIS:HD1  | 1.59                     | 0.66              |
| 1:A:809:ARG:HA   | 1:A:812:PHE:CE1  | 2.31                     | 0.66              |
| 1:A:810:LYS:HD3  | 3:H:147:VAL:HG22 | 1.76                     | 0.66              |
| 1:B:44:PHE:HE2   | 1:B:101:LEU:HD12 | 1.59                     | 0.66              |
| 1:B:153:ILE:HG23 | 1:B:682:VAL:HG21 | 1.77                     | 0.66              |
| 2:C:67:LEU:H     | 2:C:203:THR:HG23 | 1.60                     | 0.66              |
| 2:D:218:TYR:HD2  | 2:D:255:PHE:HB3  | 1.61                     | 0.66              |
| 3:H:36:ARG:NE    | 3:H:42:PRO:O     | 2.23                     | 0.66              |
| 1:A:47:ALA:HB2   | 1:A:61:LEU:HD23  | 1.75                     | 0.66              |
| 1:A:163:SER:HA   | 1:A:167:ASP:HB2  | 1.76                     | 0.66              |
| 1:A:566:HIS:HB3  | 1:A:569:PHE:HB3  | 1.78                     | 0.66              |
| 1:B:402:ILE:HG13 | 1:B:606:ASN:HD22 | 1.59                     | 0.66              |
| 1:B:445:ARG:HD3  | 1:B:448:LYS:HD2  | 1.76                     | 0.66              |
| 2:C:217:CYS:O    | 2:C:254:ARG:NH2  | 2.29                     | 0.66              |
| 2:D:24:ASP:HB2   | 2:D:340:TRP:CH2  | 2.27                     | 0.66              |
| 2:D:262:PHE:HA   | 2:D:274:ILE:HG22 | 1.75                     | 0.66              |
| 1:A:79:ASN:ND2   | 1:A:92:LEU:HB3   | 2.11                     | 0.66              |
| 1:A:178:GLU:HG3  | 1:A:242:ASN:HB2  | 1.77                     | 0.66              |
| 1:A:194:LEU:O    | 1:A:198:ALA:N    | 2.27                     | 0.66              |
| 1:A:219:GLU:HG3  | 1:A:220:LEU:HG   | 1.76                     | 0.66              |
| 2:D:14:SER:OG    | 2:D:73:HIS:N     | 2.28                     | 0.66              |
| 2:D:88:HIS:O     | 2:D:93:GLU:N     | 2.16                     | 0.66              |
| 2:D:262:PHE:HB3  | 2:D:275:HIS:CE1  | 2.30                     | 0.66              |
| 1:A:345:THR:O    | 1:A:349:GLN:N    | 2.19                     | 0.66              |
| 1:A:456:GLN:HG3  | 1:A:458:ALA:H    | 1.59                     | 0.66              |
| 2:D:105:LEU:HD21 | 2:D:123:MET:SD   | 2.34                     | 0.66              |
| 2:D:106:THR:HG21 | 2:D:339:VAL:HG12 | 1.77                     | 0.66              |
| 2:D:123:MET:SD   | 2:D:129:VAL:HG21 | 2.36                     | 0.66              |
| 2:D:220:ALA:HB2  | 2:D:255:PHE:HB2  | 1.77                     | 0.66              |
| 3:E:107:GLU:O    | 3:E:111:VAL:HG22 | 1.96                     | 0.66              |
| 1:A:185:GLU:O    | 1:A:189:LYS:NZ   | 2.25                     | 0.66              |
| 1:A:362:LEU:HD23 | 1:A:365:ILE:HD12 | 1.78                     | 0.66              |
| 1:B:437:ARG:NH2  | 1:B:605:LEU:HD21 | 2.09                     | 0.66              |
| 2:C:12:ASN:HA    | 2:C:17:VAL:HG22  | 1.78                     | 0.66              |
| 2:C:220:ALA:HB2  | 2:C:255:PHE:HB2  | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:277:ALA:HB1  | 1:A:435:PHE:HB3  | 1.77                     | 0.66              |
| 1:A:586:TYR:HH   | 1:A:715:ARG:HH22 | 1.44                     | 0.66              |
| 1:B:33:LYS:HD2   | 1:B:49:ILE:HD12  | 1.78                     | 0.66              |
| 1:B:237:ALA:HB3  | 1:B:247:ARG:HG3  | 1.76                     | 0.66              |
| 1:B:244:ASN:HD21 | 1:B:326:GLN:HG3  | 1.61                     | 0.66              |
| 2:C:14:SER:HA    | 2:C:71:ILE:HB    | 1.77                     | 0.66              |
| 2:C:216:LEU:HD12 | 2:C:250:ILE:HD13 | 1.76                     | 0.66              |
| 1:A:392:GLY:HA3  | 1:A:618:ASP:H    | 1.61                     | 0.66              |
| 2:D:98:PRO:HG2   | 2:D:127:PHE:CD1  | 2.30                     | 0.66              |
| 3:E:105:GLY:N    | 3:E:136:GLY:O    | 2.28                     | 0.66              |
| 3:H:18:PHE:O     | 3:H:30:GLN:NE2   | 2.28                     | 0.66              |
| 1:A:141:TYR:HE1  | 1:A:149:MET:HB2  | 1.60                     | 0.65              |
| 1:B:59:VAL:O     | 1:B:67:LYS:HA    | 1.96                     | 0.65              |
| 1:B:135:GLU:HA   | 1:B:138:ILE:HB   | 1.77                     | 0.65              |
| 1:B:530:ARG:NH2  | 1:B:535:PRO:O    | 2.30                     | 0.65              |
| 2:C:136:ILE:HB   | 2:C:139:VAL:HB   | 1.79                     | 0.65              |
| 1:A:391:MET:HA   | 1:A:621:VAL:HG21 | 1.78                     | 0.65              |
| 1:A:801:ALA:O    | 3:H:43:THR:OG1   | 2.14                     | 0.65              |
| 1:B:4:LYS:HB2    | 1:B:10:GLU:HB2   | 1.77                     | 0.65              |
| 1:B:688:ASN:HA   | 1:B:700:LEU:HD13 | 1.77                     | 0.65              |
| 2:C:116:ARG:HH11 | 2:C:371:HIS:CE1  | 2.14                     | 0.65              |
| 2:D:106:THR:HG22 | 2:D:140:LEU:HD12 | 1.77                     | 0.65              |
| 1:B:556:VAL:HA   | 1:B:559:LEU:HD12 | 1.78                     | 0.65              |
| 2:C:70:PRO:HA    | 2:C:78:ASN:HB3   | 1.77                     | 0.65              |
| 2:C:155:SER:HB3  | 2:C:304:THR:HG23 | 1.79                     | 0.65              |
| 2:D:15:GLY:O     | 2:D:33:SER:N     | 2.29                     | 0.65              |
| 1:A:371:ARG:NH1  | 1:A:421:GLU:OE2  | 2.28                     | 0.65              |
| 1:A:683:ARG:NE   | 1:A:710:VAL:HG22 | 2.12                     | 0.65              |
| 1:B:342:MET:HA   | 1:B:449:ALA:HB3  | 1.79                     | 0.65              |
| 1:B:386:LYS:O    | 1:B:390:LEU:HG   | 1.95                     | 0.65              |
| 1:B:505:TYR:OH   | 1:B:720:GLY:HA3  | 1.96                     | 0.65              |
| 1:A:295:ALA:HB3  | 1:A:328:ASP:HB3  | 1.79                     | 0.65              |
| 1:A:348:GLU:OE2  | 1:A:445:ARG:NH2  | 2.28                     | 0.65              |
| 1:B:603:ASP:HB2  | 1:B:659:VAL:HG23 | 1.78                     | 0.65              |
| 2:C:98:PRO:HB2   | 2:C:127:PHE:HB3  | 1.79                     | 0.65              |
| 2:D:136:ILE:HD11 | 2:D:375:PHE:HB2  | 1.78                     | 0.65              |
| 3:E:44:ASN:HA    | 3:E:47:VAL:HB    | 1.76                     | 0.65              |
| 1:A:279:ARG:NH2  | 1:A:428:GLU:OE2  | 2.23                     | 0.65              |
| 1:A:419:THR:HG21 | 1:A:549:LYS:HG2  | 1.79                     | 0.65              |
| 2:C:39:ARG:NH2   | 2:C:62:ARG:O     | 2.28                     | 0.65              |
| 4:F:99:GLU:OE2   | 4:F:160:ARG:NH2  | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:72:LYS:HD2   | 1:A:75:ILE:HB    | 1.78                     | 0.65              |
| 1:A:485:THR:HG23 | 1:A:667:LEU:HD13 | 1.79                     | 0.65              |
| 1:B:345:THR:O    | 1:B:349:GLN:N    | 2.19                     | 0.65              |
| 1:B:358:SER:OG   | 1:B:434:LYS:NZ   | 2.21                     | 0.65              |
| 1:A:475:ASN:HA   | 1:A:479:GLN:HB2  | 1.79                     | 0.65              |
| 1:A:527:LEU:O    | 1:A:537:VAL:N    | 2.20                     | 0.65              |
| 1:B:160:ALA:O    | 1:B:171:GLN:HG3  | 1.96                     | 0.65              |
| 1:B:224:LEU:HD13 | 1:B:267:ILE:HG21 | 1.79                     | 0.65              |
| 1:A:58:THR:HB    | 1:A:67:LYS:HG2   | 1.78                     | 0.65              |
| 1:A:86:VAL:O     | 1:A:107:ARG:NH1  | 2.30                     | 0.65              |
| 1:A:116:TYR:CE2  | 1:A:147:HIS:HA   | 2.31                     | 0.65              |
| 1:A:294:ILE:HD11 | 1:A:313:TYR:HD2  | 1.60                     | 0.65              |
| 1:B:224:LEU:HD11 | 1:B:250:LYS:HZ2  | 1.60                     | 0.65              |
| 1:B:367:PHE:HA   | 1:B:378:MET:HB2  | 1.78                     | 0.65              |
| 1:B:416:LYS:HE2  | 2:C:333:PRO:HD2  | 1.79                     | 0.65              |
| 1:B:785:GLU:CD   | 1:B:788:ARG:HH22 | 2.04                     | 0.65              |
| 2:D:278:THR:HG21 | 2:D:297:ASN:ND2  | 2.12                     | 0.65              |
| 2:D:368:SER:O    | 2:D:371:HIS:HB2  | 1.97                     | 0.65              |
| 3:E:41:ASN:HD22  | 3:E:81:ASP:HA    | 1.60                     | 0.65              |
| 3:H:31:CYS:SG    | 3:H:72:MET:HE3   | 2.36                     | 0.65              |
| 1:A:158:ASP:OD2  | 1:A:162:ARG:NH1  | 2.30                     | 0.65              |
| 1:A:190:VAL:O    | 1:A:194:LEU:HG   | 1.97                     | 0.65              |
| 1:A:788:ARG:NH1  | 1:A:789:ASP:OD1  | 2.30                     | 0.65              |
| 1:B:116:TYR:CZ   | 1:B:151:PRO:HA   | 2.31                     | 0.65              |
| 1:B:278:ILE:HG13 | 1:B:279:ARG:H    | 1.61                     | 0.65              |
| 1:B:405:PRO:HG3  | 1:B:418:GLN:CD   | 2.22                     | 0.65              |
| 1:B:504:GLU:HA   | 1:B:507:ARG:HD2  | 1.78                     | 0.65              |
| 1:B:570:GLN:O    | 1:B:582:CYS:N    | 2.28                     | 0.65              |
| 1:B:809:ARG:NH1  | 3:E:40:GLN:O     | 2.30                     | 0.65              |
| 2:C:365:ALA:O    | 2:C:372:ARG:NH1  | 2.31                     | 0.65              |
| 4:F:159:THR:HA   | 4:F:162:LEU:HD12 | 1.79                     | 0.65              |
| 3:H:43:THR:HG22  | 3:H:45:ALA:H     | 1.62                     | 0.65              |
| 1:A:81:PRO:HA    | 1:A:84:SER:HB2   | 1.79                     | 0.64              |
| 1:A:116:TYR:OH   | 1:A:146:ARG:O    | 2.14                     | 0.64              |
| 2:C:14:SER:H     | 2:C:158:GLY:HA2  | 1.62                     | 0.64              |
| 2:D:67:LEU:HD12  | 2:D:207:GLU:HG3  | 1.78                     | 0.64              |
| 2:D:200:PHE:HD1  | 2:D:205:GLU:HB3  | 1.62                     | 0.64              |
| 1:A:138:ILE:HG23 | 1:A:193:TYR:CD1  | 2.32                     | 0.64              |
| 1:B:113:ILE:HG21 | 1:B:126:PRO:HD3  | 1.79                     | 0.64              |
| 1:B:446:VAL:O    | 1:B:450:LEU:CB   | 2.36                     | 0.64              |
| 1:B:800:GLN:HG3  | 3:E:112:LEU:HD23 | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:50:LYS:HA    | 4:G:69:LEU:HD13  | 1.77                     | 0.64              |
| 1:B:381:ASN:O    | 1:B:385:GLN:N    | 2.27                     | 0.64              |
| 2:C:131:ALA:HB1  | 2:C:356:TRP:CD1  | 2.31                     | 0.64              |
| 2:D:240:TYR:HB3  | 2:D:250:ILE:HD11 | 1.79                     | 0.64              |
| 1:B:346:GLU:O    | 1:B:350:THR:OG1  | 2.08                     | 0.64              |
| 1:B:359:VAL:HG13 | 1:B:431:ALA:HB1  | 1.79                     | 0.64              |
| 1:B:429:ALA:HB2  | 1:B:603:ASP:HA   | 1.80                     | 0.64              |
| 1:A:118:GLY:HA3  | 1:A:717:CYS:SG   | 2.37                     | 0.64              |
| 1:A:159:THR:HA   | 1:A:162:ARG:HH21 | 1.63                     | 0.64              |
| 1:A:351:SER:O    | 1:A:355:VAL:HG23 | 1.98                     | 0.64              |
| 1:A:355:VAL:HB   | 1:A:438:LEU:HD22 | 1.78                     | 0.64              |
| 1:A:702:LEU:HA   | 1:A:705:LEU:HD12 | 1.80                     | 0.64              |
| 1:A:845:THR:HB   | 4:G:75:GLU:HG2   | 1.77                     | 0.64              |
| 1:B:10:GLU:O     | 1:B:14:PHE:N     | 2.30                     | 0.64              |
| 1:B:46:ALA:H     | 1:B:63:GLU:HG2   | 1.63                     | 0.64              |
| 1:B:101:LEU:HA   | 1:B:104:LEU:HD12 | 1.78                     | 0.64              |
| 1:B:223:GLN:O    | 1:B:227:ALA:N    | 2.27                     | 0.64              |
| 1:B:704:GLN:O    | 1:B:708:ASN:N    | 2.28                     | 0.64              |
| 1:B:752:ALA:O    | 1:B:756:MET:HG3  | 1.98                     | 0.64              |
| 2:D:298:VAL:HG22 | 2:D:330:ILE:HB   | 1.78                     | 0.64              |
| 3:E:26:ILE:O     | 3:E:64:LEU:N     | 2.29                     | 0.64              |
| 1:A:362:LEU:HD21 | 1:A:398:PHE:HZ   | 1.63                     | 0.64              |
| 1:A:429:ALA:HB2  | 1:A:603:ASP:HA   | 1.79                     | 0.64              |
| 1:A:476:SER:O    | 1:A:480:LEU:N    | 2.20                     | 0.64              |
| 1:A:477:PHE:HD2  | 1:A:600:LYS:HB3  | 1.63                     | 0.64              |
| 1:B:23:PRO:O     | 1:B:792:ILE:HD13 | 1.97                     | 0.64              |
| 3:E:72:MET:HE2   | 3:E:76:ILE:HG13  | 1.79                     | 0.64              |
| 1:A:243:ASP:OD1  | 1:A:244:ASN:N    | 2.30                     | 0.64              |
| 1:B:50:LYS:HB2   | 1:B:59:VAL:HA    | 1.79                     | 0.64              |
| 1:B:385:GLN:HG3  | 1:B:395:VAL:HG21 | 1.79                     | 0.64              |
| 1:B:480:LEU:HD23 | 1:B:538:LEU:HD13 | 1.77                     | 0.64              |
| 1:B:686:ILE:HD13 | 1:B:689:HIS:HB3  | 1.78                     | 0.64              |
| 2:C:132:MET:N    | 2:C:357:ILE:O    | 2.31                     | 0.64              |
| 1:A:352:ILE:HG13 | 1:A:620:PHE:HE2  | 1.61                     | 0.64              |
| 1:A:489:LEU:HA   | 1:A:492:LEU:HD12 | 1.80                     | 0.64              |
| 1:A:754:ILE:HG12 | 1:A:769:ILE:HG13 | 1.78                     | 0.64              |
| 1:A:799:PHE:HD1  | 1:A:802:GLN:HE21 | 1.45                     | 0.64              |
| 1:B:566:HIS:HB2  | 1:B:569:PHE:HB2  | 1.79                     | 0.64              |
| 1:B:611:SER:O    | 1:B:615:GLN:N    | 2.29                     | 0.64              |
| 1:B:734:TYR:CD2  | 1:B:760:LEU:HD11 | 2.32                     | 0.64              |
| 1:A:105:ARG:HA   | 1:A:696:LEU:HD22 | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:274:LYS:HB3  | 1:A:432:LYS:HB3  | 1.80                     | 0.64              |
| 1:A:378:MET:HB2  | 1:A:399:THR:HG23 | 1.78                     | 0.64              |
| 1:B:400:ARG:HA   | 1:B:403:LEU:HD13 | 1.79                     | 0.64              |
| 2:C:75:ILE:HG13  | 2:C:177:ARG:NH2  | 2.13                     | 0.64              |
| 2:C:189:LEU:HB2  | 2:C:257:CYS:SG   | 2.38                     | 0.64              |
| 2:C:297:ASN:HD22 | 2:C:314:GLN:HE22 | 1.43                     | 0.64              |
| 3:E:132:GLU:HA   | 3:E:138:ILE:HG23 | 1.78                     | 0.64              |
| 4:F:118:HIS:HA   | 4:F:152:ASN:HD22 | 1.63                     | 0.64              |
| 1:A:49:ILE:HG21  | 1:A:52:GLU:HB2   | 1.80                     | 0.64              |
| 1:A:84:SER:HA    | 1:A:103:ASN:OD1  | 1.97                     | 0.64              |
| 1:A:294:ILE:HA   | 1:A:307:LEU:HD13 | 1.80                     | 0.64              |
| 1:A:531:PRO:HA   | 1:A:539:ALA:HB1  | 1.79                     | 0.64              |
| 2:C:15:GLY:H     | 2:C:158:GLY:HA2  | 1.63                     | 0.64              |
| 2:D:113:LYS:HA   | 2:D:371:HIS:CE1  | 2.33                     | 0.64              |
| 2:D:151:ILE:HG23 | 2:D:297:ASN:HA   | 1.81                     | 0.64              |
| 2:D:314:GLN:NE2  | 2:D:327:ILE:O    | 2.31                     | 0.64              |
| 1:A:85:LYS:H     | 1:A:103:ASN:HA   | 1.63                     | 0.63              |
| 1:A:333:GLN:O    | 1:A:337:GLU:HG2  | 1.98                     | 0.63              |
| 1:A:504:GLU:OE1  | 1:A:507:ARG:NH1  | 2.31                     | 0.63              |
| 1:B:367:PHE:N    | 1:B:424:ASP:OD1  | 2.28                     | 0.63              |
| 1:B:437:ARG:NH1  | 1:B:627:ASP:O    | 2.31                     | 0.63              |
| 1:B:681:PHE:HA   | 1:B:683:ARG:HH21 | 1.62                     | 0.63              |
| 2:C:62:ARG:NH1   | 2:C:240:TYR:OH   | 2.30                     | 0.63              |
| 2:C:220:ALA:HB1  | 2:C:223:PHE:HA   | 1.79                     | 0.63              |
| 2:D:13:GLY:HA3   | 2:D:158:GLY:HA3  | 1.78                     | 0.63              |
| 2:D:17:VAL:HG11  | 2:D:85:ILE:HG23  | 1.80                     | 0.63              |
| 2:D:134:VAL:HG23 | 2:D:374:CYS:HB2  | 1.79                     | 0.63              |
| 2:D:193:LEU:HD21 | 2:D:250:ILE:HA   | 1.80                     | 0.63              |
| 1:A:328:ASP:O    | 1:A:332:PHE:CB   | 2.47                     | 0.63              |
| 1:B:17:LYS:HD2   | 1:B:86:VAL:HA    | 1.78                     | 0.63              |
| 1:B:182:GLY:HA2  | 1:B:185:GLU:HB3  | 1.80                     | 0.63              |
| 2:C:317:ILE:O    | 2:C:327:ILE:HD12 | 1.99                     | 0.63              |
| 4:F:117:ILE:H    | 4:F:155:TYR:HE1  | 1.45                     | 0.63              |
| 1:A:107:ARG:O    | 1:A:112:LEU:N    | 2.30                     | 0.63              |
| 1:A:121:CYS:N    | 1:A:146:ARG:HH22 | 1.96                     | 0.63              |
| 1:A:409:VAL:HG22 | 2:D:24:ASP:HB3   | 1.80                     | 0.63              |
| 1:B:187:THR:OG1  | 1:B:465:ASP:OD1  | 2.12                     | 0.63              |
| 1:B:323:ILE:HB   | 1:B:331:MET:HE1  | 1.78                     | 0.63              |
| 1:B:352:ILE:HG13 | 1:B:620:PHE:HE2  | 1.60                     | 0.63              |
| 2:C:208:ILE:HG23 | 2:C:240:TYR:CE2  | 2.33                     | 0.63              |
| 2:D:73:HIS:C     | 2:D:159:VAL:HB   | 2.23                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:125:GLU:OE1  | 2:D:362:TYR:OH   | 2.07                     | 0.63              |
| 1:B:34:LEU:HB3   | 1:B:78:MET:HB3   | 1.80                     | 0.63              |
| 1:B:275:SER:O    | 1:B:279:ARG:N    | 2.31                     | 0.63              |
| 2:C:145:SER:HB3  | 2:C:330:ILE:HG21 | 1.79                     | 0.63              |
| 2:D:104:LEU:HD13 | 2:D:343:GLY:O    | 1.99                     | 0.63              |
| 1:A:182:GLY:HA2  | 1:A:185:GLU:HB3  | 1.80                     | 0.63              |
| 1:B:45:GLU:HA    | 1:B:63:GLU:HB2   | 1.80                     | 0.63              |
| 1:B:223:GLN:HB2  | 1:B:450:LEU:HG   | 1.78                     | 0.63              |
| 1:B:274:LYS:HE2  | 1:B:432:LYS:HB3  | 1.79                     | 0.63              |
| 1:B:584:LEU:HD23 | 1:B:589:LYS:HG3  | 1.80                     | 0.63              |
| 1:B:800:GLN:HE22 | 3:E:115:LEU:HB2  | 1.63                     | 0.63              |
| 2:C:24:ASP:HB2   | 2:C:340:TRP:HH2  | 1.64                     | 0.63              |
| 2:D:54:VAL:N     | 2:D:57:GLU:OE1   | 2.31                     | 0.63              |
| 1:A:102:HIS:CD2  | 1:A:105:ARG:HH22 | 2.17                     | 0.63              |
| 1:A:289:ILE:HD13 | 1:A:335:THR:HG21 | 1.81                     | 0.63              |
| 1:B:401:SER:O    | 1:B:606:ASN:ND2  | 2.28                     | 0.63              |
| 1:B:499:ILE:HD11 | 1:B:675:ARG:HH22 | 1.64                     | 0.63              |
| 1:A:251:PHE:HA   | 1:A:463:ILE:O    | 1.98                     | 0.63              |
| 1:A:285:ARG:HH12 | 1:A:288:HIS:CD2  | 2.17                     | 0.63              |
| 1:A:510:ILE:O    | 1:A:513:ASN:ND2  | 2.31                     | 0.63              |
| 1:A:559:LEU:HD22 | 1:A:569:PHE:CE2  | 2.34                     | 0.63              |
| 1:B:356:VAL:HG22 | 1:B:435:PHE:HE1  | 1.64                     | 0.63              |
| 1:B:751:GLN:HA   | 1:B:754:ILE:HB   | 1.81                     | 0.63              |
| 2:C:162:ASN:HB2  | 2:C:176:MET:HE2  | 1.81                     | 0.63              |
| 3:E:102:THR:OG1  | 3:E:137:CYS:O    | 2.15                     | 0.63              |
| 1:A:138:ILE:HG21 | 1:A:196:VAL:HB   | 1.79                     | 0.63              |
| 1:B:12:PHE:HE2   | 1:B:131:PRO:HD2  | 1.64                     | 0.63              |
| 1:B:104:LEU:HB3  | 1:B:701:VAL:HG11 | 1.80                     | 0.63              |
| 1:B:601:ASN:HA   | 1:B:659:VAL:HB   | 1.80                     | 0.63              |
| 2:C:151:ILE:HG23 | 2:C:162:ASN:HD21 | 1.63                     | 0.63              |
| 2:D:116:ARG:HH11 | 2:D:371:HIS:HA   | 1.63                     | 0.63              |
| 1:A:47:ALA:HB2   | 1:A:61:LEU:HA    | 1.81                     | 0.63              |
| 1:A:173:ILE:HG12 | 1:A:461:LEU:HD11 | 1.81                     | 0.63              |
| 1:A:256:PHE:HB2  | 1:A:459:SER:HB3  | 1.79                     | 0.63              |
| 1:A:392:GLY:O    | 1:A:617:SER:N    | 2.24                     | 0.63              |
| 1:A:488:LYS:HD3  | 1:A:525:ILE:HG21 | 1.81                     | 0.63              |
| 1:B:80:PRO:HG2   | 1:B:785:GLU:CB   | 2.29                     | 0.63              |
| 1:B:480:LEU:HD21 | 1:B:528:ILE:HG23 | 1.80                     | 0.63              |
| 2:C:219:VAL:HG13 | 2:C:262:PHE:CE2  | 2.34                     | 0.63              |
| 1:A:276:ARG:NH1  | 1:A:284:GLU:OE2  | 2.30                     | 0.62              |
| 1:A:496:THR:OG1  | 1:A:675:ARG:NH1  | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:276:ARG:HD3  | 1:B:280:GLN:HA   | 1.79                     | 0.62              |
| 1:B:357:SER:O    | 1:B:361:GLN:HG2  | 1.98                     | 0.62              |
| 1:B:508:GLU:OE2  | 1:B:773:LYS:N    | 2.29                     | 0.62              |
| 1:B:750:LYS:O    | 1:B:754:ILE:N    | 2.22                     | 0.62              |
| 1:B:799:PHE:HZ   | 3:E:143:LEU:HG   | 1.62                     | 0.62              |
| 2:C:156:GLY:HA3  | 2:C:303:THR:N    | 2.10                     | 0.62              |
| 2:D:239:SER:HA   | 2:D:249:THR:HA   | 1.81                     | 0.62              |
| 1:A:257:ASP:N    | 1:A:261:TYR:O    | 2.22                     | 0.62              |
| 1:A:446:VAL:O    | 1:A:450:LEU:HB3  | 1.98                     | 0.62              |
| 1:A:705:LEU:HD13 | 1:A:711:LEU:HD13 | 1.81                     | 0.62              |
| 1:B:305:LEU:HD23 | 1:B:354:ARG:HG3  | 1.81                     | 0.62              |
| 1:B:344:PHE:CZ   | 1:B:442:ILE:HA   | 2.33                     | 0.62              |
| 2:C:74:GLY:O     | 2:C:111:ASN:ND2  | 2.31                     | 0.62              |
| 2:C:97:ALA:O     | 2:C:100:GLU:HG2  | 1.99                     | 0.62              |
| 2:D:136:ILE:HG21 | 2:D:163:VAL:HG21 | 1.81                     | 0.62              |
| 1:A:313:TYR:HD1  | 1:A:364:ASN:HD21 | 1.46                     | 0.62              |
| 1:A:487:GLU:HG2  | 1:A:521:LEU:HB3  | 1.81                     | 0.62              |
| 1:A:586:TYR:OH   | 1:A:715:ARG:NH2  | 2.30                     | 0.62              |
| 1:B:306:LEU:HD13 | 1:B:386:LYS:HG2  | 1.82                     | 0.62              |
| 1:B:310:PHE:O    | 1:B:316:LEU:HB2  | 1.99                     | 0.62              |
| 1:B:422:GLN:NE2  | 1:B:548:PRO:O    | 2.32                     | 0.62              |
| 1:B:613:LEU:HB3  | 1:B:625:TRP:CE3  | 2.31                     | 0.62              |
| 4:G:84:MET:HG3   | 4:G:88:MET:HE3   | 1.81                     | 0.62              |
| 1:A:52:GLU:HG3   | 1:A:57:VAL:HG22  | 1.81                     | 0.62              |
| 1:A:79:ASN:OD1   | 1:A:94:CYS:N     | 2.19                     | 0.62              |
| 1:A:362:LEU:HA   | 1:A:365:ILE:HD12 | 1.82                     | 0.62              |
| 1:A:477:PHE:CE2  | 1:A:601:ASN:HB2  | 2.34                     | 0.62              |
| 1:A:491:GLN:HA   | 1:A:521:LEU:HD13 | 1.82                     | 0.62              |
| 1:A:492:LEU:HD11 | 1:A:671:MET:HA   | 1.80                     | 0.62              |
| 1:B:12:PHE:CG    | 1:B:130:LEU:HD13 | 2.35                     | 0.62              |
| 1:B:114:TYR:CE2  | 1:B:130:LEU:HD12 | 2.34                     | 0.62              |
| 1:B:198:ALA:HB3  | 1:B:262:ILE:HG13 | 1.80                     | 0.62              |
| 1:B:527:LEU:CD2  | 1:B:583:ILE:HG23 | 2.29                     | 0.62              |
| 2:D:154:ASP:N    | 2:D:161:HIS:O    | 2.31                     | 0.62              |
| 3:H:64:LEU:HD21  | 3:H:69:PHE:HA    | 1.81                     | 0.62              |
| 1:A:406:ARG:HG2  | 1:A:415:GLN:HG3  | 1.81                     | 0.62              |
| 1:B:3:GLN:N      | 1:B:150:PRO:HG2  | 2.14                     | 0.62              |
| 1:B:82:LYS:HD2   | 1:B:733:ARG:HH21 | 1.63                     | 0.62              |
| 1:B:799:PHE:CD1  | 3:E:144:VAL:HG22 | 2.33                     | 0.62              |
| 2:C:131:ALA:HA   | 2:C:358:THR:HA   | 1.81                     | 0.62              |
| 2:C:196:ARG:NH1  | 2:C:237:GLU:OE2  | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:142:LEU:HB2  | 2:D:152:VAL:HG21 | 1.82                     | 0.62              |
| 3:E:131:HIS:HD2  | 3:E:146:MET:HB2  | 1.65                     | 0.62              |
| 3:H:36:ARG:HG3   | 3:H:42:PRO:HG2   | 1.81                     | 0.62              |
| 1:A:530:ARG:HH22 | 1:A:566:HIS:CG   | 2.17                     | 0.62              |
| 1:B:278:ILE:HB   | 1:B:279:ARG:HH11 | 1.63                     | 0.62              |
| 1:B:327:GLN:HG3  | 1:B:329:ASP:H    | 1.64                     | 0.62              |
| 2:C:27:PRO:HA    | 2:C:340:TRP:CD2  | 2.35                     | 0.62              |
| 2:C:250:ILE:HG23 | 2:C:253:GLU:HB2  | 1.82                     | 0.62              |
| 2:C:299:MET:HE1  | 2:C:313:MET:HB3  | 1.81                     | 0.62              |
| 2:D:61:LYS:HG3   | 2:D:64:ILE:HG12  | 1.79                     | 0.62              |
| 2:D:147:ARG:HE   | 2:D:330:ILE:HG21 | 1.65                     | 0.62              |
| 2:D:153:LEU:HD13 | 2:D:299:MET:HE1  | 1.82                     | 0.62              |
| 2:D:196:ARG:NH2  | 2:D:198:TYR:OH   | 2.32                     | 0.62              |
| 1:A:55:ASP:O     | 1:A:57:VAL:N     | 2.33                     | 0.62              |
| 1:A:105:ARG:O    | 1:A:109:PHE:CB   | 2.48                     | 0.62              |
| 1:A:269:THR:O    | 1:A:440:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:302:ARG:HA   | 1:A:307:LEU:HD12 | 1.82                     | 0.62              |
| 1:A:721:PHE:CD1  | 1:A:775:PHE:HB3  | 2.34                     | 0.62              |
| 1:A:812:PHE:O    | 1:A:815:ARG:NH2  | 2.33                     | 0.62              |
| 1:B:76:GLN:HB2   | 1:B:98:ALA:HB3   | 1.80                     | 0.62              |
| 1:B:289:ILE:HD12 | 1:B:292:TYR:HB2  | 1.81                     | 0.62              |
| 1:B:804:ARG:NH2  | 3:E:119:MET:HG2  | 2.14                     | 0.62              |
| 2:C:212:ILE:HG23 | 2:C:216:LEU:HD12 | 1.81                     | 0.62              |
| 2:D:96:VAL:HB    | 2:D:101:HIS:CD2  | 2.34                     | 0.62              |
| 2:D:257:CYS:O    | 2:D:260:THR:OG1  | 2.16                     | 0.62              |
| 3:H:11:PHE:O     | 3:H:15:PHE:HB2   | 2.00                     | 0.62              |
| 1:A:291:TYR:HD1  | 1:A:310:PHE:CD1  | 2.17                     | 0.62              |
| 1:A:305:LEU:HB2  | 1:A:307:LEU:HG   | 1.82                     | 0.62              |
| 1:A:406:ARG:HA   | 1:A:415:GLN:HA   | 1.82                     | 0.62              |
| 1:B:89:MET:HG3   | 1:B:100:VAL:HG13 | 1.82                     | 0.62              |
| 1:B:93:THR:HG22  | 1:B:781:LEU:HD13 | 1.82                     | 0.62              |
| 1:B:193:TYR:CZ   | 1:B:197:VAL:HG21 | 2.35                     | 0.62              |
| 1:B:373:THR:HG23 | 2:C:332:PRO:HA   | 1.81                     | 0.62              |
| 2:C:28:ARG:NH2   | 2:C:94:LEU:O     | 2.32                     | 0.62              |
| 2:C:86:TRP:CE3   | 2:C:122:ILE:HG21 | 2.34                     | 0.62              |
| 3:E:15:PHE:O     | 3:E:26:ILE:HG12  | 2.00                     | 0.62              |
| 1:A:302:ARG:HG2  | 1:A:307:LEU:HD12 | 1.82                     | 0.62              |
| 1:B:162:ARG:O    | 1:B:167:ASP:N    | 2.30                     | 0.62              |
| 1:B:562:GLU:O    | 1:B:566:HIS:ND1  | 2.32                     | 0.62              |
| 2:C:300:SER:HB2  | 2:C:335:ARG:O    | 1.99                     | 0.62              |
| 4:G:99:GLU:HA    | 4:G:102:ILE:HD12 | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:296:GLY:HA3  | 1:A:329:ASP:HA   | 1.82                     | 0.62              |
| 1:B:302:ARG:HA   | 1:B:307:LEU:HB2  | 1.81                     | 0.62              |
| 1:B:803:CYS:SG   | 3:E:119:MET:HE1  | 2.40                     | 0.62              |
| 2:C:38:PRO:HA    | 2:C:65:LEU:HA    | 1.82                     | 0.62              |
| 2:C:192:ILE:HD12 | 2:C:256:ARG:HD3  | 1.80                     | 0.62              |
| 1:A:118:GLY:HA2  | 1:A:722:PRO:HB2  | 1.81                     | 0.61              |
| 1:A:141:TYR:CE1  | 1:A:155:ALA:HB2  | 2.35                     | 0.61              |
| 1:A:174:LEU:HB3  | 1:A:464:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:402:ILE:CG1  | 1:A:606:ASN:HD22 | 2.13                     | 0.61              |
| 1:B:326:GLN:HB3  | 1:B:331:MET:CE   | 2.30                     | 0.61              |
| 1:B:419:THR:O    | 1:B:422:GLN:N    | 2.33                     | 0.61              |
| 3:E:128:VAL:HA   | 3:E:143:LEU:HD13 | 1.81                     | 0.61              |
| 1:A:117:SER:HB3  | 1:A:714:ILE:HG12 | 1.82                     | 0.61              |
| 1:A:221:GLU:OE2  | 1:A:254:ILE:HG23 | 2.00                     | 0.61              |
| 1:A:685:ILE:HD11 | 1:A:710:VAL:HG21 | 1.82                     | 0.61              |
| 1:B:505:TYR:CE1  | 1:B:721:PHE:HB2  | 2.34                     | 0.61              |
| 2:C:317:ILE:C    | 2:C:327:ILE:HD12 | 2.24                     | 0.61              |
| 2:D:69:TYR:OH    | 2:D:207:GLU:OE2  | 2.09                     | 0.61              |
| 1:A:58:THR:HA    | 1:A:68:VAL:C     | 2.25                     | 0.61              |
| 1:A:234:PHE:CD1  | 1:A:289:ILE:HG21 | 2.35                     | 0.61              |
| 1:A:373:THR:OG1  | 1:A:417:ALA:O    | 2.14                     | 0.61              |
| 1:A:804:ARG:NH1  | 3:H:113:VAL:HA   | 2.16                     | 0.61              |
| 1:B:231:LEU:HB3  | 1:B:248:PHE:HZ   | 1.65                     | 0.61              |
| 1:B:339:MET:SD   | 1:B:352:ILE:HD13 | 2.41                     | 0.61              |
| 1:B:622:ALA:O    | 1:B:626:LYS:N    | 2.33                     | 0.61              |
| 1:B:805:GLY:HA2  | 3:E:36:ARG:HD3   | 1.82                     | 0.61              |
| 1:B:812:PHE:HZ   | 3:E:34:VAL:HA    | 1.64                     | 0.61              |
| 2:C:274:ILE:HG23 | 2:C:275:HIS:H    | 1.66                     | 0.61              |
| 2:D:85:ILE:HG22  | 2:D:86:TRP:CD1   | 2.35                     | 0.61              |
| 2:D:109:PRO:HD3  | 2:D:136:ILE:HG23 | 1.82                     | 0.61              |
| 2:D:174:ALA:HB2  | 2:D:284:LYS:HB2  | 1.82                     | 0.61              |
| 3:H:108:ILE:HA   | 3:H:111:VAL:HG22 | 1.80                     | 0.61              |
| 1:A:359:VAL:HA   | 1:A:362:LEU:HD12 | 1.82                     | 0.61              |
| 1:B:344:PHE:CE2  | 1:B:442:ILE:HA   | 2.35                     | 0.61              |
| 2:C:5:THR:HG21   | 2:C:352:PHE:HB3  | 1.81                     | 0.61              |
| 3:E:55:LYS:O     | 3:E:59:MET:N     | 2.28                     | 0.61              |
| 4:G:117:ILE:HD13 | 4:G:155:TYR:HB3  | 1.81                     | 0.61              |
| 1:A:194:LEU:HD22 | 1:A:256:PHE:CZ   | 2.35                     | 0.61              |
| 1:A:388:CYS:HA   | 1:A:393:ILE:HG12 | 1.82                     | 0.61              |
| 1:B:305:LEU:HD22 | 1:B:354:ARG:N    | 2.15                     | 0.61              |
| 1:B:559:LEU:HD11 | 1:B:594:ALA:HB3  | 1.80                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:353:GLN:HA   | 2:C:356:TRP:CZ3  | 2.36                     | 0.61              |
| 2:D:75:ILE:HG13  | 2:D:115:ASN:HD21 | 1.66                     | 0.61              |
| 2:D:86:TRP:HH2   | 2:D:119:MET:HG2  | 1.63                     | 0.61              |
| 1:A:103:ASN:O    | 1:A:107:ARG:HG3  | 2.00                     | 0.61              |
| 1:B:96:ASN:O     | 1:B:100:VAL:N    | 2.22                     | 0.61              |
| 1:B:132:ILE:HG13 | 1:B:152:HIS:CE1  | 2.35                     | 0.61              |
| 2:C:70:PRO:HG3   | 2:C:81:ASP:HB3   | 1.81                     | 0.61              |
| 2:C:313:MET:O    | 2:C:317:ILE:HG12 | 2.00                     | 0.61              |
| 2:D:8:LEU:N      | 2:D:102:PRO:O    | 2.30                     | 0.61              |
| 3:E:110:HIS:O    | 3:E:114:THR:N    | 2.32                     | 0.61              |
| 4:F:161:ILE:HA   | 4:F:165:GLY:H    | 1.65                     | 0.61              |
| 3:H:112:LEU:HB3  | 3:H:124:VAL:HG11 | 1.82                     | 0.61              |
| 1:A:33:LYS:HD2   | 1:A:77:LYS:HA    | 1.83                     | 0.61              |
| 1:A:35:VAL:HG22  | 1:A:75:ILE:HA    | 1.83                     | 0.61              |
| 1:A:61:LEU:HD13  | 1:A:64:ASN:HD22  | 1.64                     | 0.61              |
| 1:A:133:TYR:HD2  | 1:A:152:HIS:HE2  | 1.48                     | 0.61              |
| 1:A:273:GLU:H    | 1:A:287:PHE:HZ   | 1.46                     | 0.61              |
| 1:A:326:GLN:HB3  | 1:A:331:MET:HG3  | 1.82                     | 0.61              |
| 1:A:498:PHE:HA   | 1:A:501:GLU:HB2  | 1.80                     | 0.61              |
| 1:A:517:PHE:CD2  | 1:A:716:ILE:HG23 | 2.35                     | 0.61              |
| 1:B:187:THR:HA   | 1:B:463:ILE:HG21 | 1.81                     | 0.61              |
| 1:B:400:ARG:O    | 1:B:404:THR:N    | 2.24                     | 0.61              |
| 2:C:104:LEU:HD12 | 2:C:352:PHE:HE1  | 1.65                     | 0.61              |
| 2:C:142:LEU:HA   | 2:C:298:VAL:HG11 | 1.82                     | 0.61              |
| 2:D:5:THR:HG21   | 2:D:352:PHE:HB3  | 1.83                     | 0.61              |
| 2:D:83:GLU:O     | 2:D:127:PHE:HZ   | 1.84                     | 0.61              |
| 1:A:82:LYS:NZ    | 1:A:789:ASP:OD2  | 2.33                     | 0.61              |
| 1:A:368:LYS:N    | 1:A:377:SER:O    | 2.34                     | 0.61              |
| 1:A:706:ARG:NH1  | 1:A:712:GLU:OE2  | 2.34                     | 0.61              |
| 1:B:265:ALA:N    | 1:B:451:ASP:OD1  | 2.25                     | 0.61              |
| 1:B:348:GLU:OE2  | 1:B:445:ARG:NH1  | 2.28                     | 0.61              |
| 1:B:381:ASN:HB3  | 1:B:399:THR:HG21 | 1.83                     | 0.61              |
| 1:A:176:THR:O    | 1:A:684:CYS:N    | 2.33                     | 0.61              |
| 1:A:295:ALA:HB2  | 1:A:310:PHE:CZ   | 2.35                     | 0.61              |
| 1:A:377:SER:HA   | 1:A:403:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:753:CYS:HB3  | 1:A:769:ILE:HD11 | 1.83                     | 0.61              |
| 1:A:804:ARG:HG3  | 3:H:117:GLU:HG3  | 1.83                     | 0.61              |
| 1:B:12:PHE:CD2   | 1:B:130:LEU:HB3  | 2.36                     | 0.61              |
| 1:B:294:ILE:HB   | 1:B:310:PHE:CE1  | 2.36                     | 0.61              |
| 1:B:307:LEU:HD23 | 1:B:313:TYR:HE2  | 1.65                     | 0.61              |
| 1:B:523:PRO:HB2  | 1:B:568:LYS:HG2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:754:ILE:HG12 | 1:B:769:ILE:HG13 | 1.83                     | 0.61              |
| 2:C:70:PRO:O     | 2:C:77:THR:N     | 2.32                     | 0.61              |
| 3:E:43:THR:HG22  | 3:E:45:ALA:N     | 2.14                     | 0.61              |
| 1:A:305:LEU:HB3  | 1:A:357:SER:OG   | 2.01                     | 0.61              |
| 1:A:508:GLU:HA   | 1:A:771:GLN:HG2  | 1.82                     | 0.61              |
| 1:B:234:PHE:CE1  | 1:B:289:ILE:HG12 | 2.36                     | 0.61              |
| 4:F:65:THR:HB    | 4:F:67:GLU:HG2   | 1.82                     | 0.61              |
| 1:A:78:MET:HA    | 1:A:99:SER:HB3   | 1.83                     | 0.60              |
| 1:A:114:TYR:HE1  | 1:A:123:VAL:HG13 | 1.66                     | 0.60              |
| 1:B:378:MET:HE2  | 1:B:380:ASP:O    | 2.02                     | 0.60              |
| 1:B:840:TRP:NE1  | 4:F:75:GLU:OE2   | 2.34                     | 0.60              |
| 2:C:157:ASP:OD1  | 2:C:213:LYS:NZ   | 2.32                     | 0.60              |
| 1:A:177:GLY:HA3  | 1:A:684:CYS:HB2  | 1.83                     | 0.60              |
| 1:A:264:GLY:HA3  | 1:A:455:ARG:HD3  | 1.84                     | 0.60              |
| 1:A:488:LYS:HD3  | 1:A:525:ILE:HD13 | 1.84                     | 0.60              |
| 1:A:683:ARG:HE   | 1:A:710:VAL:HG22 | 1.66                     | 0.60              |
| 1:B:186:ASN:HB3  | 1:B:682:VAL:HG11 | 1.83                     | 0.60              |
| 1:B:271:LEU:N    | 1:B:666:GLN:HB3  | 2.15                     | 0.60              |
| 2:C:278:THR:O    | 2:C:281:SER:OG   | 2.16                     | 0.60              |
| 2:C:317:ILE:HG22 | 2:C:327:ILE:CD1  | 2.30                     | 0.60              |
| 4:G:34:LYS:HE3   | 4:G:86:LEU:HD13  | 1.82                     | 0.60              |
| 1:A:441:TRP:CH2  | 1:A:623:ASP:HB3  | 2.36                     | 0.60              |
| 1:A:575:LEU:HA   | 1:A:578:LYS:HE3  | 1.83                     | 0.60              |
| 1:A:583:ILE:HB   | 1:A:592:TYR:CD2  | 2.36                     | 0.60              |
| 1:A:593:ASN:O    | 1:A:597:TRP:NE1  | 2.34                     | 0.60              |
| 1:B:232:GLU:O    | 1:B:288:HIS:ND1  | 2.34                     | 0.60              |
| 2:C:151:ILE:N    | 2:C:296:ASN:O    | 2.35                     | 0.60              |
| 2:D:70:PRO:O     | 2:D:77:THR:N     | 2.33                     | 0.60              |
| 4:G:50:LYS:O     | 4:G:54:HIS:HB2   | 2.02                     | 0.60              |
| 1:A:224:LEU:HD22 | 1:A:252:ILE:HG12 | 1.82                     | 0.60              |
| 1:A:362:LEU:HD11 | 1:A:434:LYS:HD3  | 1.83                     | 0.60              |
| 1:A:500:LEU:O    | 1:A:504:GLU:HG2  | 2.01                     | 0.60              |
| 1:A:554:SER:HA   | 1:A:557:GLU:HB2  | 1.84                     | 0.60              |
| 1:A:584:LEU:HA   | 1:A:589:LYS:HA   | 1.84                     | 0.60              |
| 1:A:611:SER:O    | 1:A:615:GLN:N    | 2.34                     | 0.60              |
| 1:B:61:LEU:HD11  | 1:B:70:LEU:HB2   | 1.82                     | 0.60              |
| 1:B:114:TYR:CE1  | 1:B:153:ILE:HG13 | 2.35                     | 0.60              |
| 1:B:800:GLN:NE2  | 3:E:111:VAL:O    | 2.33                     | 0.60              |
| 2:C:122:ILE:O    | 2:C:127:PHE:N    | 2.34                     | 0.60              |
| 2:C:166:TYR:HB2  | 2:C:289:ILE:HG21 | 1.82                     | 0.60              |
| 2:C:294:TYR:HB3  | 2:C:327:ILE:HG12 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:305:MET:HG3  | 2:D:336:LYS:HB2  | 1.84                     | 0.60              |
| 3:H:35:MET:HG3   | 3:H:73:MET:HA    | 1.84                     | 0.60              |
| 1:A:105:ARG:O    | 1:A:109:PHE:HB2  | 2.02                     | 0.60              |
| 1:A:176:THR:HG21 | 1:A:683:ARG:HH11 | 1.66                     | 0.60              |
| 1:A:237:ALA:H    | 1:A:247:ARG:HG2  | 1.66                     | 0.60              |
| 1:A:556:VAL:HA   | 1:A:559:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:102:HIS:CD2  | 1:B:105:ARG:HE   | 2.19                     | 0.60              |
| 1:B:278:ILE:HG13 | 1:B:279:ARG:N    | 2.15                     | 0.60              |
| 1:B:288:HIS:ND1  | 1:B:323:ILE:HD11 | 2.17                     | 0.60              |
| 2:C:220:ALA:HB3  | 2:C:259:GLU:CG   | 2.31                     | 0.60              |
| 1:B:9:ASP:O      | 1:B:132:ILE:HG22 | 2.01                     | 0.60              |
| 1:B:26:GLN:HE22  | 1:B:31:ALA:HB2   | 1.65                     | 0.60              |
| 1:B:292:TYR:CE1  | 1:B:331:MET:HE3  | 2.37                     | 0.60              |
| 1:B:712:GLU:HB3  | 1:B:715:ARG:HH21 | 1.67                     | 0.60              |
| 1:B:809:ARG:HG2  | 3:E:37:ALA:HA    | 1.83                     | 0.60              |
| 2:D:214:GLU:HB3  | 2:D:215:LYS:HE3  | 1.81                     | 0.60              |
| 2:D:246:GLN:HE21 | 2:D:248:ILE:HD11 | 1.64                     | 0.60              |
| 1:A:47:ALA:HA    | 1:A:62:GLN:H     | 1.66                     | 0.60              |
| 1:A:306:LEU:HB2  | 1:A:390:LEU:HD21 | 1.84                     | 0.60              |
| 1:A:433:ALA:O    | 1:A:437:ARG:HD2  | 2.02                     | 0.60              |
| 1:B:26:GLN:NE2   | 1:B:31:ALA:HB2   | 2.16                     | 0.60              |
| 1:B:116:TYR:OH   | 1:B:146:ARG:O    | 2.09                     | 0.60              |
| 1:B:405:PRO:HA   | 1:B:608:ASN:HD22 | 1.66                     | 0.60              |
| 1:B:437:ARG:HA   | 1:B:440:ARG:HB2  | 1.82                     | 0.60              |
| 1:B:555:PHE:CE2  | 1:B:594:ALA:HB1  | 2.37                     | 0.60              |
| 2:C:59:GLN:HA    | 2:C:67:LEU:HD21  | 1.82                     | 0.60              |
| 1:A:546:TRP:HZ3  | 2:D:349:LEU:HA   | 1.67                     | 0.60              |
| 1:A:804:ARG:NH1  | 3:H:112:LEU:O    | 2.33                     | 0.60              |
| 2:C:19:ALA:C     | 2:C:340:TRP:HE1  | 2.09                     | 0.60              |
| 2:C:23:GLY:H     | 2:C:348:SER:HB2  | 1.67                     | 0.60              |
| 2:C:135:ALA:HB1  | 2:C:140:LEU:HD21 | 1.83                     | 0.60              |
| 2:C:151:ILE:HD11 | 2:C:294:TYR:HA   | 1.83                     | 0.60              |
| 2:C:258:PRO:O    | 2:C:261:LEU:HB3  | 2.01                     | 0.60              |
| 2:D:166:TYR:CD1  | 2:D:293:LEU:HD21 | 2.33                     | 0.60              |
| 1:A:190:VAL:HG11 | 1:A:461:LEU:HD22 | 1.84                     | 0.60              |
| 1:A:505:TYR:HB3  | 1:A:513:ASN:HD22 | 1.66                     | 0.60              |
| 1:A:696:LEU:HD11 | 1:A:701:VAL:HG21 | 1.83                     | 0.60              |
| 1:A:807:LEU:O    | 1:A:811:ALA:CB   | 2.50                     | 0.60              |
| 1:B:286:THR:CG2  | 1:B:316:LEU:HD23 | 2.32                     | 0.60              |
| 1:B:295:ALA:HB2  | 1:B:310:PHE:HZ   | 1.66                     | 0.60              |
| 1:B:359:VAL:HA   | 1:B:362:LEU:HD12 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:536:GLY:O    | 1:B:540:LEU:HG   | 2.02                     | 0.60              |
| 1:B:811:ALA:HB1  | 1:B:814:LYS:HE2  | 1.84                     | 0.60              |
| 2:C:167:GLU:HG2  | 2:D:40:HIS:HB3   | 1.83                     | 0.60              |
| 2:C:298:VAL:HA   | 2:C:330:ILE:HB   | 1.82                     | 0.60              |
| 2:D:120:THR:OG1  | 2:D:362:TYR:HB2  | 2.01                     | 0.60              |
| 2:D:120:THR:HG21 | 2:D:367:PRO:HA   | 1.84                     | 0.60              |
| 1:B:124:ILE:HA   | 1:B:685:ILE:HB   | 1.83                     | 0.60              |
| 1:B:138:ILE:HG13 | 1:B:154:TYR:HE2  | 1.65                     | 0.60              |
| 1:B:288:HIS:CG   | 1:B:323:ILE:HD11 | 2.37                     | 0.60              |
| 1:B:290:PHE:HD1  | 1:B:360:LEU:HG   | 1.66                     | 0.60              |
| 2:D:219:VAL:HG11 | 2:D:309:ILE:HA   | 1.83                     | 0.60              |
| 3:E:11:PHE:O     | 3:E:15:PHE:HB2   | 2.01                     | 0.60              |
| 1:A:61:LEU:HD12  | 1:A:68:VAL:HB    | 1.84                     | 0.59              |
| 1:A:141:TYR:CD1  | 1:A:155:ALA:HB2  | 2.37                     | 0.59              |
| 1:A:251:PHE:HE2  | 1:A:253:ARG:HB2  | 1.67                     | 0.59              |
| 1:A:505:TYR:OH   | 1:A:720:GLY:HA2  | 2.02                     | 0.59              |
| 1:B:168:ARG:CZ   | 1:B:258:VAL:HA   | 2.32                     | 0.59              |
| 1:B:799:PHE:HE1  | 3:E:127:LEU:HD11 | 1.67                     | 0.59              |
| 2:C:11:ASP:HA    | 2:C:106:THR:CG2  | 2.32                     | 0.59              |
| 2:C:128:ASN:HA   | 2:C:359:LYS:HE2  | 1.83                     | 0.59              |
| 1:A:116:TYR:HE1  | 1:A:156:ILE:HD11 | 1.66                     | 0.59              |
| 1:A:410:GLY:HA3  | 2:D:28:ARG:NH2   | 2.16                     | 0.59              |
| 1:A:426:ALA:HB1  | 1:A:606:ASN:HB2  | 1.84                     | 0.59              |
| 1:A:734:TYR:HA   | 1:A:737:LEU:HB3  | 1.83                     | 0.59              |
| 1:A:803:CYS:HA   | 1:A:806:TYR:HB3  | 1.83                     | 0.59              |
| 1:B:107:ARG:CG   | 1:B:112:LEU:HD12 | 2.31                     | 0.59              |
| 1:B:808:ALA:HB2  | 3:E:36:ARG:HD2   | 1.84                     | 0.59              |
| 2:C:5:THR:OG1    | 2:C:347:ALA:O    | 2.17                     | 0.59              |
| 2:C:105:LEU:HD11 | 2:C:123:MET:CG   | 2.32                     | 0.59              |
| 2:C:105:LEU:HG   | 2:C:132:MET:SD   | 2.42                     | 0.59              |
| 2:C:180:LEU:HG   | 2:C:261:LEU:HA   | 1.83                     | 0.59              |
| 2:C:261:LEU:HD22 | 2:C:303:THR:HG21 | 1.83                     | 0.59              |
| 2:D:287:ILE:O    | 2:D:291:LYS:HB2  | 2.03                     | 0.59              |
| 3:H:28:TYR:HA    | 3:H:31:CYS:SG    | 2.42                     | 0.59              |
| 1:A:161:TYR:HA   | 1:A:164:MET:HE2  | 1.85                     | 0.59              |
| 1:A:254:ILE:O    | 1:A:460:PHE:HA   | 2.02                     | 0.59              |
| 1:A:425:PHE:HB3  | 1:A:604:PRO:HD2  | 1.83                     | 0.59              |
| 1:A:510:ILE:HD13 | 1:A:721:PHE:CE2  | 2.37                     | 0.59              |
| 1:B:231:LEU:HB3  | 1:B:248:PHE:CZ   | 2.37                     | 0.59              |
| 1:B:272:LEU:HD23 | 1:B:436:GLU:HG3  | 1.85                     | 0.59              |
| 1:B:437:ARG:HD2  | 1:B:625:TRP:HD1  | 1.65                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:164:PRO:HD3  | 2:C:281:SER:HB2  | 1.84                     | 0.59              |
| 2:C:185:LEU:HG   | 2:C:257:CYS:C    | 2.27                     | 0.59              |
| 2:D:16:LEU:H     | 2:D:157:ASP:HB2  | 1.68                     | 0.59              |
| 2:D:131:ALA:HB1  | 2:D:356:TRP:CD1  | 2.38                     | 0.59              |
| 3:E:105:GLY:HA3  | 3:E:138:ILE:HG12 | 1.83                     | 0.59              |
| 1:A:161:TYR:HA   | 1:A:256:PHE:HE2  | 1.67                     | 0.59              |
| 1:A:231:LEU:HD13 | 1:A:269:THR:HG21 | 1.85                     | 0.59              |
| 1:A:737:LEU:HD21 | 1:A:760:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:805:GLY:O    | 3:H:41:ASN:HB2   | 2.02                     | 0.59              |
| 1:B:411:ARG:NE   | 2:C:93:GLU:O     | 2.35                     | 0.59              |
| 1:B:439:PHE:HA   | 1:B:442:ILE:HB   | 1.84                     | 0.59              |
| 2:C:31:PHE:HE2   | 2:C:85:ILE:HG12  | 1.66                     | 0.59              |
| 2:D:54:VAL:HB    | 2:D:88:HIS:CD2   | 2.36                     | 0.59              |
| 3:E:127:LEU:HD12 | 3:E:147:VAL:HG21 | 1.84                     | 0.59              |
| 1:A:272:LEU:HD13 | 1:A:439:PHE:CG   | 2.38                     | 0.59              |
| 1:B:5:PRO:HB3    | 1:B:14:PHE:CD2   | 2.37                     | 0.59              |
| 1:B:18:ASN:HD22  | 1:B:81:PRO:HB2   | 1.67                     | 0.59              |
| 1:B:21:ASN:H     | 1:B:82:LYS:HB3   | 1.68                     | 0.59              |
| 1:B:601:ASN:ND2  | 1:B:658:THR:HB   | 2.17                     | 0.59              |
| 2:D:86:TRP:CE3   | 2:D:123:MET:HE3  | 2.37                     | 0.59              |
| 1:A:2:SER:HB3    | 1:A:10:GLU:OE1   | 2.03                     | 0.59              |
| 1:B:257:ASP:HA   | 1:B:456:GLN:HG2  | 1.85                     | 0.59              |
| 2:D:191:LYS:HZ1  | 2:D:267:ILE:HA   | 1.67                     | 0.59              |
| 4:G:83:THR:HA    | 4:G:86:LEU:HB3   | 1.83                     | 0.59              |
| 1:A:537:VAL:HA   | 1:A:559:LEU:HD21 | 1.84                     | 0.59              |
| 1:B:7:SER:O      | 1:B:11:LYS:N     | 2.36                     | 0.59              |
| 1:B:229:PRO:O    | 1:B:232:GLU:HB2  | 2.03                     | 0.59              |
| 1:B:563:GLN:HG2  | 1:B:571:LYS:HE3  | 1.85                     | 0.59              |
| 1:B:735:GLU:HG2  | 3:E:90:GLU:HB2   | 1.83                     | 0.59              |
| 2:C:19:ALA:HB3   | 2:C:29:ALA:HB3   | 1.82                     | 0.59              |
| 2:C:20:GLY:HA3   | 2:C:340:TRP:HZ2  | 1.66                     | 0.59              |
| 2:C:165:ILE:HG22 | 2:D:43:VAL:O     | 2.03                     | 0.59              |
| 2:C:188:TYR:O    | 2:C:192:ILE:HG12 | 2.03                     | 0.59              |
| 2:D:297:ASN:ND2  | 2:D:299:MET:HE2  | 2.18                     | 0.59              |
| 1:A:156:ILE:HG21 | 1:A:682:VAL:HG23 | 1.84                     | 0.59              |
| 1:A:509:GLY:H    | 1:A:771:GLN:HE21 | 1.50                     | 0.59              |
| 1:A:527:LEU:HD22 | 1:A:568:LYS:HB2  | 1.83                     | 0.59              |
| 1:A:742:ILE:HG21 | 1:A:746:PHE:HB2  | 1.85                     | 0.59              |
| 1:A:800:GLN:NE2  | 3:H:111:VAL:O    | 2.25                     | 0.59              |
| 1:B:12:PHE:O     | 1:B:114:TYR:HB2  | 2.03                     | 0.59              |
| 1:B:113:ILE:HG12 | 1:B:126:PRO:HD3  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:124:PHE:HZ   | 2:C:132:MET:H    | 1.49                     | 0.59              |
| 2:D:35:VAL:HA    | 2:D:53:TYR:O     | 2.03                     | 0.59              |
| 2:D:75:ILE:HA    | 2:D:115:ASN:ND2  | 2.17                     | 0.59              |
| 2:D:104:LEU:HA   | 2:D:133:TYR:HB3  | 1.84                     | 0.59              |
| 4:F:82:PHE:HA    | 4:F:85:PHE:CE1   | 2.37                     | 0.59              |
| 3:H:111:VAL:HA   | 3:H:115:LEU:HB2  | 1.83                     | 0.59              |
| 1:A:45:GLU:CD    | 1:A:64:ASN:HD21  | 2.10                     | 0.59              |
| 1:A:258:VAL:H    | 1:A:456:GLN:HG2  | 1.66                     | 0.59              |
| 1:A:305:LEU:HD23 | 1:A:354:ARG:HG3  | 1.85                     | 0.59              |
| 1:B:35:VAL:C     | 1:B:78:MET:HB2   | 2.28                     | 0.59              |
| 1:B:92:LEU:HD12  | 1:B:95:LEU:HD23  | 1.85                     | 0.59              |
| 1:B:288:HIS:HB3  | 1:B:292:TYR:CE1  | 2.38                     | 0.59              |
| 1:B:532:THR:HG21 | 2:C:4:GLU:HA     | 1.83                     | 0.59              |
| 1:B:825:ILE:HG12 | 4:F:109:PHE:HB2  | 1.85                     | 0.59              |
| 2:D:131:ALA:O    | 2:D:352:PHE:HZ   | 1.86                     | 0.59              |
| 3:E:119:MET:HB2  | 3:E:124:VAL:HG13 | 1.85                     | 0.59              |
| 4:G:30:ILE:O     | 4:G:34:LYS:HG2   | 2.03                     | 0.59              |
| 1:A:114:TYR:HB2  | 1:A:151:PRO:O    | 2.02                     | 0.59              |
| 1:A:401:SER:HG   | 1:A:609:VAL:HG23 | 1.66                     | 0.59              |
| 1:A:726:VAL:HB   | 1:A:729:GLU:HG3  | 1.84                     | 0.59              |
| 1:A:834:LYS:NZ   | 4:G:144:GLU:OE2  | 2.36                     | 0.59              |
| 1:B:44:PHE:CE2   | 1:B:98:ALA:HA    | 2.37                     | 0.59              |
| 1:B:289:ILE:HA   | 1:B:292:TYR:CB   | 2.30                     | 0.59              |
| 1:B:388:CYS:HB3  | 1:B:393:ILE:O    | 2.02                     | 0.59              |
| 1:B:688:ASN:ND2  | 1:B:690:GLU:OE1  | 2.36                     | 0.59              |
| 2:C:314:GLN:HE21 | 2:C:329:ILE:HG13 | 1.68                     | 0.59              |
| 2:D:19:ALA:O     | 2:D:28:ARG:N     | 2.36                     | 0.59              |
| 4:F:126:LEU:HD22 | 4:F:133:PHE:HB2  | 1.84                     | 0.59              |
| 1:A:276:ARG:HB3  | 1:A:287:PHE:CZ   | 2.38                     | 0.58              |
| 1:A:754:ILE:HA   | 1:A:757:ILE:HD12 | 1.85                     | 0.58              |
| 1:B:26:GLN:HA    | 1:B:29:TRP:O     | 2.03                     | 0.58              |
| 1:B:135:GLU:HA   | 1:B:138:ILE:HD12 | 1.85                     | 0.58              |
| 1:B:157:ALA:HA   | 1:B:173:ILE:HD11 | 1.84                     | 0.58              |
| 1:B:530:ARG:NE   | 1:B:534:PRO:O    | 2.28                     | 0.58              |
| 1:B:533:ASN:ND2  | 2:C:353:GLN:OE1  | 2.36                     | 0.58              |
| 1:B:695:LYS:HG2  | 1:B:696:LEU:N    | 2.18                     | 0.58              |
| 1:B:764:PRO:HB3  | 1:B:768:ARG:HH11 | 1.68                     | 0.58              |
| 2:C:54:VAL:N     | 2:C:57:GLU:OE1   | 2.36                     | 0.58              |
| 2:C:192:ILE:HG21 | 2:C:256:ARG:HE   | 1.68                     | 0.58              |
| 2:C:362:TYR:HA   | 2:C:369:ILE:HG21 | 1.85                     | 0.58              |
| 3:E:50:VAL:HG21  | 3:E:76:ILE:HG12  | 1.85                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:H:15:PHE:CD1  | 3:H:26:ILE:HD13  | 2.37                     | 0.58              |
| 1:B:9:ASP:C     | 1:B:132:ILE:HG22 | 2.28                     | 0.58              |
| 1:B:59:VAL:HG21 | 1:B:75:ILE:HG12  | 1.84                     | 0.58              |
| 1:B:199:SER:HB3 | 1:B:261:TYR:HD2  | 1.67                     | 0.58              |
| 1:B:487:GLU:CD  | 1:B:585:HIS:HD1  | 2.11                     | 0.58              |
| 1:B:552:ASP:OD1 | 1:B:598:LEU:HD13 | 2.03                     | 0.58              |
| 1:B:799:PHE:CZ  | 3:E:143:LEU:HG   | 2.37                     | 0.58              |
| 2:C:367:PRO:O   | 2:C:370:VAL:HG23 | 2.03                     | 0.58              |
| 3:E:104:MET:HE3 | 3:E:107:GLU:HB3  | 1.82                     | 0.58              |
| 4:F:34:LYS:HD2  | 4:F:86:LEU:HD21  | 1.86                     | 0.58              |
| 1:A:141:TYR:CD2 | 1:A:154:TYR:HB2  | 2.38                     | 0.58              |
| 1:A:153:ILE:O   | 1:A:157:ALA:CB   | 2.52                     | 0.58              |
| 1:A:271:LEU:N   | 1:A:666:GLN:HB3  | 2.19                     | 0.58              |
| 1:A:388:CYS:HB3 | 1:A:393:ILE:O    | 2.03                     | 0.58              |
| 1:A:734:TYR:CZ  | 1:A:784:LEU:HB3  | 2.38                     | 0.58              |
| 1:A:822:MET:HA  | 1:A:825:ILE:HD12 | 1.85                     | 0.58              |
| 1:B:281:ALA:HB3 | 1:B:284:GLU:HB2  | 1.84                     | 0.58              |
| 1:B:281:ALA:HA  | 1:B:474:ILE:HD13 | 1.86                     | 0.58              |
| 1:B:286:THR:OG1 | 1:B:290:PHE:HB2  | 2.03                     | 0.58              |
| 2:C:27:PRO:HG3  | 2:C:337:TYR:CD2  | 2.38                     | 0.58              |
| 2:C:301:GLY:O   | 2:C:304:THR:OG1  | 2.20                     | 0.58              |
| 1:A:16:ASP:O    | 1:A:85:LYS:HD2   | 2.03                     | 0.58              |
| 1:A:177:GLY:HA2 | 1:A:708:ASN:OD1  | 2.03                     | 0.58              |
| 1:A:193:TYR:CD2 | 1:A:194:LEU:HD23 | 2.28                     | 0.58              |
| 1:A:257:ASP:HA  | 1:A:456:GLN:HB3  | 1.84                     | 0.58              |
| 1:A:328:ASP:O   | 1:A:332:PHE:HB3  | 2.03                     | 0.58              |
| 1:A:501:GLU:OE2 | 1:A:721:PHE:N    | 2.35                     | 0.58              |
| 1:A:815:ARG:HA  | 1:A:818:GLN:HG3  | 1.86                     | 0.58              |
| 1:B:309:GLY:N   | 1:B:312:ASN:HB2  | 2.17                     | 0.58              |
| 1:B:373:THR:OG1 | 1:B:549:LYS:NZ   | 2.36                     | 0.58              |
| 1:B:721:PHE:O   | 1:B:724:ARG:NH2  | 2.37                     | 0.58              |
| 2:C:50:LYS:HG2  | 2:C:51:ASP:H     | 1.67                     | 0.58              |
| 3:E:87:ASP:HA   | 3:E:90:GLU:HG2   | 1.85                     | 0.58              |
| 3:E:121:GLU:HA  | 3:E:124:VAL:HG22 | 1.83                     | 0.58              |
| 4:F:77:PRO:O    | 4:F:84:MET:HE1   | 2.04                     | 0.58              |
| 3:H:133:ASP:OD2 | 3:H:133:ASP:N    | 2.35                     | 0.58              |
| 1:A:138:ILE:CD1 | 1:A:192:GLN:HG3  | 2.31                     | 0.58              |
| 1:A:237:ALA:O   | 1:A:245:SER:OG   | 2.20                     | 0.58              |
| 1:A:480:LEU:HA  | 1:A:592:TYR:CE1  | 2.37                     | 0.58              |
| 1:A:621:VAL:O   | 1:A:625:TRP:HE3  | 1.87                     | 0.58              |
| 1:A:844:PHE:HE2 | 4:G:87:THR:HG23  | 1.68                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:847:VAL:HG11 | 4:F:62:LYS:HB2   | 1.85                     | 0.58              |
| 1:B:95:LEU:O     | 1:B:718:ARG:NH1  | 2.37                     | 0.58              |
| 1:B:100:VAL:HG11 | 1:B:714:ILE:HD13 | 1.85                     | 0.58              |
| 1:B:133:TYR:HA   | 1:B:154:TYR:CZ   | 2.38                     | 0.58              |
| 1:B:177:GLY:HA2  | 1:B:707:CYS:SG   | 2.43                     | 0.58              |
| 1:B:223:GLN:HB3  | 1:B:342:MET:HE1  | 1.85                     | 0.58              |
| 2:C:9:VAL:HA     | 2:C:104:LEU:HB3  | 1.85                     | 0.58              |
| 2:C:192:ILE:HG13 | 2:C:253:GLU:HB3  | 1.84                     | 0.58              |
| 2:D:11:ASP:HB3   | 2:D:18:LYS:HD3   | 1.85                     | 0.58              |
| 2:D:132:MET:N    | 2:D:357:ILE:O    | 2.36                     | 0.58              |
| 3:E:15:PHE:CD2   | 3:E:26:ILE:HD13  | 2.38                     | 0.58              |
| 1:A:70:LEU:HB3   | 1:A:75:ILE:HD11  | 1.86                     | 0.58              |
| 1:A:408:LYS:HG3  | 1:A:413:VAL:HG22 | 1.85                     | 0.58              |
| 1:B:93:THR:HB    | 1:B:781:LEU:HB3  | 1.86                     | 0.58              |
| 1:B:171:GLN:OE1  | 1:B:680:ASN:ND2  | 2.34                     | 0.58              |
| 1:B:717:CYS:SG   | 1:B:722:PRO:HA   | 2.43                     | 0.58              |
| 2:C:94:LEU:C     | 2:C:96:VAL:H     | 2.12                     | 0.58              |
| 2:C:304:THR:HG22 | 2:C:309:ILE:HG12 | 1.84                     | 0.58              |
| 2:D:32:PRO:O     | 2:D:55:GLY:HA2   | 2.03                     | 0.58              |
| 3:E:109:ARG:HG3  | 3:E:128:VAL:HG21 | 1.85                     | 0.58              |
| 4:F:132:ARG:NH1  | 4:F:133:PHE:O    | 2.35                     | 0.58              |
| 1:A:469:PHE:CZ   | 1:A:586:TYR:HB3  | 2.38                     | 0.58              |
| 1:A:571:LYS:HG3  | 1:A:577:ASP:CB   | 2.33                     | 0.58              |
| 1:A:826:GLN:HA   | 4:G:60:MET:HE1   | 1.84                     | 0.58              |
| 1:B:543:GLU:HA   | 1:B:546:TRP:CD2  | 2.38                     | 0.58              |
| 1:B:766:LEU:O    | 1:B:776:PHE:HA   | 2.03                     | 0.58              |
| 1:B:804:ARG:NH2  | 3:E:117:GLU:O    | 2.37                     | 0.58              |
| 2:C:37:ARG:NH2   | 2:C:81:ASP:OD1   | 2.37                     | 0.58              |
| 2:C:314:GLN:NE2  | 2:C:329:ILE:HG13 | 2.18                     | 0.58              |
| 2:D:79:TRP:CE3   | 2:D:122:ILE:HG12 | 2.34                     | 0.58              |
| 2:D:86:TRP:HZ3   | 2:D:122:ILE:HB   | 1.68                     | 0.58              |
| 2:D:153:LEU:HD11 | 2:D:274:ILE:CG1  | 2.32                     | 0.58              |
| 2:D:218:TYR:HD1  | 2:D:307:PRO:HG2  | 1.68                     | 0.58              |
| 4:F:116:PHE:HB3  | 4:F:154:ASN:HA   | 1.86                     | 0.58              |
| 1:A:34:LEU:HA    | 1:A:47:ALA:O     | 2.04                     | 0.58              |
| 1:A:280:GLN:O    | 1:A:600:LYS:NZ   | 2.36                     | 0.58              |
| 1:A:733:ARG:HH21 | 1:A:734:TYR:HH   | 1.49                     | 0.58              |
| 1:B:25:ALA:HB2   | 1:B:82:LYS:HE2   | 1.86                     | 0.58              |
| 1:B:152:HIS:CG   | 1:B:154:TYR:H    | 2.21                     | 0.58              |
| 2:C:8:LEU:HD22   | 2:C:94:LEU:HD22  | 1.86                     | 0.58              |
| 2:C:188:TYR:CZ   | 2:C:266:PHE:HB3  | 2.39                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:133:TYR:CE2  | 2:D:135:ALA:HB2  | 2.39                     | 0.58              |
| 4:F:50:LYS:HZ2   | 4:F:69:LEU:HB3   | 1.68                     | 0.58              |
| 1:A:351:SER:HA   | 1:A:354:ARG:HD2  | 1.86                     | 0.58              |
| 1:A:387:VAL:HG11 | 1:A:398:PHE:CE1  | 2.39                     | 0.58              |
| 1:A:503:GLU:OE2  | 1:A:507:ARG:NH2  | 2.36                     | 0.58              |
| 1:A:541:LEU:HA   | 1:A:555:PHE:HB2  | 1.84                     | 0.58              |
| 1:A:804:ARG:HE   | 3:H:119:MET:N    | 2.01                     | 0.58              |
| 1:A:848:LYS:HD3  | 4:G:84:MET:HE1   | 1.86                     | 0.58              |
| 1:B:114:TYR:CE2  | 1:B:132:ILE:HD11 | 2.39                     | 0.58              |
| 1:B:153:ILE:O    | 1:B:157:ALA:CB   | 2.50                     | 0.58              |
| 1:B:757:ILE:HG23 | 1:B:762:LEU:HB2  | 1.84                     | 0.58              |
| 2:C:227:MET:HG3  | 2:C:252:ASN:HD22 | 1.69                     | 0.58              |
| 2:C:262:PHE:HE1  | 2:C:313:MET:HG2  | 1.68                     | 0.58              |
| 2:D:19:ALA:HB2   | 2:D:89:THR:HA    | 1.86                     | 0.58              |
| 2:D:37:ARG:HB2   | 2:D:68:LYS:HZ2   | 1.69                     | 0.58              |
| 2:D:86:TRP:HB2   | 2:D:127:PHE:CE2  | 2.39                     | 0.58              |
| 3:E:93:ARG:NH2   | 3:E:103:VAL:HG13 | 2.18                     | 0.58              |
| 1:A:32:LYS:HD2   | 1:A:49:ILE:HB    | 1.84                     | 0.58              |
| 1:A:146:ARG:HG3  | 1:A:156:ILE:HG13 | 1.85                     | 0.58              |
| 1:A:290:PHE:CB   | 1:A:316:LEU:HD21 | 2.32                     | 0.58              |
| 1:A:336:LEU:HA   | 1:A:339:MET:HE3  | 1.85                     | 0.58              |
| 1:B:89:MET:HG2   | 1:B:117:SER:HA   | 1.85                     | 0.58              |
| 1:B:332:PHE:O    | 1:B:335:THR:HB   | 2.04                     | 0.58              |
| 1:B:391:MET:HB3  | 1:B:621:VAL:HG11 | 1.85                     | 0.58              |
| 1:B:732:GLN:HA   | 1:B:744:LYS:HB2  | 1.86                     | 0.58              |
| 1:B:404:THR:HA   | 1:B:417:ALA:HB1  | 1.86                     | 0.57              |
| 1:B:604:PRO:HB3  | 1:B:655:MET:HG3  | 1.86                     | 0.57              |
| 1:B:763:ASP:OD1  | 1:B:766:LEU:N    | 2.24                     | 0.57              |
| 1:B:793:THR:O    | 1:B:797:ILE:HG13 | 2.04                     | 0.57              |
| 2:D:142:LEU:HD21 | 2:D:148:THR:HA   | 1.86                     | 0.57              |
| 2:D:356:TRP:C    | 2:D:373:LYS:HG2  | 2.29                     | 0.57              |
| 3:E:28:TYR:HE1   | 3:E:64:LEU:HD13  | 1.69                     | 0.57              |
| 3:H:43:THR:HB    | 3:H:46:GLU:HG2   | 1.84                     | 0.57              |
| 1:A:114:TYR:CE1  | 1:A:123:VAL:HG22 | 2.39                     | 0.57              |
| 1:A:170:ASP:OD2  | 1:A:460:PHE:N    | 2.37                     | 0.57              |
| 1:A:344:PHE:CE1  | 1:A:352:ILE:HD11 | 2.39                     | 0.57              |
| 1:B:250:LYS:HG3  | 1:B:465:ASP:HB2  | 1.86                     | 0.57              |
| 1:B:545:CYS:SG   | 1:B:598:LEU:HG   | 2.44                     | 0.57              |
| 1:B:766:LEU:HA   | 1:B:777:ARG:HG3  | 1.86                     | 0.57              |
| 2:C:76:ILE:HB    | 2:C:115:ASN:HB3  | 1.86                     | 0.57              |
| 2:D:2:GLU:O      | 2:D:5:THR:HA     | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:73:HIS:HB2   | 2:D:183:ARG:HH21 | 1.69                     | 0.57              |
| 1:A:42:HIS:ND1   | 1:A:699:HIS:HA   | 2.20                     | 0.57              |
| 1:A:125:ASN:HB3  | 1:A:686:ILE:HD13 | 1.85                     | 0.57              |
| 1:A:133:TYR:HA   | 1:A:154:TYR:CE2  | 2.40                     | 0.57              |
| 1:A:266:ASN:HD21 | 1:A:447:ASN:HB3  | 1.67                     | 0.57              |
| 1:A:491:GLN:OE1  | 1:A:522:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:807:LEU:O    | 3:H:126:GLN:NE2  | 2.37                     | 0.57              |
| 1:B:145:LYS:NZ   | 1:B:159:THR:O    | 2.37                     | 0.57              |
| 1:B:292:TYR:CZ   | 1:B:331:MET:HB3  | 2.39                     | 0.57              |
| 1:B:344:PHE:HB3  | 1:B:349:GLN:HG3  | 1.87                     | 0.57              |
| 1:B:411:ARG:NH2  | 2:C:92:ASN:O     | 2.37                     | 0.57              |
| 2:D:57:GLU:O     | 2:D:60:SER:OG    | 2.21                     | 0.57              |
| 2:D:86:TRP:CZ3   | 2:D:122:ILE:HB   | 2.39                     | 0.57              |
| 2:D:123:MET:O    | 2:D:129:VAL:N    | 2.26                     | 0.57              |
| 1:A:229:PRO:O    | 1:A:233:ALA:N    | 2.37                     | 0.57              |
| 1:A:407:ILE:HG21 | 2:D:25:ASP:HB2   | 1.87                     | 0.57              |
| 1:A:468:GLY:O    | 1:A:486:ASN:ND2  | 2.37                     | 0.57              |
| 1:B:154:TYR:CZ   | 1:B:193:TYR:HB2  | 2.39                     | 0.57              |
| 1:B:306:LEU:O    | 1:B:361:GLN:NE2  | 2.37                     | 0.57              |
| 3:E:46:GLU:HA    | 3:E:49:LYS:CG    | 2.32                     | 0.57              |
| 1:A:139:ASP:O    | 1:A:144:LYS:NZ   | 2.27                     | 0.57              |
| 1:B:546:TRP:CE3  | 2:C:4:GLU:HG2    | 2.40                     | 0.57              |
| 2:D:68:LYS:HG3   | 2:D:81:ASP:OD2   | 2.05                     | 0.57              |
| 2:D:358:THR:H    | 2:D:361:GLU:CD   | 2.13                     | 0.57              |
| 1:A:79:ASN:H     | 1:A:99:SER:HB3   | 1.69                     | 0.57              |
| 1:A:129:GLN:HA   | 1:A:133:TYR:HD1  | 1.69                     | 0.57              |
| 1:A:269:THR:OG1  | 1:A:443:LEU:HD22 | 2.05                     | 0.57              |
| 1:A:546:TRP:CD1  | 1:A:657:ARG:HG3  | 2.40                     | 0.57              |
| 1:A:731:ARG:NH1  | 1:A:746:PHE:O    | 2.35                     | 0.57              |
| 1:A:809:ARG:HA   | 1:A:812:PHE:CZ   | 2.39                     | 0.57              |
| 1:B:78:MET:HA    | 1:B:99:SER:HB2   | 1.86                     | 0.57              |
| 1:B:127:TYR:CE1  | 1:B:181:ALA:HA   | 2.39                     | 0.57              |
| 1:B:269:THR:H    | 1:B:443:LEU:HD21 | 1.69                     | 0.57              |
| 1:B:391:MET:HA   | 1:B:621:VAL:HG21 | 1.86                     | 0.57              |
| 1:B:498:PHE:HA   | 1:B:517:PHE:HD2  | 1.69                     | 0.57              |
| 1:B:808:ALA:HB3  | 3:E:36:ARG:HD2   | 1.87                     | 0.57              |
| 2:C:32:PRO:O     | 2:C:55:GLY:HA2   | 2.05                     | 0.57              |
| 2:D:92:ASN:HA    | 2:D:95:ARG:CZ    | 2.35                     | 0.57              |
| 2:D:189:LEU:HD21 | 2:D:212:ILE:HG22 | 1.86                     | 0.57              |
| 2:D:219:VAL:HA   | 2:D:258:PRO:HB2  | 1.86                     | 0.57              |
| 4:F:81:ASN:O     | 4:F:85:PHE:N     | 2.25                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:153:ILE:O    | 1:A:157:ALA:HB3  | 2.04                     | 0.57              |
| 1:A:252:ILE:HG23 | 1:A:267:ILE:HG22 | 1.85                     | 0.57              |
| 1:B:422:GLN:HA   | 1:B:425:PHE:HB2  | 1.85                     | 0.57              |
| 1:B:484:TYR:CE1  | 1:B:525:ILE:HG23 | 2.35                     | 0.57              |
| 1:B:530:ARG:HB3  | 1:B:536:GLY:N    | 2.19                     | 0.57              |
| 1:B:731:ARG:NH2  | 1:B:749:GLY:HA2  | 2.20                     | 0.57              |
| 2:C:167:GLU:CG   | 2:D:40:HIS:HB3   | 2.35                     | 0.57              |
| 2:C:190:MET:HG3  | 2:C:200:PHE:HB2  | 1.87                     | 0.57              |
| 2:D:83:GLU:HA    | 2:D:127:PHE:HE2  | 1.68                     | 0.57              |
| 2:D:123:MET:HE2  | 2:D:123:MET:HA   | 1.86                     | 0.57              |
| 2:D:222:ASP:HB2  | 2:D:225:ASN:ND2  | 2.19                     | 0.57              |
| 1:A:85:LYS:HG2   | 1:A:107:ARG:HG2  | 1.87                     | 0.57              |
| 1:A:172:SER:HB3  | 1:A:677:THR:HG21 | 1.87                     | 0.57              |
| 1:A:224:LEU:HA   | 1:A:227:ALA:HB3  | 1.85                     | 0.57              |
| 1:B:115:THR:O    | 1:B:122:VAL:HB   | 2.05                     | 0.57              |
| 1:B:152:HIS:HB3  | 1:B:155:ALA:H    | 1.70                     | 0.57              |
| 1:B:163:SER:O    | 1:B:169:GLU:N    | 2.22                     | 0.57              |
| 1:B:290:PHE:CB   | 1:B:316:LEU:HD21 | 2.35                     | 0.57              |
| 1:B:315:PHE:HB2  | 1:B:360:LEU:HD23 | 1.87                     | 0.57              |
| 1:B:731:ARG:HH22 | 1:B:749:GLY:HA2  | 1.67                     | 0.57              |
| 1:B:799:PHE:CD2  | 3:E:112:LEU:HD21 | 2.39                     | 0.57              |
| 2:C:32:PRO:HD2   | 2:C:56:ASP:N     | 2.19                     | 0.57              |
| 2:C:189:LEU:HD23 | 2:C:213:LYS:HB2  | 1.86                     | 0.57              |
| 2:D:166:TYR:HD2  | 2:D:167:GLU:HG2  | 1.70                     | 0.57              |
| 2:D:262:PHE:CZ   | 2:D:312:ARG:HG2  | 2.40                     | 0.57              |
| 1:A:129:GLN:HA   | 1:A:133:TYR:CD1  | 2.40                     | 0.57              |
| 1:A:129:GLN:HG3  | 1:A:133:TYR:HD1  | 1.70                     | 0.57              |
| 1:A:153:ILE:HG23 | 1:A:682:VAL:HG21 | 1.87                     | 0.57              |
| 1:A:556:VAL:HA   | 1:A:559:LEU:HB2  | 1.87                     | 0.57              |
| 1:A:776:PHE:HB3  | 1:A:781:LEU:HB2  | 1.87                     | 0.57              |
| 1:B:108:TYR:CE1  | 1:B:113:ILE:HG13 | 2.40                     | 0.57              |
| 2:C:19:ALA:HB2   | 2:C:89:THR:HA    | 1.85                     | 0.57              |
| 2:D:151:ILE:O    | 2:D:297:ASN:HA   | 2.04                     | 0.57              |
| 2:D:351:THR:HB   | 2:D:355:MET:HE2  | 1.87                     | 0.57              |
| 3:H:109:ARG:HG2  | 3:H:124:VAL:HG23 | 1.87                     | 0.57              |
| 1:A:111:GLY:O    | 1:A:113:ILE:N    | 2.37                     | 0.57              |
| 1:A:370:GLU:HB2  | 1:A:374:ASP:OD1  | 2.05                     | 0.57              |
| 2:C:87:HIS:O     | 2:C:92:ASN:N     | 2.38                     | 0.57              |
| 1:B:388:CYS:SG   | 1:B:395:VAL:HA   | 2.44                     | 0.56              |
| 2:C:226:GLU:CB   | 2:C:236:LEU:HD13 | 2.35                     | 0.56              |
| 4:F:67:GLU:HB3   | 4:G:137:GLU:HG3  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:117:SER:HB2  | 1:A:120:PHE:CD2  | 2.39                     | 0.56              |
| 1:A:161:TYR:CZ   | 1:A:197:VAL:HG12 | 2.40                     | 0.56              |
| 1:A:275:SER:H    | 1:A:663:TYR:HH   | 1.52                     | 0.56              |
| 1:A:688:ASN:HB3  | 1:A:692:ARG:HB2  | 1.86                     | 0.56              |
| 1:B:12:PHE:CZ    | 1:B:130:LEU:HD22 | 2.40                     | 0.56              |
| 1:B:126:PRO:HG3  | 1:B:130:LEU:HD11 | 1.87                     | 0.56              |
| 1:B:508:GLU:HB3  | 1:B:770:GLY:HA3  | 1.86                     | 0.56              |
| 2:C:120:THR:OG1  | 2:C:370:VAL:HG22 | 2.05                     | 0.56              |
| 2:C:169:TYR:OH   | 2:D:43:VAL:N     | 2.23                     | 0.56              |
| 2:C:352:PHE:CE2  | 2:C:356:TRP:HB3  | 2.40                     | 0.56              |
| 2:D:70:PRO:HB3   | 2:D:81:ASP:C     | 2.29                     | 0.56              |
| 2:D:82:MET:HE3   | 2:D:86:TRP:CZ2   | 2.40                     | 0.56              |
| 1:A:104:LEU:CD2  | 1:A:122:VAL:HG11 | 2.36                     | 0.56              |
| 1:A:179:SER:HB3  | 1:A:467:ALA:N    | 2.20                     | 0.56              |
| 1:A:290:PHE:CD1  | 1:A:356:VAL:HG13 | 2.40                     | 0.56              |
| 1:A:377:SER:HA   | 1:A:403:LEU:HD13 | 1.86                     | 0.56              |
| 1:A:502:GLN:HA   | 1:A:505:TYR:CD2  | 2.40                     | 0.56              |
| 1:A:568:LYS:HD3  | 1:A:584:LEU:HD12 | 1.86                     | 0.56              |
| 1:A:616:SER:OG   | 1:A:621:VAL:HG12 | 2.05                     | 0.56              |
| 1:B:57:VAL:HG21  | 1:B:72:LYS:HG2   | 1.86                     | 0.56              |
| 1:B:266:ASN:ND2  | 1:B:447:ASN:HB3  | 2.20                     | 0.56              |
| 1:B:291:TYR:CE1  | 1:B:316:LEU:HB3  | 2.40                     | 0.56              |
| 1:B:294:ILE:HG22 | 1:B:302:ARG:CZ   | 2.36                     | 0.56              |
| 1:B:326:GLN:HB3  | 1:B:331:MET:HE2  | 1.87                     | 0.56              |
| 1:B:368:LYS:N    | 1:B:377:SER:O    | 2.37                     | 0.56              |
| 1:B:731:ARG:HH11 | 1:B:752:ALA:HB3  | 1.70                     | 0.56              |
| 2:D:107:GLU:HG3  | 2:D:111:ASN:HD22 | 1.70                     | 0.56              |
| 3:E:36:ARG:HG2   | 3:E:42:PRO:HG2   | 1.85                     | 0.56              |
| 1:A:171:GLN:NE2  | 1:A:678:ASN:HB3  | 2.20                     | 0.56              |
| 1:A:291:TYR:CG   | 1:A:316:LEU:HD22 | 2.40                     | 0.56              |
| 1:A:366:VAL:HG22 | 1:A:380:ASP:HB3  | 1.87                     | 0.56              |
| 1:A:443:LEU:HA   | 1:A:446:VAL:HB   | 1.88                     | 0.56              |
| 1:A:552:ASP:OD2  | 1:A:598:LEU:N    | 2.38                     | 0.56              |
| 1:A:820:THR:O    | 1:A:824:VAL:HG23 | 2.06                     | 0.56              |
| 1:B:25:ALA:H     | 1:B:789:ASP:HB3  | 1.70                     | 0.56              |
| 1:B:264:GLY:HA3  | 1:B:455:ARG:HD2  | 1.88                     | 0.56              |
| 1:B:276:ARG:NH1  | 1:B:284:GLU:HB3  | 2.20                     | 0.56              |
| 1:B:368:LYS:O    | 1:B:377:SER:HB2  | 2.06                     | 0.56              |
| 2:C:12:ASN:OD1   | 2:C:106:THR:N    | 2.38                     | 0.56              |
| 2:C:183:ARG:HH22 | 2:C:210:ARG:HD2  | 1.69                     | 0.56              |
| 2:D:86:TRP:CH2   | 2:D:119:MET:HA   | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:64:LEU:HD21  | 3:H:72:MET:HG2   | 1.87                     | 0.56              |
| 1:A:55:ASP:OD2   | 1:A:72:LYS:HG2   | 2.05                     | 0.56              |
| 1:A:571:LYS:HG3  | 1:A:577:ASP:HB3  | 1.88                     | 0.56              |
| 1:A:756:MET:HA   | 1:A:759:ALA:HB3  | 1.86                     | 0.56              |
| 1:B:13:LEU:HD23  | 1:B:132:ILE:HD12 | 1.88                     | 0.56              |
| 1:B:263:VAL:HB   | 1:B:455:ARG:HA   | 1.88                     | 0.56              |
| 1:B:294:ILE:HD13 | 1:B:308:GLU:O    | 2.05                     | 0.56              |
| 1:B:395:VAL:O    | 1:B:399:THR:OG1  | 2.22                     | 0.56              |
| 1:B:407:ILE:HD11 | 1:B:418:GLN:HA   | 1.87                     | 0.56              |
| 2:C:50:LYS:HB3   | 2:C:53:TYR:CZ    | 2.39                     | 0.56              |
| 2:C:68:LYS:C     | 2:C:69:TYR:HD1   | 2.14                     | 0.56              |
| 2:C:75:ILE:HG13  | 2:C:177:ARG:HH22 | 1.69                     | 0.56              |
| 2:C:108:ALA:HA   | 2:C:161:HIS:CE1  | 2.41                     | 0.56              |
| 2:C:294:TYR:CG   | 2:C:327:ILE:HG12 | 2.40                     | 0.56              |
| 2:D:218:TYR:C    | 2:D:258:PRO:HG2  | 2.30                     | 0.56              |
| 4:F:36:ALA:O     | 4:F:40:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:57:VAL:HG12  | 1:A:59:VAL:HG13  | 1.87                     | 0.56              |
| 1:A:278:ILE:HG13 | 1:A:279:ARG:HG2  | 1.88                     | 0.56              |
| 1:A:430:LEU:O    | 1:A:434:LYS:HG3  | 2.06                     | 0.56              |
| 1:B:288:HIS:CE1  | 1:B:323:ILE:HD11 | 2.41                     | 0.56              |
| 1:B:464:LEU:HD13 | 1:B:674:LEU:HD21 | 1.87                     | 0.56              |
| 1:B:721:PHE:CG   | 1:B:775:PHE:HB3  | 2.41                     | 0.56              |
| 2:C:301:GLY:H    | 2:C:336:LYS:HA   | 1.70                     | 0.56              |
| 2:C:304:THR:HA   | 2:C:309:ILE:HG21 | 1.86                     | 0.56              |
| 2:D:14:SER:N     | 2:D:158:GLY:HA2  | 2.20                     | 0.56              |
| 2:D:144:ALA:HB2  | 2:D:338:SER:O    | 2.05                     | 0.56              |
| 3:E:105:GLY:O    | 3:E:109:ARG:HB2  | 2.04                     | 0.56              |
| 1:A:411:ARG:HE   | 2:D:94:LEU:HD23  | 1.71                     | 0.56              |
| 1:A:517:PHE:HB3  | 1:A:715:ARG:HH12 | 1.71                     | 0.56              |
| 1:A:807:LEU:HD11 | 3:H:127:LEU:HD22 | 1.86                     | 0.56              |
| 1:B:256:PHE:HB2  | 1:B:459:SER:OG   | 2.05                     | 0.56              |
| 1:B:263:VAL:HG21 | 1:B:456:GLN:H    | 1.70                     | 0.56              |
| 1:B:517:PHE:CG   | 1:B:716:ILE:HG23 | 2.40                     | 0.56              |
| 1:B:540:LEU:HD12 | 1:B:559:LEU:HD23 | 1.85                     | 0.56              |
| 2:C:79:TRP:HB3   | 2:C:118:LYS:HD3  | 1.86                     | 0.56              |
| 2:C:105:LEU:HB2  | 2:C:119:MET:HE2  | 1.87                     | 0.56              |
| 2:D:12:ASN:HD22  | 2:D:82:MET:HE1   | 1.71                     | 0.56              |
| 2:D:86:TRP:CZ2   | 2:D:105:LEU:HD13 | 2.40                     | 0.56              |
| 2:D:124:PHE:CD2  | 2:D:362:TYR:HB3  | 2.41                     | 0.56              |
| 1:A:105:ARG:HA   | 1:A:696:LEU:HD13 | 1.86                     | 0.56              |
| 1:A:119:LEU:HD13 | 1:A:500:LEU:HB2  | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:612:LEU:HA   | 1:A:615:GLN:HB2  | 1.87                     | 0.56              |
| 1:B:58:THR:HA    | 1:B:68:VAL:O     | 2.05                     | 0.56              |
| 1:B:141:TYR:CE1  | 1:B:149:MET:HB2  | 2.41                     | 0.56              |
| 1:B:768:ARG:H    | 1:B:774:ILE:HG22 | 1.69                     | 0.56              |
| 2:C:109:PRO:HD2  | 2:C:161:HIS:CG   | 2.41                     | 0.56              |
| 1:A:89:MET:HE3   | 1:A:115:THR:HG23 | 1.88                     | 0.56              |
| 1:A:159:THR:HA   | 1:A:162:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:224:LEU:CD2  | 1:A:252:ILE:HG12 | 2.36                     | 0.56              |
| 1:A:291:TYR:CD1  | 1:A:316:LEU:HD22 | 2.41                     | 0.56              |
| 1:A:292:TYR:CD1  | 1:A:328:ASP:HA   | 2.41                     | 0.56              |
| 1:A:609:VAL:HG13 | 1:A:612:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:834:LYS:NZ   | 4:G:161:ILE:HG23 | 2.21                     | 0.56              |
| 1:B:276:ARG:NH2  | 1:B:479:GLN:HE22 | 2.03                     | 0.56              |
| 1:B:290:PHE:CD1  | 1:B:360:LEU:HG   | 2.41                     | 0.56              |
| 1:B:468:GLY:O    | 1:B:486:ASN:ND2  | 2.39                     | 0.56              |
| 1:B:481:CYS:HB3  | 1:B:663:TYR:HB3  | 1.87                     | 0.56              |
| 1:B:542:ASP:HA   | 1:B:658:THR:HG21 | 1.86                     | 0.56              |
| 3:E:20:ARG:HG2   | 3:E:30:GLN:NE2   | 2.20                     | 0.56              |
| 1:A:243:ASP:OD2  | 1:A:325:ALA:HB3  | 2.06                     | 0.56              |
| 1:A:313:TYR:OH   | 1:A:361:GLN:NE2  | 2.39                     | 0.56              |
| 1:B:95:LEU:H     | 1:B:778:THR:HB   | 1.71                     | 0.56              |
| 1:B:434:LYS:HE3  | 1:B:625:TRP:CH2  | 2.41                     | 0.56              |
| 1:B:476:SER:O    | 1:B:480:LEU:N    | 2.28                     | 0.56              |
| 1:B:478:GLU:OE1  | 1:B:600:LYS:NZ   | 2.38                     | 0.56              |
| 2:C:120:THR:HA   | 2:C:132:MET:CE   | 2.36                     | 0.56              |
| 2:C:155:SER:O    | 2:C:303:THR:N    | 2.39                     | 0.56              |
| 2:C:352:PHE:CD2  | 2:C:356:TRP:HE3  | 2.23                     | 0.56              |
| 2:D:136:ILE:O    | 2:D:140:LEU:N    | 2.32                     | 0.56              |
| 2:D:221:LEU:HD23 | 2:D:312:ARG:HB2  | 1.88                     | 0.56              |
| 1:A:157:ALA:HA   | 1:A:173:ILE:HG13 | 1.88                     | 0.55              |
| 1:B:60:GLU:O     | 1:B:62:GLN:HG3   | 2.06                     | 0.55              |
| 1:B:411:ARG:CZ   | 2:C:93:GLU:HA    | 2.37                     | 0.55              |
| 1:B:562:GLU:HB3  | 1:B:566:HIS:CE1  | 2.41                     | 0.55              |
| 2:C:14:SER:OG    | 2:C:74:GLY:N     | 2.28                     | 0.55              |
| 2:C:352:PHE:HD2  | 2:C:356:TRP:HE3  | 1.53                     | 0.55              |
| 2:D:124:PHE:CG   | 2:D:359:LYS:HA   | 2.41                     | 0.55              |
| 2:D:282:ILE:HG12 | 2:D:293:LEU:C    | 2.31                     | 0.55              |
| 1:A:89:MET:O     | 1:A:95:LEU:HD22  | 2.06                     | 0.55              |
| 1:A:114:TYR:HD1  | 1:A:123:VAL:HA   | 1.70                     | 0.55              |
| 1:A:256:PHE:HA   | 1:A:262:ILE:HA   | 1.88                     | 0.55              |
| 1:A:765:ASN:O    | 1:A:777:ARG:NH2  | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:17:LYS:NZ    | 1:B:18:ASN:O     | 2.37                     | 0.55              |
| 1:B:143:GLY:C    | 1:B:144:LYS:HD3  | 2.31                     | 0.55              |
| 1:B:311:ASN:ND2  | 1:B:316:LEU:O    | 2.39                     | 0.55              |
| 1:B:560:ILE:HG23 | 1:B:571:LYS:HE2  | 1.87                     | 0.55              |
| 1:B:724:ARG:HG2  | 1:B:775:PHE:CD1  | 2.41                     | 0.55              |
| 2:D:85:ILE:O     | 2:D:89:THR:OG1   | 2.18                     | 0.55              |
| 2:D:150:GLY:N    | 2:D:165:ILE:HB   | 2.19                     | 0.55              |
| 2:D:152:VAL:HG13 | 2:D:298:VAL:HB   | 1.88                     | 0.55              |
| 2:D:219:VAL:HG13 | 2:D:262:PHE:CE2  | 2.41                     | 0.55              |
| 3:E:79:ASN:OD1   | 3:E:80:LYS:N     | 2.37                     | 0.55              |
| 4:F:66:ASP:O     | 4:F:70:GLU:HG2   | 2.06                     | 0.55              |
| 4:F:80:ILE:HB    | 4:F:85:PHE:HB3   | 1.88                     | 0.55              |
| 3:H:16:GLN:HG2   | 3:H:24:GLY:HA2   | 1.89                     | 0.55              |
| 1:A:53:LYS:HB2   | 1:A:56:GLU:HB2   | 1.87                     | 0.55              |
| 1:A:285:ARG:NH1  | 1:A:288:HIS:CD2  | 2.75                     | 0.55              |
| 1:A:613:LEU:O    | 1:A:616:SER:OG   | 2.16                     | 0.55              |
| 1:A:810:LYS:HE3  | 3:H:146:MET:HE1  | 1.88                     | 0.55              |
| 1:B:12:PHE:CE2   | 1:B:131:PRO:HD2  | 2.41                     | 0.55              |
| 1:B:313:TYR:CD1  | 1:B:360:LEU:HB3  | 2.42                     | 0.55              |
| 1:B:368:LYS:O    | 1:B:420:LYS:HG2  | 2.07                     | 0.55              |
| 1:B:397:ASP:HA   | 1:B:400:ARG:HH12 | 1.71                     | 0.55              |
| 1:B:437:ARG:HB2  | 1:B:625:TRP:CD1  | 2.40                     | 0.55              |
| 1:B:845:THR:HA   | 1:B:848:LYS:HD3  | 1.88                     | 0.55              |
| 3:E:90:GLU:O     | 3:E:94:VAL:HG22  | 2.07                     | 0.55              |
| 3:H:103:VAL:HG23 | 3:H:138:ILE:HB   | 1.89                     | 0.55              |
| 3:H:119:MET:HG3  | 3:H:120:THR:H    | 1.72                     | 0.55              |
| 1:A:362:LEU:CD1  | 1:A:434:LYS:HD3  | 2.37                     | 0.55              |
| 1:B:10:GLU:HA    | 1:B:13:LEU:HB2   | 1.88                     | 0.55              |
| 1:B:130:LEU:C    | 1:B:132:ILE:H    | 2.14                     | 0.55              |
| 2:C:124:PHE:HB3  | 2:C:359:LYS:HG3  | 1.87                     | 0.55              |
| 2:C:369:ILE:O    | 2:C:373:LYS:N    | 2.40                     | 0.55              |
| 2:D:27:PRO:HA    | 2:D:340:TRP:CE2  | 2.41                     | 0.55              |
| 2:D:189:LEU:HD21 | 2:D:212:ILE:CG2  | 2.36                     | 0.55              |
| 1:A:230:ILE:O    | 1:A:234:PHE:N    | 2.28                     | 0.55              |
| 1:A:527:LEU:HD11 | 1:A:566:HIS:HB3  | 1.87                     | 0.55              |
| 1:B:701:VAL:O    | 1:B:705:LEU:HG   | 2.07                     | 0.55              |
| 1:B:702:LEU:HD11 | 1:B:711:LEU:HD13 | 1.88                     | 0.55              |
| 2:C:90:PHE:HB2   | 2:C:98:PRO:HD3   | 1.89                     | 0.55              |
| 2:C:237:GLU:CA   | 2:C:250:ILE:O    | 2.51                     | 0.55              |
| 4:F:126:LEU:HD13 | 4:F:133:PHE:H    | 1.72                     | 0.55              |
| 1:A:394:ASN:ND2  | 1:A:396:THR:OG1  | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:475:ASN:ND2  | 1:A:479:GLN:O    | 2.38                     | 0.55              |
| 1:A:496:THR:HB   | 1:A:681:PHE:CE1  | 2.41                     | 0.55              |
| 1:A:530:ARG:HH22 | 1:A:566:HIS:CD2  | 2.24                     | 0.55              |
| 1:A:752:ALA:O    | 1:A:756:MET:HG3  | 2.06                     | 0.55              |
| 1:A:767:TYR:HB3  | 1:A:776:PHE:CD1  | 2.42                     | 0.55              |
| 1:A:844:PHE:HD2  | 4:G:88:MET:HA    | 1.72                     | 0.55              |
| 1:B:220:LEU:HD22 | 1:B:452:LYS:N    | 2.22                     | 0.55              |
| 1:B:342:MET:CG   | 1:B:446:VAL:HA   | 2.37                     | 0.55              |
| 2:C:28:ARG:NH1   | 2:C:94:LEU:HD23  | 2.22                     | 0.55              |
| 2:C:317:ILE:HG22 | 2:C:327:ILE:HD13 | 1.88                     | 0.55              |
| 2:D:105:LEU:HD12 | 2:D:134:VAL:HG13 | 1.89                     | 0.55              |
| 2:D:253:GLU:HA   | 2:D:256:ARG:HD2  | 1.89                     | 0.55              |
| 2:D:302:GLY:HA2  | 2:D:336:LYS:HG3  | 1.88                     | 0.55              |
| 3:H:71:PRO:O     | 3:H:75:THR:HG22  | 2.06                     | 0.55              |
| 1:A:29:TRP:HA    | 1:A:34:LEU:HD22  | 1.87                     | 0.55              |
| 1:A:234:PHE:CZ   | 1:A:289:ILE:HG12 | 2.42                     | 0.55              |
| 1:A:488:LYS:HG3  | 1:A:671:MET:HG3  | 1.89                     | 0.55              |
| 1:B:156:ILE:HG23 | 1:B:680:ASN:HB3  | 1.89                     | 0.55              |
| 1:B:241:LYS:NZ   | 1:B:703:GLU:OE2  | 2.38                     | 0.55              |
| 1:B:313:TYR:OH   | 1:B:361:GLN:NE2  | 2.40                     | 0.55              |
| 1:B:367:PHE:CD2  | 1:B:403:LEU:HD12 | 2.40                     | 0.55              |
| 2:C:124:PHE:CG   | 2:C:359:LYS:HA   | 2.42                     | 0.55              |
| 2:D:34:ILE:O     | 2:D:55:GLY:N     | 2.39                     | 0.55              |
| 4:F:131:ASP:OD1  | 4:F:131:ASP:N    | 2.39                     | 0.55              |
| 1:A:97:GLU:OE1   | 1:A:101:LEU:HD12 | 2.07                     | 0.55              |
| 1:A:134:SER:H    | 1:A:154:TYR:HE2  | 1.54                     | 0.55              |
| 1:A:220:LEU:CD1  | 1:A:452:LYS:HB2  | 2.37                     | 0.55              |
| 1:A:434:LYS:HG2  | 1:A:625:TRP:CZ2  | 2.42                     | 0.55              |
| 1:A:546:TRP:NE1  | 1:A:657:ARG:HG3  | 2.21                     | 0.55              |
| 1:A:737:LEU:HA   | 1:A:791:LYS:HG2  | 1.87                     | 0.55              |
| 1:B:362:LEU:HA   | 1:B:365:ILE:HD12 | 1.88                     | 0.55              |
| 1:B:365:ILE:HG21 | 1:B:398:PHE:CE2  | 2.40                     | 0.55              |
| 1:B:508:GLU:CG   | 1:B:773:LYS:HB2  | 2.36                     | 0.55              |
| 2:C:66:THR:OG1   | 2:C:68:LYS:NZ    | 2.38                     | 0.55              |
| 2:D:193:LEU:HD21 | 2:D:250:ILE:HG23 | 1.89                     | 0.55              |
| 3:E:119:MET:SD   | 3:E:124:VAL:HG12 | 2.46                     | 0.55              |
| 4:F:34:LYS:HD3   | 4:F:82:PHE:HE1   | 1.71                     | 0.55              |
| 3:H:20:ARG:HG2   | 3:H:30:GLN:HE22  | 1.71                     | 0.55              |
| 3:H:83:GLY:HA3   | 3:H:88:TYR:CE1   | 2.41                     | 0.55              |
| 1:A:35:VAL:CG2   | 1:A:47:ALA:HB3   | 2.37                     | 0.55              |
| 1:A:47:ALA:CB    | 1:A:61:LEU:HA    | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:TYR:OH   | 1:A:150:PRO:O    | 2.24                     | 0.55              |
| 1:A:244:ASN:HA   | 1:A:288:HIS:CE1  | 2.39                     | 0.55              |
| 1:A:527:LEU:HD12 | 1:A:530:ARG:NH2  | 2.21                     | 0.55              |
| 1:A:570:GLN:N    | 1:A:582:CYS:O    | 2.21                     | 0.55              |
| 1:A:598:LEU:HG   | 1:A:602:MET:HB2  | 1.88                     | 0.55              |
| 1:B:35:VAL:CG2   | 1:B:47:ALA:H     | 2.20                     | 0.55              |
| 1:B:46:ALA:N     | 1:B:102:HIS:HE1  | 2.04                     | 0.55              |
| 1:B:286:THR:HG23 | 1:B:316:LEU:HD23 | 1.88                     | 0.55              |
| 1:B:291:TYR:HD1  | 1:B:310:PHE:CD1  | 2.25                     | 0.55              |
| 1:B:438:LEU:HD12 | 1:B:624:LEU:HD22 | 1.87                     | 0.55              |
| 1:B:735:GLU:CD   | 1:B:744:LYS:H    | 2.15                     | 0.55              |
| 1:B:799:PHE:CE1  | 3:E:144:VAL:HG22 | 2.42                     | 0.55              |
| 1:B:803:CYS:HB3  | 3:E:119:MET:HE1  | 1.89                     | 0.55              |
| 2:C:59:GLN:HB3   | 2:C:62:ARG:NH2   | 2.22                     | 0.55              |
| 2:C:218:TYR:C    | 2:C:258:PRO:HG2  | 2.31                     | 0.55              |
| 2:D:1:ASP:N      | 2:D:353:GLN:HG2  | 2.22                     | 0.55              |
| 2:D:119:MET:SD   | 2:D:134:VAL:HG11 | 2.46                     | 0.55              |
| 2:D:198:TYR:HB3  | 2:D:248:ILE:HG23 | 1.89                     | 0.55              |
| 1:A:35:VAL:HG13  | 1:A:74:ASP:C     | 2.32                     | 0.55              |
| 1:A:194:LEU:HB2  | 1:A:262:ILE:HD11 | 1.87                     | 0.55              |
| 1:A:540:LEU:HD13 | 1:A:559:LEU:HA   | 1.89                     | 0.55              |
| 1:B:26:GLN:NE2   | 1:B:790:LEU:HB2  | 2.21                     | 0.55              |
| 1:B:79:ASN:CG    | 1:B:94:CYS:H     | 2.15                     | 0.55              |
| 1:B:141:TYR:HE1  | 1:B:149:MET:HB2  | 1.72                     | 0.55              |
| 1:B:165:LEU:HD13 | 1:B:259:THR:HA   | 1.89                     | 0.55              |
| 1:B:175:CYS:HB2  | 1:B:464:LEU:O    | 2.07                     | 0.55              |
| 1:B:190:VAL:HG11 | 1:B:461:LEU:HD21 | 1.87                     | 0.55              |
| 1:B:504:GLU:HB3  | 1:B:724:ARG:HE   | 1.71                     | 0.55              |
| 1:B:757:ILE:HD13 | 1:B:767:TYR:CD2  | 2.42                     | 0.55              |
| 2:C:185:LEU:HD21 | 2:C:303:THR:HG23 | 1.89                     | 0.55              |
| 2:C:219:VAL:HG11 | 2:C:309:ILE:HA   | 1.89                     | 0.55              |
| 2:C:358:THR:N    | 2:C:361:GLU:HB2  | 2.22                     | 0.55              |
| 2:D:123:MET:HA   | 2:D:127:PHE:HB2  | 1.87                     | 0.55              |
| 2:D:299:MET:O    | 2:D:335:ARG:NE   | 2.40                     | 0.55              |
| 1:A:141:TYR:HD2  | 1:A:154:TYR:HB2  | 1.70                     | 0.54              |
| 1:A:154:TYR:CD1  | 1:A:193:TYR:HB2  | 2.43                     | 0.54              |
| 1:A:227:ALA:HA   | 1:A:446:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:273:GLU:O    | 1:A:276:ARG:N    | 2.41                     | 0.54              |
| 1:A:728:GLN:NE2  | 1:A:732:GLN:HG3  | 2.22                     | 0.54              |
| 1:B:228:ASN:OD1  | 1:B:250:LYS:NZ   | 2.23                     | 0.54              |
| 1:B:292:TYR:CD1  | 1:B:328:ASP:HA   | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:800:GLN:HG2  | 3:E:112:LEU:HA   | 1.88                     | 0.54              |
| 1:B:806:TYR:HB2  | 3:E:147:VAL:O    | 2.07                     | 0.54              |
| 2:C:76:ILE:O     | 2:C:115:ASN:ND2  | 2.39                     | 0.54              |
| 3:E:28:TYR:CE1   | 3:E:64:LEU:HD13  | 2.42                     | 0.54              |
| 1:A:580:GLU:HB3  | 1:A:593:ASN:HD22 | 1.72                     | 0.54              |
| 1:B:291:TYR:CG   | 1:B:316:LEU:HD22 | 2.42                     | 0.54              |
| 1:B:301:MET:O    | 1:B:305:LEU:HG   | 2.07                     | 0.54              |
| 1:B:305:LEU:HB2  | 1:B:307:LEU:HG   | 1.87                     | 0.54              |
| 1:B:536:GLY:O    | 1:B:540:LEU:N    | 2.40                     | 0.54              |
| 2:C:113:LYS:O    | 2:C:117:GLU:HG3  | 2.08                     | 0.54              |
| 2:D:35:VAL:HG22  | 2:D:54:VAL:HA    | 1.87                     | 0.54              |
| 2:D:105:LEU:HB2  | 2:D:134:VAL:HG12 | 1.89                     | 0.54              |
| 2:D:107:GLU:HB3  | 2:D:374:CYS:SG   | 2.47                     | 0.54              |
| 2:D:200:PHE:CD1  | 2:D:205:GLU:HB3  | 2.42                     | 0.54              |
| 2:D:351:THR:O    | 2:D:355:MET:N    | 2.40                     | 0.54              |
| 1:A:179:SER:OG   | 1:A:246:SER:N    | 2.40                     | 0.54              |
| 1:A:223:GLN:HB2  | 1:A:450:LEU:HA   | 1.90                     | 0.54              |
| 1:A:247:ARG:NH2  | 1:A:470:GLU:OE1  | 2.37                     | 0.54              |
| 1:A:357:SER:HB2  | 1:A:390:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:491:GLN:N    | 1:A:521:LEU:HD22 | 2.23                     | 0.54              |
| 1:A:523:PRO:O    | 1:A:527:LEU:HB2  | 2.07                     | 0.54              |
| 1:B:190:VAL:HB   | 1:B:463:ILE:HD13 | 1.88                     | 0.54              |
| 1:B:447:ASN:HA   | 1:B:450:LEU:HB3  | 1.89                     | 0.54              |
| 1:B:718:ARG:O    | 1:B:777:ARG:NH1  | 2.39                     | 0.54              |
| 2:D:20:GLY:N     | 2:D:340:TRP:HE1  | 2.05                     | 0.54              |
| 2:D:223:PHE:CG   | 2:D:259:GLU:HG3  | 2.42                     | 0.54              |
| 3:E:127:LEU:CD1  | 3:E:147:VAL:HG21 | 2.38                     | 0.54              |
| 4:F:48:ILE:HB    | 4:F:80:ILE:HD11  | 1.89                     | 0.54              |
| 4:F:109:PHE:CE1  | 4:F:125:LEU:HD13 | 2.43                     | 0.54              |
| 3:H:64:LEU:CD2   | 3:H:72:MET:HG2   | 2.38                     | 0.54              |
| 1:A:108:TYR:HD2  | 1:A:696:LEU:HB2  | 1.71                     | 0.54              |
| 1:A:114:TYR:CD2  | 1:A:152:HIS:HA   | 2.42                     | 0.54              |
| 1:B:164:MET:HB3  | 1:B:459:SER:OG   | 2.08                     | 0.54              |
| 1:B:221:GLU:H    | 1:B:221:GLU:CD   | 2.11                     | 0.54              |
| 1:B:705:LEU:HB3  | 1:B:711:LEU:N    | 2.22                     | 0.54              |
| 1:B:802:GLN:N    | 3:E:82:GLN:HG3   | 2.23                     | 0.54              |
| 2:C:20:GLY:C     | 2:C:94:LEU:HD21  | 2.33                     | 0.54              |
| 2:C:154:ASP:HB3  | 2:C:161:HIS:CD2  | 2.42                     | 0.54              |
| 2:C:369:ILE:HD12 | 2:C:372:ARG:HB2  | 1.90                     | 0.54              |
| 2:D:294:TYR:HB3  | 2:D:326:LYS:O    | 2.07                     | 0.54              |
| 4:G:52:ASP:O     | 4:G:56:MET:HG2   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:GLU:HA    | 1:A:100:VAL:HB   | 1.88                     | 0.54              |
| 1:A:290:PHE:C    | 1:A:316:LEU:HD11 | 2.33                     | 0.54              |
| 1:A:313:TYR:CD2  | 1:A:360:LEU:HB3  | 2.43                     | 0.54              |
| 1:A:521:LEU:HG   | 1:A:586:TYR:CG   | 2.43                     | 0.54              |
| 1:A:524:CYS:O    | 1:A:528:ILE:HG12 | 2.08                     | 0.54              |
| 1:B:23:PRO:CB    | 3:E:94:VAL:HB    | 2.37                     | 0.54              |
| 1:B:109:PHE:CE1  | 1:B:696:LEU:HB3  | 2.42                     | 0.54              |
| 1:B:295:ALA:HB2  | 1:B:310:PHE:CZ   | 2.42                     | 0.54              |
| 1:B:387:VAL:O    | 1:B:391:MET:HG2  | 2.07                     | 0.54              |
| 1:B:530:ARG:O    | 1:B:536:GLY:N    | 2.19                     | 0.54              |
| 1:B:606:ASN:HB3  | 1:B:609:VAL:HB   | 1.89                     | 0.54              |
| 2:C:212:ILE:HD13 | 2:C:250:ILE:HD11 | 1.90                     | 0.54              |
| 2:C:310:ALA:O    | 2:C:329:ILE:HD12 | 2.07                     | 0.54              |
| 2:D:78:ASN:CB    | 2:D:81:ASP:HB2   | 2.34                     | 0.54              |
| 2:D:83:GLU:HA    | 2:D:127:PHE:CE2  | 2.43                     | 0.54              |
| 3:E:12:LYS:HD3   | 3:E:66:PHE:CG    | 2.42                     | 0.54              |
| 1:A:141:TYR:HA   | 1:A:144:LYS:HB2  | 1.88                     | 0.54              |
| 1:A:254:ILE:HG22 | 1:A:256:PHE:HE1  | 1.72                     | 0.54              |
| 1:B:127:TYR:CG   | 1:B:691:LYS:HA   | 2.42                     | 0.54              |
| 1:B:174:LEU:HD12 | 1:B:683:ARG:HH22 | 1.72                     | 0.54              |
| 1:B:188:LYS:HA   | 1:B:191:ILE:HB   | 1.90                     | 0.54              |
| 1:B:393:ILE:HG21 | 1:B:613:LEU:HA   | 1.89                     | 0.54              |
| 1:B:687:PRO:HB2  | 1:B:695:LYS:O    | 2.08                     | 0.54              |
| 1:B:795:VAL:HG21 | 3:E:91:GLY:HA3   | 1.89                     | 0.54              |
| 2:C:79:TRP:HE3   | 2:C:122:ILE:HD11 | 1.71                     | 0.54              |
| 4:F:64:PRO:HB2   | 4:F:68:TYR:CD1   | 2.42                     | 0.54              |
| 1:A:108:TYR:CZ   | 1:A:687:PRO:HG3  | 2.42                     | 0.54              |
| 1:A:237:ALA:HA   | 1:A:288:HIS:CD2  | 2.42                     | 0.54              |
| 1:A:609:VAL:HA   | 1:A:612:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:705:LEU:O    | 1:A:710:VAL:N    | 2.41                     | 0.54              |
| 1:B:25:ALA:H     | 1:B:789:ASP:CG   | 2.15                     | 0.54              |
| 1:B:153:ILE:HD13 | 1:B:186:ASN:HA   | 1.90                     | 0.54              |
| 1:B:323:ILE:HD12 | 1:B:331:MET:SD   | 2.48                     | 0.54              |
| 1:B:541:LEU:HB2  | 1:B:555:PHE:CZ   | 2.41                     | 0.54              |
| 2:C:14:SER:N     | 2:C:158:GLY:HA2  | 2.22                     | 0.54              |
| 2:C:141:SER:HB3  | 2:C:300:SER:HB3  | 1.88                     | 0.54              |
| 2:C:157:ASP:N    | 2:C:302:GLY:HA3  | 2.22                     | 0.54              |
| 2:D:151:ILE:HD12 | 2:D:282:ILE:HG13 | 1.89                     | 0.54              |
| 2:D:315:LYS:NZ   | 2:D:316:GLU:OE2  | 2.37                     | 0.54              |
| 2:D:317:ILE:CG2  | 2:D:327:ILE:HD13 | 2.34                     | 0.54              |
| 4:F:138:VAL:HA   | 4:F:141:MET:HE2  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:83:GLY:HA3   | 3:H:88:TYR:CZ    | 2.43                     | 0.54              |
| 1:A:108:TYR:HE2  | 1:A:695:LYS:C    | 2.16                     | 0.54              |
| 1:A:129:GLN:HG3  | 1:A:133:TYR:HB2  | 1.89                     | 0.54              |
| 1:A:293:LEU:HD11 | 1:A:305:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:400:ARG:HH12 | 1:A:406:ARG:NH1  | 2.04                     | 0.54              |
| 1:A:480:LEU:HD21 | 1:A:538:LEU:HD22 | 1.89                     | 0.54              |
| 1:A:537:VAL:O    | 1:A:555:PHE:HE1  | 1.91                     | 0.54              |
| 1:A:547:PHE:HE1  | 2:D:349:LEU:HD21 | 1.72                     | 0.54              |
| 1:A:806:TYR:CZ   | 3:H:147:VAL:HB   | 2.42                     | 0.54              |
| 1:B:273:GLU:N    | 1:B:287:PHE:HZ   | 2.05                     | 0.54              |
| 1:B:812:PHE:CZ   | 3:E:37:ALA:HB3   | 2.43                     | 0.54              |
| 2:C:156:GLY:CA   | 2:C:182:GLY:H    | 2.21                     | 0.54              |
| 2:D:56:ASP:HA    | 2:D:59:GLN:HG2   | 1.89                     | 0.54              |
| 2:D:133:TYR:CE1  | 2:D:373:LYS:HG3  | 2.43                     | 0.54              |
| 2:D:165:ILE:HD12 | 2:D:169:TYR:CD2  | 2.42                     | 0.54              |
| 2:D:189:LEU:HD12 | 2:D:253:GLU:HB3  | 1.90                     | 0.54              |
| 4:G:93:LEU:HB3   | 4:G:163:LYS:NZ   | 2.23                     | 0.54              |
| 3:H:84:CYS:O     | 3:H:88:TYR:N     | 2.28                     | 0.54              |
| 1:A:250:LYS:HE3  | 1:A:269:THR:HG22 | 1.89                     | 0.54              |
| 1:A:846:LYS:HD3  | 4:G:75:GLU:HG3   | 1.90                     | 0.54              |
| 1:B:176:THR:C    | 1:B:183:LYS:HE3  | 2.33                     | 0.54              |
| 1:B:508:GLU:OE2  | 1:B:771:GLN:N    | 2.41                     | 0.54              |
| 1:B:517:PHE:HB3  | 1:B:716:ILE:HG12 | 1.90                     | 0.54              |
| 1:B:538:LEU:HD23 | 1:B:664:LYS:HE3  | 1.90                     | 0.54              |
| 1:B:573:LYS:HG3  | 1:B:576:LYS:H    | 1.72                     | 0.54              |
| 2:C:224:GLU:N    | 2:C:224:GLU:OE1  | 2.41                     | 0.54              |
| 2:D:225:ASN:O    | 2:D:229:THR:HG23 | 2.07                     | 0.54              |
| 3:H:127:LEU:O    | 3:H:131:HIS:ND1  | 2.40                     | 0.54              |
| 1:A:114:TYR:CD1  | 1:A:123:VAL:HG22 | 2.42                     | 0.54              |
| 1:A:560:ILE:HA   | 1:A:563:GLN:HE21 | 1.73                     | 0.54              |
| 1:B:122:VAL:HG13 | 1:B:685:ILE:HD13 | 1.90                     | 0.54              |
| 1:B:514:PHE:HE2  | 1:B:721:PHE:CD2  | 2.25                     | 0.54              |
| 1:B:822:MET:O    | 1:B:826:GLN:HG3  | 2.08                     | 0.54              |
| 2:C:26:ALA:HA    | 2:C:341:ILE:HG12 | 1.91                     | 0.54              |
| 2:C:124:PHE:CZ   | 2:C:132:MET:HB3  | 2.43                     | 0.54              |
| 1:A:44:PHE:CD1   | 1:A:98:ALA:HA    | 2.39                     | 0.53              |
| 1:A:46:ALA:HB3   | 1:A:63:GLU:HG3   | 1.90                     | 0.53              |
| 1:A:239:THR:HA   | 1:A:284:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:294:ILE:CD1  | 1:A:316:LEU:HD12 | 2.35                     | 0.53              |
| 1:A:331:MET:HA   | 1:A:334:GLU:HG2  | 1.90                     | 0.53              |
| 1:A:724:ARG:HA   | 1:A:775:PHE:HA   | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:810:LYS:HB2  | 3:H:147:VAL:CG1  | 2.37                     | 0.53              |
| 1:B:66:LYS:HD3   | 1:B:68:VAL:HG21  | 1.89                     | 0.53              |
| 1:B:80:PRO:O     | 1:B:83:PHE:N     | 2.31                     | 0.53              |
| 1:B:142:LYS:NZ   | 1:B:197:VAL:O    | 2.37                     | 0.53              |
| 1:B:186:ASN:O    | 1:B:189:LYS:HB2  | 2.08                     | 0.53              |
| 1:B:223:GLN:CB   | 1:B:450:LEU:HA   | 2.38                     | 0.53              |
| 1:B:248:PHE:HB2  | 1:B:270:TYR:O    | 2.08                     | 0.53              |
| 1:B:253:ARG:NE   | 1:B:255:ASN:OD1  | 2.41                     | 0.53              |
| 1:B:300:GLN:NE2  | 1:B:304:ASP:OD2  | 2.40                     | 0.53              |
| 2:C:159:VAL:HG13 | 2:C:161:HIS:CE1  | 2.42                     | 0.53              |
| 2:C:236:LEU:HD23 | 2:C:254:ARG:HH12 | 1.73                     | 0.53              |
| 2:C:261:LEU:HD22 | 2:C:303:THR:CG2  | 2.39                     | 0.53              |
| 2:C:279:TYR:OH   | 2:C:294:TYR:OH   | 2.26                     | 0.53              |
| 2:C:282:ILE:HA   | 2:C:293:LEU:HD12 | 1.91                     | 0.53              |
| 2:C:286:ASP:O    | 2:C:290:ARG:N    | 2.28                     | 0.53              |
| 3:E:38:LEU:HB2   | 3:E:40:GLN:HE22  | 1.73                     | 0.53              |
| 3:E:103:VAL:CG2  | 3:E:140:TYR:HB3  | 2.38                     | 0.53              |
| 3:H:32:GLY:HA2   | 3:H:72:MET:HE1   | 1.90                     | 0.53              |
| 1:A:114:TYR:HB3  | 1:A:121:CYS:SG   | 2.49                     | 0.53              |
| 1:A:398:PHE:HA   | 1:A:609:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:407:ILE:HD11 | 1:A:418:GLN:OE1  | 2.09                     | 0.53              |
| 1:A:437:ARG:HG2  | 1:A:627:ASP:HB3  | 1.89                     | 0.53              |
| 1:A:807:LEU:O    | 1:A:811:ALA:HB2  | 2.08                     | 0.53              |
| 1:B:290:PHE:HB2  | 1:B:316:LEU:HD21 | 1.90                     | 0.53              |
| 1:B:425:PHE:CD2  | 1:B:602:MET:HG2  | 2.43                     | 0.53              |
| 1:B:537:VAL:HA   | 1:B:540:LEU:HD12 | 1.89                     | 0.53              |
| 1:B:763:ASP:O    | 1:B:767:TYR:N    | 2.32                     | 0.53              |
| 2:C:118:LYS:O    | 2:C:122:ILE:HB   | 2.08                     | 0.53              |
| 2:C:127:PHE:O    | 2:C:129:VAL:N    | 2.41                     | 0.53              |
| 2:C:291:LYS:HA   | 2:C:294:TYR:CD2  | 2.42                     | 0.53              |
| 2:D:120:THR:HB   | 2:D:370:VAL:CG2  | 2.37                     | 0.53              |
| 2:D:150:GLY:HA3  | 2:D:296:ASN:HB2  | 1.91                     | 0.53              |
| 3:E:36:ARG:HA    | 3:E:42:PRO:HD2   | 1.89                     | 0.53              |
| 3:E:96:ASP:OD1   | 3:E:98:GLU:HG2   | 2.07                     | 0.53              |
| 3:H:92:LEU:HD22  | 3:H:103:VAL:HG21 | 1.90                     | 0.53              |
| 1:A:104:LEU:CD1  | 1:A:705:LEU:HD11 | 2.38                     | 0.53              |
| 1:A:168:ARG:HH22 | 1:A:458:ALA:C    | 2.15                     | 0.53              |
| 1:A:253:ARG:HG3  | 1:A:460:PHE:CD2  | 2.43                     | 0.53              |
| 1:A:402:ILE:HD11 | 1:A:609:VAL:HG11 | 1.89                     | 0.53              |
| 1:A:537:VAL:HG21 | 1:A:583:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:586:TYR:OH   | 1:A:712:GLU:HB3  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:ALA:O    | 1:A:834:LYS:HB3  | 2.08                     | 0.53              |
| 1:B:158:ASP:OD1  | 1:B:193:TYR:OH   | 2.26                     | 0.53              |
| 1:B:274:LYS:O    | 1:B:277:ALA:HB3  | 2.07                     | 0.53              |
| 2:C:8:LEU:HD13   | 2:C:94:LEU:HD13  | 1.89                     | 0.53              |
| 2:D:37:ARG:HD3   | 2:D:51:ASP:HB3   | 1.90                     | 0.53              |
| 2:D:369:ILE:HD12 | 2:D:372:ARG:HD2  | 1.90                     | 0.53              |
| 3:E:68:GLN:HA    | 3:E:71:PRO:HD2   | 1.91                     | 0.53              |
| 3:E:93:ARG:HH11  | 3:E:100:ASN:N    | 2.07                     | 0.53              |
| 3:H:15:PHE:O     | 3:H:26:ILE:HG12  | 2.09                     | 0.53              |
| 1:A:309:GLY:H    | 1:A:312:ASN:HB2  | 1.73                     | 0.53              |
| 1:A:484:TYR:OH   | 1:A:529:GLU:OE1  | 2.21                     | 0.53              |
| 1:B:95:LEU:HD22  | 1:B:714:ILE:HG23 | 1.89                     | 0.53              |
| 1:B:352:ILE:O    | 1:B:356:VAL:HG23 | 2.07                     | 0.53              |
| 1:B:355:VAL:HG21 | 1:B:624:LEU:CD1  | 2.38                     | 0.53              |
| 1:B:476:SER:H    | 1:B:479:GLN:HB2  | 1.73                     | 0.53              |
| 1:B:822:MET:HB2  | 4:F:129:MET:HE1  | 1.90                     | 0.53              |
| 2:C:54:VAL:HG22  | 2:C:84:LYS:HB3   | 1.89                     | 0.53              |
| 2:C:189:LEU:HA   | 2:C:192:ILE:HD11 | 1.91                     | 0.53              |
| 2:D:78:ASN:CG    | 2:D:81:ASP:H     | 2.16                     | 0.53              |
| 3:E:12:LYS:HB2   | 3:E:66:PHE:CZ    | 2.43                     | 0.53              |
| 3:E:36:ARG:HG2   | 3:E:42:PRO:HD2   | 1.90                     | 0.53              |
| 4:F:103:ARG:NH2  | 4:F:159:THR:OG1  | 2.42                     | 0.53              |
| 3:H:32:GLY:CA    | 3:H:47:VAL:HG13  | 2.33                     | 0.53              |
| 1:A:8:ASP:HA     | 1:A:11:LYS:HB3   | 1.91                     | 0.53              |
| 1:A:17:LYS:HB3   | 1:A:86:VAL:HA    | 1.90                     | 0.53              |
| 1:A:198:ALA:C    | 1:A:262:ILE:H    | 2.16                     | 0.53              |
| 1:A:354:ARG:O    | 1:A:358:SER:HB2  | 2.09                     | 0.53              |
| 1:A:543:GLU:HG3  | 2:D:349:LEU:HD22 | 1.91                     | 0.53              |
| 1:A:583:ILE:HG22 | 1:A:585:HIS:ND1  | 2.24                     | 0.53              |
| 1:A:728:GLN:HE22 | 1:A:745:GLY:HA2  | 1.73                     | 0.53              |
| 1:B:15:VAL:HG21  | 1:B:87:GLU:HB2   | 1.91                     | 0.53              |
| 1:B:278:ILE:O    | 1:B:280:GLN:NE2  | 2.42                     | 0.53              |
| 1:B:510:ILE:HG22 | 1:B:512:TRP:H    | 1.72                     | 0.53              |
| 1:B:555:PHE:CZ   | 1:B:594:ALA:HB1  | 2.44                     | 0.53              |
| 1:B:601:ASN:HD21 | 1:B:658:THR:HB   | 1.72                     | 0.53              |
| 1:B:729:GLU:O    | 1:B:733:ARG:HG2  | 2.08                     | 0.53              |
| 1:B:781:LEU:O    | 1:B:785:GLU:HG2  | 2.09                     | 0.53              |
| 2:C:66:THR:C     | 2:C:67:LEU:HD12  | 2.33                     | 0.53              |
| 2:C:76:ILE:HD12  | 2:C:119:MET:HG2  | 1.91                     | 0.53              |
| 2:D:37:ARG:HH21  | 2:D:52:SER:HA    | 1.74                     | 0.53              |
| 2:D:117:GLU:HA   | 2:D:367:PRO:CB   | 2.37                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:331:ALA:HA   | 2:D:335:ARG:HH21 | 1.73                     | 0.53              |
| 2:D:357:ILE:HG13 | 2:D:373:LYS:HB3  | 1.91                     | 0.53              |
| 3:E:141:GLU:HB3  | 3:E:145:ARG:NH2  | 2.23                     | 0.53              |
| 3:H:88:TYR:HB3   | 3:H:144:VAL:HG11 | 1.89                     | 0.53              |
| 1:A:533:ASN:CG   | 1:A:565:ASN:HB3  | 2.33                     | 0.53              |
| 1:A:620:PHE:CZ   | 1:A:624:LEU:HD12 | 2.43                     | 0.53              |
| 1:B:2:SER:O      | 1:B:10:GLU:HB3   | 2.09                     | 0.53              |
| 1:B:49:ILE:HA    | 1:B:59:VAL:HG12  | 1.91                     | 0.53              |
| 1:B:142:LYS:HB2  | 1:B:197:VAL:HG22 | 1.89                     | 0.53              |
| 1:B:145:LYS:HG3  | 1:B:162:ARG:NH2  | 2.24                     | 0.53              |
| 1:B:426:ALA:HB1  | 1:B:606:ASN:HB2  | 1.90                     | 0.53              |
| 1:B:510:ILE:HD12 | 1:B:768:ARG:HB3  | 1.90                     | 0.53              |
| 1:B:556:VAL:HG11 | 1:B:579:THR:HA   | 1.91                     | 0.53              |
| 2:C:15:GLY:N     | 2:C:158:GLY:HA2  | 2.23                     | 0.53              |
| 2:C:178:LEU:HD22 | 2:C:274:ILE:HA   | 1.90                     | 0.53              |
| 2:D:7:ALA:HB3    | 2:D:347:ALA:HB1  | 1.91                     | 0.53              |
| 2:D:185:LEU:HD21 | 2:D:261:LEU:HB2  | 1.89                     | 0.53              |
| 1:A:53:LYS:NZ    | 1:A:56:GLU:O     | 2.42                     | 0.53              |
| 1:B:160:ALA:HA   | 1:B:171:GLN:HG3  | 1.90                     | 0.53              |
| 1:B:441:TRP:CH2  | 1:B:623:ASP:HB3  | 2.43                     | 0.53              |
| 1:B:531:PRO:C    | 1:B:535:PRO:HB3  | 2.34                     | 0.53              |
| 1:B:734:TYR:HE2  | 1:B:784:LEU:HB3  | 1.72                     | 0.53              |
| 1:B:792:ILE:HG12 | 3:E:94:VAL:CG2   | 2.39                     | 0.53              |
| 2:C:16:LEU:HD23  | 2:C:32:PRO:HA    | 1.90                     | 0.53              |
| 2:C:46:GLY:O     | 2:C:61:LYS:NZ    | 2.42                     | 0.53              |
| 2:C:62:ARG:HB3   | 2:C:204:ALA:HB1  | 1.89                     | 0.53              |
| 2:C:334:GLU:O    | 2:C:338:SER:HB3  | 2.08                     | 0.53              |
| 2:D:11:ASP:CG    | 2:D:339:VAL:HB   | 2.34                     | 0.53              |
| 2:D:118:LYS:HB3  | 2:D:122:ILE:HD11 | 1.90                     | 0.53              |
| 2:D:303:THR:HA   | 2:D:306:TYR:CZ   | 2.43                     | 0.53              |
| 3:E:47:VAL:HG12  | 3:E:48:MET:SD    | 2.49                     | 0.53              |
| 1:A:138:ILE:HA   | 1:A:154:TYR:HB3  | 1.91                     | 0.53              |
| 1:A:224:LEU:HD22 | 1:A:252:ILE:HG21 | 1.91                     | 0.53              |
| 1:A:471:ILE:HG13 | 1:A:483:ASN:ND2  | 2.23                     | 0.53              |
| 1:B:12:PHE:HA    | 1:B:112:LEU:HA   | 1.91                     | 0.53              |
| 1:B:77:LYS:HD2   | 1:B:782:ALA:HB3  | 1.91                     | 0.53              |
| 1:B:218:GLY:HA3  | 1:B:262:ILE:HG21 | 1.91                     | 0.53              |
| 1:B:500:LEU:O    | 1:B:504:GLU:HG2  | 2.08                     | 0.53              |
| 1:B:517:PHE:HB3  | 1:B:716:ILE:HD13 | 1.91                     | 0.53              |
| 1:B:521:LEU:HG   | 1:B:586:TYR:CG   | 2.44                     | 0.53              |
| 1:B:594:ALA:HA   | 1:B:597:TRP:CE2  | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:189:LEU:HG   | 2:C:209:VAL:HG13 | 1.90                     | 0.53              |
| 2:C:291:LYS:HZ3  | 2:C:325:MET:HE2  | 1.73                     | 0.53              |
| 2:C:358:THR:H    | 2:C:361:GLU:CD   | 2.16                     | 0.53              |
| 2:D:71:ILE:HG12  | 2:D:76:ILE:HA    | 1.91                     | 0.53              |
| 2:D:94:LEU:HB3   | 2:D:96:VAL:HG22  | 1.90                     | 0.53              |
| 3:H:43:THR:HG21  | 3:H:117:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:232:GLU:O    | 1:A:236:ASN:HB2  | 2.08                     | 0.53              |
| 1:A:309:GLY:N    | 1:A:312:ASN:HB2  | 2.24                     | 0.53              |
| 1:A:605:LEU:O    | 1:A:655:MET:N    | 2.42                     | 0.53              |
| 1:A:834:LYS:HG3  | 4:G:144:GLU:OE1  | 2.09                     | 0.53              |
| 1:B:35:VAL:CG2   | 1:B:75:ILE:HA    | 2.39                     | 0.53              |
| 1:B:35:VAL:HG11  | 1:B:74:ASP:C     | 2.34                     | 0.53              |
| 1:B:44:PHE:CD2   | 1:B:98:ALA:HA    | 2.44                     | 0.53              |
| 1:B:195:ALA:HA   | 1:B:262:ILE:HD12 | 1.90                     | 0.53              |
| 1:B:224:LEU:HD11 | 1:B:250:LYS:NZ   | 2.23                     | 0.53              |
| 1:B:554:SER:HA   | 1:B:557:GLU:HB2  | 1.90                     | 0.53              |
| 2:C:286:ASP:N    | 2:C:289:ILE:HB   | 2.23                     | 0.53              |
| 3:E:28:TYR:N     | 3:E:59:MET:O     | 2.42                     | 0.53              |
| 4:G:85:PHE:HA    | 4:G:88:MET:HB2   | 1.90                     | 0.53              |
| 3:H:4:SER:O      | 3:H:8:THR:OG1    | 2.26                     | 0.53              |
| 3:H:58:GLU:HG3   | 3:H:62:LYS:HB3   | 1.91                     | 0.53              |
| 1:A:90:ALA:O     | 1:A:723:ASN:ND2  | 2.33                     | 0.53              |
| 1:A:114:TYR:CE2  | 1:A:133:TYR:HE2  | 2.27                     | 0.53              |
| 1:A:411:ARG:HH21 | 2:D:94:LEU:HD23  | 1.74                     | 0.53              |
| 1:A:550:ALA:HB3  | 1:A:602:MET:SD   | 2.49                     | 0.53              |
| 1:B:10:GLU:HG3   | 1:B:137:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:294:ILE:HD11 | 1:B:313:TYR:HD2  | 1.74                     | 0.53              |
| 1:B:355:VAL:HG22 | 1:B:625:TRP:CH2  | 2.44                     | 0.53              |
| 1:B:685:ILE:HG12 | 1:B:705:LEU:HD23 | 1.90                     | 0.53              |
| 1:B:687:PRO:O    | 1:B:695:LYS:NZ   | 2.41                     | 0.53              |
| 2:C:153:LEU:HD21 | 2:C:155:SER:HB2  | 1.91                     | 0.53              |
| 2:D:18:LYS:HB3   | 2:D:27:PRO:HB3   | 1.91                     | 0.53              |
| 2:D:75:ILE:HA    | 2:D:115:ASN:CG   | 2.33                     | 0.53              |
| 2:D:124:PHE:HD2  | 2:D:362:TYR:HB3  | 1.74                     | 0.53              |
| 2:D:180:LEU:HD22 | 2:D:264:PRO:HG3  | 1.91                     | 0.53              |
| 3:H:48:MET:HE3   | 3:H:59:MET:SD    | 2.49                     | 0.53              |
| 1:A:123:VAL:HG11 | 1:A:186:ASN:OD1  | 2.09                     | 0.52              |
| 1:A:176:THR:HG21 | 1:A:683:ARG:NH1  | 2.23                     | 0.52              |
| 1:A:256:PHE:HB3  | 1:A:261:TYR:N    | 2.24                     | 0.52              |
| 1:A:624:LEU:HD22 | 1:A:625:TRP:CH2  | 2.44                     | 0.52              |
| 1:A:685:ILE:HA   | 1:A:704:GLN:HB3  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:807:LEU:HD21 | 3:H:127:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:845:THR:HG23 | 4:G:92:LYS:NZ    | 2.23                     | 0.52              |
| 1:B:51:GLU:O     | 1:B:57:VAL:HA    | 2.09                     | 0.52              |
| 1:B:352:ILE:HA   | 1:B:438:LEU:HD11 | 1.90                     | 0.52              |
| 1:B:362:LEU:HB2  | 1:B:431:ALA:HB2  | 1.90                     | 0.52              |
| 1:B:841:TRP:CH2  | 4:F:162:LEU:HA   | 2.44                     | 0.52              |
| 2:C:9:VAL:HG22   | 2:C:104:LEU:HB3  | 1.90                     | 0.52              |
| 2:C:214:GLU:C    | 2:C:215:LYS:HD2  | 2.34                     | 0.52              |
| 3:E:42:PRO:HG3   | 3:E:76:ILE:HD12  | 1.90                     | 0.52              |
| 1:A:124:ILE:HG21 | 1:A:696:LEU:HD12 | 1.91                     | 0.52              |
| 1:B:78:MET:HG3   | 1:B:84:SER:OG    | 2.09                     | 0.52              |
| 1:B:154:TYR:CE1  | 1:B:193:TYR:HB2  | 2.44                     | 0.52              |
| 1:B:234:PHE:CD2  | 1:B:442:ILE:HD13 | 2.44                     | 0.52              |
| 1:B:430:LEU:O    | 1:B:434:LYS:CB   | 2.52                     | 0.52              |
| 1:B:794:ASP:HA   | 1:B:797:ILE:HD12 | 1.91                     | 0.52              |
| 2:C:76:ILE:HD12  | 2:C:119:MET:CG   | 2.39                     | 0.52              |
| 2:C:219:VAL:HA   | 2:C:258:PRO:HB2  | 1.92                     | 0.52              |
| 2:C:314:GLN:HE22 | 2:C:327:ILE:HG22 | 1.74                     | 0.52              |
| 2:D:166:TYR:CD2  | 2:D:289:ILE:HG23 | 2.44                     | 0.52              |
| 3:H:102:THR:HA   | 3:H:140:TYR:H    | 1.74                     | 0.52              |
| 1:A:101:LEU:HD13 | 1:A:698:ALA:HB1  | 1.90                     | 0.52              |
| 1:A:266:ASN:ND2  | 1:A:447:ASN:HB3  | 2.25                     | 0.52              |
| 1:A:477:PHE:HE1  | 1:A:538:LEU:HD21 | 1.75                     | 0.52              |
| 1:A:485:THR:HA   | 1:A:667:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:526:GLU:HA   | 1:A:529:GLU:HB3  | 1.91                     | 0.52              |
| 1:B:316:LEU:HG   | 1:B:360:LEU:HD21 | 1.92                     | 0.52              |
| 2:C:122:ILE:HG23 | 2:C:126:THR:HB   | 1.92                     | 0.52              |
| 2:C:185:LEU:HB3  | 2:C:257:CYS:HB3  | 1.92                     | 0.52              |
| 2:D:137:GLN:HG3  | 2:D:339:VAL:HG11 | 1.90                     | 0.52              |
| 3:E:40:GLN:HG2   | 3:E:76:ILE:HG22  | 1.91                     | 0.52              |
| 4:G:29:GLN:NE2   | 4:G:94:ASN:OD1   | 2.29                     | 0.52              |
| 1:A:12:PHE:C     | 1:A:132:ILE:HG21 | 2.35                     | 0.52              |
| 1:A:66:LYS:HB3   | 1:A:68:VAL:HG23  | 1.91                     | 0.52              |
| 1:A:137:ILE:HB   | 1:A:154:TYR:CD2  | 2.44                     | 0.52              |
| 1:A:310:PHE:CZ   | 1:A:321:VAL:HG13 | 2.44                     | 0.52              |
| 1:A:484:TYR:HE1  | 1:A:525:ILE:HG23 | 1.75                     | 0.52              |
| 1:A:683:ARG:HH21 | 1:A:710:VAL:HA   | 1.74                     | 0.52              |
| 1:B:291:TYR:HB3  | 1:B:328:ASP:CG   | 2.35                     | 0.52              |
| 1:B:293:LEU:HD21 | 1:B:353:LEU:O    | 2.08                     | 0.52              |
| 1:B:799:PHE:HE2  | 3:E:108:ILE:HD11 | 1.75                     | 0.52              |
| 2:C:14:SER:HB2   | 2:C:158:GLY:O    | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:133:TYR:HB2  | 2:C:356:TRP:HA   | 1.90                     | 0.52              |
| 2:C:155:SER:HA   | 2:C:160:THR:HG23 | 1.92                     | 0.52              |
| 2:D:326:LYS:C    | 2:D:327:ILE:HG13 | 2.34                     | 0.52              |
| 1:A:100:VAL:HA   | 1:A:103:ASN:ND2  | 2.25                     | 0.52              |
| 1:A:466:ILE:HD12 | 1:A:670:LEU:HD23 | 1.91                     | 0.52              |
| 1:A:760:LEU:HB3  | 1:A:762:LEU:HG   | 1.92                     | 0.52              |
| 1:A:762:LEU:HB2  | 1:A:767:TYR:OH   | 2.08                     | 0.52              |
| 1:A:795:VAL:HG11 | 3:H:90:GLU:HB3   | 1.91                     | 0.52              |
| 1:B:141:TYR:CE2  | 1:B:152:HIS:HD2  | 2.28                     | 0.52              |
| 1:B:406:ARG:H    | 1:B:608:ASN:ND2  | 2.03                     | 0.52              |
| 1:B:734:TYR:CD2  | 1:B:737:LEU:HD12 | 2.44                     | 0.52              |
| 1:B:804:ARG:HD2  | 3:E:43:THR:HG23  | 1.91                     | 0.52              |
| 2:C:120:THR:HG23 | 2:C:124:PHE:CE2  | 2.45                     | 0.52              |
| 2:C:192:ILE:HD12 | 2:C:253:GLU:HA   | 1.91                     | 0.52              |
| 2:D:113:LYS:O    | 2:D:117:GLU:HG3  | 2.08                     | 0.52              |
| 4:F:128:THR:HG23 | 4:F:129:MET:HG2  | 1.89                     | 0.52              |
| 1:A:56:GLU:HA    | 1:A:69:THR:HG23  | 1.91                     | 0.52              |
| 1:A:532:THR:HG22 | 1:A:533:ASN:N    | 2.21                     | 0.52              |
| 1:A:582:CYS:O    | 1:A:583:ILE:HG13 | 2.09                     | 0.52              |
| 1:B:18:ASN:HB3   | 1:B:81:PRO:HB2   | 1.92                     | 0.52              |
| 1:B:273:GLU:O    | 1:B:276:ARG:N    | 2.43                     | 0.52              |
| 1:B:282:LYS:H    | 1:B:474:ILE:HG21 | 1.74                     | 0.52              |
| 1:B:598:LEU:O    | 1:B:602:MET:N    | 2.32                     | 0.52              |
| 1:B:668:THR:O    | 1:B:672:THR:HG23 | 2.10                     | 0.52              |
| 2:C:103:THR:O    | 2:C:132:MET:HA   | 2.10                     | 0.52              |
| 2:C:178:LEU:HG   | 2:C:180:LEU:H    | 1.75                     | 0.52              |
| 2:C:219:VAL:HG21 | 2:C:309:ILE:HB   | 1.91                     | 0.52              |
| 2:C:314:GLN:HB2  | 2:C:329:ILE:HD12 | 1.91                     | 0.52              |
| 2:D:98:PRO:HB3   | 2:D:103:THR:HG21 | 1.90                     | 0.52              |
| 2:D:122:ILE:HG22 | 2:D:127:PHE:CE2  | 2.45                     | 0.52              |
| 2:D:279:TYR:HA   | 2:D:282:ILE:HD12 | 1.91                     | 0.52              |
| 3:E:11:PHE:CE2   | 3:E:73:MET:HE2   | 2.45                     | 0.52              |
| 3:E:46:GLU:O     | 3:E:50:VAL:HG13  | 2.10                     | 0.52              |
| 4:G:42:GLN:HG2   | 4:G:52:ASP:HB3   | 1.91                     | 0.52              |
| 4:G:146:PRO:HD2  | 4:G:153:PHE:HE2  | 1.73                     | 0.52              |
| 3:H:33:ASP:O     | 3:H:36:ARG:HB2   | 2.10                     | 0.52              |
| 3:H:102:THR:OG1  | 3:H:137:CYS:HB3  | 2.09                     | 0.52              |
| 1:A:6:LEU:HD23   | 1:A:6:LEU:H      | 1.74                     | 0.52              |
| 1:A:198:ALA:HB3  | 1:A:262:ILE:HG13 | 1.91                     | 0.52              |
| 1:A:285:ARG:NH1  | 1:A:288:HIS:HA   | 2.23                     | 0.52              |
| 1:A:809:ARG:HB2  | 3:H:41:ASN:CB    | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:489:LEU:HD13 | 1:B:674:LEU:HD11 | 1.91                     | 0.52              |
| 2:D:12:ASN:HD22  | 2:D:86:TRP:HZ2   | 1.57                     | 0.52              |
| 2:D:73:HIS:CE1   | 2:D:179:ASP:HA   | 2.45                     | 0.52              |
| 3:E:109:ARG:NH2  | 3:E:132:GLU:OE2  | 2.43                     | 0.52              |
| 3:E:128:VAL:HA   | 3:E:143:LEU:CD1  | 2.39                     | 0.52              |
| 3:H:49:LYS:HA    | 3:H:53:ASN:HD22  | 1.75                     | 0.52              |
| 1:A:15:VAL:HG23  | 1:A:150:PRO:HB3  | 1.91                     | 0.52              |
| 1:A:23:PRO:HG2   | 1:A:793:THR:HG22 | 1.91                     | 0.52              |
| 1:A:138:ILE:CG1  | 1:A:193:TYR:HA   | 2.40                     | 0.52              |
| 1:A:728:GLN:NE2  | 1:A:745:GLY:HA2  | 2.24                     | 0.52              |
| 1:A:834:LYS:HZ2  | 4:G:161:ILE:HG23 | 1.75                     | 0.52              |
| 1:B:238:LYS:HB2  | 1:B:285:ARG:HD3  | 1.92                     | 0.52              |
| 1:B:291:TYR:CD1  | 1:B:316:LEU:HD22 | 2.45                     | 0.52              |
| 1:B:408:LYS:HA   | 1:B:413:VAL:HG13 | 1.92                     | 0.52              |
| 1:B:728:GLN:HE22 | 1:B:745:GLY:H    | 1.58                     | 0.52              |
| 1:B:795:VAL:HG13 | 3:E:88:TYR:HA    | 1.91                     | 0.52              |
| 1:B:832:TYR:OH   | 4:F:141:MET:SD   | 2.55                     | 0.52              |
| 2:C:261:LEU:HD11 | 2:C:274:ILE:HD12 | 1.91                     | 0.52              |
| 2:C:280:ASN:HA   | 2:C:283:MET:HE2  | 1.90                     | 0.52              |
| 2:D:34:ILE:HD11  | 2:D:210:ARG:HD3  | 1.91                     | 0.52              |
| 2:D:120:THR:HB   | 2:D:370:VAL:HG21 | 1.92                     | 0.52              |
| 4:F:160:ARG:HG3  | 4:F:165:GLY:HA3  | 1.92                     | 0.52              |
| 3:H:3:PHE:HB3    | 3:H:7:GLN:NE2    | 2.24                     | 0.52              |
| 1:A:185:GLU:O    | 1:A:189:LYS:HG2  | 2.08                     | 0.52              |
| 1:A:232:GLU:HA   | 1:A:236:ASN:CG   | 2.35                     | 0.52              |
| 1:A:402:ILE:HG13 | 1:A:609:VAL:HG21 | 1.90                     | 0.52              |
| 1:A:700:LEU:O    | 1:A:703:GLU:HB3  | 2.10                     | 0.52              |
| 1:B:95:LEU:H     | 1:B:778:THR:CB   | 2.23                     | 0.52              |
| 1:B:164:MET:SD   | 1:B:461:LEU:HB2  | 2.50                     | 0.52              |
| 1:B:182:GLY:HA3  | 1:B:684:CYS:HB3  | 1.92                     | 0.52              |
| 1:B:290:PHE:O    | 1:B:316:LEU:HD11 | 2.10                     | 0.52              |
| 1:B:367:PHE:CE2  | 1:B:403:LEU:HD12 | 2.45                     | 0.52              |
| 1:B:411:ARG:HG3  | 2:C:28:ARG:HE    | 1.75                     | 0.52              |
| 1:B:602:MET:HG3  | 1:B:604:PRO:HD3  | 1.92                     | 0.52              |
| 1:B:688:ASN:HD22 | 1:B:692:ARG:HD2  | 1.74                     | 0.52              |
| 1:B:722:PRO:O    | 1:B:724:ARG:NH1  | 2.41                     | 0.52              |
| 1:B:739:ALA:HB2  | 1:B:756:MET:HG2  | 1.91                     | 0.52              |
| 1:B:754:ILE:O    | 1:B:758:LYS:HG2  | 2.10                     | 0.52              |
| 1:B:757:ILE:HG22 | 1:B:758:LYS:HD3  | 1.92                     | 0.52              |
| 2:C:86:TRP:NE1   | 2:C:105:LEU:HD13 | 2.25                     | 0.52              |
| 2:C:318:THR:HG22 | 2:C:327:ILE:H    | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:120:THR:HA   | 2:D:132:MET:HE3  | 1.92                     | 0.52              |
| 2:D:304:THR:O    | 2:D:309:ILE:HG21 | 2.09                     | 0.52              |
| 3:E:86:GLU:HA    | 3:E:89:VAL:HG22  | 1.92                     | 0.52              |
| 3:E:88:TYR:CD2   | 3:E:144:VAL:HG11 | 2.45                     | 0.52              |
| 1:A:338:ALA:HA   | 1:A:341:ILE:HD12 | 1.91                     | 0.52              |
| 1:B:101:LEU:HD21 | 1:B:702:LEU:HB2  | 1.91                     | 0.52              |
| 1:B:514:PHE:CG   | 1:B:720:GLY:HA2  | 2.45                     | 0.52              |
| 1:B:750:LYS:HE3  | 1:B:771:GLN:HA   | 1.92                     | 0.52              |
| 1:B:768:ARG:NH2  | 1:B:769:ILE:HB   | 2.25                     | 0.52              |
| 2:C:67:LEU:HD22  | 2:C:207:GLU:CB   | 2.40                     | 0.52              |
| 2:C:86:TRP:HB3   | 2:C:123:MET:HE1  | 1.91                     | 0.52              |
| 2:D:9:VAL:HA     | 2:D:104:LEU:O    | 2.10                     | 0.52              |
| 2:D:107:GLU:HB2  | 2:D:119:MET:SD   | 2.50                     | 0.52              |
| 2:D:275:HIS:HB2  | 2:D:317:ILE:HD13 | 1.91                     | 0.52              |
| 2:D:350:SER:O    | 2:D:354:GLN:HG2  | 2.10                     | 0.52              |
| 1:A:165:LEU:HD22 | 1:A:260:GLY:HA3  | 1.92                     | 0.51              |
| 1:A:187:THR:HG23 | 1:A:463:ILE:HG21 | 1.92                     | 0.51              |
| 1:A:407:ILE:HD11 | 1:A:418:GLN:CD   | 2.35                     | 0.51              |
| 1:A:541:LEU:HB2  | 1:A:555:PHE:CG   | 2.45                     | 0.51              |
| 1:A:757:ILE:O    | 1:A:761:GLU:N    | 2.42                     | 0.51              |
| 1:A:848:LYS:HE2  | 4:G:87:THR:HG21  | 1.91                     | 0.51              |
| 1:B:13:LEU:HD21  | 1:B:152:HIS:CG   | 2.45                     | 0.51              |
| 1:B:108:TYR:OH   | 1:B:694:GLY:N    | 2.43                     | 0.51              |
| 1:B:145:LYS:H    | 1:B:148:GLU:CD   | 2.18                     | 0.51              |
| 1:B:229:PRO:HA   | 1:B:232:GLU:HB2  | 1.92                     | 0.51              |
| 1:B:559:LEU:HB3  | 1:B:569:PHE:HZ   | 1.75                     | 0.51              |
| 1:B:616:SER:HB2  | 1:B:622:ALA:HB2  | 1.92                     | 0.51              |
| 1:B:723:ASN:O    | 1:B:724:ARG:HG3  | 2.10                     | 0.51              |
| 1:B:734:TYR:HA   | 1:B:737:LEU:HB2  | 1.92                     | 0.51              |
| 1:B:734:TYR:CE2  | 1:B:784:LEU:HB3  | 2.45                     | 0.51              |
| 2:D:53:TYR:CE2   | 2:D:65:LEU:HD21  | 2.45                     | 0.51              |
| 2:D:90:PHE:HZ    | 2:D:105:LEU:HD23 | 1.74                     | 0.51              |
| 2:D:313:MET:O    | 2:D:316:GLU:HB2  | 2.10                     | 0.51              |
| 1:A:83:PHE:HB2   | 1:A:92:LEU:HD23  | 1.93                     | 0.51              |
| 1:A:86:VAL:HG23  | 1:A:89:MET:HE2   | 1.92                     | 0.51              |
| 1:A:477:PHE:HE2  | 1:A:659:VAL:HG23 | 1.75                     | 0.51              |
| 1:B:231:LEU:HD11 | 1:B:267:ILE:HD12 | 1.93                     | 0.51              |
| 1:B:407:ILE:HG12 | 1:B:655:MET:HE1  | 1.91                     | 0.51              |
| 1:B:527:LEU:HD22 | 1:B:568:LYS:C    | 2.35                     | 0.51              |
| 2:C:12:ASN:HB2   | 2:C:71:ILE:HD11  | 1.91                     | 0.51              |
| 2:D:12:ASN:ND2   | 2:D:86:TRP:HZ2   | 2.08                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:78:ASN:O     | 2:D:82:MET:N     | 2.43                     | 0.51              |
| 2:D:192:ILE:HD12 | 2:D:256:ARG:HD3  | 1.92                     | 0.51              |
| 2:D:208:ILE:HG23 | 2:D:240:TYR:CE2  | 2.45                     | 0.51              |
| 3:E:4:SER:OG     | 3:E:7:GLN:OE1    | 2.24                     | 0.51              |
| 1:A:59:VAL:HG23  | 1:A:61:LEU:HG    | 1.92                     | 0.51              |
| 1:A:368:LYS:HB2  | 1:A:376:ALA:CA   | 2.40                     | 0.51              |
| 1:A:416:LYS:HE3  | 2:D:334:GLU:HB3  | 1.92                     | 0.51              |
| 1:A:534:PRO:HB2  | 1:A:562:GLU:CG   | 2.40                     | 0.51              |
| 1:A:657:ARG:H    | 1:A:657:ARG:HD2  | 1.75                     | 0.51              |
| 1:A:710:VAL:O    | 1:A:714:ILE:HG13 | 2.10                     | 0.51              |
| 1:A:728:GLN:HA   | 1:A:731:ARG:HE   | 1.76                     | 0.51              |
| 1:A:821:ALA:O    | 1:A:825:ILE:HG13 | 2.11                     | 0.51              |
| 1:B:727:PHE:HB3  | 1:B:731:ARG:HH22 | 1.75                     | 0.51              |
| 1:B:776:PHE:HB3  | 1:B:781:LEU:HD11 | 1.92                     | 0.51              |
| 2:C:16:LEU:HD12  | 2:C:336:LYS:HD2  | 1.91                     | 0.51              |
| 2:C:86:TRP:HZ3   | 2:C:122:ILE:HD13 | 1.75                     | 0.51              |
| 2:C:257:CYS:O    | 2:C:260:THR:OG1  | 2.17                     | 0.51              |
| 2:C:365:ALA:HB1  | 2:C:372:ARG:HH11 | 1.75                     | 0.51              |
| 2:D:108:ALA:HB2  | 2:D:159:VAL:HG11 | 1.90                     | 0.51              |
| 2:D:118:LYS:O    | 2:D:122:ILE:HG13 | 2.11                     | 0.51              |
| 2:D:171:LEU:HB2  | 2:D:174:ALA:HB3  | 1.92                     | 0.51              |
| 3:E:32:GLY:CA    | 3:E:47:VAL:HG13  | 2.34                     | 0.51              |
| 3:H:97:LYS:NZ    | 3:H:111:VAL:HG11 | 2.26                     | 0.51              |
| 1:A:77:LYS:H     | 1:A:96:ASN:HD22  | 1.58                     | 0.51              |
| 1:A:113:ILE:HG23 | 1:A:124:ILE:O    | 2.11                     | 0.51              |
| 1:A:156:ILE:CG2  | 1:A:173:ILE:HD12 | 2.37                     | 0.51              |
| 1:A:434:LYS:HA   | 1:A:625:TRP:HE1  | 1.74                     | 0.51              |
| 1:A:444:THR:O    | 1:A:448:LYS:HG3  | 2.11                     | 0.51              |
| 1:A:504:GLU:HG3  | 1:A:721:PHE:O    | 2.09                     | 0.51              |
| 1:B:146:ARG:N    | 1:B:159:THR:OG1  | 2.43                     | 0.51              |
| 2:C:53:TYR:HB3   | 2:C:57:GLU:C     | 2.34                     | 0.51              |
| 2:C:113:LYS:HG3  | 2:C:371:HIS:NE2  | 2.26                     | 0.51              |
| 2:C:370:VAL:O    | 2:C:374:CYS:N    | 2.22                     | 0.51              |
| 2:D:12:ASN:OD1   | 2:D:12:ASN:N     | 2.37                     | 0.51              |
| 2:D:140:LEU:HD22 | 2:D:342:GLY:C    | 2.35                     | 0.51              |
| 2:D:361:GLU:CB   | 2:D:369:ILE:HG12 | 2.30                     | 0.51              |
| 1:A:92:LEU:HD22  | 1:A:99:SER:HB2   | 1.93                     | 0.51              |
| 1:A:142:LYS:HA   | 1:A:193:TYR:OH   | 2.11                     | 0.51              |
| 1:A:186:ASN:O    | 1:A:190:VAL:HG23 | 2.09                     | 0.51              |
| 1:A:256:PHE:N    | 1:A:256:PHE:CD1  | 2.78                     | 0.51              |
| 1:A:342:MET:HB3  | 1:A:445:ARG:C    | 2.36                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:488:LYS:HB2  | 1:A:667:LEU:HD21 | 1.92                     | 0.51              |
| 1:B:101:LEU:HD23 | 1:B:104:LEU:HD13 | 1.92                     | 0.51              |
| 1:B:251:PHE:CE1  | 1:B:268:GLU:HB3  | 2.45                     | 0.51              |
| 1:B:510:ILE:HA   | 1:B:768:ARG:HG3  | 1.93                     | 0.51              |
| 1:B:802:GLN:NE2  | 3:E:148:LEU:HA   | 2.25                     | 0.51              |
| 1:B:837:ASN:ND2  | 4:F:137:GLU:OE2  | 2.40                     | 0.51              |
| 2:D:258:PRO:O    | 2:D:261:LEU:HB3  | 2.10                     | 0.51              |
| 3:E:3:PHE:HE2    | 3:E:11:PHE:HZ    | 1.58                     | 0.51              |
| 4:F:105:ALA:HA   | 4:F:108:CYS:SG   | 2.51                     | 0.51              |
| 3:H:35:MET:SD    | 3:H:73:MET:HB2   | 2.51                     | 0.51              |
| 1:A:484:TYR:HA   | 1:A:585:HIS:NE2  | 2.25                     | 0.51              |
| 1:A:811:ALA:HB2  | 3:H:126:GLN:CD   | 2.35                     | 0.51              |
| 1:B:194:LEU:HD13 | 1:B:256:PHE:CZ   | 2.42                     | 0.51              |
| 1:B:358:SER:HB2  | 1:B:387:VAL:HG23 | 1.91                     | 0.51              |
| 1:B:539:ALA:O    | 1:B:543:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:585:HIS:CD2  | 1:B:590:VAL:HB   | 2.41                     | 0.51              |
| 1:B:735:GLU:HG3  | 1:B:743:PRO:HA   | 1.93                     | 0.51              |
| 1:B:796:ILE:HB   | 3:E:115:LEU:HD12 | 1.91                     | 0.51              |
| 2:C:86:TRP:CZ3   | 2:C:122:ILE:HD13 | 2.46                     | 0.51              |
| 2:D:72:GLU:HB2   | 2:D:77:THR:HG21  | 1.92                     | 0.51              |
| 3:E:105:GLY:CA   | 3:E:138:ILE:HG12 | 2.39                     | 0.51              |
| 3:H:56:SER:HA    | 3:H:59:MET:SD    | 2.51                     | 0.51              |
| 3:H:111:VAL:HA   | 3:H:115:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:95:LEU:C     | 1:A:718:ARG:HH21 | 2.18                     | 0.51              |
| 1:A:104:LEU:O    | 1:A:696:LEU:HD13 | 2.11                     | 0.51              |
| 1:A:249:GLY:HA3  | 1:A:670:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:301:MET:O    | 1:A:305:LEU:N    | 2.41                     | 0.51              |
| 1:B:272:LEU:N    | 1:B:666:GLN:OE1  | 2.42                     | 0.51              |
| 1:B:393:ILE:HD12 | 1:B:612:LEU:HD23 | 1.92                     | 0.51              |
| 1:B:470:GLU:OE1  | 1:B:470:GLU:HA   | 2.11                     | 0.51              |
| 1:B:586:TYR:OH   | 1:B:712:GLU:HB3  | 2.11                     | 0.51              |
| 1:B:726:VAL:O    | 1:B:730:PHE:N    | 2.37                     | 0.51              |
| 2:C:24:ASP:HB2   | 2:C:340:TRP:CH2  | 2.44                     | 0.51              |
| 2:C:180:LEU:HD21 | 2:C:260:THR:O    | 2.10                     | 0.51              |
| 2:C:220:ALA:N    | 2:C:259:GLU:OE2  | 2.43                     | 0.51              |
| 2:C:223:PHE:HD1  | 2:C:255:PHE:HD2  | 1.59                     | 0.51              |
| 4:F:100:ASP:OD1  | 4:F:101:VAL:N    | 2.40                     | 0.51              |
| 3:H:139:ASN:HB3  | 3:H:142:GLU:HB3  | 1.92                     | 0.51              |
| 1:A:137:ILE:HB   | 1:A:154:TYR:HD2  | 1.76                     | 0.51              |
| 1:A:344:PHE:HE1  | 1:A:441:TRP:CD1  | 2.28                     | 0.51              |
| 1:A:425:PHE:CD2  | 1:A:602:MET:HG2  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:675:ARG:C    | 1:A:677:THR:H    | 2.18                     | 0.51              |
| 1:A:806:TYR:OH   | 3:H:148:LEU:N    | 2.44                     | 0.51              |
| 1:B:138:ILE:CG2  | 1:B:197:VAL:HG23 | 2.39                     | 0.51              |
| 1:B:527:LEU:HA   | 1:B:566:HIS:HD2  | 1.75                     | 0.51              |
| 1:B:746:PHE:HD2  | 1:B:752:ALA:HB2  | 1.75                     | 0.51              |
| 2:C:163:VAL:HG22 | 2:C:175:ILE:HD13 | 1.92                     | 0.51              |
| 2:D:15:GLY:HA3   | 2:D:157:ASP:HB3  | 1.93                     | 0.51              |
| 2:D:37:ARG:HB2   | 2:D:68:LYS:NZ    | 2.26                     | 0.51              |
| 2:D:103:THR:OG1  | 2:D:123:MET:SD   | 2.50                     | 0.51              |
| 2:D:105:LEU:HB2  | 2:D:134:VAL:CG1  | 2.40                     | 0.51              |
| 2:D:355:MET:HA   | 2:D:373:LYS:HD2  | 1.92                     | 0.51              |
| 2:D:365:ALA:HB3  | 2:D:369:ILE:HB   | 1.93                     | 0.51              |
| 3:E:70:LEU:O     | 3:E:74:GLN:HG2   | 2.11                     | 0.51              |
| 3:E:141:GLU:HB3  | 3:E:145:ARG:HH22 | 1.75                     | 0.51              |
| 1:A:2:SER:HA     | 1:A:141:TYR:OH   | 2.10                     | 0.51              |
| 1:A:119:LEU:CD1  | 1:A:500:LEU:HB2  | 2.40                     | 0.51              |
| 1:A:272:LEU:CD2  | 1:A:436:GLU:HA   | 2.40                     | 0.51              |
| 1:B:48:SER:O     | 1:B:50:LYS:HG2   | 2.10                     | 0.51              |
| 1:B:156:ILE:HG21 | 1:B:682:VAL:HG23 | 1.93                     | 0.51              |
| 1:B:291:TYR:CD2  | 1:B:316:LEU:HD22 | 2.46                     | 0.51              |
| 1:B:514:PHE:HB2  | 1:B:720:GLY:HA2  | 1.92                     | 0.51              |
| 2:C:277:THR:HG22 | 2:C:280:ASN:HD22 | 1.76                     | 0.51              |
| 2:D:153:LEU:HD12 | 2:D:278:THR:OG1  | 2.10                     | 0.51              |
| 3:H:93:ARG:HD3   | 3:H:140:TYR:OH   | 2.11                     | 0.51              |
| 1:A:293:LEU:HD21 | 1:A:305:LEU:HD13 | 1.92                     | 0.51              |
| 1:A:616:SER:HB2  | 1:A:622:ALA:HB2  | 1.92                     | 0.51              |
| 1:B:9:ASP:HB3    | 1:B:137:ILE:HD11 | 1.93                     | 0.51              |
| 1:B:12:PHE:HD1   | 1:B:111:GLY:O    | 1.94                     | 0.51              |
| 1:B:32:LYS:HB3   | 1:B:49:ILE:N     | 2.25                     | 0.51              |
| 1:B:126:PRO:HB2  | 1:B:128:LYS:HG2  | 1.93                     | 0.51              |
| 1:B:171:GLN:NE2  | 1:B:678:ASN:HB3  | 2.20                     | 0.51              |
| 1:B:175:CYS:H    | 1:B:464:LEU:HB3  | 1.76                     | 0.51              |
| 1:B:291:TYR:CE1  | 1:B:321:VAL:HA   | 2.46                     | 0.51              |
| 1:B:313:TYR:HE1  | 1:B:361:GLN:CD   | 2.19                     | 0.51              |
| 1:B:561:GLN:HB2  | 1:B:562:GLU:OE1  | 2.11                     | 0.51              |
| 1:B:736:ILE:HG12 | 1:B:792:ILE:HG13 | 1.93                     | 0.51              |
| 2:C:109:PRO:HG3  | 2:C:136:ILE:HG22 | 1.93                     | 0.51              |
| 2:D:2:GLU:OE1    | 2:D:6:THR:OG1    | 2.22                     | 0.51              |
| 2:D:34:ILE:HG12  | 2:D:69:TYR:CE2   | 2.46                     | 0.51              |
| 3:E:104:MET:N    | 3:E:107:GLU:HG2  | 2.26                     | 0.51              |
| 1:A:34:LEU:HD12  | 1:A:47:ALA:O     | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:126:PRO:HB2  | 1:A:128:LYS:CG   | 2.41                     | 0.50              |
| 1:A:296:GLY:CA   | 1:A:329:ASP:HA   | 2.41                     | 0.50              |
| 1:A:327:GLN:HG2  | 1:A:329:ASP:H    | 1.76                     | 0.50              |
| 1:A:357:SER:O    | 1:A:361:GLN:HG2  | 2.11                     | 0.50              |
| 1:A:530:ARG:NH2  | 1:A:536:GLY:HA2  | 2.26                     | 0.50              |
| 1:A:736:ILE:HG12 | 1:A:792:ILE:HG12 | 1.92                     | 0.50              |
| 1:A:844:PHE:HA   | 4:F:62:LYS:HB3   | 1.93                     | 0.50              |
| 1:B:17:LYS:HA    | 1:B:85:LYS:HE3   | 1.92                     | 0.50              |
| 1:B:18:ASN:ND2   | 1:B:81:PRO:HB2   | 2.27                     | 0.50              |
| 1:B:29:TRP:HZ2   | 1:B:34:LEU:N     | 1.97                     | 0.50              |
| 1:B:144:LYS:HB3  | 1:B:149:MET:HG2  | 1.94                     | 0.50              |
| 1:B:365:ILE:HB   | 1:B:427:ILE:HD12 | 1.92                     | 0.50              |
| 1:B:583:ILE:HD12 | 1:B:592:TYR:CD2  | 2.46                     | 0.50              |
| 1:B:669:LYS:O    | 1:B:673:THR:HG23 | 2.12                     | 0.50              |
| 2:C:17:VAL:HG11  | 2:C:85:ILE:HG23  | 1.93                     | 0.50              |
| 2:C:137:GLN:HB3  | 2:C:161:HIS:NE2  | 2.27                     | 0.50              |
| 2:C:223:PHE:CE1  | 2:C:256:ARG:HG2  | 2.46                     | 0.50              |
| 3:H:7:GLN:HA     | 3:H:10:GLU:HB2   | 1.93                     | 0.50              |
| 1:A:132:ILE:HG13 | 1:A:133:TYR:CE2  | 2.46                     | 0.50              |
| 1:A:136:LYS:O    | 1:A:140:MET:N    | 2.22                     | 0.50              |
| 1:A:342:MET:N    | 1:A:342:MET:SD   | 2.83                     | 0.50              |
| 1:A:344:PHE:CE1  | 1:A:441:TRP:HD1  | 2.29                     | 0.50              |
| 1:B:289:ILE:HG13 | 1:B:356:VAL:HG11 | 1.93                     | 0.50              |
| 2:C:153:LEU:HA   | 2:C:161:HIS:O    | 2.11                     | 0.50              |
| 2:C:299:MET:HG3  | 2:C:329:ILE:HG23 | 1.94                     | 0.50              |
| 2:C:370:VAL:HG12 | 2:C:374:CYS:O    | 2.11                     | 0.50              |
| 2:D:20:GLY:C     | 2:D:94:LEU:HD21  | 2.37                     | 0.50              |
| 2:D:86:TRP:CE2   | 2:D:105:LEU:HD22 | 2.46                     | 0.50              |
| 2:D:223:PHE:CD1  | 2:D:259:GLU:HG3  | 2.47                     | 0.50              |
| 2:D:368:SER:O    | 2:D:372:ARG:N    | 2.43                     | 0.50              |
| 3:E:41:ASN:ND2   | 3:E:81:ASP:HA    | 2.26                     | 0.50              |
| 4:F:74:SER:O     | 4:G:129:MET:HE3  | 2.12                     | 0.50              |
| 1:A:10:GLU:HG2   | 1:A:137:ILE:CD1  | 2.41                     | 0.50              |
| 1:A:104:LEU:HD11 | 1:A:705:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:127:TYR:OH   | 1:A:686:ILE:HD12 | 2.10                     | 0.50              |
| 1:A:230:ILE:HG22 | 1:A:234:PHE:CD2  | 2.46                     | 0.50              |
| 1:A:294:ILE:HB   | 1:A:310:PHE:CE1  | 2.46                     | 0.50              |
| 1:A:730:PHE:HB3  | 1:A:753:CYS:SG   | 2.50                     | 0.50              |
| 1:B:107:ARG:O    | 1:B:112:LEU:N    | 2.38                     | 0.50              |
| 1:B:161:TYR:HB2  | 1:B:193:TYR:HE2  | 1.76                     | 0.50              |
| 1:B:191:ILE:HD13 | 1:B:221:GLU:HB3  | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:339:MET:HE3  | 1:B:349:GLN:HG2  | 1.92                     | 0.50              |
| 1:B:762:LEU:HD22 | 1:B:780:VAL:HG21 | 1.93                     | 0.50              |
| 2:C:294:TYR:HA   | 2:C:327:ILE:HG23 | 1.93                     | 0.50              |
| 2:C:299:MET:HE1  | 2:C:313:MET:HE3  | 1.93                     | 0.50              |
| 2:D:86:TRP:HH2   | 2:D:119:MET:HA   | 1.75                     | 0.50              |
| 2:D:218:TYR:CE2  | 2:D:220:ALA:HA   | 2.47                     | 0.50              |
| 2:D:297:ASN:ND2  | 2:D:317:ILE:HG13 | 2.24                     | 0.50              |
| 3:E:64:LEU:HD21  | 3:E:69:PHE:HA    | 1.92                     | 0.50              |
| 4:F:106:PHE:HB3  | 4:F:155:TYR:CE1  | 2.47                     | 0.50              |
| 3:H:11:PHE:CZ    | 3:H:73:MET:HE3   | 2.47                     | 0.50              |
| 1:A:42:HIS:HB2   | 1:A:101:LEU:CD1  | 2.41                     | 0.50              |
| 1:A:83:PHE:CE2   | 1:A:782:ALA:HB1  | 2.46                     | 0.50              |
| 1:A:269:THR:C    | 1:A:440:ARG:HH12 | 2.19                     | 0.50              |
| 1:A:275:SER:O    | 1:A:279:ARG:N    | 2.31                     | 0.50              |
| 1:A:344:PHE:CE1  | 1:A:441:TRP:CD1  | 2.99                     | 0.50              |
| 1:A:494:ASN:ND2  | 1:A:586:TYR:OH   | 2.32                     | 0.50              |
| 1:A:541:LEU:HG   | 1:A:601:ASN:OD1  | 2.11                     | 0.50              |
| 1:A:704:GLN:HB3  | 1:A:708:ASN:ND2  | 2.26                     | 0.50              |
| 1:B:485:THR:CA   | 1:B:667:LEU:HD13 | 2.40                     | 0.50              |
| 1:B:517:PHE:HB3  | 1:B:716:ILE:CG1  | 2.41                     | 0.50              |
| 1:B:815:ARG:HA   | 3:E:20:ARG:HH22  | 1.76                     | 0.50              |
| 2:C:147:ARG:HE   | 2:C:330:ILE:HG21 | 1.75                     | 0.50              |
| 2:D:14:SER:HA    | 2:D:71:ILE:O     | 2.12                     | 0.50              |
| 2:D:98:PRO:CB    | 2:D:127:PHE:HB3  | 2.38                     | 0.50              |
| 2:D:294:TYR:HD1  | 2:D:327:ILE:HD11 | 1.76                     | 0.50              |
| 3:E:28:TYR:CE1   | 3:E:51:LEU:HD22  | 2.46                     | 0.50              |
| 3:E:128:VAL:HG22 | 3:E:143:LEU:HD21 | 1.93                     | 0.50              |
| 4:G:91:GLU:HA    | 4:G:94:ASN:HB2   | 1.94                     | 0.50              |
| 3:H:4:SER:OG     | 3:H:7:GLN:OE1    | 2.19                     | 0.50              |
| 1:A:13:LEU:HD11  | 1:A:151:PRO:O    | 2.12                     | 0.50              |
| 1:A:15:VAL:HG21  | 1:A:87:GLU:HG2   | 1.93                     | 0.50              |
| 1:A:563:GLN:HA   | 1:A:566:HIS:ND1  | 2.27                     | 0.50              |
| 1:A:687:PRO:HB2  | 1:A:695:LYS:O    | 2.12                     | 0.50              |
| 1:A:730:PHE:CE2  | 1:A:757:ILE:HG13 | 2.47                     | 0.50              |
| 1:B:266:ASN:HD21 | 1:B:447:ASN:HB3  | 1.76                     | 0.50              |
| 1:B:570:GLN:CB   | 1:B:582:CYS:HB2  | 2.37                     | 0.50              |
| 2:C:17:VAL:HG11  | 2:C:85:ILE:CG2   | 2.41                     | 0.50              |
| 2:C:120:THR:CG2  | 2:C:362:TYR:HB2  | 2.41                     | 0.50              |
| 2:C:214:GLU:HA   | 2:C:306:TYR:CE1  | 2.45                     | 0.50              |
| 2:D:70:PRO:HB2   | 2:D:82:MET:SD    | 2.51                     | 0.50              |
| 2:D:183:ARG:NH1  | 2:D:184:ASP:OD1  | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:29:GLN:HA    | 4:F:32:GLU:HG2   | 1.92                     | 0.50              |
| 3:H:84:CYS:HB3   | 3:H:87:ASP:HB2   | 1.94                     | 0.50              |
| 3:H:103:VAL:HG22 | 3:H:140:TYR:HB3  | 1.93                     | 0.50              |
| 1:A:8:ASP:OD1    | 1:A:11:LYS:HB3   | 2.12                     | 0.50              |
| 1:A:51:GLU:HB3   | 1:A:58:THR:OG1   | 2.12                     | 0.50              |
| 1:A:275:SER:OG   | 1:A:478:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:438:LEU:O    | 1:A:442:ILE:HG12 | 2.11                     | 0.50              |
| 1:B:76:GLN:HB3   | 1:B:96:ASN:HB3   | 1.92                     | 0.50              |
| 1:B:294:ILE:HA   | 1:B:307:LEU:HD13 | 1.93                     | 0.50              |
| 1:B:420:LYS:HA   | 1:B:423:ALA:HB3  | 1.93                     | 0.50              |
| 2:C:149:THR:HA   | 2:C:165:ILE:HG21 | 1.93                     | 0.50              |
| 2:C:185:LEU:HG   | 2:C:257:CYS:O    | 2.11                     | 0.50              |
| 2:C:188:TYR:CE2  | 2:C:192:ILE:HD13 | 2.46                     | 0.50              |
| 2:C:207:GLU:OE1  | 2:C:210:ARG:NE   | 2.44                     | 0.50              |
| 2:D:155:SER:HB3  | 2:D:160:THR:HA   | 1.92                     | 0.50              |
| 3:E:128:VAL:O    | 3:E:132:GLU:HG3  | 2.12                     | 0.50              |
| 4:G:100:ASP:OD1  | 4:G:101:VAL:N    | 2.41                     | 0.50              |
| 3:H:70:LEU:HA    | 3:H:73:MET:HG3   | 1.93                     | 0.50              |
| 1:A:199:SER:H    | 1:A:261:TYR:HD1  | 1.58                     | 0.50              |
| 1:A:251:PHE:HB3  | 1:A:673:THR:HG21 | 1.94                     | 0.50              |
| 1:A:342:MET:O    | 1:A:445:ARG:HG3  | 2.11                     | 0.50              |
| 1:A:399:THR:CG2  | 1:A:403:LEU:HD21 | 2.41                     | 0.50              |
| 1:A:789:ASP:O    | 1:A:793:THR:HG23 | 2.11                     | 0.50              |
| 1:B:57:VAL:HG12  | 1:B:59:VAL:CG1   | 2.39                     | 0.50              |
| 1:B:108:TYR:HB3  | 1:B:696:LEU:HD13 | 1.93                     | 0.50              |
| 1:B:338:ALA:O    | 1:B:342:MET:HG2  | 2.11                     | 0.50              |
| 1:B:517:PHE:HB3  | 1:B:716:ILE:CD1  | 2.41                     | 0.50              |
| 1:B:705:LEU:O    | 1:B:709:GLY:N    | 2.45                     | 0.50              |
| 2:C:101:HIS:O    | 2:C:129:VAL:HG13 | 2.12                     | 0.50              |
| 2:C:123:MET:SD   | 2:C:129:VAL:HG21 | 2.52                     | 0.50              |
| 2:C:189:LEU:HD21 | 2:C:212:ILE:HG22 | 1.94                     | 0.50              |
| 2:D:70:PRO:HG3   | 2:D:85:ILE:HG12  | 1.94                     | 0.50              |
| 2:D:79:TRP:HB2   | 2:D:122:ILE:HD11 | 1.92                     | 0.50              |
| 2:D:368:SER:HA   | 2:D:371:HIS:HD2  | 1.76                     | 0.50              |
| 3:E:65:ASN:OD1   | 3:E:68:GLN:HB2   | 2.12                     | 0.50              |
| 4:F:125:LEU:HD12 | 4:F:129:MET:HG3  | 1.94                     | 0.50              |
| 1:A:126:PRO:HB2  | 1:A:128:LYS:HG3  | 1.94                     | 0.50              |
| 1:A:156:ILE:HG22 | 1:A:173:ILE:HG23 | 1.93                     | 0.50              |
| 1:A:177:GLY:O    | 1:A:468:GLY:N    | 2.40                     | 0.50              |
| 1:A:342:MET:HG3  | 1:A:446:VAL:HA   | 1.94                     | 0.50              |
| 1:A:555:PHE:CZ   | 1:A:559:LEU:HD11 | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:737:LEU:CD2  | 1:A:760:LEU:HD21 | 2.42                     | 0.50              |
| 1:B:18:ASN:ND2   | 1:B:28:ASP:OD2   | 2.45                     | 0.50              |
| 1:B:35:VAL:HG13  | 1:B:76:GLN:H     | 1.77                     | 0.50              |
| 1:B:101:LEU:HD11 | 1:B:702:LEU:CB   | 2.39                     | 0.50              |
| 1:B:233:ALA:HB2  | 1:B:335:THR:OG1  | 2.12                     | 0.50              |
| 2:C:166:TYR:CD2  | 2:C:285:CYS:HA   | 2.47                     | 0.50              |
| 2:D:41:GLN:HG2   | 2:D:51:ASP:OD1   | 2.11                     | 0.50              |
| 2:D:98:PRO:HG2   | 2:D:127:PHE:CG   | 2.46                     | 0.50              |
| 2:D:297:ASN:O    | 2:D:329:ILE:HG12 | 2.11                     | 0.50              |
| 3:E:93:ARG:HH22  | 3:E:103:VAL:HG13 | 1.76                     | 0.50              |
| 3:H:146:MET:O    | 3:H:150:GLY:N    | 2.42                     | 0.50              |
| 1:A:2:SER:N      | 1:A:137:ILE:HG23 | 2.27                     | 0.50              |
| 1:A:241:LYS:NZ   | 1:A:707:CYS:SG   | 2.75                     | 0.50              |
| 1:A:253:ARG:HG3  | 1:A:460:PHE:CG   | 2.47                     | 0.50              |
| 1:A:276:ARG:HB2  | 1:A:478:GLU:HG2  | 1.94                     | 0.50              |
| 1:A:508:GLU:HB2  | 1:A:510:ILE:HG13 | 1.94                     | 0.50              |
| 1:B:45:GLU:HB2   | 1:B:61:LEU:HD22  | 1.94                     | 0.50              |
| 1:B:282:LYS:O    | 1:B:284:GLU:HG3  | 2.12                     | 0.50              |
| 1:B:314:THR:N    | 1:B:364:ASN:HD21 | 2.10                     | 0.50              |
| 1:B:659:VAL:HG22 | 1:B:662:LEU:HD12 | 1.94                     | 0.50              |
| 1:B:796:ILE:HG21 | 3:E:111:VAL:CG2  | 2.42                     | 0.50              |
| 1:B:797:ILE:HG12 | 3:E:116:GLY:N    | 2.27                     | 0.50              |
| 2:C:44:MET:HE1   | 2:C:64:ILE:HB    | 1.93                     | 0.50              |
| 1:A:356:VAL:HG23 | 1:A:438:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:404:THR:OG1  | 1:A:415:GLN:NE2  | 2.45                     | 0.49              |
| 1:B:42:HIS:N     | 1:B:101:LEU:HD13 | 2.27                     | 0.49              |
| 1:B:95:LEU:H     | 1:B:778:THR:CG2  | 2.24                     | 0.49              |
| 1:B:121:CYS:HB2  | 1:B:156:ILE:HD13 | 1.94                     | 0.49              |
| 1:B:323:ILE:HG22 | 1:B:324:PRO:O    | 2.12                     | 0.49              |
| 1:B:384:ALA:HA   | 1:B:387:VAL:HG12 | 1.93                     | 0.49              |
| 1:B:444:THR:O    | 1:B:448:LYS:HG3  | 2.11                     | 0.49              |
| 1:B:575:LEU:HA   | 1:B:578:LYS:HE3  | 1.92                     | 0.49              |
| 2:C:135:ALA:HB3  | 2:C:140:LEU:HD11 | 1.94                     | 0.49              |
| 2:C:365:ALA:HB3  | 2:C:369:ILE:HB   | 1.93                     | 0.49              |
| 3:E:18:PHE:CZ    | 3:E:30:GLN:HG2   | 2.47                     | 0.49              |
| 3:E:97:LYS:N     | 3:E:97:LYS:HD2   | 2.26                     | 0.49              |
| 4:G:54:HIS:NE2   | 4:G:64:PRO:O     | 2.43                     | 0.49              |
| 3:H:80:LYS:HA    | 3:H:82:GLN:OE1   | 2.12                     | 0.49              |
| 1:A:13:LEU:HD13  | 1:A:132:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:95:LEU:HB2   | 1:A:718:ARG:HE   | 1.77                     | 0.49              |
| 1:A:339:MET:SD   | 1:A:349:GLN:HG2  | 2.52                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:434:LYS:HG2  | 1:A:625:TRP:CE2  | 2.47                     | 0.49              |
| 1:B:59:VAL:HG23  | 1:B:61:LEU:HG    | 1.94                     | 0.49              |
| 1:B:92:LEU:HD11  | 1:B:103:ASN:HD21 | 1.78                     | 0.49              |
| 1:B:296:GLY:HA2  | 1:B:329:ASP:HA   | 1.94                     | 0.49              |
| 1:B:521:LEU:HG   | 1:B:586:TYR:CD1  | 2.47                     | 0.49              |
| 1:B:806:TYR:CZ   | 3:E:131:HIS:HE1  | 2.30                     | 0.49              |
| 2:D:23:GLY:N     | 2:D:344:SER:O    | 2.35                     | 0.49              |
| 2:D:100:GLU:N    | 2:D:130:PRO:HD3  | 2.27                     | 0.49              |
| 2:D:227:MET:HG3  | 2:D:252:ASN:CB   | 2.42                     | 0.49              |
| 2:D:257:CYS:HB2  | 2:D:258:PRO:HD3  | 1.94                     | 0.49              |
| 3:E:79:ASN:C     | 3:E:81:ASP:H     | 2.20                     | 0.49              |
| 3:H:85:PHE:HA    | 3:H:88:TYR:HB2   | 1.94                     | 0.49              |
| 1:A:92:LEU:HD11  | 1:A:103:ASN:ND2  | 2.24                     | 0.49              |
| 1:A:113:ILE:CG2  | 1:A:126:PRO:HD3  | 2.42                     | 0.49              |
| 1:A:361:GLN:HE22 | 1:A:386:LYS:HD3  | 1.77                     | 0.49              |
| 1:A:843:LEU:HD23 | 4:F:65:THR:HA    | 1.93                     | 0.49              |
| 1:B:156:ILE:CG2  | 1:B:680:ASN:HB3  | 2.43                     | 0.49              |
| 1:B:271:LEU:HD11 | 1:B:485:THR:HG21 | 1.93                     | 0.49              |
| 1:B:361:GLN:OE1  | 1:B:386:LYS:HD3  | 2.12                     | 0.49              |
| 1:B:502:GLN:HB3  | 1:B:506:GLN:NE2  | 2.28                     | 0.49              |
| 1:B:677:THR:O    | 1:B:679:PRO:HD3  | 2.12                     | 0.49              |
| 1:B:727:PHE:HB3  | 1:B:731:ARG:NH2  | 2.27                     | 0.49              |
| 1:B:785:GLU:O    | 1:B:788:ARG:HG2  | 2.12                     | 0.49              |
| 1:B:844:PHE:O    | 1:B:848:LYS:HG3  | 2.12                     | 0.49              |
| 2:C:13:GLY:O     | 2:C:71:ILE:HD12  | 2.11                     | 0.49              |
| 2:C:109:PRO:HB2  | 2:C:175:ILE:HG21 | 1.94                     | 0.49              |
| 2:C:157:ASP:H    | 2:C:302:GLY:HA3  | 1.78                     | 0.49              |
| 2:C:303:THR:HA   | 2:C:306:TYR:CD2  | 2.48                     | 0.49              |
| 2:D:106:THR:HG22 | 2:D:140:LEU:CD1  | 2.43                     | 0.49              |
| 2:D:108:ALA:HB1  | 2:D:161:HIS:CD2  | 2.47                     | 0.49              |
| 2:D:163:VAL:HG22 | 2:D:175:ILE:HD11 | 1.94                     | 0.49              |
| 4:F:109:PHE:CZ   | 4:F:125:LEU:HB2  | 2.47                     | 0.49              |
| 3:H:96:ASP:OD2   | 3:H:99:GLY:N     | 2.46                     | 0.49              |
| 3:H:104:MET:HB2  | 3:H:107:GLU:CB   | 2.40                     | 0.49              |
| 3:H:139:ASN:O    | 3:H:143:LEU:N    | 2.35                     | 0.49              |
| 1:A:2:SER:HB2    | 1:A:137:ILE:HG23 | 1.94                     | 0.49              |
| 1:A:34:LEU:HB3   | 1:A:78:MET:O     | 2.12                     | 0.49              |
| 1:A:168:ARG:HH12 | 1:A:459:SER:N    | 2.09                     | 0.49              |
| 1:A:175:CYS:HB3  | 1:A:183:LYS:HA   | 1.93                     | 0.49              |
| 1:A:342:MET:C    | 1:A:445:ARG:HG3  | 2.38                     | 0.49              |
| 1:A:389:HIS:CD2  | 1:A:390:LEU:HD23 | 2.43                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:447:ASN:HA   | 1:A:450:LEU:HB3  | 1.93                     | 0.49              |
| 1:A:559:LEU:O    | 1:A:563:GLN:HB3  | 2.13                     | 0.49              |
| 1:B:242:ASN:ND2  | 1:B:691:LYS:HE2  | 2.27                     | 0.49              |
| 1:B:257:ASP:HA   | 1:B:456:GLN:HB3  | 1.95                     | 0.49              |
| 1:B:269:THR:HG23 | 1:B:443:LEU:HD13 | 1.92                     | 0.49              |
| 1:B:283:ASP:HA   | 1:B:320:HIS:NE2  | 2.27                     | 0.49              |
| 1:B:388:CYS:HA   | 1:B:393:ILE:HG12 | 1.94                     | 0.49              |
| 1:B:418:GLN:NE2  | 1:B:423:ALA:HA   | 2.28                     | 0.49              |
| 1:B:514:PHE:CB   | 1:B:720:GLY:HA2  | 2.43                     | 0.49              |
| 2:C:207:GLU:OE2  | 2:C:210:ARG:HD3  | 2.12                     | 0.49              |
| 2:C:347:ALA:HA   | 2:C:352:PHE:CB   | 2.35                     | 0.49              |
| 2:D:20:GLY:HA2   | 2:D:28:ARG:HD2   | 1.95                     | 0.49              |
| 2:D:54:VAL:CG2   | 2:D:84:LYS:HB3   | 2.41                     | 0.49              |
| 2:D:62:ARG:HB3   | 2:D:204:ALA:HA   | 1.94                     | 0.49              |
| 3:E:113:VAL:HG13 | 3:E:124:VAL:HG11 | 1.94                     | 0.49              |
| 4:F:106:PHE:CE2  | 4:F:153:PHE:HE2  | 2.31                     | 0.49              |
| 1:A:132:ILE:O    | 1:A:137:ILE:HG21 | 2.12                     | 0.49              |
| 1:A:173:ILE:CG1  | 1:A:461:LEU:HD11 | 2.41                     | 0.49              |
| 1:A:193:TYR:CD2  | 1:A:193:TYR:C    | 2.90                     | 0.49              |
| 1:A:313:TYR:HE1  | 1:A:361:GLN:CD   | 2.21                     | 0.49              |
| 1:A:425:PHE:CG   | 1:A:602:MET:HG2  | 2.47                     | 0.49              |
| 1:A:509:GLY:H    | 1:A:771:GLN:NE2  | 2.09                     | 0.49              |
| 1:A:823:LYS:HE3  | 3:H:10:GLU:HG3   | 1.92                     | 0.49              |
| 1:B:530:ARG:O    | 1:B:539:ALA:HB3  | 2.11                     | 0.49              |
| 1:B:568:LYS:HA   | 1:B:584:LEU:HD12 | 1.94                     | 0.49              |
| 2:C:214:GLU:HA   | 2:C:306:TYR:HE1  | 1.77                     | 0.49              |
| 2:C:274:ILE:HG23 | 2:C:275:HIS:N    | 2.26                     | 0.49              |
| 2:C:326:LYS:HD2  | 2:C:327:ILE:N    | 2.28                     | 0.49              |
| 3:E:50:VAL:O     | 3:E:75:THR:OG1   | 2.28                     | 0.49              |
| 3:H:70:LEU:O     | 3:H:73:MET:HG3   | 2.12                     | 0.49              |
| 1:A:138:ILE:HG13 | 1:A:154:TYR:CD2  | 2.48                     | 0.49              |
| 1:A:231:LEU:HD12 | 1:A:250:LYS:HZ1  | 1.77                     | 0.49              |
| 1:A:411:ARG:NE   | 2:D:28:ARG:HD3   | 2.28                     | 0.49              |
| 1:A:735:GLU:HB2  | 1:A:756:MET:SD   | 2.53                     | 0.49              |
| 1:B:95:LEU:HD12  | 1:B:722:PRO:CB   | 2.43                     | 0.49              |
| 1:B:153:ILE:HG12 | 1:B:682:VAL:HG13 | 1.95                     | 0.49              |
| 1:B:176:THR:HG21 | 1:B:490:GLN:OE1  | 2.11                     | 0.49              |
| 1:B:270:TYR:O    | 1:B:271:LEU:HB2  | 2.12                     | 0.49              |
| 1:B:293:LEU:O    | 1:B:297:ALA:HB3  | 2.12                     | 0.49              |
| 1:B:389:HIS:CD2  | 1:B:390:LEU:HD23 | 2.42                     | 0.49              |
| 1:B:508:GLU:OE2  | 1:B:772:SER:N    | 2.33                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:686:ILE:H    | 1:B:704:GLN:HG3  | 1.78                     | 0.49              |
| 1:B:725:ILE:HG13 | 1:B:781:LEU:CD2  | 2.43                     | 0.49              |
| 2:C:289:ILE:HD11 | 2:D:64:ILE:HG21  | 1.95                     | 0.49              |
| 2:D:73:HIS:HB2   | 2:D:183:ARG:NH2  | 2.27                     | 0.49              |
| 3:E:104:MET:HB2  | 3:E:107:GLU:HG2  | 1.94                     | 0.49              |
| 3:H:140:TYR:CE2  | 3:H:141:GLU:HG3  | 2.48                     | 0.49              |
| 1:A:504:GLU:HB2  | 1:A:721:PHE:HB2  | 1.95                     | 0.49              |
| 1:A:730:PHE:CG   | 1:A:774:ILE:HD12 | 2.47                     | 0.49              |
| 1:B:194:LEU:CB   | 1:B:262:ILE:HD11 | 2.43                     | 0.49              |
| 1:B:502:GLN:HE22 | 1:B:513:ASN:HB3  | 1.77                     | 0.49              |
| 1:B:537:VAL:HG22 | 1:B:569:PHE:CE2  | 2.48                     | 0.49              |
| 1:B:683:ARG:HG3  | 1:B:710:VAL:HG21 | 1.94                     | 0.49              |
| 1:B:767:TYR:CE2  | 1:B:769:ILE:HG12 | 2.47                     | 0.49              |
| 2:C:279:TYR:HH   | 2:C:294:TYR:HH   | 1.59                     | 0.49              |
| 2:D:291:LYS:HA   | 2:D:294:TYR:HD2  | 1.78                     | 0.49              |
| 2:D:305:MET:SD   | 2:D:335:ARG:HB3  | 2.53                     | 0.49              |
| 3:E:11:PHE:HE2   | 3:E:73:MET:HE2   | 1.77                     | 0.49              |
| 3:H:10:GLU:HA    | 3:H:13:GLU:HG2   | 1.95                     | 0.49              |
| 3:H:25:LYS:HE3   | 3:H:65:ASN:HB2   | 1.94                     | 0.49              |
| 3:H:55:LYS:HG2   | 3:H:58:GLU:HB2   | 1.94                     | 0.49              |
| 3:H:92:LEU:HD13  | 3:H:140:TYR:HB2  | 1.95                     | 0.49              |
| 1:A:241:LYS:NZ   | 1:A:469:PHE:O    | 2.46                     | 0.49              |
| 1:A:248:PHE:CZ   | 1:A:250:LYS:HD2  | 2.48                     | 0.49              |
| 1:A:469:PHE:HA   | 1:A:486:ASN:HD22 | 1.78                     | 0.49              |
| 1:A:624:LEU:HD22 | 1:A:625:TRP:CZ3  | 2.47                     | 0.49              |
| 1:A:764:PRO:HG2  | 1:A:769:ILE:HG12 | 1.94                     | 0.49              |
| 1:B:44:PHE:C     | 1:B:102:HIS:HE2  | 2.21                     | 0.49              |
| 1:B:53:LYS:HE2   | 1:B:56:GLU:HG2   | 1.93                     | 0.49              |
| 1:B:114:TYR:CE2  | 1:B:123:VAL:HG13 | 2.48                     | 0.49              |
| 1:B:146:ARG:HG3  | 1:B:156:ILE:HD11 | 1.93                     | 0.49              |
| 1:B:562:GLU:HA   | 1:B:565:ASN:OD1  | 2.13                     | 0.49              |
| 1:B:828:ASN:HD22 | 4:F:105:ALA:HB2  | 1.78                     | 0.49              |
| 2:C:17:VAL:C     | 2:C:18:LYS:HD3   | 2.38                     | 0.49              |
| 2:C:92:ASN:HA    | 2:C:95:ARG:CZ    | 2.43                     | 0.49              |
| 2:C:114:ALA:O    | 2:C:118:LYS:HG3  | 2.13                     | 0.49              |
| 2:C:357:ILE:HG13 | 2:C:373:LYS:HB3  | 1.94                     | 0.49              |
| 2:D:13:GLY:O     | 2:D:33:SER:OG    | 2.29                     | 0.49              |
| 3:E:66:PHE:CE2   | 3:E:69:PHE:HD2   | 2.30                     | 0.49              |
| 1:A:47:ALA:HB1   | 1:A:59:VAL:HB    | 1.95                     | 0.49              |
| 1:A:269:THR:OG1  | 1:A:440:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:551:THR:HA   | 1:A:598:LEU:HD22 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:4:LYS:NZ     | 1:B:10:GLU:OE1   | 2.30                     | 0.49              |
| 1:B:49:ILE:HA    | 1:B:59:VAL:CG1   | 2.43                     | 0.49              |
| 1:B:238:LYS:HG2  | 1:B:239:THR:N    | 2.28                     | 0.49              |
| 1:B:274:LYS:CE   | 1:B:432:LYS:HB3  | 2.43                     | 0.49              |
| 1:B:367:PHE:H    | 1:B:424:ASP:CG   | 2.19                     | 0.49              |
| 1:B:527:LEU:HG   | 1:B:528:ILE:HD13 | 1.94                     | 0.49              |
| 1:B:541:LEU:HD11 | 1:B:601:ASN:HB3  | 1.95                     | 0.49              |
| 1:B:547:PHE:HD2  | 1:B:549:LYS:H    | 1.61                     | 0.49              |
| 1:B:556:VAL:HG21 | 1:B:579:THR:HA   | 1.94                     | 0.49              |
| 2:C:37:ARG:HG2   | 2:C:51:ASP:O     | 2.13                     | 0.49              |
| 2:C:90:PHE:HA    | 2:C:94:LEU:HD12  | 1.95                     | 0.49              |
| 2:C:98:PRO:CB    | 2:C:127:PHE:HB3  | 2.43                     | 0.49              |
| 2:C:132:MET:O    | 2:C:357:ILE:N    | 2.45                     | 0.49              |
| 2:D:124:PHE:HE1  | 2:D:129:VAL:HB   | 1.78                     | 0.49              |
| 2:D:160:THR:HG22 | 2:D:176:MET:HE3  | 1.93                     | 0.49              |
| 2:D:192:ILE:HB   | 2:D:256:ARG:HH11 | 1.77                     | 0.49              |
| 1:A:42:HIS:HB3   | 1:A:44:PHE:CZ    | 2.47                     | 0.49              |
| 1:A:276:ARG:HE   | 1:A:478:GLU:HG2  | 1.77                     | 0.49              |
| 1:A:529:GLU:HA   | 1:A:664:LYS:HD3  | 1.95                     | 0.49              |
| 1:A:799:PHE:HA   | 1:A:802:GLN:NE2  | 2.28                     | 0.49              |
| 1:B:5:PRO:HD3    | 1:B:14:PHE:CD1   | 2.48                     | 0.49              |
| 1:B:183:LYS:HE2  | 1:B:466:ILE:O    | 2.12                     | 0.49              |
| 1:B:194:LEU:HD22 | 1:B:256:PHE:CZ   | 2.48                     | 0.49              |
| 1:B:469:PHE:HB2  | 1:B:707:CYS:CA   | 2.38                     | 0.49              |
| 1:B:535:PRO:HB2  | 1:B:540:LEU:HD23 | 1.95                     | 0.49              |
| 1:B:802:GLN:CD   | 3:E:148:LEU:HA   | 2.37                     | 0.49              |
| 2:C:19:ALA:O     | 2:C:28:ARG:HB3   | 2.12                     | 0.49              |
| 2:C:152:VAL:HB   | 2:C:163:VAL:HB   | 1.94                     | 0.49              |
| 2:D:66:THR:C     | 2:D:67:LEU:HD23  | 2.38                     | 0.49              |
| 3:E:41:ASN:O     | 3:E:82:GLN:NE2   | 2.45                     | 0.49              |
| 3:E:110:HIS:CD2  | 3:E:114:THR:HG21 | 2.48                     | 0.49              |
| 1:A:220:LEU:HD13 | 1:A:452:LYS:HB2  | 1.95                     | 0.48              |
| 1:A:267:ILE:N    | 1:A:450:LEU:HD21 | 2.27                     | 0.48              |
| 1:A:291:TYR:OH   | 1:A:318:ASN:HB3  | 2.13                     | 0.48              |
| 1:A:416:LYS:HG3  | 2:D:334:GLU:HB2  | 1.95                     | 0.48              |
| 1:A:547:PHE:CE1  | 2:D:349:LEU:HD21 | 2.48                     | 0.48              |
| 1:B:161:TYR:HA   | 1:B:164:MET:CE   | 2.42                     | 0.48              |
| 1:B:171:GLN:HA   | 1:B:677:THR:HB   | 1.95                     | 0.48              |
| 1:B:302:ARG:CA   | 1:B:307:LEU:HB2  | 2.42                     | 0.48              |
| 1:B:351:SER:HG   | 1:B:621:VAL:HG23 | 1.78                     | 0.48              |
| 1:B:401:SER:C    | 1:B:606:ASN:HD21 | 2.19                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:584:LEU:HA   | 1:B:589:LYS:HA   | 1.95                     | 0.48              |
| 2:C:61:LYS:O     | 2:C:65:LEU:N     | 2.46                     | 0.48              |
| 2:C:143:TYR:CZ   | 2:C:346:LEU:HD21 | 2.48                     | 0.48              |
| 2:C:178:LEU:HG   | 2:C:180:LEU:HB3  | 1.95                     | 0.48              |
| 2:C:286:ASP:HB2  | 2:C:289:ILE:HG13 | 1.95                     | 0.48              |
| 2:C:304:THR:HB   | 2:C:335:ARG:NE   | 2.21                     | 0.48              |
| 2:D:11:ASP:HA    | 2:D:106:THR:CG2  | 2.42                     | 0.48              |
| 2:D:38:PRO:HB2   | 2:D:41:GLN:HG3   | 1.95                     | 0.48              |
| 2:D:279:TYR:OH   | 2:D:322:PRO:HD3  | 2.13                     | 0.48              |
| 2:D:361:GLU:C    | 2:D:369:ILE:HG21 | 2.38                     | 0.48              |
| 4:G:153:PHE:CZ   | 4:G:158:PHE:HB2  | 2.49                     | 0.48              |
| 3:H:28:TYR:HB3   | 3:H:51:LEU:HD13  | 1.95                     | 0.48              |
| 1:A:12:PHE:CD1   | 1:A:111:GLY:HA3  | 2.40                     | 0.48              |
| 1:A:90:ALA:HB1   | 1:A:722:PRO:HG2  | 1.96                     | 0.48              |
| 1:A:180:GLY:HA3  | 1:A:244:ASN:O    | 2.13                     | 0.48              |
| 1:A:378:MET:HE1  | 1:A:398:PHE:CD2  | 2.48                     | 0.48              |
| 1:B:29:TRP:CE3   | 1:B:80:PRO:HA    | 2.48                     | 0.48              |
| 1:B:44:PHE:CE2   | 1:B:101:LEU:HD12 | 2.46                     | 0.48              |
| 1:B:194:LEU:O    | 1:B:198:ALA:N    | 2.38                     | 0.48              |
| 1:B:194:LEU:HB3  | 1:B:256:PHE:CZ   | 2.48                     | 0.48              |
| 1:B:219:GLU:O    | 1:B:222:LYS:HB2  | 2.13                     | 0.48              |
| 1:B:438:LEU:HG   | 1:B:442:ILE:HD12 | 1.95                     | 0.48              |
| 1:B:497:MET:HE3  | 1:B:501:GLU:HG2  | 1.95                     | 0.48              |
| 1:B:573:LYS:HE2  | 1:B:575:LEU:H    | 1.76                     | 0.48              |
| 2:C:117:GLU:CA   | 2:C:367:PRO:HB2  | 2.41                     | 0.48              |
| 2:D:67:LEU:HD12  | 2:D:207:GLU:CB   | 2.43                     | 0.48              |
| 2:D:124:PHE:CE2  | 2:D:357:ILE:HG22 | 2.48                     | 0.48              |
| 4:F:64:PRO:HB2   | 4:F:68:TYR:HD1   | 1.78                     | 0.48              |
| 1:A:13:LEU:HD22  | 1:A:152:HIS:CD2  | 2.42                     | 0.48              |
| 1:A:15:VAL:CG2   | 1:A:107:ARG:HH12 | 2.27                     | 0.48              |
| 1:A:171:GLN:HE22 | 1:A:678:ASN:HB3  | 1.76                     | 0.48              |
| 1:A:242:ASN:O    | 1:A:245:SER:HB3  | 2.12                     | 0.48              |
| 1:A:255:ASN:OD1  | 1:A:455:ARG:NH1  | 2.47                     | 0.48              |
| 1:A:302:ARG:HB3  | 1:A:307:LEU:HB2  | 1.94                     | 0.48              |
| 1:A:342:MET:HA   | 1:A:449:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:488:LYS:HD2  | 1:A:491:GLN:NE2  | 2.28                     | 0.48              |
| 1:B:70:LEU:HG    | 1:B:71:SER:N     | 2.28                     | 0.48              |
| 1:B:116:TYR:HA   | 1:B:120:PHE:O    | 2.13                     | 0.48              |
| 1:B:487:GLU:HB3  | 1:B:525:ILE:HG12 | 1.95                     | 0.48              |
| 1:B:835:LEU:HD13 | 4:F:162:LEU:HD22 | 1.94                     | 0.48              |
| 2:C:11:ASP:O     | 2:C:17:VAL:HA    | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:220:ALA:HB1  | 2:D:223:PHE:HA   | 1.95                     | 0.48              |
| 4:F:118:HIS:HB2  | 4:F:121:HIS:HB2  | 1.95                     | 0.48              |
| 3:H:55:LYS:NZ    | 3:H:58:GLU:OE1   | 2.45                     | 0.48              |
| 1:A:193:TYR:CZ   | 1:A:197:VAL:HG21 | 2.49                     | 0.48              |
| 1:A:305:LEU:HD22 | 1:A:354:ARG:N    | 2.28                     | 0.48              |
| 1:A:339:MET:C    | 1:A:344:PHE:HB2  | 2.37                     | 0.48              |
| 1:A:685:ILE:HG23 | 1:A:704:GLN:HB2  | 1.95                     | 0.48              |
| 1:B:35:VAL:HB    | 1:B:45:GLU:O     | 2.13                     | 0.48              |
| 1:B:57:VAL:HB    | 1:B:75:ILE:CD1   | 2.40                     | 0.48              |
| 1:B:430:LEU:HD21 | 1:B:613:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:498:PHE:CD1  | 1:B:516:ASP:HA   | 2.48                     | 0.48              |
| 1:B:508:GLU:CD   | 1:B:772:SER:H    | 2.16                     | 0.48              |
| 2:C:142:LEU:HD11 | 2:C:149:THR:N    | 2.28                     | 0.48              |
| 2:C:218:TYR:CE2  | 2:C:220:ALA:HA   | 2.48                     | 0.48              |
| 2:D:104:LEU:HD12 | 2:D:352:PHE:CD1  | 2.42                     | 0.48              |
| 2:D:291:LYS:HG3  | 2:D:325:MET:HB3  | 1.95                     | 0.48              |
| 1:A:89:MET:HG2   | 1:A:116:TYR:O    | 2.14                     | 0.48              |
| 1:A:108:TYR:OH   | 1:A:694:GLY:N    | 2.47                     | 0.48              |
| 1:A:127:TYR:CD2  | 1:A:691:LYS:HA   | 2.48                     | 0.48              |
| 1:A:274:LYS:HE3  | 1:A:433:ALA:HA   | 1.94                     | 0.48              |
| 1:A:475:ASN:HD21 | 1:A:483:ASN:CG   | 2.21                     | 0.48              |
| 1:A:570:GLN:HG3  | 1:A:589:LYS:HD2  | 1.95                     | 0.48              |
| 1:A:711:LEU:HA   | 1:A:714:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:754:ILE:HG22 | 1:A:758:LYS:HE3  | 1.94                     | 0.48              |
| 1:A:809:ARG:HH22 | 3:H:148:LEU:HD12 | 1.78                     | 0.48              |
| 1:B:290:PHE:C    | 1:B:316:LEU:HD11 | 2.38                     | 0.48              |
| 1:B:416:LYS:HB2  | 2:C:26:ALA:HB2   | 1.96                     | 0.48              |
| 1:B:540:LEU:O    | 1:B:544:GLU:HG2  | 2.14                     | 0.48              |
| 1:B:785:GLU:HA   | 1:B:788:ARG:NH1  | 2.28                     | 0.48              |
| 2:C:82:MET:HB3   | 2:C:86:TRP:CZ3   | 2.48                     | 0.48              |
| 2:C:226:GLU:HG3  | 2:C:255:PHE:CE2  | 2.49                     | 0.48              |
| 2:D:124:PHE:HA   | 2:D:128:ASN:HA   | 1.96                     | 0.48              |
| 2:D:130:PRO:O    | 2:D:358:THR:HG23 | 2.14                     | 0.48              |
| 4:F:35:GLU:O     | 4:F:39:MET:HG3   | 2.14                     | 0.48              |
| 1:A:230:ILE:HG21 | 1:A:339:MET:HG3  | 1.96                     | 0.48              |
| 1:A:717:CYS:HB3  | 1:A:722:PRO:HG3  | 1.94                     | 0.48              |
| 1:A:731:ARG:CZ   | 1:A:749:GLY:HA2  | 2.43                     | 0.48              |
| 1:A:750:LYS:O    | 1:A:754:ILE:HG13 | 2.14                     | 0.48              |
| 1:A:837:ASN:HB2  | 4:G:143:ARG:HH22 | 1.79                     | 0.48              |
| 1:B:132:ILE:HA   | 1:B:137:ILE:HG13 | 1.96                     | 0.48              |
| 1:B:418:GLN:CB   | 1:B:422:GLN:HB2  | 2.41                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:485:THR:HA   | 1:B:667:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:498:PHE:HB2  | 1:B:517:PHE:H    | 1.79                     | 0.48              |
| 2:C:317:ILE:HG22 | 2:C:327:ILE:HD12 | 1.96                     | 0.48              |
| 2:D:70:PRO:HG3   | 2:D:85:ILE:CG1   | 2.43                     | 0.48              |
| 2:D:180:LEU:HD13 | 2:D:264:PRO:HB3  | 1.95                     | 0.48              |
| 3:E:27:LEU:HD12  | 3:E:63:THR:HG22  | 1.94                     | 0.48              |
| 3:H:36:ARG:HA    | 3:H:42:PRO:HD2   | 1.96                     | 0.48              |
| 1:A:43:GLY:N     | 1:A:698:ALA:HB3  | 2.29                     | 0.48              |
| 1:A:79:ASN:HD22  | 1:A:92:LEU:HD22  | 1.78                     | 0.48              |
| 1:A:175:CYS:SG   | 1:A:186:ASN:HB2  | 2.53                     | 0.48              |
| 1:A:234:PHE:CG   | 1:A:442:ILE:HG13 | 2.49                     | 0.48              |
| 1:A:250:LYS:CG   | 1:A:465:ASP:HB2  | 2.44                     | 0.48              |
| 1:A:469:PHE:CZ   | 1:A:487:GLU:HA   | 2.47                     | 0.48              |
| 1:A:744:LYS:HG2  | 3:H:93:ARG:HE    | 1.77                     | 0.48              |
| 1:A:751:GLN:NE2  | 1:A:751:GLN:O    | 2.47                     | 0.48              |
| 1:B:42:HIS:HA    | 1:B:699:HIS:CA   | 2.43                     | 0.48              |
| 1:B:101:LEU:HD23 | 1:B:104:LEU:CD1  | 2.44                     | 0.48              |
| 1:B:102:HIS:CG   | 1:B:105:ARG:HH21 | 2.32                     | 0.48              |
| 1:B:119:LEU:C    | 1:B:146:ARG:HH21 | 2.21                     | 0.48              |
| 1:B:420:LYS:HA   | 1:B:423:ALA:CB   | 2.44                     | 0.48              |
| 2:C:124:PHE:CD1  | 2:C:359:LYS:HA   | 2.49                     | 0.48              |
| 2:C:200:PHE:HZ   | 2:C:248:ILE:HD12 | 1.78                     | 0.48              |
| 2:D:117:GLU:HG2  | 2:D:367:PRO:HB2  | 1.96                     | 0.48              |
| 2:D:124:PHE:CE1  | 2:D:129:VAL:HB   | 2.49                     | 0.48              |
| 2:D:134:VAL:HG21 | 2:D:370:VAL:HG13 | 1.95                     | 0.48              |
| 2:D:218:TYR:CD1  | 2:D:307:PRO:HG2  | 2.49                     | 0.48              |
| 2:D:220:ALA:O    | 2:D:312:ARG:NH1  | 2.47                     | 0.48              |
| 2:D:345:ILE:O    | 2:D:349:LEU:HG   | 2.14                     | 0.48              |
| 3:E:11:PHE:CE2   | 3:E:73:MET:HB2   | 2.49                     | 0.48              |
| 4:G:93:LEU:HB3   | 4:G:163:LYS:HZ1  | 1.77                     | 0.48              |
| 3:H:125:GLU:HA   | 3:H:128:VAL:HG22 | 1.96                     | 0.48              |
| 1:A:19:PHE:HA    | 1:A:82:LYS:HA    | 1.95                     | 0.48              |
| 1:A:178:GLU:HB3  | 1:A:181:ALA:O    | 2.13                     | 0.48              |
| 1:A:254:ILE:CD1  | 1:A:463:ILE:HD11 | 2.43                     | 0.48              |
| 1:A:293:LEU:HD11 | 1:A:305:LEU:CD1  | 2.43                     | 0.48              |
| 1:B:56:GLU:HG3   | 1:B:69:THR:CG2   | 2.44                     | 0.48              |
| 1:B:391:MET:HA   | 1:B:391:MET:HE2  | 1.94                     | 0.48              |
| 1:B:392:GLY:HA3  | 1:B:618:ASP:N    | 2.25                     | 0.48              |
| 1:B:481:CYS:SG   | 1:B:663:TYR:HD2  | 2.37                     | 0.48              |
| 1:B:505:TYR:HE1  | 1:B:721:PHE:HB2  | 1.78                     | 0.48              |
| 1:B:531:PRO:HA   | 1:B:539:ALA:CB   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:8:LEU:HB2    | 2:C:103:THR:HA   | 1.96                     | 0.48              |
| 2:C:156:GLY:C    | 2:C:182:GLY:H    | 2.21                     | 0.48              |
| 2:C:188:TYR:CE2  | 2:C:266:PHE:HB3  | 2.48                     | 0.48              |
| 2:D:178:LEU:HD11 | 2:D:272:ALA:O    | 2.13                     | 0.48              |
| 3:E:112:LEU:HD13 | 3:E:127:LEU:HD21 | 1.96                     | 0.48              |
| 4:G:35:GLU:O     | 4:G:39:MET:HG3   | 2.14                     | 0.48              |
| 1:A:13:LEU:HB2   | 1:A:132:ILE:HG21 | 1.96                     | 0.48              |
| 1:A:44:PHE:CG    | 1:A:74:ASP:HA    | 2.48                     | 0.48              |
| 1:A:113:ILE:HG21 | 1:A:126:PRO:HD3  | 1.96                     | 0.48              |
| 1:A:127:TYR:CG   | 1:A:691:LYS:HA   | 2.48                     | 0.48              |
| 1:A:251:PHE:CE1  | 1:A:268:GLU:HB3  | 2.49                     | 0.48              |
| 1:B:92:LEU:HD11  | 1:B:103:ASN:ND2  | 2.29                     | 0.48              |
| 1:B:126:PRO:C    | 1:B:128:LYS:H    | 2.22                     | 0.48              |
| 1:B:165:LEU:O    | 1:B:168:ARG:HD2  | 2.14                     | 0.48              |
| 1:B:397:ASP:HA   | 1:B:400:ARG:NH1  | 2.29                     | 0.48              |
| 3:E:8:THR:HG23   | 3:E:70:LEU:HD11  | 1.96                     | 0.48              |
| 3:H:42:PRO:HA    | 3:H:46:GLU:CD    | 2.39                     | 0.48              |
| 1:A:220:LEU:HB2  | 1:A:265:ALA:HB3  | 1.96                     | 0.48              |
| 1:A:263:VAL:HG21 | 1:A:456:GLN:HB3  | 1.96                     | 0.48              |
| 1:A:285:ARG:HD2  | 1:A:322:PRO:O    | 2.13                     | 0.48              |
| 1:B:29:TRP:CG    | 1:B:30:SER:H     | 2.32                     | 0.48              |
| 1:B:220:LEU:HD13 | 1:B:452:LYS:H    | 1.79                     | 0.48              |
| 1:B:392:GLY:C    | 1:B:617:SER:H    | 2.21                     | 0.48              |
| 1:B:437:ARG:NH1  | 1:B:625:TRP:HB3  | 2.29                     | 0.48              |
| 1:B:768:ARG:O    | 1:B:774:ILE:HA   | 2.14                     | 0.48              |
| 1:B:812:PHE:CE1  | 3:E:34:VAL:HA    | 2.48                     | 0.48              |
| 2:C:44:MET:HE3   | 2:C:47:MET:HB3   | 1.96                     | 0.48              |
| 2:C:288:ASP:O    | 2:C:291:LYS:HB3  | 2.14                     | 0.48              |
| 2:D:20:GLY:H     | 2:D:94:LEU:HD11  | 1.78                     | 0.48              |
| 1:A:35:VAL:HB    | 1:A:45:GLU:O     | 2.14                     | 0.47              |
| 1:A:480:LEU:HD22 | 1:A:597:TRP:CH2  | 2.49                     | 0.47              |
| 1:A:744:LYS:NZ   | 3:H:96:ASP:O     | 2.33                     | 0.47              |
| 1:B:85:LYS:HD3   | 1:B:106:GLU:HB2  | 1.96                     | 0.47              |
| 1:B:129:GLN:HG3  | 1:B:189:LYS:HE2  | 1.96                     | 0.47              |
| 1:B:243:ASP:OD1  | 1:B:244:ASN:N    | 2.47                     | 0.47              |
| 1:B:276:ARG:HH22 | 1:B:479:GLN:HE22 | 1.61                     | 0.47              |
| 1:B:477:PHE:HE1  | 1:B:660:GLY:HA2  | 1.78                     | 0.47              |
| 1:B:504:GLU:HB3  | 1:B:775:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:744:LYS:HE2  | 3:E:99:GLY:HA3   | 1.95                     | 0.47              |
| 1:B:826:GLN:CG   | 4:F:129:MET:HB3  | 2.40                     | 0.47              |
| 2:C:99:GLU:HG3   | 2:C:127:PHE:C    | 2.38                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:219:VAL:HG13 | 2:C:262:PHE:CZ   | 2.49                     | 0.47              |
| 2:C:220:ALA:HB1  | 2:C:223:PHE:CA   | 2.45                     | 0.47              |
| 2:D:357:ILE:HG12 | 2:D:370:VAL:HA   | 1.96                     | 0.47              |
| 3:E:93:ARG:NH1   | 3:E:100:ASN:OD1  | 2.47                     | 0.47              |
| 4:F:25:PHE:HB2   | 4:F:30:ILE:HD11  | 1.96                     | 0.47              |
| 4:F:117:ILE:N    | 4:F:155:TYR:HE1  | 2.11                     | 0.47              |
| 3:H:90:GLU:O     | 3:H:94:VAL:HG22  | 2.13                     | 0.47              |
| 3:H:108:ILE:O    | 3:H:112:LEU:N    | 2.47                     | 0.47              |
| 1:A:257:ASP:O    | 1:A:260:GLY:N    | 2.45                     | 0.47              |
| 1:A:267:ILE:HG12 | 1:A:450:LEU:CD2  | 2.44                     | 0.47              |
| 1:A:620:PHE:CE2  | 1:A:624:LEU:HD12 | 2.48                     | 0.47              |
| 1:B:55:ASP:OD1   | 1:B:72:LYS:N     | 2.46                     | 0.47              |
| 1:B:405:PRO:HA   | 1:B:608:ASN:ND2  | 2.28                     | 0.47              |
| 1:B:443:LEU:CA   | 1:B:446:VAL:HB   | 2.44                     | 0.47              |
| 1:B:477:PHE:HB2  | 1:B:597:TRP:CG   | 2.49                     | 0.47              |
| 1:B:742:ILE:HD11 | 1:B:755:LEU:HD12 | 1.95                     | 0.47              |
| 2:C:140:LEU:O    | 2:C:342:GLY:HA3  | 2.14                     | 0.47              |
| 2:D:21:PHE:O     | 2:D:344:SER:HB3  | 2.14                     | 0.47              |
| 2:D:137:GLN:HA   | 2:D:339:VAL:HG13 | 1.96                     | 0.47              |
| 2:D:174:ALA:O    | 2:D:281:SER:HB2  | 2.14                     | 0.47              |
| 3:E:29:SER:HB3   | 3:E:60:ASN:OD1   | 2.14                     | 0.47              |
| 3:H:123:GLU:O    | 3:H:126:GLN:NE2  | 2.47                     | 0.47              |
| 1:A:50:LYS:HG2   | 1:A:60:GLU:HB2   | 1.97                     | 0.47              |
| 1:A:116:TYR:CE1  | 1:A:156:ILE:HD11 | 2.48                     | 0.47              |
| 1:A:120:PHE:HZ   | 1:A:497:MET:HE3  | 1.79                     | 0.47              |
| 1:A:290:PHE:HA   | 1:A:356:VAL:CG1  | 2.44                     | 0.47              |
| 1:A:295:ALA:HB3  | 1:A:328:ASP:CB   | 2.44                     | 0.47              |
| 1:A:532:THR:HG23 | 2:D:350:SER:HB3  | 1.96                     | 0.47              |
| 1:A:744:LYS:HG2  | 3:H:93:ARG:NE    | 2.28                     | 0.47              |
| 1:A:847:VAL:O    | 1:A:850:LEU:HG   | 2.15                     | 0.47              |
| 1:B:142:LYS:HD2  | 1:B:197:VAL:HG22 | 1.97                     | 0.47              |
| 1:B:361:GLN:O    | 1:B:365:ILE:HG13 | 2.14                     | 0.47              |
| 1:B:502:GLN:HB3  | 1:B:506:GLN:HE22 | 1.79                     | 0.47              |
| 1:B:533:ASN:H    | 2:C:353:GLN:NE2  | 2.10                     | 0.47              |
| 1:B:806:TYR:CZ   | 3:E:131:HIS:CE1  | 3.02                     | 0.47              |
| 2:C:94:LEU:C     | 2:C:96:VAL:N     | 2.72                     | 0.47              |
| 2:C:120:THR:HG23 | 2:C:124:PHE:CD2  | 2.50                     | 0.47              |
| 2:C:289:ILE:HA   | 2:C:292:ASP:OD2  | 2.14                     | 0.47              |
| 2:C:336:LYS:HE3  | 2:C:337:TYR:CZ   | 2.50                     | 0.47              |
| 2:D:76:ILE:HD13  | 2:D:82:MET:HG3   | 1.97                     | 0.47              |
| 2:D:136:ILE:HG22 | 2:D:139:VAL:H    | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:217:CYS:HA   | 2:D:254:ARG:HB3  | 1.95                     | 0.47              |
| 3:E:107:GLU:O    | 3:E:110:HIS:HB3  | 2.14                     | 0.47              |
| 1:A:107:ARG:NE   | 1:A:115:THR:OG1  | 2.47                     | 0.47              |
| 1:A:441:TRP:HE1  | 1:A:445:ARG:NH2  | 2.10                     | 0.47              |
| 1:A:688:ASN:HB2  | 1:A:695:LYS:NZ   | 2.30                     | 0.47              |
| 1:B:362:LEU:HA   | 1:B:365:ILE:CD1  | 2.45                     | 0.47              |
| 1:B:536:GLY:C    | 1:B:540:LEU:HG   | 2.39                     | 0.47              |
| 1:B:731:ARG:HD2  | 1:B:746:PHE:H    | 1.80                     | 0.47              |
| 1:B:734:TYR:HD2  | 1:B:737:LEU:HB2  | 1.79                     | 0.47              |
| 2:C:73:HIS:NE2   | 2:C:183:ARG:HB2  | 2.29                     | 0.47              |
| 2:C:213:LYS:O    | 2:C:215:LYS:N    | 2.48                     | 0.47              |
| 2:C:275:HIS:CD2  | 2:C:316:GLU:HB3  | 2.50                     | 0.47              |
| 2:D:219:VAL:HG21 | 2:D:309:ILE:HB   | 1.95                     | 0.47              |
| 2:D:300:SER:HA   | 2:D:335:ARG:CG   | 2.42                     | 0.47              |
| 3:E:3:PHE:HE2    | 3:E:11:PHE:CZ    | 2.31                     | 0.47              |
| 3:H:48:MET:HA    | 3:H:51:LEU:HD12  | 1.96                     | 0.47              |
| 1:A:26:GLN:HG3   | 1:A:786:GLU:HB3  | 1.97                     | 0.47              |
| 1:A:34:LEU:C     | 1:A:78:MET:HB3   | 2.39                     | 0.47              |
| 1:A:272:LEU:HD13 | 1:A:439:PHE:CD2  | 2.48                     | 0.47              |
| 1:A:393:ILE:HD13 | 1:A:613:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:511:GLU:OE1  | 1:A:511:GLU:N    | 2.37                     | 0.47              |
| 1:A:555:PHE:HE2  | 1:A:594:ALA:HB2  | 1.80                     | 0.47              |
| 1:A:657:ARG:NH1  | 2:D:4:GLU:OE1    | 2.47                     | 0.47              |
| 1:A:844:PHE:H    | 4:G:92:LYS:HE3   | 1.80                     | 0.47              |
| 1:B:272:LEU:HD21 | 1:B:439:PHE:HB3  | 1.94                     | 0.47              |
| 1:B:328:ASP:O    | 1:B:332:PHE:CB   | 2.63                     | 0.47              |
| 1:B:339:MET:SD   | 1:B:352:ILE:HG21 | 2.54                     | 0.47              |
| 1:B:355:VAL:HG22 | 1:B:625:TRP:HH2  | 1.79                     | 0.47              |
| 1:B:686:ILE:CD1  | 1:B:689:HIS:HB3  | 2.45                     | 0.47              |
| 1:B:800:GLN:NE2  | 3:E:115:LEU:HB2  | 2.28                     | 0.47              |
| 2:C:252:ASN:N    | 2:C:252:ASN:OD1  | 2.45                     | 0.47              |
| 2:C:297:ASN:HD22 | 2:C:314:GLN:NE2  | 2.12                     | 0.47              |
| 2:D:14:SER:H     | 2:D:158:GLY:HA2  | 1.79                     | 0.47              |
| 2:D:74:GLY:N     | 2:D:159:VAL:HB   | 2.29                     | 0.47              |
| 2:D:274:ILE:CD1  | 2:D:313:MET:HE1  | 2.43                     | 0.47              |
| 3:H:128:VAL:HG12 | 3:H:138:ILE:HG13 | 1.96                     | 0.47              |
| 1:A:129:GLN:HG3  | 1:A:133:TYR:CD1  | 2.49                     | 0.47              |
| 1:A:145:LYS:HB2  | 1:A:148:GLU:CD   | 2.38                     | 0.47              |
| 1:A:400:ARG:NH2  | 1:A:401:SER:HB3  | 2.30                     | 0.47              |
| 1:A:447:ASN:HA   | 1:A:450:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:704:GLN:HA   | 1:A:707:CYS:SG   | 2.54                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:736:ILE:O    | 1:A:791:LYS:HG2  | 2.15                     | 0.47              |
| 1:B:80:PRO:O     | 1:B:82:LYS:N     | 2.48                     | 0.47              |
| 1:B:269:THR:H    | 1:B:443:LEU:CD2  | 2.26                     | 0.47              |
| 1:B:272:LEU:HD22 | 1:B:440:ARG:NH1  | 2.29                     | 0.47              |
| 1:B:400:ARG:O    | 1:B:404:THR:OG1  | 2.32                     | 0.47              |
| 1:B:437:ARG:NH2  | 1:B:610:THR:HG21 | 2.28                     | 0.47              |
| 1:B:675:ARG:NH1  | 1:B:679:PRO:HG2  | 2.29                     | 0.47              |
| 2:C:208:ILE:O    | 2:C:212:ILE:HG13 | 2.15                     | 0.47              |
| 2:D:200:PHE:HZ   | 2:D:248:ILE:HG21 | 1.80                     | 0.47              |
| 2:D:230:ALA:O    | 2:D:251:GLY:HA3  | 2.13                     | 0.47              |
| 3:E:28:TYR:HA    | 3:E:31:CYS:SG    | 2.54                     | 0.47              |
| 3:H:19:ASP:OD2   | 3:H:24:GLY:N     | 2.48                     | 0.47              |
| 3:H:20:ARG:HG2   | 3:H:30:GLN:NE2   | 2.29                     | 0.47              |
| 3:H:31:CYS:SG    | 3:H:64:LEU:HD22  | 2.54                     | 0.47              |
| 1:A:108:TYR:CD2  | 1:A:696:LEU:HD12 | 2.50                     | 0.47              |
| 1:A:113:ILE:HG13 | 1:A:130:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:154:TYR:HE1  | 1:A:189:LYS:O    | 1.98                     | 0.47              |
| 1:A:158:ASP:HB2  | 1:A:193:TYR:CE1  | 2.50                     | 0.47              |
| 1:A:294:ILE:HD12 | 1:A:310:PHE:HA   | 1.95                     | 0.47              |
| 1:A:418:GLN:OE1  | 1:A:422:GLN:HG3  | 2.15                     | 0.47              |
| 1:A:469:PHE:HB2  | 1:A:707:CYS:O    | 2.15                     | 0.47              |
| 1:A:585:HIS:HB2  | 1:A:590:VAL:HG23 | 1.96                     | 0.47              |
| 1:A:776:PHE:CD1  | 1:A:781:LEU:HA   | 2.50                     | 0.47              |
| 1:A:807:LEU:HA   | 1:A:807:LEU:HD23 | 1.48                     | 0.47              |
| 1:B:25:ALA:H     | 1:B:789:ASP:CB   | 2.27                     | 0.47              |
| 1:B:33:LYS:N     | 1:B:49:ILE:H     | 2.12                     | 0.47              |
| 1:B:66:LYS:HB3   | 1:B:68:VAL:HG23  | 1.97                     | 0.47              |
| 1:B:156:ILE:CG2  | 1:B:682:VAL:HG23 | 2.45                     | 0.47              |
| 1:B:269:THR:O    | 1:B:440:ARG:NH2  | 2.47                     | 0.47              |
| 1:B:278:ILE:HD12 | 1:B:279:ARG:HD3  | 1.95                     | 0.47              |
| 1:B:290:PHE:O    | 1:B:294:ILE:HG13 | 2.15                     | 0.47              |
| 1:B:342:MET:C    | 1:B:445:ARG:HG3  | 2.40                     | 0.47              |
| 1:B:367:PHE:CE2  | 1:B:402:ILE:HB   | 2.49                     | 0.47              |
| 1:B:368:LYS:HE2  | 1:B:378:MET:HA   | 1.96                     | 0.47              |
| 1:B:501:GLU:HB3  | 1:B:505:TYR:OH   | 2.15                     | 0.47              |
| 1:B:537:VAL:HG12 | 1:B:597:TRP:HZ3  | 1.80                     | 0.47              |
| 2:C:20:GLY:HA3   | 2:C:340:TRP:HE1  | 1.80                     | 0.47              |
| 2:C:103:THR:H    | 2:C:129:VAL:HG11 | 1.79                     | 0.47              |
| 2:C:133:TYR:CE1  | 2:C:135:ALA:HA   | 2.50                     | 0.47              |
| 2:C:181:ALA:C    | 2:C:185:LEU:HD13 | 2.40                     | 0.47              |
| 2:C:285:CYS:O    | 2:C:290:ARG:NH2  | 2.46                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:291:LYS:NZ   | 2:C:325:MET:HG2  | 2.30                     | 0.47              |
| 2:C:294:TYR:CB   | 2:C:327:ILE:HG12 | 2.45                     | 0.47              |
| 2:D:11:ASP:OD2   | 2:D:339:VAL:HB   | 2.15                     | 0.47              |
| 2:D:70:PRO:HD3   | 2:D:81:ASP:HB3   | 1.97                     | 0.47              |
| 2:D:79:TRP:O     | 2:D:83:GLU:HG3   | 2.15                     | 0.47              |
| 2:D:107:GLU:HB3  | 2:D:134:VAL:HB   | 1.97                     | 0.47              |
| 2:D:114:ALA:HB1  | 2:D:118:LYS:HE3  | 1.97                     | 0.47              |
| 2:D:153:LEU:HD22 | 2:D:299:MET:SD   | 2.54                     | 0.47              |
| 2:D:279:TYR:O    | 2:D:282:ILE:HB   | 2.15                     | 0.47              |
| 2:D:282:ILE:HA   | 2:D:293:LEU:HB3  | 1.97                     | 0.47              |
| 2:D:301:GLY:C    | 2:D:336:LYS:HA   | 2.40                     | 0.47              |
| 2:D:347:ALA:HA   | 2:D:352:PHE:HB2  | 1.97                     | 0.47              |
| 3:E:49:LYS:O     | 3:E:53:ASN:ND2   | 2.48                     | 0.47              |
| 3:H:108:ILE:HG21 | 3:H:127:LEU:HD23 | 1.96                     | 0.47              |
| 3:H:125:GLU:O    | 3:H:128:VAL:N    | 2.48                     | 0.47              |
| 1:A:233:ALA:O    | 1:A:289:ILE:N    | 2.34                     | 0.47              |
| 1:A:246:SER:HB3  | 1:A:248:PHE:O    | 2.14                     | 0.47              |
| 1:A:255:ASN:HB3  | 1:A:457:GLY:CA   | 2.42                     | 0.47              |
| 1:A:376:ALA:HB3  | 1:A:403:LEU:O    | 2.14                     | 0.47              |
| 1:A:398:PHE:HA   | 1:A:609:VAL:HG22 | 1.96                     | 0.47              |
| 1:A:473:GLU:HG2  | 1:A:474:ILE:H    | 1.78                     | 0.47              |
| 1:A:480:LEU:HD11 | 1:A:528:ILE:HD12 | 1.95                     | 0.47              |
| 1:A:500:LEU:O    | 1:A:503:GLU:HB3  | 2.14                     | 0.47              |
| 1:A:505:TYR:CZ   | 1:A:514:PHE:HD2  | 2.33                     | 0.47              |
| 1:A:521:LEU:HG   | 1:A:586:TYR:CD1  | 2.50                     | 0.47              |
| 1:A:705:LEU:HA   | 1:A:710:VAL:HB   | 1.96                     | 0.47              |
| 1:A:813:ALA:CB   | 1:A:815:ARG:HG2  | 2.41                     | 0.47              |
| 1:B:257:ASP:HA   | 1:B:456:GLN:CG   | 2.45                     | 0.47              |
| 1:B:315:PHE:O    | 1:B:316:LEU:HB2  | 2.14                     | 0.47              |
| 1:B:796:ILE:HG21 | 3:E:111:VAL:HG23 | 1.95                     | 0.47              |
| 2:C:86:TRP:CZ2   | 2:C:105:LEU:HD13 | 2.50                     | 0.47              |
| 2:D:34:ILE:HD13  | 2:D:207:GLU:CD   | 2.40                     | 0.47              |
| 2:D:218:TYR:CD2  | 2:D:255:PHE:HB3  | 2.47                     | 0.47              |
| 3:E:15:PHE:HA    | 3:E:34:VAL:HG11  | 1.96                     | 0.47              |
| 3:E:55:LYS:NZ    | 3:E:58:GLU:HB2   | 2.29                     | 0.47              |
| 3:E:120:THR:OG1  | 3:E:123:GLU:HB2  | 2.14                     | 0.47              |
| 3:H:11:PHE:CD1   | 3:H:38:LEU:HD13  | 2.50                     | 0.47              |
| 1:A:153:ILE:HD13 | 1:A:186:ASN:HA   | 1.97                     | 0.47              |
| 1:A:328:ASP:O    | 1:A:332:PHE:HB2  | 2.14                     | 0.47              |
| 1:A:435:PHE:HD1  | 1:A:438:LEU:HD23 | 1.73                     | 0.47              |
| 1:A:704:GLN:OE1  | 1:A:708:ASN:ND2  | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:846:LYS:HD2  | 1:A:846:LYS:HA   | 1.74                     | 0.47              |
| 1:B:50:LYS:N     | 1:B:59:VAL:HG12  | 2.27                     | 0.47              |
| 1:B:280:GLN:CG   | 1:B:286:THR:HG22 | 2.44                     | 0.47              |
| 1:B:393:ILE:HG21 | 1:B:613:LEU:HD23 | 1.97                     | 0.47              |
| 1:B:527:LEU:HA   | 1:B:566:HIS:CD2  | 2.49                     | 0.47              |
| 1:B:683:ARG:HB3  | 1:B:708:ASN:HD22 | 1.80                     | 0.47              |
| 1:B:696:LEU:HD11 | 1:B:701:VAL:HG21 | 1.97                     | 0.47              |
| 2:D:67:LEU:HD12  | 2:D:207:GLU:CG   | 2.44                     | 0.47              |
| 2:D:133:TYR:HA   | 2:D:357:ILE:HD12 | 1.97                     | 0.47              |
| 2:D:219:VAL:HA   | 2:D:258:PRO:CB   | 2.45                     | 0.47              |
| 2:D:314:GLN:NE2  | 2:D:318:THR:HG23 | 2.30                     | 0.47              |
| 1:A:4:LYS:HB2    | 1:A:10:GLU:CG    | 2.45                     | 0.47              |
| 1:A:105:ARG:CA   | 1:A:696:LEU:HD22 | 2.44                     | 0.47              |
| 1:A:250:LYS:HG2  | 1:A:465:ASP:HB2  | 1.97                     | 0.47              |
| 1:A:274:LYS:O    | 1:A:277:ALA:CB   | 2.52                     | 0.47              |
| 1:A:355:VAL:HG22 | 1:A:625:TRP:CH2  | 2.50                     | 0.47              |
| 1:A:484:TYR:CE1  | 1:A:525:ILE:HG23 | 2.50                     | 0.47              |
| 1:A:527:LEU:CD2  | 1:A:583:ILE:HG23 | 2.41                     | 0.47              |
| 1:A:552:ASP:HB3  | 1:A:594:ALA:HB1  | 1.96                     | 0.47              |
| 1:B:58:THR:HG22  | 1:B:67:LYS:HG2   | 1.97                     | 0.47              |
| 1:B:322:PRO:HA   | 1:B:328:ASP:OD1  | 2.16                     | 0.47              |
| 1:B:536:GLY:HA2  | 1:B:566:HIS:CD2  | 2.49                     | 0.47              |
| 1:B:681:PHE:HA   | 1:B:683:ARG:NH2  | 2.30                     | 0.47              |
| 1:B:836:ARG:HD3  | 4:F:158:PHE:CZ   | 2.50                     | 0.47              |
| 2:C:188:TYR:OH   | 2:C:256:ARG:NH2  | 2.40                     | 0.47              |
| 2:C:192:ILE:HG21 | 2:C:256:ARG:NE   | 2.28                     | 0.47              |
| 2:C:279:TYR:CD1  | 2:C:282:ILE:HB   | 2.50                     | 0.47              |
| 2:D:134:VAL:CG2  | 2:D:370:VAL:HG13 | 2.45                     | 0.47              |
| 2:D:309:ILE:HD11 | 2:D:313:MET:HE2  | 1.96                     | 0.47              |
| 3:E:41:ASN:HB2   | 3:E:82:GLN:HG2   | 1.95                     | 0.47              |
| 4:G:30:ILE:HA    | 4:G:33:PHE:CD2   | 2.49                     | 0.47              |
| 3:H:28:TYR:CE1   | 3:H:64:LEU:HB2   | 2.50                     | 0.47              |
| 3:H:124:VAL:O    | 3:H:127:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:18:ASN:HB3   | 1:A:81:PRO:O     | 2.15                     | 0.46              |
| 1:A:25:ALA:HB2   | 1:A:789:ASP:OD2  | 2.15                     | 0.46              |
| 1:A:291:TYR:CE1  | 1:A:316:LEU:HB3  | 2.50                     | 0.46              |
| 1:A:399:THR:HG22 | 1:A:403:LEU:HD21 | 1.95                     | 0.46              |
| 1:A:480:LEU:HD11 | 1:A:528:ILE:HG23 | 1.97                     | 0.46              |
| 1:A:560:ILE:HA   | 1:A:563:GLN:NE2  | 2.29                     | 0.46              |
| 1:A:845:THR:HG23 | 4:G:92:LYS:HZ1   | 1.81                     | 0.46              |
| 1:B:97:GLU:HA    | 1:B:100:VAL:HB   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:238:LYS:HE2  | 1:B:324:PRO:CG   | 2.44                     | 0.46              |
| 1:B:291:TYR:CD1  | 1:B:316:LEU:HD13 | 2.50                     | 0.46              |
| 1:B:297:ALA:HA   | 1:B:332:PHE:CE2  | 2.49                     | 0.46              |
| 2:C:75:ILE:HA    | 2:C:111:ASN:HD21 | 1.80                     | 0.46              |
| 2:C:140:LEU:HB3  | 2:C:339:VAL:O    | 2.15                     | 0.46              |
| 2:C:314:GLN:OE1  | 2:C:327:ILE:HB   | 2.15                     | 0.46              |
| 2:D:96:VAL:HB    | 2:D:101:HIS:NE2  | 2.29                     | 0.46              |
| 2:D:97:ALA:O     | 2:D:101:HIS:HB2  | 2.15                     | 0.46              |
| 2:D:139:VAL:O    | 2:D:142:LEU:HB3  | 2.15                     | 0.46              |
| 2:D:151:ILE:N    | 2:D:296:ASN:O    | 2.48                     | 0.46              |
| 2:D:274:ILE:HG23 | 2:D:275:HIS:N    | 2.30                     | 0.46              |
| 3:E:28:TYR:CE2   | 3:E:58:GLU:HG2   | 2.50                     | 0.46              |
| 3:E:109:ARG:HG2  | 3:E:124:VAL:HG23 | 1.96                     | 0.46              |
| 3:E:109:ARG:O    | 3:E:113:VAL:HG22 | 2.15                     | 0.46              |
| 3:E:133:ASP:O    | 3:E:135:ASN:N    | 2.48                     | 0.46              |
| 4:G:34:LYS:HZ2   | 4:G:86:LEU:HB2   | 1.79                     | 0.46              |
| 1:A:15:VAL:HG22  | 1:A:112:LEU:HD13 | 1.97                     | 0.46              |
| 1:A:198:ALA:HA   | 1:A:260:GLY:O    | 2.14                     | 0.46              |
| 1:A:331:MET:O    | 1:A:335:THR:OG1  | 2.21                     | 0.46              |
| 1:A:336:LEU:HD22 | 1:A:349:GLN:HB3  | 1.95                     | 0.46              |
| 1:A:355:VAL:HG13 | 1:A:625:TRP:CH2  | 2.50                     | 0.46              |
| 1:B:160:ALA:HB1  | 1:B:461:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:275:SER:H    | 1:B:663:TYR:HH   | 1.55                     | 0.46              |
| 1:B:327:GLN:HE21 | 1:B:329:ASP:H    | 1.63                     | 0.46              |
| 1:B:537:VAL:HG11 | 1:B:583:ILE:HD11 | 1.98                     | 0.46              |
| 1:B:583:ILE:HB   | 1:B:592:TYR:CD2  | 2.50                     | 0.46              |
| 1:B:736:ILE:HD11 | 1:B:791:LYS:HG3  | 1.97                     | 0.46              |
| 2:C:103:THR:OG1  | 2:C:129:VAL:HG21 | 2.15                     | 0.46              |
| 2:C:104:LEU:HD21 | 2:C:140:LEU:HD11 | 1.97                     | 0.46              |
| 2:C:166:TYR:OH   | 2:C:284:LYS:HB3  | 2.15                     | 0.46              |
| 2:C:287:ILE:O    | 2:C:290:ARG:HG2  | 2.15                     | 0.46              |
| 2:C:314:GLN:HE21 | 2:C:329:ILE:N    | 2.13                     | 0.46              |
| 2:D:100:GLU:H    | 2:D:130:PRO:HD3  | 1.80                     | 0.46              |
| 2:D:151:ILE:CD1  | 2:D:282:ILE:HG13 | 2.45                     | 0.46              |
| 2:D:212:ILE:HG21 | 2:D:250:ILE:HG12 | 1.97                     | 0.46              |
| 2:D:357:ILE:HG12 | 2:D:370:VAL:HG22 | 1.97                     | 0.46              |
| 3:E:50:VAL:HG21  | 3:E:76:ILE:CG1   | 2.46                     | 0.46              |
| 3:E:93:ARG:NH1   | 3:E:101:GLY:H    | 2.13                     | 0.46              |
| 3:H:25:LYS:HA    | 3:H:64:LEU:O     | 2.15                     | 0.46              |
| 1:A:122:VAL:HG12 | 1:A:124:ILE:HG13 | 1.98                     | 0.46              |
| 1:A:123:VAL:HG21 | 1:A:682:VAL:HG13 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:336:LEU:O    | 1:A:339:MET:HB2  | 2.14                     | 0.46              |
| 1:A:411:ARG:NE   | 2:D:94:LEU:HA    | 2.30                     | 0.46              |
| 1:A:443:LEU:O    | 1:A:446:VAL:HB   | 2.15                     | 0.46              |
| 1:A:527:LEU:HD23 | 1:A:583:ILE:CG2  | 2.40                     | 0.46              |
| 1:B:135:GLU:HG2  | 1:B:196:VAL:HG21 | 1.97                     | 0.46              |
| 1:B:237:ALA:HB1  | 1:B:285:ARG:O    | 2.14                     | 0.46              |
| 1:B:547:PHE:HB3  | 1:B:549:LYS:O    | 2.15                     | 0.46              |
| 1:B:566:HIS:CE1  | 1:B:569:PHE:CD2  | 3.04                     | 0.46              |
| 2:C:217:CYS:SG   | 2:C:257:CYS:HB2  | 2.56                     | 0.46              |
| 2:D:112:PRO:HD2  | 2:D:115:ASN:ND2  | 2.30                     | 0.46              |
| 2:D:123:MET:O    | 2:D:128:ASN:N    | 2.49                     | 0.46              |
| 2:D:192:ILE:HB   | 2:D:256:ARG:NH1  | 2.30                     | 0.46              |
| 2:D:279:TYR:CZ   | 2:D:321:ALA:HA   | 2.49                     | 0.46              |
| 2:D:358:THR:O    | 2:D:361:GLU:HB2  | 2.15                     | 0.46              |
| 3:H:46:GLU:O     | 3:H:50:VAL:HG13  | 2.16                     | 0.46              |
| 3:H:123:GLU:HA   | 3:H:126:GLN:HE21 | 1.79                     | 0.46              |
| 1:A:315:PHE:O    | 1:A:316:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:355:VAL:HG22 | 1:A:625:TRP:HH2  | 1.81                     | 0.46              |
| 1:A:361:GLN:NE2  | 1:A:386:LYS:HD3  | 2.31                     | 0.46              |
| 1:A:409:VAL:HG13 | 2:D:24:ASP:HB3   | 1.96                     | 0.46              |
| 1:A:434:LYS:HG2  | 1:A:625:TRP:NE1  | 2.30                     | 0.46              |
| 1:A:773:LYS:HB2  | 1:A:775:PHE:CD1  | 2.50                     | 0.46              |
| 1:B:77:LYS:O     | 1:B:79:ASN:ND2   | 2.49                     | 0.46              |
| 1:B:165:LEU:HD13 | 1:B:259:THR:C    | 2.40                     | 0.46              |
| 1:B:280:GLN:NE2  | 1:B:286:THR:HG22 | 2.30                     | 0.46              |
| 2:C:69:TYR:OH    | 2:C:207:GLU:OE2  | 2.22                     | 0.46              |
| 2:D:10:CYS:SG    | 2:D:12:ASN:HB3   | 2.56                     | 0.46              |
| 2:D:50:LYS:O     | 2:D:53:TYR:OH    | 2.21                     | 0.46              |
| 2:D:124:PHE:CD2  | 2:D:359:LYS:HA   | 2.50                     | 0.46              |
| 2:D:219:VAL:HG13 | 2:D:262:PHE:HE2  | 1.79                     | 0.46              |
| 2:D:361:GLU:O    | 2:D:365:ALA:HB3  | 2.15                     | 0.46              |
| 3:E:43:THR:HB    | 3:E:46:GLU:CD    | 2.40                     | 0.46              |
| 3:H:15:PHE:CG    | 3:H:26:ILE:HD13  | 2.49                     | 0.46              |
| 1:A:7:SER:OG     | 1:A:136:LYS:NZ   | 2.48                     | 0.46              |
| 1:A:18:ASN:N     | 1:A:84:SER:O     | 2.40                     | 0.46              |
| 1:A:95:LEU:HB2   | 1:A:718:ARG:NE   | 2.31                     | 0.46              |
| 1:A:136:LYS:HG3  | 1:A:137:ILE:H    | 1.81                     | 0.46              |
| 1:A:263:VAL:HG21 | 1:A:456:GLN:N    | 2.30                     | 0.46              |
| 1:A:344:PHE:CZ   | 1:A:442:ILE:HA   | 2.50                     | 0.46              |
| 1:A:438:LEU:N    | 1:A:624:LEU:HD21 | 2.31                     | 0.46              |
| 1:A:543:GLU:HA   | 1:A:546:TRP:CD2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:667:LEU:C    | 1:A:667:LEU:HD12 | 2.40                     | 0.46              |
| 1:A:807:LEU:CD1  | 3:H:127:LEU:HB2  | 2.45                     | 0.46              |
| 1:B:46:ALA:O     | 1:B:62:GLN:HB2   | 2.15                     | 0.46              |
| 1:B:102:HIS:CE1  | 1:B:105:ARG:HH21 | 2.33                     | 0.46              |
| 1:B:114:TYR:OH   | 1:B:189:LYS:HE3  | 2.16                     | 0.46              |
| 1:B:799:PHE:CE2  | 3:E:108:ILE:HD11 | 2.49                     | 0.46              |
| 2:C:107:GLU:OE1  | 2:C:116:ARG:HG2  | 2.16                     | 0.46              |
| 2:C:144:ALA:HB2  | 2:C:342:GLY:N    | 2.31                     | 0.46              |
| 2:C:145:SER:OG   | 2:C:332:PRO:HG3  | 2.15                     | 0.46              |
| 2:C:278:THR:O    | 2:C:282:ILE:HG13 | 2.16                     | 0.46              |
| 2:C:282:ILE:HG21 | 2:C:294:TYR:CE1  | 2.51                     | 0.46              |
| 2:D:5:THR:C      | 2:D:7:ALA:N      | 2.73                     | 0.46              |
| 2:D:58:ALA:HB1   | 2:D:67:LEU:HD13  | 1.97                     | 0.46              |
| 2:D:118:LYS:O    | 2:D:119:MET:C    | 2.57                     | 0.46              |
| 2:D:140:LEU:HA   | 2:D:140:LEU:HD23 | 1.55                     | 0.46              |
| 3:E:3:PHE:N      | 3:E:74:GLN:HE22  | 2.14                     | 0.46              |
| 3:H:7:GLN:O      | 3:H:11:PHE:N     | 2.45                     | 0.46              |
| 1:A:117:SER:O    | 1:A:119:LEU:N    | 2.45                     | 0.46              |
| 1:A:718:ARG:HA   | 1:A:778:THR:HB   | 1.97                     | 0.46              |
| 1:A:750:LYS:HG3  | 1:A:769:ILE:HG23 | 1.98                     | 0.46              |
| 1:B:87:GLU:HA    | 1:B:107:ARG:NH1  | 2.30                     | 0.46              |
| 1:B:114:TYR:CZ   | 1:B:132:ILE:HD11 | 2.51                     | 0.46              |
| 1:B:730:PHE:CD1  | 1:B:774:ILE:HD12 | 2.50                     | 0.46              |
| 1:B:760:LEU:HD13 | 1:B:762:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:781:LEU:HD23 | 1:B:781:LEU:HA   | 1.59                     | 0.46              |
| 1:B:792:ILE:HG23 | 3:E:91:GLY:O     | 2.15                     | 0.46              |
| 2:C:12:ASN:HB2   | 2:C:71:ILE:CD1   | 2.46                     | 0.46              |
| 2:C:120:THR:HG21 | 2:C:369:ILE:CG2  | 2.45                     | 0.46              |
| 2:D:30:VAL:HG21  | 2:D:337:TYR:CZ   | 2.51                     | 0.46              |
| 2:D:138:ALA:HB3  | 2:D:163:VAL:HG23 | 1.98                     | 0.46              |
| 2:D:213:LYS:HE2  | 2:D:306:TYR:OH   | 2.16                     | 0.46              |
| 3:E:133:ASP:OD1  | 3:E:138:ILE:HA   | 2.16                     | 0.46              |
| 1:A:89:MET:HE1   | 1:A:103:ASN:HB3  | 1.98                     | 0.46              |
| 1:A:159:THR:O    | 1:A:163:SER:OG   | 2.25                     | 0.46              |
| 1:A:219:GLU:HA   | 1:A:222:LYS:HD2  | 1.97                     | 0.46              |
| 1:A:263:VAL:HG21 | 1:A:456:GLN:H    | 1.79                     | 0.46              |
| 1:A:298:SER:OG   | 1:A:301:MET:HG3  | 2.16                     | 0.46              |
| 1:A:362:LEU:HA   | 1:A:365:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:403:LEU:O    | 1:A:423:ALA:HB2  | 2.15                     | 0.46              |
| 1:A:508:GLU:CG   | 1:A:770:GLY:HA3  | 2.42                     | 0.46              |
| 1:A:592:TYR:HB3  | 1:A:597:TRP:CZ2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:737:LEU:HD22 | 1:A:788:ARG:N    | 2.31                     | 0.46              |
| 1:B:26:GLN:HE21  | 1:B:786:GLU:C    | 2.21                     | 0.46              |
| 1:B:127:TYR:CD1  | 1:B:691:LYS:HA   | 2.50                     | 0.46              |
| 1:B:342:MET:O    | 1:B:445:ARG:HG3  | 2.16                     | 0.46              |
| 1:B:517:PHE:CD2  | 1:B:716:ILE:HG23 | 2.50                     | 0.46              |
| 1:B:527:LEU:HD13 | 1:B:569:PHE:HB2  | 1.98                     | 0.46              |
| 1:B:528:ILE:HD11 | 1:B:583:ILE:HG21 | 1.98                     | 0.46              |
| 1:B:657:ARG:HH21 | 1:B:662:LEU:HA   | 1.79                     | 0.46              |
| 1:B:659:VAL:HA   | 1:B:662:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:666:GLN:HA   | 1:B:669:LYS:HE3  | 1.96                     | 0.46              |
| 1:B:808:ALA:HA   | 1:B:815:ARG:HH22 | 1.79                     | 0.46              |
| 2:C:16:LEU:HD22  | 2:C:30:VAL:HG12  | 1.97                     | 0.46              |
| 2:C:105:LEU:HD12 | 2:C:119:MET:CB   | 2.40                     | 0.46              |
| 2:C:142:LEU:HB2  | 2:C:152:VAL:HG13 | 1.98                     | 0.46              |
| 2:C:286:ASP:H    | 2:C:289:ILE:HB   | 1.81                     | 0.46              |
| 2:C:346:LEU:O    | 2:C:351:THR:OG1  | 2.33                     | 0.46              |
| 2:D:160:THR:HB   | 2:D:178:LEU:HB3  | 1.97                     | 0.46              |
| 2:D:368:SER:O    | 2:D:372:ARG:HG3  | 2.16                     | 0.46              |
| 3:E:21:THR:OG1   | 3:E:23:ASP:OD1   | 2.33                     | 0.46              |
| 3:E:40:GLN:HB3   | 3:E:42:PRO:HD3   | 1.97                     | 0.46              |
| 3:H:108:ILE:HG23 | 3:H:112:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:61:LEU:HD11  | 1:A:70:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:153:ILE:H    | 1:A:153:ILE:HG13 | 1.39                     | 0.46              |
| 1:A:236:ASN:OD1  | 1:A:248:PHE:HE1  | 1.99                     | 0.46              |
| 1:A:302:ARG:O    | 1:A:306:LEU:N    | 2.49                     | 0.46              |
| 1:A:471:ILE:HG13 | 1:A:483:ASN:HD21 | 1.79                     | 0.46              |
| 1:A:531:PRO:O    | 1:A:535:PRO:HG3  | 2.16                     | 0.46              |
| 1:A:720:GLY:O    | 1:A:722:PRO:HD3  | 2.15                     | 0.46              |
| 1:B:33:LYS:HB3   | 1:B:77:LYS:HG3   | 1.97                     | 0.46              |
| 1:B:249:GLY:HA2  | 1:B:466:ILE:HA   | 1.97                     | 0.46              |
| 1:B:358:SER:HB3  | 1:B:390:LEU:HB2  | 1.97                     | 0.46              |
| 1:B:685:ILE:HG12 | 1:B:705:LEU:CD2  | 2.46                     | 0.46              |
| 1:B:804:ARG:HH21 | 3:E:119:MET:HG2  | 1.81                     | 0.46              |
| 1:B:814:LYS:O    | 1:B:817:GLN:HG3  | 2.15                     | 0.46              |
| 2:C:18:LYS:HD2   | 2:C:30:VAL:HG13  | 1.97                     | 0.46              |
| 2:C:189:LEU:HD11 | 2:C:250:ILE:HG23 | 1.97                     | 0.46              |
| 2:C:218:TYR:CD2  | 2:C:220:ALA:HA   | 2.51                     | 0.46              |
| 2:D:305:MET:HG3  | 2:D:336:LYS:N    | 2.31                     | 0.46              |
| 2:D:346:LEU:HD23 | 2:D:349:LEU:HD12 | 1.98                     | 0.46              |
| 2:D:357:ILE:HG23 | 2:D:369:ILE:HG23 | 1.97                     | 0.46              |
| 3:E:55:LYS:HG3   | 3:E:57:ASP:HB3   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:89:VAL:O     | 3:E:93:ARG:HG2   | 2.15                     | 0.46              |
| 1:A:35:VAL:HG22  | 1:A:75:ILE:HG23  | 1.97                     | 0.46              |
| 1:A:116:TYR:CE1  | 1:A:151:PRO:HA   | 2.51                     | 0.46              |
| 1:A:283:ASP:HB3  | 1:A:473:GLU:HG3  | 1.97                     | 0.46              |
| 1:A:409:VAL:HG13 | 2:D:24:ASP:CB    | 2.45                     | 0.46              |
| 1:A:466:ILE:HG12 | 1:A:467:ALA:N    | 2.30                     | 0.46              |
| 1:A:734:TYR:CD1  | 1:A:760:LEU:HD11 | 2.51                     | 0.46              |
| 1:A:783:HIS:O    | 1:A:787:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:51:GLU:HB2   | 1:B:58:THR:HB    | 1.97                     | 0.46              |
| 1:B:102:HIS:CD2  | 1:B:105:ARG:HH21 | 2.34                     | 0.46              |
| 1:B:194:LEU:HD12 | 1:B:254:ILE:HD12 | 1.98                     | 0.46              |
| 1:B:240:VAL:HG21 | 1:B:473:GLU:OE1  | 2.16                     | 0.46              |
| 2:C:123:MET:O    | 2:C:128:ASN:N    | 2.49                     | 0.46              |
| 2:D:27:PRO:HA    | 2:D:340:TRP:CZ2  | 2.51                     | 0.46              |
| 2:D:332:PRO:HD2  | 2:D:335:ARG:HE   | 1.81                     | 0.46              |
| 1:A:11:LYS:CE    | 1:A:16:ASP:HB2   | 2.46                     | 0.46              |
| 1:A:28:ASP:HB2   | 1:A:81:PRO:HD2   | 1.97                     | 0.46              |
| 1:A:50:LYS:N     | 1:A:58:THR:O     | 2.38                     | 0.46              |
| 1:A:124:ILE:HG21 | 1:A:696:LEU:CD1  | 2.46                     | 0.46              |
| 1:A:451:ASP:OD2  | 1:A:455:ARG:NE   | 2.46                     | 0.46              |
| 1:A:524:CYS:SG   | 1:A:568:LYS:HB3  | 2.56                     | 0.46              |
| 1:B:87:GLU:HB3   | 1:B:91:GLU:OE1   | 2.16                     | 0.46              |
| 1:B:351:SER:O    | 1:B:355:VAL:HG23 | 2.16                     | 0.46              |
| 2:C:312:ARG:HH11 | 2:C:315:LYS:NZ   | 2.14                     | 0.46              |
| 2:D:3:ASP:OD2    | 2:D:4:GLU:N      | 2.45                     | 0.46              |
| 2:D:86:TRP:CH2   | 2:D:119:MET:HG2  | 2.48                     | 0.46              |
| 2:D:218:TYR:O    | 2:D:258:PRO:HG2  | 2.15                     | 0.46              |
| 2:D:257:CYS:O    | 2:D:260:THR:N    | 2.48                     | 0.46              |
| 3:H:85:PHE:HA    | 3:H:88:TYR:CD2   | 2.50                     | 0.46              |
| 1:A:116:TYR:HD1  | 1:A:120:PHE:O    | 1.99                     | 0.45              |
| 1:A:190:VAL:CG1  | 1:A:463:ILE:HG12 | 2.44                     | 0.45              |
| 1:A:247:ARG:HB3  | 1:A:482:ILE:HD11 | 1.99                     | 0.45              |
| 1:A:477:PHE:HD1  | 1:A:480:LEU:HD23 | 1.80                     | 0.45              |
| 1:A:493:PHE:O    | 1:A:497:MET:HG3  | 2.16                     | 0.45              |
| 1:A:497:MET:N    | 1:A:681:PHE:HZ   | 2.14                     | 0.45              |
| 1:A:742:ILE:HD12 | 1:A:746:PHE:CD1  | 2.51                     | 0.45              |
| 1:A:819:LEU:HA   | 1:A:822:MET:HG2  | 1.98                     | 0.45              |
| 1:B:89:MET:C     | 1:B:95:LEU:HD21  | 2.40                     | 0.45              |
| 1:B:141:TYR:O    | 1:B:144:LYS:N    | 2.43                     | 0.45              |
| 1:B:161:TYR:OH   | 1:B:260:GLY:O    | 2.21                     | 0.45              |
| 1:B:290:PHE:HA   | 1:B:356:VAL:CG1  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:309:GLY:H    | 1:B:312:ASN:HB2  | 1.80                     | 0.45              |
| 1:B:314:THR:H    | 1:B:364:ASN:HD21 | 1.63                     | 0.45              |
| 1:B:441:TRP:HB3  | 1:B:624:LEU:HD23 | 1.97                     | 0.45              |
| 1:B:496:THR:C    | 1:B:681:PHE:HZ   | 2.24                     | 0.45              |
| 1:B:618:ASP:O    | 1:B:621:VAL:HB   | 2.16                     | 0.45              |
| 2:C:20:GLY:HA3   | 2:C:340:TRP:NE1  | 2.32                     | 0.45              |
| 2:C:22:ALA:HB2   | 2:C:347:ALA:CB   | 2.45                     | 0.45              |
| 2:D:20:GLY:HA2   | 2:D:28:ARG:HB2   | 1.98                     | 0.45              |
| 2:D:73:HIS:C     | 2:D:75:ILE:H     | 2.23                     | 0.45              |
| 2:D:76:ILE:HD11  | 2:D:119:MET:CG   | 2.46                     | 0.45              |
| 2:D:145:SER:HB2  | 2:D:147:ARG:CD   | 2.45                     | 0.45              |
| 2:D:212:ILE:HG12 | 2:D:216:LEU:HD13 | 1.97                     | 0.45              |
| 3:E:113:VAL:HG23 | 3:E:114:THR:HG23 | 1.97                     | 0.45              |
| 1:A:79:ASN:CG    | 1:A:92:LEU:HB3   | 2.40                     | 0.45              |
| 1:A:79:ASN:N     | 1:A:99:SER:HB3   | 2.31                     | 0.45              |
| 1:A:273:GLU:N    | 1:A:287:PHE:HZ   | 2.13                     | 0.45              |
| 1:A:391:MET:HB3  | 1:A:621:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:528:ILE:HD11 | 1:A:583:ILE:HG21 | 1.98                     | 0.45              |
| 1:A:547:PHE:HB2  | 1:A:549:LYS:O    | 2.17                     | 0.45              |
| 1:A:624:LEU:HB3  | 1:A:625:TRP:CE3  | 2.50                     | 0.45              |
| 1:A:727:PHE:CE1  | 1:A:774:ILE:HG13 | 2.52                     | 0.45              |
| 1:A:834:LYS:HG3  | 4:G:144:GLU:CD   | 2.42                     | 0.45              |
| 1:A:840:TRP:HA   | 1:A:840:TRP:CE3  | 2.51                     | 0.45              |
| 1:B:42:HIS:HA    | 1:B:699:HIS:N    | 2.31                     | 0.45              |
| 1:B:56:GLU:HA    | 1:B:69:THR:HG23  | 1.98                     | 0.45              |
| 1:B:358:SER:OG   | 1:B:391:MET:SD   | 2.74                     | 0.45              |
| 1:B:569:PHE:CE1  | 1:B:581:PHE:HB2  | 2.50                     | 0.45              |
| 1:B:572:SER:O    | 1:B:577:ASP:HB3  | 2.16                     | 0.45              |
| 2:C:87:HIS:ND1   | 2:C:127:PHE:HE1  | 2.13                     | 0.45              |
| 2:C:176:MET:SD   | 2:C:277:THR:OG1  | 2.56                     | 0.45              |
| 2:C:189:LEU:HD13 | 2:C:253:GLU:O    | 2.16                     | 0.45              |
| 2:C:236:LEU:O    | 2:C:254:ARG:HD3  | 2.16                     | 0.45              |
| 2:D:111:ASN:HB3  | 2:D:115:ASN:HD22 | 1.80                     | 0.45              |
| 2:D:117:GLU:O    | 2:D:120:THR:HG22 | 2.16                     | 0.45              |
| 2:D:124:PHE:HE2  | 2:D:357:ILE:HG22 | 1.81                     | 0.45              |
| 2:D:151:ILE:HG12 | 2:D:162:ASN:OD1  | 2.16                     | 0.45              |
| 2:D:189:LEU:HG   | 2:D:209:VAL:HG13 | 1.97                     | 0.45              |
| 2:D:192:ILE:HD12 | 2:D:253:GLU:HA   | 1.98                     | 0.45              |
| 4:F:145:ALA:O    | 4:F:149:LYS:NZ   | 2.50                     | 0.45              |
| 4:G:157:GLU:O    | 4:G:161:ILE:HG12 | 2.16                     | 0.45              |
| 3:H:28:TYR:CB    | 3:H:51:LEU:HD13  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:50:LYS:CG    | 1:A:60:GLU:HB2   | 2.46                     | 0.45              |
| 1:A:82:LYS:HB2   | 1:A:82:LYS:HE3   | 1.75                     | 0.45              |
| 1:A:105:ARG:O    | 1:A:109:PHE:HB3  | 2.15                     | 0.45              |
| 1:A:153:ILE:HG12 | 1:A:682:VAL:CG2  | 2.47                     | 0.45              |
| 1:A:293:LEU:CD1  | 1:A:297:ALA:HB2  | 2.46                     | 0.45              |
| 1:A:441:TRP:HZ3  | 1:A:626:LYS:HD3  | 1.82                     | 0.45              |
| 1:A:524:CYS:SG   | 1:A:584:LEU:C    | 2.99                     | 0.45              |
| 1:A:527:LEU:HD21 | 1:A:569:PHE:CA   | 2.47                     | 0.45              |
| 1:B:95:LEU:H     | 1:B:778:THR:HG21 | 1.82                     | 0.45              |
| 1:B:194:LEU:HB2  | 1:B:262:ILE:HD11 | 1.99                     | 0.45              |
| 1:B:272:LEU:HB2  | 1:B:440:ARG:NH2  | 2.32                     | 0.45              |
| 1:B:704:GLN:NE2  | 1:B:707:CYS:SG   | 2.89                     | 0.45              |
| 2:C:44:MET:HB2   | 2:C:47:MET:HG2   | 1.97                     | 0.45              |
| 2:C:98:PRO:O     | 2:C:129:VAL:HA   | 2.16                     | 0.45              |
| 2:C:124:PHE:CE1  | 2:C:129:VAL:HB   | 2.52                     | 0.45              |
| 2:C:237:GLU:HB2  | 2:C:251:GLY:HA2  | 1.98                     | 0.45              |
| 3:E:113:VAL:O    | 3:E:118:LYS:HD2  | 2.16                     | 0.45              |
| 3:H:15:PHE:CZ    | 3:H:69:PHE:HB2   | 2.52                     | 0.45              |
| 3:H:92:LEU:HB3   | 3:H:140:TYR:HB2  | 1.97                     | 0.45              |
| 3:H:112:LEU:HB3  | 3:H:124:VAL:CG1  | 2.47                     | 0.45              |
| 1:A:89:MET:SD    | 1:A:103:ASN:ND2  | 2.77                     | 0.45              |
| 1:A:123:VAL:HG11 | 1:A:186:ASN:HD21 | 1.81                     | 0.45              |
| 1:A:165:LEU:HD13 | 1:A:259:THR:C    | 2.40                     | 0.45              |
| 1:A:179:SER:O    | 1:A:245:SER:HA   | 2.17                     | 0.45              |
| 1:A:257:ASP:N    | 1:A:263:VAL:HG22 | 2.31                     | 0.45              |
| 1:A:351:SER:HA   | 1:A:354:ARG:HB2  | 1.97                     | 0.45              |
| 1:A:488:LYS:CB   | 1:A:667:LEU:HD11 | 2.30                     | 0.45              |
| 1:A:533:ASN:ND2  | 1:A:565:ASN:O    | 2.48                     | 0.45              |
| 1:A:806:TYR:HD1  | 1:A:809:ARG:HH21 | 1.64                     | 0.45              |
| 1:B:33:LYS:HB3   | 1:B:77:LYS:HA    | 1.99                     | 0.45              |
| 1:B:181:ALA:HB1  | 1:B:686:ILE:HG13 | 1.99                     | 0.45              |
| 1:B:274:LYS:HD3  | 1:B:659:VAL:HG13 | 1.98                     | 0.45              |
| 1:B:471:ILE:HD12 | 1:B:703:GLU:HG2  | 1.98                     | 0.45              |
| 1:B:488:LYS:NZ   | 1:B:525:ILE:HG21 | 2.32                     | 0.45              |
| 1:B:530:ARG:HH22 | 1:B:566:HIS:CG   | 2.34                     | 0.45              |
| 2:C:34:ILE:HD11  | 2:C:183:ARG:HH12 | 1.82                     | 0.45              |
| 2:C:317:ILE:O    | 2:C:320:LEU:N    | 2.50                     | 0.45              |
| 2:D:124:PHE:HZ   | 2:D:357:ILE:O    | 2.00                     | 0.45              |
| 3:E:23:ASP:OD1   | 3:E:23:ASP:N     | 2.49                     | 0.45              |
| 3:E:128:VAL:C    | 3:E:132:GLU:HG3  | 2.42                     | 0.45              |
| 1:A:195:ALA:HA   | 1:A:262:ILE:HD12 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:532:THR:HG21 | 2:D:353:GLN:CD   | 2.40                     | 0.45              |
| 1:A:563:GLN:HA   | 1:A:566:HIS:CG   | 2.52                     | 0.45              |
| 1:A:563:GLN:HE22 | 1:A:571:LYS:HD3  | 1.81                     | 0.45              |
| 1:A:838:TRP:HB2  | 4:G:143:ARG:NH1  | 2.31                     | 0.45              |
| 1:B:124:ILE:HG21 | 1:B:696:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:158:ASP:OD2  | 1:B:162:ARG:NE   | 2.49                     | 0.45              |
| 1:B:178:GLU:CD   | 1:B:241:LYS:HB2  | 2.41                     | 0.45              |
| 1:B:362:LEU:HD22 | 1:B:430:LEU:HB3  | 1.98                     | 0.45              |
| 1:B:400:ARG:O    | 1:B:403:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:732:GLN:HA   | 1:B:744:LYS:HD2  | 1.97                     | 0.45              |
| 1:B:781:LEU:O    | 1:B:784:LEU:HB2  | 2.15                     | 0.45              |
| 1:B:808:ALA:HB2  | 3:E:36:ARG:HH11  | 1.81                     | 0.45              |
| 2:C:285:CYS:HB3  | 2:C:289:ILE:CG2  | 2.46                     | 0.45              |
| 2:D:217:CYS:SG   | 2:D:258:PRO:HD3  | 2.57                     | 0.45              |
| 2:D:223:PHE:HE1  | 2:D:256:ARG:HG3  | 1.82                     | 0.45              |
| 2:D:312:ARG:O    | 2:D:316:GLU:HG2  | 2.16                     | 0.45              |
| 1:A:9:ASP:HA     | 1:A:131:PRO:HG2  | 1.98                     | 0.45              |
| 1:A:13:LEU:HD21  | 1:A:151:PRO:O    | 2.17                     | 0.45              |
| 1:A:48:SER:HB2   | 1:A:60:GLU:HB3   | 1.99                     | 0.45              |
| 1:A:133:TYR:HD2  | 1:A:152:HIS:NE2  | 2.12                     | 0.45              |
| 1:A:164:MET:O    | 1:A:168:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:169:GLU:O    | 1:A:171:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:221:GLU:HG2  | 1:A:254:ILE:CD1  | 2.47                     | 0.45              |
| 1:A:276:ARG:O    | 1:A:286:THR:HB   | 2.17                     | 0.45              |
| 1:A:440:ARG:HD3  | 1:A:440:ARG:HA   | 1.70                     | 0.45              |
| 1:A:477:PHE:HZ   | 1:A:660:GLY:HA2  | 1.82                     | 0.45              |
| 1:A:535:PRO:HB2  | 1:A:540:LEU:HG   | 1.97                     | 0.45              |
| 1:B:29:TRP:CG    | 1:B:30:SER:N     | 2.85                     | 0.45              |
| 1:B:45:GLU:HA    | 1:B:63:GLU:CB    | 2.46                     | 0.45              |
| 1:B:93:THR:O     | 1:B:781:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:113:ILE:HG23 | 1:B:124:ILE:O    | 2.17                     | 0.45              |
| 1:B:163:SER:OG   | 1:B:171:GLN:NE2  | 2.49                     | 0.45              |
| 1:B:296:GLY:CA   | 1:B:329:ASP:HA   | 2.47                     | 0.45              |
| 1:B:706:ARG:NH1  | 1:B:712:GLU:OE2  | 2.49                     | 0.45              |
| 1:B:850:LEU:HD13 | 4:F:53:LEU:HD23  | 1.97                     | 0.45              |
| 2:C:19:ALA:O     | 2:C:340:TRP:NE1  | 2.49                     | 0.45              |
| 2:D:83:GLU:HG2   | 2:D:122:ILE:HG23 | 1.98                     | 0.45              |
| 2:D:112:PRO:HD2  | 2:D:115:ASN:HD21 | 1.81                     | 0.45              |
| 2:D:262:PHE:CE2  | 2:D:312:ARG:HG2  | 2.52                     | 0.45              |
| 3:E:55:LYS:HG2   | 3:E:58:GLU:H     | 1.81                     | 0.45              |
| 3:E:93:ARG:NE    | 3:E:93:ARG:HA    | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:57:VAL:CG1   | 1:A:59:VAL:HG13  | 2.46                     | 0.45              |
| 1:A:361:GLN:HA   | 1:A:364:ASN:ND2  | 2.31                     | 0.45              |
| 1:A:546:TRP:CE3  | 2:D:349:LEU:HD23 | 2.52                     | 0.45              |
| 1:A:781:LEU:O    | 1:A:785:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:806:TYR:O    | 1:A:809:ARG:HB3  | 2.17                     | 0.45              |
| 1:B:116:TYR:CD1  | 1:B:151:PRO:HB3  | 2.52                     | 0.45              |
| 1:B:247:ARG:HG3  | 1:B:276:ARG:NH1  | 2.32                     | 0.45              |
| 1:B:282:LYS:HD3  | 1:B:474:ILE:HB   | 1.99                     | 0.45              |
| 1:B:285:ARG:HG2  | 1:B:320:HIS:O    | 2.17                     | 0.45              |
| 1:B:342:MET:HG3  | 1:B:446:VAL:HA   | 1.99                     | 0.45              |
| 1:B:424:ASP:O    | 1:B:428:GLU:HG3  | 2.17                     | 0.45              |
| 1:B:429:ALA:HA   | 1:B:432:LYS:HE3  | 1.98                     | 0.45              |
| 1:B:440:ARG:HD3  | 1:B:440:ARG:HA   | 1.72                     | 0.45              |
| 1:B:498:PHE:CG   | 1:B:516:ASP:HA   | 2.52                     | 0.45              |
| 1:B:511:GLU:HB2  | 1:B:512:TRP:CE2  | 2.52                     | 0.45              |
| 1:B:538:LEU:O    | 1:B:541:LEU:HB3  | 2.17                     | 0.45              |
| 1:B:731:ARG:HG3  | 1:B:753:CYS:SG   | 2.57                     | 0.45              |
| 1:B:742:ILE:HG22 | 1:B:756:MET:HE3  | 1.99                     | 0.45              |
| 1:B:757:ILE:HD13 | 1:B:767:TYR:CG   | 2.51                     | 0.45              |
| 1:B:757:ILE:HD12 | 1:B:769:ILE:HD11 | 1.99                     | 0.45              |
| 2:C:20:GLY:HA3   | 2:C:340:TRP:CE2  | 2.50                     | 0.45              |
| 2:C:61:LYS:O     | 2:C:64:ILE:N     | 2.42                     | 0.45              |
| 2:C:180:LEU:HD21 | 2:C:264:PRO:HG3  | 1.98                     | 0.45              |
| 2:C:314:GLN:OE1  | 2:C:318:THR:HG23 | 2.16                     | 0.45              |
| 2:C:368:SER:HB2  | 2:C:372:ARG:CZ   | 2.47                     | 0.45              |
| 2:D:43:VAL:HA    | 2:D:47:MET:SD    | 2.57                     | 0.45              |
| 2:D:59:GLN:OE1   | 2:D:207:GLU:HB3  | 2.16                     | 0.45              |
| 2:D:190:MET:N    | 2:D:209:VAL:HG11 | 2.31                     | 0.45              |
| 2:D:314:GLN:OE1  | 2:D:329:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:120:PHE:HE2  | 1:A:714:ILE:N    | 2.15                     | 0.45              |
| 1:A:237:ALA:HB3  | 1:A:276:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:309:GLY:H    | 1:A:312:ASN:HD22 | 1.65                     | 0.45              |
| 1:A:472:PHE:HE2  | 1:A:479:GLN:NE2  | 2.15                     | 0.45              |
| 1:B:291:TYR:HB3  | 1:B:328:ASP:OD1  | 2.17                     | 0.45              |
| 1:B:510:ILE:HA   | 1:B:768:ARG:CG   | 2.47                     | 0.45              |
| 1:B:686:ILE:HG23 | 1:B:688:ASN:C    | 2.41                     | 0.45              |
| 1:B:840:TRP:CG   | 4:F:92:LYS:HZ3   | 2.35                     | 0.45              |
| 2:C:98:PRO:O     | 2:C:129:VAL:HG22 | 2.16                     | 0.45              |
| 2:C:237:GLU:CG   | 2:C:251:GLY:HA2  | 2.46                     | 0.45              |
| 2:C:279:TYR:HD1  | 2:C:282:ILE:HB   | 1.82                     | 0.45              |
| 2:D:8:LEU:HB2    | 2:D:103:THR:HG22 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:32:PRO:HD2   | 2:D:56:ASP:N     | 2.31                     | 0.45              |
| 2:D:71:ILE:HG12  | 2:D:76:ILE:HG12  | 1.99                     | 0.45              |
| 2:D:113:LYS:HA   | 2:D:371:HIS:HE1  | 1.78                     | 0.45              |
| 2:D:369:ILE:O    | 2:D:373:LYS:N    | 2.50                     | 0.45              |
| 3:E:70:LEU:HA    | 3:E:73:MET:HG3   | 1.98                     | 0.45              |
| 3:E:131:HIS:CB   | 3:E:143:LEU:HA   | 2.45                     | 0.45              |
| 4:F:40:ILE:HG22  | 4:F:52:ASP:HB3   | 1.99                     | 0.45              |
| 3:H:50:VAL:CG2   | 3:H:72:MET:HE2   | 2.46                     | 0.45              |
| 1:A:247:ARG:HH22 | 1:A:470:GLU:CD   | 2.23                     | 0.45              |
| 1:A:384:ALA:HB1  | 1:A:398:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:484:TYR:CE2  | 1:A:664:LYS:HG2  | 2.52                     | 0.45              |
| 1:A:537:VAL:HG13 | 1:A:559:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:543:GLU:HA   | 1:A:546:TRP:CE2  | 2.52                     | 0.45              |
| 1:A:583:ILE:HB   | 1:A:592:TYR:CE2  | 2.52                     | 0.45              |
| 1:A:583:ILE:HB   | 1:A:592:TYR:HD2  | 1.79                     | 0.45              |
| 1:A:614:ASN:HB2  | 1:A:625:TRP:O    | 2.17                     | 0.45              |
| 1:B:3:GLN:H      | 1:B:150:PRO:HG2  | 1.81                     | 0.45              |
| 1:B:224:LEU:HA   | 1:B:450:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:302:ARG:HG2  | 1:B:307:LEU:CD1  | 2.46                     | 0.45              |
| 1:B:496:THR:HB   | 1:B:681:PHE:CZ   | 2.52                     | 0.45              |
| 1:B:524:CYS:HA   | 1:B:568:LYS:HB2  | 1.99                     | 0.45              |
| 1:B:535:PRO:HG2  | 1:B:543:GLU:OE1  | 2.17                     | 0.45              |
| 1:B:836:ARG:HH11 | 4:F:158:PHE:HZ   | 1.65                     | 0.45              |
| 2:C:39:ARG:HG2   | 2:C:66:THR:HG23  | 1.99                     | 0.45              |
| 2:C:115:ASN:O    | 2:C:119:MET:HG3  | 2.17                     | 0.45              |
| 2:C:220:ALA:HB3  | 2:C:259:GLU:CD   | 2.41                     | 0.45              |
| 2:D:73:HIS:HE1   | 2:D:178:LEU:O    | 2.00                     | 0.45              |
| 2:D:185:LEU:HB2  | 2:D:213:LYS:HE3  | 1.99                     | 0.45              |
| 2:D:274:ILE:HG23 | 2:D:275:HIS:H    | 1.81                     | 0.45              |
| 4:F:123:ARG:O    | 4:F:127:THR:HG23 | 2.16                     | 0.45              |
| 1:A:145:LYS:N    | 1:A:162:ARG:HH12 | 2.14                     | 0.45              |
| 1:A:236:ASN:HD22 | 1:A:244:ASN:C    | 2.25                     | 0.45              |
| 1:A:281:ALA:HB3  | 1:A:284:GLU:CD   | 2.42                     | 0.45              |
| 1:A:348:GLU:HG3  | 1:A:620:PHE:CD1  | 2.52                     | 0.45              |
| 1:A:371:ARG:O    | 1:A:371:ARG:NE   | 2.50                     | 0.45              |
| 1:A:402:ILE:HG21 | 1:A:427:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:416:LYS:O    | 1:A:418:GLN:N    | 2.50                     | 0.45              |
| 1:A:549:LYS:NZ   | 2:D:145:SER:HB3  | 2.32                     | 0.45              |
| 1:A:702:LEU:HD11 | 1:A:711:LEU:HD22 | 1.98                     | 0.45              |
| 1:B:90:ALA:HA    | 1:B:95:LEU:HD11  | 1.99                     | 0.45              |
| 1:B:95:LEU:HD12  | 1:B:722:PRO:HB2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:116:TYR:CE1  | 1:B:151:PRO:HA   | 2.51                     | 0.45              |
| 1:B:367:PHE:HE2  | 1:B:399:THR:O    | 2.00                     | 0.45              |
| 1:B:385:GLN:HA   | 1:B:395:VAL:HB   | 1.99                     | 0.45              |
| 1:B:530:ARG:HH22 | 1:B:566:HIS:CD2  | 2.34                     | 0.45              |
| 1:B:620:PHE:HA   | 1:B:623:ASP:OD2  | 2.17                     | 0.45              |
| 1:B:793:THR:HG22 | 1:B:797:ILE:HD11 | 1.99                     | 0.45              |
| 2:C:31:PHE:CZ    | 2:C:88:HIS:HB3   | 2.52                     | 0.45              |
| 2:C:70:PRO:HB2   | 2:C:82:MET:CG    | 2.46                     | 0.45              |
| 2:C:135:ALA:CB   | 2:C:140:LEU:HD11 | 2.47                     | 0.45              |
| 2:C:252:ASN:O    | 2:C:256:ARG:HG3  | 2.17                     | 0.45              |
| 2:D:133:TYR:CZ   | 2:D:355:MET:HB3  | 2.52                     | 0.45              |
| 3:E:50:VAL:HB    | 3:E:75:THR:OG1   | 2.17                     | 0.45              |
| 3:E:109:ARG:CZ   | 3:E:125:GLU:HG2  | 2.47                     | 0.45              |
| 3:H:33:ASP:HA    | 3:H:36:ARG:CD    | 2.36                     | 0.45              |
| 1:A:470:GLU:HB3  | 1:A:472:PHE:HZ   | 1.79                     | 0.44              |
| 1:A:551:THR:HG1  | 1:A:554:SER:H    | 1.55                     | 0.44              |
| 1:B:2:SER:O      | 1:B:13:LEU:HB3   | 2.18                     | 0.44              |
| 1:B:23:PRO:HG3   | 1:B:733:ARG:HA   | 1.99                     | 0.44              |
| 1:B:727:PHE:H    | 1:B:773:LYS:HA   | 1.82                     | 0.44              |
| 1:B:730:PHE:CZ   | 1:B:757:ILE:HG13 | 2.52                     | 0.44              |
| 1:B:743:PRO:O    | 1:B:746:PHE:HB2  | 2.18                     | 0.44              |
| 2:C:38:PRO:HD2   | 2:C:41:GLN:OE1   | 2.17                     | 0.44              |
| 2:C:120:THR:HA   | 2:C:132:MET:HE1  | 1.98                     | 0.44              |
| 2:C:193:LEU:O    | 2:C:198:TYR:N    | 2.46                     | 0.44              |
| 2:C:205:GLU:HA   | 2:C:208:ILE:HD12 | 2.00                     | 0.44              |
| 2:C:224:GLU:HA   | 2:C:227:MET:HB3  | 1.98                     | 0.44              |
| 2:C:282:ILE:HG23 | 2:C:293:LEU:HD12 | 1.99                     | 0.44              |
| 2:D:198:TYR:CD1  | 2:D:248:ILE:HA   | 2.51                     | 0.44              |
| 3:H:36:ARG:HH12  | 3:H:119:MET:HE2  | 1.81                     | 0.44              |
| 1:A:61:LEU:HD23  | 1:A:61:LEU:HA    | 1.82                     | 0.44              |
| 1:A:291:TYR:CD2  | 1:A:316:LEU:HD22 | 2.52                     | 0.44              |
| 1:A:293:LEU:CD1  | 1:A:353:LEU:HB3  | 2.47                     | 0.44              |
| 1:A:480:LEU:HD13 | 1:A:597:TRP:CH2  | 2.53                     | 0.44              |
| 1:A:540:LEU:HD11 | 1:A:566:HIS:CE1  | 2.52                     | 0.44              |
| 1:A:603:ASP:HB3  | 1:A:658:THR:HA   | 2.00                     | 0.44              |
| 1:B:26:GLN:CD    | 1:B:790:LEU:HB2  | 2.42                     | 0.44              |
| 1:B:79:ASN:ND2   | 1:B:94:CYS:HB2   | 2.25                     | 0.44              |
| 1:B:129:GLN:HE22 | 1:B:188:LYS:HD3  | 1.82                     | 0.44              |
| 1:B:156:ILE:HG22 | 1:B:173:ILE:HD13 | 1.99                     | 0.44              |
| 1:B:176:THR:HG22 | 1:B:683:ARG:HH11 | 1.83                     | 0.44              |
| 1:B:275:SER:OG   | 1:B:478:GLU:HB3  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:280:GLN:HE21 | 1:B:286:THR:HG22 | 1.81                     | 0.44              |
| 1:B:314:THR:OG1  | 1:B:364:ASN:ND2  | 2.50                     | 0.44              |
| 1:B:331:MET:HE3  | 1:B:331:MET:HB2  | 1.61                     | 0.44              |
| 1:B:505:TYR:O    | 1:B:510:ILE:HB   | 2.17                     | 0.44              |
| 1:B:538:LEU:HD23 | 1:B:664:LYS:HG3  | 1.99                     | 0.44              |
| 1:B:621:VAL:HG13 | 1:B:625:TRP:HZ3  | 1.77                     | 0.44              |
| 1:B:675:ARG:C    | 1:B:677:THR:H    | 2.26                     | 0.44              |
| 1:B:720:GLY:O    | 1:B:777:ARG:NH1  | 2.50                     | 0.44              |
| 1:B:733:ARG:HB3  | 1:B:788:ARG:CZ   | 2.47                     | 0.44              |
| 1:B:811:ALA:O    | 1:B:814:LYS:HG2  | 2.18                     | 0.44              |
| 2:C:116:ARG:O    | 2:C:370:VAL:HG21 | 2.17                     | 0.44              |
| 2:C:262:PHE:CZ   | 2:C:309:ILE:HD12 | 2.52                     | 0.44              |
| 2:C:356:TRP:CD1  | 2:C:358:THR:HG1  | 2.35                     | 0.44              |
| 2:D:138:ALA:HB1  | 2:D:152:VAL:O    | 2.17                     | 0.44              |
| 2:D:225:ASN:ND2  | 2:D:225:ASN:H    | 2.15                     | 0.44              |
| 3:E:18:PHE:CE2   | 3:E:30:GLN:HA    | 2.52                     | 0.44              |
| 3:E:44:ASN:O     | 3:E:48:MET:HG2   | 2.16                     | 0.44              |
| 3:E:71:PRO:O     | 3:E:75:THR:HG23  | 2.17                     | 0.44              |
| 3:H:61:LEU:HD12  | 3:H:62:LYS:N     | 2.33                     | 0.44              |
| 3:H:102:THR:HG22 | 3:H:139:ASN:HA   | 1.98                     | 0.44              |
| 1:A:121:CYS:HB3  | 1:A:682:VAL:HA   | 1.99                     | 0.44              |
| 1:A:135:GLU:O    | 1:A:138:ILE:HB   | 2.16                     | 0.44              |
| 1:A:160:ALA:O    | 1:A:161:TYR:C    | 2.60                     | 0.44              |
| 1:A:238:LYS:HE3  | 1:A:238:LYS:HB3  | 1.87                     | 0.44              |
| 1:A:294:ILE:CD1  | 1:A:313:TYR:HD2  | 2.27                     | 0.44              |
| 1:A:305:LEU:HD22 | 1:A:353:LEU:C    | 2.43                     | 0.44              |
| 1:A:469:PHE:HB2  | 1:A:707:CYS:CA   | 2.48                     | 0.44              |
| 1:A:733:ARG:HB3  | 1:A:788:ARG:HD3  | 1.99                     | 0.44              |
| 1:B:554:SER:O    | 1:B:558:LYS:HG2  | 2.17                     | 0.44              |
| 1:B:803:CYS:CB   | 3:E:119:MET:HE1  | 2.46                     | 0.44              |
| 1:B:833:LEU:O    | 1:B:837:ASN:ND2  | 2.51                     | 0.44              |
| 2:C:21:PHE:O     | 2:C:344:SER:HB3  | 2.17                     | 0.44              |
| 2:C:86:TRP:NE1   | 2:C:105:LEU:HD22 | 2.33                     | 0.44              |
| 2:C:182:GLY:HA2  | 2:C:185:LEU:HD22 | 1.98                     | 0.44              |
| 2:D:4:GLU:O      | 2:D:6:THR:N      | 2.51                     | 0.44              |
| 2:D:104:LEU:HD22 | 2:D:343:GLY:HA2  | 1.98                     | 0.44              |
| 2:D:222:ASP:HB2  | 2:D:225:ASN:HD22 | 1.82                     | 0.44              |
| 2:D:279:TYR:CE1  | 2:D:321:ALA:HA   | 2.52                     | 0.44              |
| 3:E:51:LEU:HD21  | 3:E:72:MET:SD    | 2.58                     | 0.44              |
| 1:A:156:ILE:HG12 | 1:A:681:PHE:O    | 2.18                     | 0.44              |
| 1:A:355:VAL:HA   | 1:A:391:MET:HE1  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:367:PHE:O    | 1:A:369:LYS:HE3  | 2.16                     | 0.44              |
| 1:A:576:LYS:HB3  | 1:A:576:LYS:HE2  | 1.65                     | 0.44              |
| 1:A:766:LEU:HD12 | 1:A:780:VAL:HG23 | 1.99                     | 0.44              |
| 1:B:130:LEU:O    | 1:B:132:ILE:N    | 2.50                     | 0.44              |
| 1:B:133:TYR:HB3  | 1:B:189:LYS:NZ   | 2.33                     | 0.44              |
| 1:B:163:SER:OG   | 1:B:169:GLU:HB3  | 2.17                     | 0.44              |
| 1:B:290:PHE:HA   | 1:B:356:VAL:HG12 | 1.99                     | 0.44              |
| 1:B:397:ASP:O    | 1:B:401:SER:OG   | 2.30                     | 0.44              |
| 1:B:400:ARG:NH1  | 1:B:400:ARG:HB3  | 2.33                     | 0.44              |
| 1:B:796:ILE:HD13 | 3:E:111:VAL:HG21 | 2.00                     | 0.44              |
| 1:B:812:PHE:O    | 1:B:816:GLN:HG2  | 2.17                     | 0.44              |
| 1:B:850:LEU:HD23 | 4:F:39:MET:HE1   | 1.99                     | 0.44              |
| 1:B:851:LEU:HB2  | 4:F:164:HIS:CD2  | 2.52                     | 0.44              |
| 2:C:156:GLY:O    | 2:C:181:ALA:HB1  | 2.18                     | 0.44              |
| 2:C:208:ILE:HD11 | 2:C:242:LEU:HD22 | 1.98                     | 0.44              |
| 2:C:253:GLU:HA   | 2:C:256:ARG:HB2  | 1.98                     | 0.44              |
| 2:D:227:MET:HG3  | 2:D:252:ASN:HB3  | 1.98                     | 0.44              |
| 3:E:31:CYS:O     | 3:E:34:VAL:HB    | 2.18                     | 0.44              |
| 3:H:27:LEU:HB2   | 3:H:30:GLN:HB2   | 1.99                     | 0.44              |
| 3:H:55:LYS:O     | 3:H:59:MET:HG3   | 2.17                     | 0.44              |
| 3:H:88:TYR:HE2   | 3:H:148:LEU:HD13 | 1.82                     | 0.44              |
| 1:A:23:PRO:O     | 1:A:789:ASP:HB3  | 2.18                     | 0.44              |
| 1:A:162:ARG:HE   | 1:A:162:ARG:HB2  | 1.53                     | 0.44              |
| 1:A:233:ALA:CA   | 1:A:288:HIS:HB2  | 2.35                     | 0.44              |
| 1:A:265:ALA:O    | 1:A:450:LEU:HG   | 2.17                     | 0.44              |
| 1:A:365:ILE:HD13 | 1:A:398:PHE:CE2  | 2.52                     | 0.44              |
| 1:A:475:ASN:HD22 | 1:A:592:TYR:HE1  | 1.65                     | 0.44              |
| 1:A:527:LEU:HA   | 1:A:530:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:584:LEU:HD23 | 1:A:589:LYS:HB2  | 2.00                     | 0.44              |
| 1:B:15:VAL:HG12  | 1:B:17:LYS:HG2   | 1.99                     | 0.44              |
| 1:B:165:LEU:HB2  | 1:B:260:GLY:CA   | 2.45                     | 0.44              |
| 1:B:502:GLN:HE22 | 1:B:513:ASN:CB   | 2.30                     | 0.44              |
| 1:B:583:ILE:O    | 1:B:585:HIS:N    | 2.49                     | 0.44              |
| 1:B:614:ASN:CG   | 1:B:626:LYS:HA   | 2.42                     | 0.44              |
| 1:B:806:TYR:CD2  | 3:E:147:VAL:HG22 | 2.52                     | 0.44              |
| 1:B:840:TRP:CD1  | 4:F:92:LYS:HZ3   | 2.35                     | 0.44              |
| 2:C:1:ASP:N      | 2:C:6:THR:HB     | 2.33                     | 0.44              |
| 2:C:8:LEU:HD11   | 2:C:96:VAL:HG23  | 1.98                     | 0.44              |
| 2:C:32:PRO:HB3   | 2:C:34:ILE:HD12  | 1.99                     | 0.44              |
| 2:C:78:ASN:CG    | 2:C:81:ASP:HB2   | 2.42                     | 0.44              |
| 2:C:192:ILE:HG12 | 2:C:192:ILE:H    | 1.56                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:1:ASP:H3     | 2:D:353:GLN:HG2  | 1.82                     | 0.44              |
| 2:D:122:ILE:HG22 | 2:D:127:PHE:CD2  | 2.53                     | 0.44              |
| 2:D:239:SER:HA   | 2:D:248:ILE:O    | 2.18                     | 0.44              |
| 4:G:101:VAL:HA   | 4:G:104:ASN:HD22 | 1.82                     | 0.44              |
| 3:H:25:LYS:HB3   | 3:H:63:THR:HG23  | 1.98                     | 0.44              |
| 1:A:95:LEU:HG    | 1:A:718:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:194:LEU:HD12 | 1:A:254:ILE:CD1  | 2.43                     | 0.44              |
| 1:A:239:THR:HG21 | 1:A:472:PHE:CZ   | 2.53                     | 0.44              |
| 1:A:267:ILE:H    | 1:A:450:LEU:CD2  | 2.27                     | 0.44              |
| 1:A:336:LEU:HB3  | 1:A:349:GLN:OE1  | 2.18                     | 0.44              |
| 1:A:344:PHE:CE2  | 1:A:445:ARG:HB3  | 2.53                     | 0.44              |
| 1:A:530:ARG:HH12 | 1:A:566:HIS:HA   | 1.82                     | 0.44              |
| 1:A:800:GLN:HE22 | 3:H:115:LEU:HB3  | 1.83                     | 0.44              |
| 1:B:29:TRP:CZ3   | 1:B:786:GLU:HG2  | 2.52                     | 0.44              |
| 1:B:80:PRO:HA    | 1:B:81:PRO:HD3   | 1.92                     | 0.44              |
| 1:B:122:VAL:CG2  | 1:B:710:VAL:HG11 | 2.48                     | 0.44              |
| 1:B:241:LYS:HB3  | 1:B:689:HIS:HB2  | 2.00                     | 0.44              |
| 1:B:577:ASP:HA   | 1:B:580:GLU:O    | 2.18                     | 0.44              |
| 1:B:807:LEU:HD12 | 3:E:123:GLU:HA   | 1.99                     | 0.44              |
| 2:C:275:HIS:HA   | 2:C:313:MET:HE1  | 1.98                     | 0.44              |
| 2:D:47:MET:HE2   | 2:D:49:GLN:N     | 2.29                     | 0.44              |
| 2:D:53:TYR:HB3   | 2:D:57:GLU:HB3   | 2.00                     | 0.44              |
| 2:D:142:LEU:HD12 | 2:D:152:VAL:HG21 | 1.99                     | 0.44              |
| 2:D:156:GLY:O    | 2:D:303:THR:HG23 | 2.18                     | 0.44              |
| 2:D:213:LYS:C    | 2:D:213:LYS:HD3  | 2.41                     | 0.44              |
| 3:E:27:LEU:HD22  | 3:E:30:GLN:OE1   | 2.18                     | 0.44              |
| 4:G:27:GLN:H     | 4:G:27:GLN:CD    | 2.26                     | 0.44              |
| 3:H:15:PHE:CE2   | 3:H:26:ILE:HB    | 2.52                     | 0.44              |
| 1:A:61:LEU:O     | 1:A:65:GLY:CA    | 2.63                     | 0.44              |
| 1:A:126:PRO:C    | 1:A:128:LYS:H    | 2.25                     | 0.44              |
| 1:A:173:ILE:CD1  | 1:A:680:ASN:HB2  | 2.47                     | 0.44              |
| 1:A:391:MET:HA   | 1:A:621:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:485:THR:HA   | 1:A:667:LEU:CD1  | 2.46                     | 0.44              |
| 1:A:521:LEU:HD21 | 1:A:586:TYR:CD2  | 2.53                     | 0.44              |
| 1:A:674:LEU:O    | 1:A:679:PRO:HG3  | 2.17                     | 0.44              |
| 1:B:12:PHE:CE2   | 1:B:130:LEU:HB3  | 2.53                     | 0.44              |
| 1:B:234:PHE:HB2  | 1:B:439:PHE:HD1  | 1.82                     | 0.44              |
| 1:B:280:GLN:NE2  | 1:B:315:PHE:HB3  | 2.33                     | 0.44              |
| 1:B:313:TYR:CD2  | 1:B:360:LEU:HD13 | 2.53                     | 0.44              |
| 1:B:510:ILE:HD12 | 1:B:775:PHE:HB2  | 1.98                     | 0.44              |
| 2:C:12:ASN:HD21  | 2:C:105:LEU:HB3  | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:116:ARG:HH12 | 2:C:375:PHE:HD2  | 1.66                     | 0.44              |
| 2:C:149:THR:HG23 | 2:D:45:VAL:HG22  | 1.99                     | 0.44              |
| 2:C:198:TYR:CE1  | 2:C:248:ILE:HA   | 2.53                     | 0.44              |
| 2:D:221:LEU:CD2  | 2:D:312:ARG:HB2  | 2.47                     | 0.44              |
| 2:D:230:ALA:HB2  | 2:D:236:LEU:HB2  | 1.99                     | 0.44              |
| 2:D:330:ILE:HD13 | 2:D:330:ILE:HA   | 1.91                     | 0.44              |
| 3:E:11:PHE:HB3   | 3:E:69:PHE:CE2   | 2.52                     | 0.44              |
| 3:E:92:LEU:HD23  | 3:E:95:PHE:CD2   | 2.52                     | 0.44              |
| 3:E:135:ASN:ND2  | 3:E:137:CYS:HB3  | 2.33                     | 0.44              |
| 3:H:92:LEU:HD22  | 3:H:140:TYR:HB2  | 2.00                     | 0.44              |
| 1:A:124:ILE:HG23 | 1:A:701:VAL:HG22 | 1.99                     | 0.44              |
| 1:A:294:ILE:HD11 | 1:A:360:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:344:PHE:CZ   | 1:A:441:TRP:HD1  | 2.36                     | 0.44              |
| 1:A:441:TRP:CD1  | 1:A:620:PHE:HE1  | 2.36                     | 0.44              |
| 1:A:517:PHE:HB2  | 1:A:716:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:527:LEU:HG   | 1:A:537:VAL:HG23 | 1.98                     | 0.44              |
| 1:B:79:ASN:HB3   | 1:B:80:PRO:HD2   | 1.99                     | 0.44              |
| 1:B:494:ASN:HD22 | 1:B:521:LEU:HD11 | 1.81                     | 0.44              |
| 1:B:516:ASP:HB3  | 1:B:519:LEU:HG   | 2.00                     | 0.44              |
| 1:B:568:LYS:O    | 1:B:584:LEU:HG   | 2.18                     | 0.44              |
| 1:B:725:ILE:HG23 | 1:B:729:GLU:HG2  | 2.00                     | 0.44              |
| 2:C:145:SER:O    | 2:C:147:ARG:NE   | 2.50                     | 0.44              |
| 2:C:153:LEU:HD11 | 2:C:274:ILE:HD11 | 1.98                     | 0.44              |
| 2:C:237:GLU:HG3  | 2:C:250:ILE:C    | 2.43                     | 0.44              |
| 2:C:259:GLU:HG3  | 2:C:263:GLN:HE21 | 1.82                     | 0.44              |
| 2:D:15:GLY:C     | 2:D:33:SER:H     | 2.24                     | 0.44              |
| 2:D:124:PHE:CZ   | 2:D:132:MET:HB3  | 2.52                     | 0.44              |
| 2:D:236:LEU:O    | 2:D:254:ARG:HD3  | 2.17                     | 0.44              |
| 3:E:96:ASP:HB2   | 3:E:103:VAL:HG12 | 1.99                     | 0.44              |
| 3:H:50:VAL:HG23  | 3:H:51:LEU:HG    | 1.99                     | 0.44              |
| 1:A:77:LYS:H     | 1:A:96:ASN:ND2   | 2.15                     | 0.44              |
| 1:A:113:ILE:HD12 | 1:A:126:PRO:HB3  | 2.00                     | 0.44              |
| 1:A:243:ASP:HB2  | 1:A:324:PRO:O    | 2.17                     | 0.44              |
| 1:A:365:ILE:HG12 | 1:A:384:ALA:N    | 2.33                     | 0.44              |
| 1:A:452:LYS:HB3  | 1:A:454:LYS:O    | 2.17                     | 0.44              |
| 1:A:484:TYR:CZ   | 1:A:667:LEU:HD23 | 2.53                     | 0.44              |
| 1:A:804:ARG:HD3  | 1:A:804:ARG:HA   | 1.73                     | 0.44              |
| 1:A:806:TYR:HE1  | 3:H:148:LEU:HA   | 1.82                     | 0.44              |
| 1:A:811:ALA:HB2  | 3:H:126:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:838:TRP:CE3  | 1:A:840:TRP:HB2  | 2.52                     | 0.44              |
| 1:B:101:LEU:HD22 | 1:B:698:ALA:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:127:TYR:CD2  | 1:B:691:LYS:HA   | 2.53                     | 0.44              |
| 1:B:402:ILE:CG1  | 1:B:609:VAL:HG21 | 2.41                     | 0.44              |
| 1:B:583:ILE:HG22 | 1:B:585:HIS:CD2  | 2.53                     | 0.44              |
| 1:B:584:LEU:HD23 | 1:B:589:LYS:CG   | 2.47                     | 0.44              |
| 1:B:686:ILE:HB   | 1:B:704:GLN:HG2  | 2.00                     | 0.44              |
| 1:B:797:ILE:HA   | 1:B:800:GLN:CD   | 2.42                     | 0.44              |
| 1:B:804:ARG:HG2  | 3:E:123:GLU:OE2  | 2.18                     | 0.44              |
| 1:B:847:VAL:HG11 | 4:F:72:MET:HE2   | 2.00                     | 0.44              |
| 2:C:40:HIS:HB2   | 2:C:44:MET:SD    | 2.57                     | 0.44              |
| 2:C:227:MET:HA   | 2:C:252:ASN:HB3  | 2.00                     | 0.44              |
| 2:C:305:MET:HG3  | 2:C:336:LYS:HE2  | 2.00                     | 0.44              |
| 2:D:29:ALA:HB3   | 2:D:93:GLU:HB3   | 2.00                     | 0.44              |
| 2:D:129:VAL:O    | 2:D:359:LYS:HB2  | 2.17                     | 0.44              |
| 2:D:164:PRO:HB2  | 2:D:293:LEU:HD13 | 2.00                     | 0.44              |
| 2:D:218:TYR:HE2  | 2:D:226:GLU:CD   | 2.25                     | 0.44              |
| 1:A:7:SER:OG     | 1:A:10:GLU:HG3   | 2.18                     | 0.43              |
| 1:A:108:TYR:CD1  | 1:A:113:ILE:HD12 | 2.53                     | 0.43              |
| 1:A:173:ILE:H    | 1:A:461:LEU:HD21 | 1.82                     | 0.43              |
| 1:A:291:TYR:HB3  | 1:A:328:ASP:OD2  | 2.18                     | 0.43              |
| 1:A:321:VAL:HB   | 1:A:322:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:349:GLN:HA   | 1:A:352:ILE:HB   | 2.00                     | 0.43              |
| 1:A:406:ARG:O    | 1:A:655:MET:HG3  | 2.18                     | 0.43              |
| 1:A:441:TRP:CE2  | 1:A:620:PHE:HE1  | 2.36                     | 0.43              |
| 1:B:16:ASP:O     | 1:B:85:LYS:HB3   | 2.18                     | 0.43              |
| 1:B:288:HIS:HB3  | 1:B:292:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:306:LEU:CB   | 1:B:390:LEU:HD21 | 2.44                     | 0.43              |
| 1:B:356:VAL:HG22 | 1:B:435:PHE:CE1  | 2.50                     | 0.43              |
| 1:B:493:PHE:HD1  | 1:B:683:ARG:CZ   | 2.31                     | 0.43              |
| 1:B:496:THR:HB   | 1:B:681:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:580:GLU:HG2  | 1:B:581:PHE:H    | 1.83                     | 0.43              |
| 1:B:738:ALA:O    | 1:B:759:ALA:HB3  | 2.18                     | 0.43              |
| 1:B:837:ASN:HB3  | 4:F:137:GLU:HG2  | 2.00                     | 0.43              |
| 2:C:20:GLY:N     | 2:C:340:TRP:HE1  | 2.16                     | 0.43              |
| 2:C:80:ASP:O     | 2:C:84:LYS:HG2   | 2.18                     | 0.43              |
| 2:C:171:LEU:C    | 2:C:173:HIS:H    | 2.26                     | 0.43              |
| 2:D:33:SER:HB3   | 2:D:70:PRO:HG2   | 2.00                     | 0.43              |
| 2:D:105:LEU:HD11 | 2:D:123:MET:CG   | 2.46                     | 0.43              |
| 2:D:123:MET:HE2  | 2:D:127:PHE:HB2  | 2.00                     | 0.43              |
| 2:D:282:ILE:HG21 | 2:D:294:TYR:CD1  | 2.53                     | 0.43              |
| 3:E:14:ALA:HB3   | 3:E:38:LEU:HD11  | 2.00                     | 0.43              |
| 3:H:128:VAL:O    | 3:H:132:GLU:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:SER:HB2  | 1:A:171:GLN:HG3  | 2.00                     | 0.43              |
| 1:A:220:LEU:O    | 1:A:450:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:234:PHE:CB   | 1:A:439:PHE:HD1  | 2.31                     | 0.43              |
| 1:A:362:LEU:CD2  | 1:A:398:PHE:HZ   | 2.28                     | 0.43              |
| 1:A:378:MET:SD   | 1:A:399:THR:HA   | 2.57                     | 0.43              |
| 1:A:496:THR:HB   | 1:A:681:PHE:HE1  | 1.81                     | 0.43              |
| 1:A:539:ALA:HB2  | 1:A:664:LYS:NZ   | 2.33                     | 0.43              |
| 1:B:52:GLU:HG3   | 1:B:57:VAL:HG13  | 2.00                     | 0.43              |
| 1:B:87:GLU:O     | 1:B:116:TYR:N    | 2.50                     | 0.43              |
| 1:B:187:THR:HA   | 1:B:463:ILE:CG2  | 2.47                     | 0.43              |
| 1:B:229:PRO:CB   | 1:B:334:GLU:HB3  | 2.48                     | 0.43              |
| 1:B:231:LEU:HA   | 1:B:439:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:276:ARG:HD2  | 1:B:285:ARG:O    | 2.17                     | 0.43              |
| 1:B:292:TYR:CE2  | 1:B:331:MET:HB3  | 2.53                     | 0.43              |
| 1:B:367:PHE:HE1  | 1:B:427:ILE:HD11 | 1.82                     | 0.43              |
| 1:B:409:VAL:HG12 | 2:C:25:ASP:H     | 1.82                     | 0.43              |
| 1:B:530:ARG:HG2  | 1:B:535:PRO:HA   | 2.00                     | 0.43              |
| 1:B:563:GLN:HA   | 1:B:566:HIS:HD1  | 1.83                     | 0.43              |
| 1:B:623:ASP:O    | 1:B:626:LYS:HE3  | 2.18                     | 0.43              |
| 1:B:733:ARG:HB3  | 1:B:788:ARG:NH2  | 2.33                     | 0.43              |
| 1:B:792:ILE:HG12 | 3:E:94:VAL:HG23  | 2.00                     | 0.43              |
| 1:B:803:CYS:CB   | 3:E:127:LEU:HD22 | 2.47                     | 0.43              |
| 2:C:17:VAL:HG21  | 2:C:85:ILE:HG21  | 1.99                     | 0.43              |
| 2:C:75:ILE:O     | 2:C:77:THR:HG23  | 2.17                     | 0.43              |
| 2:C:122:ILE:HG22 | 2:C:123:MET:HE2  | 2.00                     | 0.43              |
| 2:D:68:LYS:HE2   | 2:D:81:ASP:OD1   | 2.18                     | 0.43              |
| 2:D:123:MET:O    | 2:D:129:VAL:HG23 | 2.18                     | 0.43              |
| 2:D:185:LEU:HG   | 2:D:257:CYS:O    | 2.17                     | 0.43              |
| 2:D:259:GLU:O    | 2:D:263:GLN:N    | 2.50                     | 0.43              |
| 2:D:358:THR:CG2  | 2:D:360:GLN:HG3  | 2.49                     | 0.43              |
| 3:E:25:LYS:HA    | 3:E:64:LEU:O     | 2.18                     | 0.43              |
| 3:E:33:ASP:O     | 3:E:36:ARG:HB2   | 2.18                     | 0.43              |
| 3:E:119:MET:HE2  | 3:E:123:GLU:HG2  | 1.99                     | 0.43              |
| 4:F:96:THR:HG22  | 4:F:97:ASP:OD2   | 2.17                     | 0.43              |
| 4:F:142:TYR:CZ   | 4:F:149:LYS:HG3  | 2.53                     | 0.43              |
| 1:A:13:LEU:HA    | 1:A:13:LEU:HD12  | 1.71                     | 0.43              |
| 1:A:163:SER:HA   | 1:A:167:ASP:CB   | 2.45                     | 0.43              |
| 1:A:288:HIS:HB3  | 1:A:292:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:306:LEU:O    | 1:A:361:GLN:NE2  | 2.52                     | 0.43              |
| 1:A:340:THR:HA   | 1:A:344:PHE:O    | 2.17                     | 0.43              |
| 1:A:394:ASN:HB3  | 1:A:612:LEU:HD11 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:466:ILE:HG21 | 1:A:489:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:487:GLU:HB2  | 1:A:585:HIS:HD2  | 1.83                     | 0.43              |
| 1:A:807:LEU:HD21 | 3:H:127:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:834:LYS:HE3  | 4:G:165:GLY:N    | 2.32                     | 0.43              |
| 1:B:15:VAL:HG13  | 1:B:107:ARG:NH1  | 2.33                     | 0.43              |
| 1:B:85:LYS:N     | 1:B:103:ASN:OD1  | 2.47                     | 0.43              |
| 1:B:183:LYS:HB3  | 1:B:465:ASP:HA   | 2.00                     | 0.43              |
| 1:B:284:GLU:OE2  | 1:B:479:GLN:NE2  | 2.51                     | 0.43              |
| 1:B:291:TYR:HD1  | 1:B:310:PHE:HD1  | 1.63                     | 0.43              |
| 1:B:361:GLN:CD   | 1:B:386:LYS:HB3  | 2.42                     | 0.43              |
| 1:B:512:TRP:HD1  | 1:B:721:PHE:HE2  | 1.66                     | 0.43              |
| 1:B:546:TRP:CZ3  | 2:C:4:GLU:HG2    | 2.53                     | 0.43              |
| 1:B:782:ALA:HA   | 1:B:785:GLU:CG   | 2.48                     | 0.43              |
| 1:B:807:LEU:HD23 | 1:B:807:LEU:HA   | 1.58                     | 0.43              |
| 1:B:836:ARG:HD3  | 4:F:158:PHE:HZ   | 1.81                     | 0.43              |
| 2:C:103:THR:O    | 2:C:132:MET:HG2  | 2.19                     | 0.43              |
| 2:C:139:VAL:HG23 | 2:C:163:VAL:HG21 | 2.01                     | 0.43              |
| 3:E:11:PHE:HB3   | 3:E:69:PHE:HE2   | 1.84                     | 0.43              |
| 3:E:29:SER:HB2   | 3:E:59:MET:SD    | 2.59                     | 0.43              |
| 1:A:339:MET:HB3  | 1:A:344:PHE:HB2  | 2.01                     | 0.43              |
| 1:A:436:GLU:O    | 1:A:440:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:487:GLU:OE2  | 1:A:524:CYS:HB2  | 2.17                     | 0.43              |
| 1:B:104:LEU:HA   | 1:B:115:THR:HG21 | 2.00                     | 0.43              |
| 1:B:224:LEU:CD2  | 1:B:252:ILE:HG12 | 2.47                     | 0.43              |
| 1:B:237:ALA:CB   | 1:B:276:ARG:HG2  | 2.49                     | 0.43              |
| 1:B:301:MET:HE1  | 1:B:336:LEU:HD11 | 1.99                     | 0.43              |
| 1:B:313:TYR:HB3  | 1:B:360:LEU:HD22 | 2.00                     | 0.43              |
| 1:B:540:LEU:HB2  | 1:B:555:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:731:ARG:HD2  | 1:B:746:PHE:N    | 2.32                     | 0.43              |
| 1:B:839:GLN:HE22 | 4:G:97:ASP:CG    | 2.25                     | 0.43              |
| 2:C:350:SER:HA   | 2:C:353:GLN:HE21 | 1.83                     | 0.43              |
| 2:D:113:LYS:HG3  | 2:D:371:HIS:NE2  | 2.33                     | 0.43              |
| 2:D:275:HIS:CD2  | 2:D:316:GLU:HB3  | 2.53                     | 0.43              |
| 4:G:123:ARG:HD3  | 4:G:123:ARG:HA   | 1.74                     | 0.43              |
| 3:H:27:LEU:HD13  | 3:H:30:GLN:NE2   | 2.33                     | 0.43              |
| 3:H:30:GLN:O     | 3:H:34:VAL:HG23  | 2.18                     | 0.43              |
| 3:H:136:GLY:O    | 3:H:138:ILE:N    | 2.52                     | 0.43              |
| 1:A:108:TYR:HE1  | 1:A:126:PRO:HB3  | 1.83                     | 0.43              |
| 1:A:141:TYR:CE2  | 1:A:152:HIS:HB3  | 2.53                     | 0.43              |
| 1:A:164:MET:HG2  | 1:A:169:GLU:O    | 2.18                     | 0.43              |
| 1:A:228:ASN:HA   | 1:A:250:LYS:NZ   | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:473:GLU:HG2  | 1:A:474:ILE:N    | 2.34                     | 0.43              |
| 1:A:484:TYR:HB2  | 1:A:528:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:660:GLY:O    | 1:A:664:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:138:ILE:HG22 | 1:B:139:ASP:OD1  | 2.18                     | 0.43              |
| 1:B:178:GLU:OE1  | 1:B:241:LYS:HB2  | 2.19                     | 0.43              |
| 1:B:306:LEU:HB3  | 1:B:386:LYS:NZ   | 2.34                     | 0.43              |
| 1:B:365:ILE:HG22 | 1:B:367:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:670:LEU:HD12 | 1:B:673:THR:OG1  | 2.19                     | 0.43              |
| 2:C:71:ILE:HG12  | 2:C:76:ILE:HG12  | 2.00                     | 0.43              |
| 2:C:75:ILE:HG12  | 2:C:112:PRO:HD2  | 2.00                     | 0.43              |
| 2:C:345:ILE:HD13 | 2:C:345:ILE:HA   | 1.82                     | 0.43              |
| 2:D:34:ILE:HG12  | 2:D:69:TYR:CD2   | 2.54                     | 0.43              |
| 2:D:71:ILE:HD11  | 2:D:119:MET:HE2  | 2.01                     | 0.43              |
| 2:D:178:LEU:O    | 2:D:180:LEU:N    | 2.51                     | 0.43              |
| 2:D:242:LEU:O    | 2:D:244:ASP:N    | 2.43                     | 0.43              |
| 3:E:14:ALA:HA    | 3:E:17:LEU:HB2   | 1.99                     | 0.43              |
| 4:F:116:PHE:HA   | 4:F:155:TYR:CE1  | 2.54                     | 0.43              |
| 4:F:150:LYS:NZ   | 4:F:152:ASN:HB3  | 2.32                     | 0.43              |
| 1:A:104:LEU:HD13 | 1:A:701:VAL:HG12 | 2.01                     | 0.43              |
| 1:A:132:ILE:HA   | 1:A:137:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:276:ARG:HB3  | 1:A:287:PHE:CE2  | 2.54                     | 0.43              |
| 1:A:316:LEU:HA   | 1:A:316:LEU:HD23 | 1.60                     | 0.43              |
| 1:A:388:CYS:SG   | 1:A:393:ILE:HG13 | 2.58                     | 0.43              |
| 1:A:746:PHE:HB3  | 1:A:752:ALA:HB1  | 2.01                     | 0.43              |
| 1:A:813:ALA:HB3  | 1:A:815:ARG:CG   | 2.42                     | 0.43              |
| 1:B:89:MET:SD    | 1:B:103:ASN:HB2  | 2.58                     | 0.43              |
| 1:B:136:LYS:O    | 1:B:140:MET:HB2  | 2.18                     | 0.43              |
| 1:B:153:ILE:HD12 | 1:B:189:LYS:HG3  | 2.00                     | 0.43              |
| 1:B:168:ARG:NH2  | 1:B:459:SER:HB3  | 2.34                     | 0.43              |
| 1:B:231:LEU:HD22 | 1:B:439:PHE:HZ   | 1.83                     | 0.43              |
| 1:B:246:SER:HB3  | 1:B:248:PHE:O    | 2.18                     | 0.43              |
| 1:B:520:ASP:OD2  | 1:B:715:ARG:NH1  | 2.40                     | 0.43              |
| 1:B:543:GLU:OE2  | 1:B:558:LYS:NZ   | 2.45                     | 0.43              |
| 1:B:543:GLU:OE2  | 2:C:350:SER:OG   | 2.36                     | 0.43              |
| 1:B:620:PHE:CE2  | 1:B:624:LEU:HD11 | 2.54                     | 0.43              |
| 1:B:686:ILE:N    | 1:B:704:GLN:HG3  | 2.34                     | 0.43              |
| 1:B:730:PHE:HE1  | 1:B:776:PHE:CZ   | 2.37                     | 0.43              |
| 1:B:734:TYR:HD2  | 1:B:737:LEU:HD12 | 1.84                     | 0.43              |
| 1:B:832:TYR:HE1  | 4:F:158:PHE:HE2  | 1.66                     | 0.43              |
| 2:C:38:PRO:HB3   | 2:C:65:LEU:HD22  | 2.01                     | 0.43              |
| 2:C:157:ASP:HB2  | 2:C:302:GLY:HA3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:287:ILE:HG23 | 2:C:325:MET:HE1  | 1.99                     | 0.43              |
| 2:D:8:LEU:HD11   | 2:D:96:VAL:HG23  | 2.00                     | 0.43              |
| 2:D:10:CYS:SG    | 2:D:17:VAL:HG13  | 2.58                     | 0.43              |
| 3:E:30:GLN:O     | 3:E:34:VAL:HG23  | 2.18                     | 0.43              |
| 4:F:143:ARG:HG3  | 4:F:144:GLU:HG2  | 2.00                     | 0.43              |
| 3:H:50:VAL:HG21  | 3:H:72:MET:HE2   | 2.01                     | 0.43              |
| 1:A:15:VAL:HG21  | 1:A:87:GLU:HA    | 2.00                     | 0.43              |
| 1:A:254:ILE:HG22 | 1:A:256:PHE:CE1  | 2.51                     | 0.43              |
| 1:A:263:VAL:HG12 | 1:A:454:LYS:NZ   | 2.33                     | 0.43              |
| 1:A:358:SER:OG   | 1:A:387:VAL:HG13 | 2.18                     | 0.43              |
| 1:A:364:ASN:HB2  | 1:A:383:ALA:HB1  | 2.00                     | 0.43              |
| 1:A:528:ILE:HA   | 1:A:537:VAL:HB   | 2.00                     | 0.43              |
| 1:A:611:SER:O    | 1:A:615:GLN:HG3  | 2.18                     | 0.43              |
| 1:A:758:LYS:C    | 1:A:761:GLU:H    | 2.27                     | 0.43              |
| 1:A:790:LEU:O    | 1:A:793:THR:OG1  | 2.30                     | 0.43              |
| 1:A:840:TRP:CH2  | 4:G:92:LYS:HA    | 2.53                     | 0.43              |
| 1:B:45:GLU:HA    | 1:B:63:GLU:CG    | 2.48                     | 0.43              |
| 1:B:103:ASN:O    | 1:B:107:ARG:HB2  | 2.19                     | 0.43              |
| 1:B:105:ARG:HG3  | 1:B:696:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:161:TYR:HE2  | 1:B:165:LEU:HD23 | 1.83                     | 0.43              |
| 1:B:407:ILE:HD12 | 1:B:416:LYS:O    | 2.19                     | 0.43              |
| 1:B:534:PRO:HB3  | 1:B:562:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:801:ALA:HA   | 1:B:804:ARG:NH1  | 2.34                     | 0.43              |
| 1:B:822:MET:HE1  | 3:E:20:ARG:HD2   | 2.01                     | 0.43              |
| 2:C:28:ARG:CZ    | 2:C:94:LEU:HA    | 2.49                     | 0.43              |
| 2:C:153:LEU:HB3  | 2:C:299:MET:HA   | 2.01                     | 0.43              |
| 2:D:47:MET:HE3   | 2:D:47:MET:HB2   | 1.84                     | 0.43              |
| 2:D:118:LYS:O    | 2:D:121:GLN:N    | 2.51                     | 0.43              |
| 2:D:128:ASN:HA   | 2:D:359:LYS:HD2  | 2.00                     | 0.43              |
| 2:D:217:CYS:SG   | 2:D:257:CYS:HB2  | 2.59                     | 0.43              |
| 2:D:362:TYR:N    | 2:D:369:ILE:HG21 | 2.33                     | 0.43              |
| 3:E:109:ARG:HE   | 3:E:128:VAL:HB   | 1.84                     | 0.43              |
| 3:E:131:HIS:HD2  | 3:E:146:MET:CB   | 2.31                     | 0.43              |
| 3:H:131:HIS:CD2  | 3:H:143:LEU:HA   | 2.53                     | 0.43              |
| 1:A:12:PHE:HB3   | 1:A:130:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:79:ASN:HB2   | 1:A:92:LEU:HD22  | 2.01                     | 0.43              |
| 1:A:175:CYS:HB2  | 1:A:464:LEU:O    | 2.19                     | 0.43              |
| 1:A:367:PHE:HB3  | 1:A:376:ALA:O    | 2.18                     | 0.43              |
| 1:A:416:LYS:HE2  | 2:D:333:PRO:HB2  | 2.00                     | 0.43              |
| 1:A:480:LEU:HD22 | 1:A:597:TRP:CZ3  | 2.54                     | 0.43              |
| 1:A:757:ILE:HD11 | 1:A:774:ILE:HD11 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:GLU:HA   | 1:B:236:ASN:CB   | 2.38                     | 0.43              |
| 1:B:416:LYS:HD2  | 2:C:25:ASP:HB3   | 2.00                     | 0.43              |
| 1:B:501:GLU:O    | 1:B:504:GLU:HB2  | 2.18                     | 0.43              |
| 2:C:38:PRO:HD3   | 2:C:53:TYR:CE1   | 2.53                     | 0.43              |
| 2:C:50:LYS:HB3   | 2:C:53:TYR:CE1   | 2.54                     | 0.43              |
| 2:C:211:ASP:O    | 2:C:215:LYS:HG2  | 2.19                     | 0.43              |
| 2:D:86:TRP:CH2   | 2:D:105:LEU:HD13 | 2.53                     | 0.43              |
| 2:D:94:LEU:O     | 2:D:96:VAL:HG22  | 2.19                     | 0.43              |
| 2:D:328:LYS:HG2  | 2:D:329:ILE:N    | 2.32                     | 0.43              |
| 3:E:25:LYS:C     | 3:E:63:THR:HB    | 2.43                     | 0.43              |
| 4:F:150:LYS:HZ3  | 4:F:152:ASN:HB3  | 1.83                     | 0.43              |
| 4:G:92:LYS:O     | 4:G:93:LEU:HD22  | 2.19                     | 0.43              |
| 4:G:153:PHE:CE1  | 4:G:158:PHE:HB2  | 2.54                     | 0.43              |
| 1:A:12:PHE:O     | 1:A:112:LEU:HA   | 2.18                     | 0.43              |
| 1:A:230:ILE:CG2  | 1:A:339:MET:HG3  | 2.49                     | 0.43              |
| 1:A:241:LYS:O    | 1:A:689:HIS:HB2  | 2.18                     | 0.43              |
| 1:A:272:LEU:HD22 | 1:A:439:PHE:CD2  | 2.54                     | 0.43              |
| 1:A:273:GLU:HB2  | 1:A:276:ARG:CB   | 2.48                     | 0.43              |
| 1:A:305:LEU:HA   | 1:A:390:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:480:LEU:HA   | 1:A:592:TYR:HE1  | 1.84                     | 0.43              |
| 1:A:527:LEU:HD21 | 1:A:569:PHE:N    | 2.34                     | 0.43              |
| 1:A:531:PRO:HA   | 1:A:539:ALA:CB   | 2.47                     | 0.43              |
| 1:A:563:GLN:C    | 1:A:566:HIS:H    | 2.27                     | 0.43              |
| 1:A:570:GLN:O    | 1:A:582:CYS:N    | 2.43                     | 0.43              |
| 1:B:70:LEU:HG    | 1:B:71:SER:H     | 1.82                     | 0.43              |
| 1:B:230:ILE:HD11 | 1:B:338:ALA:C    | 2.44                     | 0.43              |
| 1:B:539:ALA:HB2  | 1:B:664:LYS:NZ   | 2.33                     | 0.43              |
| 1:B:612:LEU:HD12 | 1:B:615:GLN:HB2  | 2.00                     | 0.43              |
| 1:B:722:PRO:HG2  | 1:B:778:THR:HG23 | 2.01                     | 0.43              |
| 2:C:7:ALA:HB3    | 2:C:347:ALA:HB1  | 2.00                     | 0.43              |
| 2:C:132:MET:HB3  | 2:C:132:MET:HE3  | 1.79                     | 0.43              |
| 2:C:144:ALA:HB3  | 2:C:338:SER:HB2  | 2.00                     | 0.43              |
| 2:C:359:LYS:HB3  | 2:C:360:GLN:OE1  | 2.18                     | 0.43              |
| 2:D:9:VAL:HB     | 2:D:340:TRP:NE1  | 2.34                     | 0.43              |
| 2:D:10:CYS:HB2   | 2:D:90:PHE:CZ    | 2.54                     | 0.43              |
| 2:D:116:ARG:HB2  | 2:D:371:HIS:NE2  | 2.34                     | 0.43              |
| 2:D:189:LEU:HA   | 2:D:192:ILE:CD1  | 2.44                     | 0.43              |
| 3:E:36:ARG:NE    | 3:E:47:VAL:HG21  | 2.27                     | 0.43              |
| 4:F:160:ARG:O    | 4:F:165:GLY:N    | 2.52                     | 0.43              |
| 3:H:86:GLU:HA    | 3:H:89:VAL:HG22  | 2.00                     | 0.43              |
| 3:H:95:PHE:HA    | 3:H:97:LYS:HE2   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:238:LYS:HB2  | 1:A:285:ARG:HD3  | 2.00                     | 0.43              |
| 1:A:241:LYS:HB2  | 1:A:472:PHE:HE1  | 1.83                     | 0.43              |
| 1:A:272:LEU:HD23 | 1:A:436:GLU:HA   | 2.01                     | 0.43              |
| 1:A:411:ARG:CZ   | 2:D:28:ARG:HH11  | 2.31                     | 0.43              |
| 1:A:566:HIS:CB   | 1:A:569:PHE:HB3  | 2.47                     | 0.43              |
| 1:A:725:ILE:HB   | 1:A:776:PHE:CD2  | 2.54                     | 0.43              |
| 1:B:2:SER:HA     | 1:B:150:PRO:HB2  | 2.01                     | 0.43              |
| 1:B:74:ASP:OD1   | 1:B:74:ASP:N     | 2.52                     | 0.43              |
| 1:B:76:GLN:HE22  | 1:B:97:GLU:HG2   | 1.84                     | 0.43              |
| 1:B:247:ARG:HH12 | 1:B:472:PHE:HE2  | 1.67                     | 0.43              |
| 1:B:351:SER:OG   | 1:B:621:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:425:PHE:C    | 1:B:604:PRO:HD2  | 2.43                     | 0.43              |
| 1:B:658:THR:H    | 1:B:658:THR:HG23 | 1.57                     | 0.43              |
| 1:B:722:PRO:HB2  | 1:B:778:THR:HG23 | 2.00                     | 0.43              |
| 2:C:162:ASN:CG   | 2:C:278:THR:HG23 | 2.44                     | 0.43              |
| 2:C:303:THR:HG23 | 2:C:306:TYR:HD2  | 1.84                     | 0.43              |
| 2:D:286:ASP:O    | 2:D:290:ARG:N    | 2.46                     | 0.43              |
| 3:E:29:SER:HB2   | 3:E:59:MET:HG2   | 2.01                     | 0.43              |
| 4:G:28:SER:O     | 4:G:31:GLN:HG3   | 2.19                     | 0.43              |
| 3:H:12:LYS:HG2   | 3:H:66:PHE:CZ    | 2.54                     | 0.43              |
| 1:A:14:PHE:HA    | 1:A:150:PRO:HG2  | 2.01                     | 0.42              |
| 1:A:160:ALA:CB   | 1:A:171:GLN:HB2  | 2.49                     | 0.42              |
| 1:A:252:ILE:HB   | 1:A:463:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:477:PHE:CZ   | 1:A:660:GLY:HA2  | 2.54                     | 0.42              |
| 1:A:675:ARG:NH2  | 1:A:679:PRO:HD2  | 2.34                     | 0.42              |
| 1:B:87:GLU:CD    | 1:B:150:PRO:HA   | 2.44                     | 0.42              |
| 1:B:227:ALA:O    | 1:B:231:LEU:HG   | 2.19                     | 0.42              |
| 1:B:238:LYS:HE3  | 1:B:320:HIS:CE1  | 2.54                     | 0.42              |
| 1:B:374:ASP:O    | 1:B:419:THR:HA   | 2.19                     | 0.42              |
| 1:B:477:PHE:HB3  | 1:B:600:LYS:NZ   | 2.33                     | 0.42              |
| 1:B:484:TYR:O    | 1:B:487:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:696:LEU:HD11 | 1:B:701:VAL:CG2  | 2.49                     | 0.42              |
| 2:D:50:LYS:HE2   | 2:D:50:LYS:HB3   | 1.85                     | 0.42              |
| 2:D:53:TYR:C     | 2:D:57:GLU:HB2   | 2.44                     | 0.42              |
| 2:D:240:TYR:O    | 2:D:248:ILE:HB   | 2.19                     | 0.42              |
| 3:E:27:LEU:HD13  | 3:E:30:GLN:NE2   | 2.34                     | 0.42              |
| 4:G:32:GLU:HA    | 4:G:35:GLU:HG3   | 2.01                     | 0.42              |
| 1:A:60:GLU:O     | 1:A:62:GLN:N     | 2.52                     | 0.42              |
| 1:A:101:LEU:HD23 | 1:A:104:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:234:PHE:CD1  | 1:A:442:ILE:HG13 | 2.53                     | 0.42              |
| 1:A:237:ALA:HB1  | 1:A:285:ARG:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:ARG:NH2  | 1:A:315:PHE:HE1  | 2.17                     | 0.42              |
| 1:A:292:TYR:HD1  | 1:A:328:ASP:HA   | 1.82                     | 0.42              |
| 1:A:387:VAL:O    | 1:A:391:MET:HG2  | 2.19                     | 0.42              |
| 1:A:464:LEU:HD11 | 1:A:466:ILE:HG22 | 2.01                     | 0.42              |
| 1:A:497:MET:HE2  | 1:A:497:MET:HB2  | 1.94                     | 0.42              |
| 1:A:573:LYS:HD3  | 1:A:575:LEU:H    | 1.84                     | 0.42              |
| 1:A:693:ALA:C    | 1:A:695:LYS:H    | 2.27                     | 0.42              |
| 1:A:752:ALA:HA   | 1:A:755:LEU:HB2  | 2.01                     | 0.42              |
| 1:A:844:PHE:CD1  | 4:F:62:LYS:HB3   | 2.54                     | 0.42              |
| 1:B:58:THR:HA    | 1:B:68:VAL:C     | 2.43                     | 0.42              |
| 1:B:351:SER:CB   | 1:B:620:PHE:HB3  | 2.49                     | 0.42              |
| 1:B:468:GLY:O    | 1:B:470:GLU:HG2  | 2.20                     | 0.42              |
| 1:B:504:GLU:O    | 1:B:507:ARG:HB2  | 2.19                     | 0.42              |
| 1:B:804:ARG:HG2  | 3:E:123:GLU:CD   | 2.43                     | 0.42              |
| 2:C:1:ASP:H3     | 2:C:6:THR:HB     | 1.84                     | 0.42              |
| 2:C:10:CYS:SG    | 2:C:86:TRP:CD1   | 3.10                     | 0.42              |
| 2:C:36:GLY:CA    | 2:C:53:TYR:HB2   | 2.50                     | 0.42              |
| 2:C:125:GLU:OE2  | 2:C:362:TYR:OH   | 2.25                     | 0.42              |
| 2:C:159:VAL:HG22 | 2:C:161:HIS:CE1  | 2.53                     | 0.42              |
| 2:C:217:CYS:SG   | 2:C:258:PRO:HD3  | 2.59                     | 0.42              |
| 4:F:68:TYR:CD1   | 4:G:95:GLY:HA3   | 2.54                     | 0.42              |
| 3:H:15:PHE:CE2   | 3:H:31:CYS:HB2   | 2.47                     | 0.42              |
| 3:H:41:ASN:OD1   | 3:H:82:GLN:HG3   | 2.18                     | 0.42              |
| 3:H:122:GLU:O    | 3:H:126:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:15:VAL:HG22  | 1:A:107:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:66:LYS:HB2   | 1:A:66:LYS:HE3   | 1.69                     | 0.42              |
| 1:A:291:TYR:CE1  | 1:A:310:PHE:HB3  | 2.55                     | 0.42              |
| 1:A:292:TYR:HA   | 1:A:328:ASP:CA   | 2.49                     | 0.42              |
| 1:A:365:ILE:HG21 | 1:A:384:ALA:HB2  | 2.00                     | 0.42              |
| 1:A:391:MET:CA   | 1:A:621:VAL:HG11 | 2.49                     | 0.42              |
| 1:A:434:LYS:HA   | 1:A:625:TRP:NE1  | 2.33                     | 0.42              |
| 1:A:477:PHE:CE2  | 1:A:659:VAL:HG23 | 2.53                     | 0.42              |
| 1:B:104:LEU:CD2  | 1:B:122:VAL:HG11 | 2.50                     | 0.42              |
| 1:B:237:ALA:O    | 1:B:247:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:274:LYS:HG2  | 1:B:663:TYR:OH   | 2.19                     | 0.42              |
| 1:B:556:VAL:HG22 | 1:B:559:LEU:HD12 | 2.01                     | 0.42              |
| 1:B:723:ASN:C    | 1:B:724:ARG:HG3  | 2.44                     | 0.42              |
| 1:B:825:ILE:HA   | 4:F:105:ALA:HB1  | 2.02                     | 0.42              |
| 2:C:8:LEU:HB3    | 2:C:90:PHE:CD1   | 2.54                     | 0.42              |
| 2:C:11:ASP:HA    | 2:C:106:THR:HG23 | 1.99                     | 0.42              |
| 2:C:19:ALA:HB1   | 2:C:94:LEU:HG    | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:79:TRP:CD1   | 2:C:118:LYS:HG2  | 2.55                     | 0.42              |
| 2:C:90:PHE:CE1   | 2:C:103:THR:HB   | 2.55                     | 0.42              |
| 2:D:15:GLY:N     | 2:D:157:ASP:O    | 2.53                     | 0.42              |
| 2:D:247:VAL:O    | 2:D:248:ILE:HD13 | 2.19                     | 0.42              |
| 3:E:91:GLY:HA2   | 3:E:94:VAL:HG22  | 2.00                     | 0.42              |
| 3:E:103:VAL:HG21 | 3:E:108:ILE:HD13 | 2.00                     | 0.42              |
| 3:E:142:GLU:HA   | 3:E:145:ARG:HG2  | 2.01                     | 0.42              |
| 3:H:46:GLU:CD    | 3:H:81:ASP:HB3   | 2.44                     | 0.42              |
| 1:A:188:LYS:CG   | 1:A:189:LYS:HZ2  | 2.33                     | 0.42              |
| 1:A:194:LEU:HB3  | 1:A:256:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:238:LYS:HE2  | 1:A:320:HIS:CD2  | 2.55                     | 0.42              |
| 1:A:252:ILE:HB   | 1:A:463:ILE:HB   | 2.00                     | 0.42              |
| 1:A:398:PHE:HA   | 1:A:609:VAL:HG21 | 2.02                     | 0.42              |
| 1:A:487:GLU:O    | 1:A:521:LEU:HD22 | 2.20                     | 0.42              |
| 1:A:695:LYS:HZ3  | 1:A:697:ASP:HB2  | 1.85                     | 0.42              |
| 1:A:742:ILE:HD12 | 1:A:746:PHE:CE1  | 2.55                     | 0.42              |
| 1:B:95:LEU:HD22  | 1:B:714:ILE:CG2  | 2.49                     | 0.42              |
| 1:B:174:LEU:HB2  | 1:B:683:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:342:MET:SD   | 1:B:446:VAL:HA   | 2.59                     | 0.42              |
| 1:B:411:ARG:H    | 2:C:28:ARG:CG    | 2.17                     | 0.42              |
| 1:B:571:LYS:HD3  | 1:B:577:ASP:OD2  | 2.19                     | 0.42              |
| 1:B:585:HIS:CD2  | 1:B:592:TYR:HE2  | 2.36                     | 0.42              |
| 1:B:683:ARG:CB   | 1:B:685:ILE:HD11 | 2.49                     | 0.42              |
| 2:C:104:LEU:HD12 | 2:C:352:PHE:CE1  | 2.48                     | 0.42              |
| 2:C:108:ALA:O    | 2:C:111:ASN:HB2  | 2.20                     | 0.42              |
| 2:C:134:VAL:HB   | 2:C:370:VAL:HG13 | 2.00                     | 0.42              |
| 2:C:305:MET:SD   | 2:C:336:LYS:HB2  | 2.60                     | 0.42              |
| 2:C:358:THR:OG1  | 2:C:361:GLU:OE1  | 2.35                     | 0.42              |
| 2:D:153:LEU:HG   | 2:D:176:MET:HE1  | 2.00                     | 0.42              |
| 2:D:208:ILE:HG12 | 2:D:240:TYR:OH   | 2.18                     | 0.42              |
| 2:D:369:ILE:HA   | 2:D:372:ARG:HB2  | 2.02                     | 0.42              |
| 4:F:29:GLN:NE2   | 4:F:94:ASN:HD21  | 2.09                     | 0.42              |
| 3:H:35:MET:HG3   | 3:H:76:ILE:HG13  | 2.01                     | 0.42              |
| 1:A:43:GLY:HA2   | 1:A:105:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:103:ASN:C    | 1:A:107:ARG:HG3  | 2.45                     | 0.42              |
| 1:A:113:ILE:HG13 | 1:A:126:PRO:HG3  | 2.02                     | 0.42              |
| 1:A:137:ILE:O    | 1:A:141:TYR:N    | 2.52                     | 0.42              |
| 1:A:145:LYS:HA   | 1:A:162:ARG:NH2  | 2.32                     | 0.42              |
| 1:A:194:LEU:HB3  | 1:A:256:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:288:HIS:CG   | 1:A:323:ILE:HD11 | 2.54                     | 0.42              |
| 1:A:315:PHE:CD2  | 1:A:359:VAL:HG12 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:504:GLU:HA   | 1:A:507:ARG:HD2  | 2.02                     | 0.42              |
| 1:A:541:LEU:HD21 | 1:A:601:ASN:HB3  | 2.02                     | 0.42              |
| 1:A:586:TYR:CZ   | 1:A:712:GLU:HB3  | 2.55                     | 0.42              |
| 1:A:734:TYR:CG   | 1:A:760:LEU:HD11 | 2.55                     | 0.42              |
| 1:A:812:PHE:HE1  | 3:H:36:ARG:HB3   | 1.84                     | 0.42              |
| 1:B:124:ILE:HG21 | 1:B:696:LEU:CD1  | 2.50                     | 0.42              |
| 1:B:164:MET:O    | 1:B:168:ARG:HA   | 2.18                     | 0.42              |
| 1:B:177:GLY:CA   | 1:B:704:GLN:HE22 | 2.33                     | 0.42              |
| 1:B:343:GLY:O    | 1:B:445:ARG:NH1  | 2.50                     | 0.42              |
| 1:B:491:GLN:N    | 1:B:521:LEU:HD22 | 2.33                     | 0.42              |
| 1:B:742:ILE:HG23 | 1:B:746:PHE:CD2  | 2.53                     | 0.42              |
| 2:C:116:ARG:HB3  | 2:C:370:VAL:CB   | 2.49                     | 0.42              |
| 2:C:116:ARG:NH1  | 2:C:375:PHE:HD2  | 2.16                     | 0.42              |
| 2:C:198:TYR:HB3  | 2:C:200:PHE:CE2  | 2.54                     | 0.42              |
| 2:C:227:MET:HG3  | 2:C:252:ASN:ND2  | 2.34                     | 0.42              |
| 2:D:7:ALA:HB3    | 2:D:347:ALA:CB   | 2.48                     | 0.42              |
| 1:A:141:TYR:HH   | 1:A:150:PRO:C    | 2.26                     | 0.42              |
| 1:A:168:ARG:NH2  | 1:A:458:ALA:O    | 2.36                     | 0.42              |
| 1:A:238:LYS:HA   | 1:A:243:ASP:O    | 2.20                     | 0.42              |
| 1:A:278:ILE:HD11 | 1:A:599:THR:O    | 2.20                     | 0.42              |
| 1:A:738:ALA:CB   | 1:A:759:ALA:HB1  | 2.50                     | 0.42              |
| 1:B:153:ILE:HA   | 1:B:682:VAL:HG22 | 2.01                     | 0.42              |
| 1:B:243:ASP:HB2  | 1:B:323:ILE:HG23 | 2.00                     | 0.42              |
| 1:B:244:ASN:HA   | 1:B:323:ILE:HD13 | 2.02                     | 0.42              |
| 1:B:248:PHE:CG   | 1:B:269:THR:HB   | 2.54                     | 0.42              |
| 1:B:253:ARG:HG3  | 1:B:460:PHE:HB2  | 2.00                     | 0.42              |
| 1:B:343:GLY:C    | 1:B:445:ARG:HH11 | 2.27                     | 0.42              |
| 1:B:365:ILE:HD13 | 1:B:384:ALA:HA   | 2.00                     | 0.42              |
| 1:B:498:PHE:O    | 1:B:502:GLN:HG2  | 2.20                     | 0.42              |
| 1:B:715:ARG:NH1  | 1:B:719:GLN:HG3  | 2.35                     | 0.42              |
| 2:C:79:TRP:HB2   | 2:C:122:ILE:CD1  | 2.50                     | 0.42              |
| 2:C:118:LYS:HA   | 2:C:121:GLN:NE2  | 2.34                     | 0.42              |
| 2:D:48:GLY:C     | 2:D:50:LYS:H     | 2.27                     | 0.42              |
| 2:D:90:PHE:CD2   | 2:D:98:PRO:HG3   | 2.55                     | 0.42              |
| 2:D:116:ARG:HB3  | 2:D:370:VAL:CG1  | 2.50                     | 0.42              |
| 2:D:334:GLU:HB3  | 2:D:341:ILE:HD11 | 2.02                     | 0.42              |
| 4:F:76:ALA:HB1   | 4:F:84:MET:HE3   | 2.00                     | 0.42              |
| 3:H:15:PHE:HA    | 3:H:34:VAL:HG21  | 2.00                     | 0.42              |
| 3:H:138:ILE:HG22 | 3:H:143:LEU:HB2  | 2.00                     | 0.42              |
| 1:A:130:LEU:O    | 1:A:133:TYR:N    | 2.45                     | 0.42              |
| 1:A:292:TYR:CB   | 1:A:332:PHE:HB2  | 2.40                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:357:SER:O    | 1:A:360:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:469:PHE:O    | 1:A:707:CYS:HB2  | 2.19                     | 0.42              |
| 1:A:728:GLN:HE21 | 1:A:732:GLN:HG3  | 1.85                     | 0.42              |
| 1:B:306:LEU:HA   | 1:B:306:LEU:HD23 | 1.78                     | 0.42              |
| 1:B:399:THR:HG22 | 1:B:403:LEU:CD1  | 2.50                     | 0.42              |
| 1:B:464:LEU:HB2  | 1:B:674:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:581:PHE:HE2  | 1:B:583:ILE:HG13 | 1.84                     | 0.42              |
| 1:B:748:ASP:CG   | 1:B:751:GLN:HB3  | 2.45                     | 0.42              |
| 2:C:10:CYS:SG    | 2:C:12:ASN:HB3   | 2.59                     | 0.42              |
| 2:C:11:ASP:OD2   | 2:C:339:VAL:HB   | 2.19                     | 0.42              |
| 2:C:237:GLU:HG3  | 2:C:251:GLY:HA2  | 2.02                     | 0.42              |
| 2:D:11:ASP:HB2   | 2:D:340:TRP:HB2  | 2.01                     | 0.42              |
| 2:D:124:PHE:CD1  | 2:D:359:LYS:HA   | 2.55                     | 0.42              |
| 2:D:133:TYR:CG   | 2:D:356:TRP:HA   | 2.54                     | 0.42              |
| 2:D:155:SER:HB3  | 2:D:160:THR:HG23 | 2.02                     | 0.42              |
| 2:D:212:ILE:HD13 | 2:D:250:ILE:HG12 | 2.02                     | 0.42              |
| 2:D:317:ILE:HB   | 2:D:327:ILE:HG21 | 2.01                     | 0.42              |
| 4:F:37:PHE:HD1   | 4:F:48:ILE:HG12  | 1.85                     | 0.42              |
| 4:G:37:PHE:O     | 4:G:40:ILE:HG22  | 2.20                     | 0.42              |
| 3:H:89:VAL:HA    | 3:H:140:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:18:ASN:O     | 1:A:82:LYS:HA    | 2.20                     | 0.42              |
| 1:A:123:VAL:CG2  | 1:A:682:VAL:HG13 | 2.49                     | 0.42              |
| 1:A:226:GLN:O    | 1:A:338:ALA:HB1  | 2.18                     | 0.42              |
| 1:A:355:VAL:CG1  | 1:A:438:LEU:HB2  | 2.46                     | 0.42              |
| 1:A:469:PHE:HB2  | 1:A:707:CYS:HA   | 2.02                     | 0.42              |
| 1:A:743:PRO:HB2  | 3:H:93:ARG:NE    | 2.35                     | 0.42              |
| 1:B:94:CYS:SG    | 1:B:782:ALA:HB3  | 2.60                     | 0.42              |
| 1:B:104:LEU:HD23 | 1:B:115:THR:OG1  | 2.19                     | 0.42              |
| 1:B:158:ASP:OD1  | 1:B:162:ARG:HG3  | 2.19                     | 0.42              |
| 1:B:369:LYS:HG2  | 1:B:420:LYS:HB3  | 2.01                     | 0.42              |
| 1:B:408:LYS:HG3  | 1:B:413:VAL:HG22 | 2.00                     | 0.42              |
| 1:B:470:GLU:HB3  | 1:B:472:PHE:CD2  | 2.55                     | 0.42              |
| 1:B:535:PRO:O    | 1:B:540:LEU:HD21 | 2.19                     | 0.42              |
| 1:B:681:PHE:HD1  | 1:B:683:ARG:HH21 | 1.68                     | 0.42              |
| 1:B:744:LYS:NZ   | 3:E:94:VAL:HA    | 2.35                     | 0.42              |
| 1:B:781:LEU:HD23 | 1:B:784:LEU:HD12 | 2.01                     | 0.42              |
| 1:B:809:ARG:HE   | 3:E:150:GLY:C    | 2.28                     | 0.42              |
| 1:B:818:GLN:HB2  | 3:E:20:ARG:HH12  | 1.84                     | 0.42              |
| 2:C:123:MET:HG3  | 2:C:132:MET:CG   | 2.44                     | 0.42              |
| 2:C:136:ILE:O    | 2:C:140:LEU:HG   | 2.19                     | 0.42              |
| 2:C:142:LEU:HD13 | 2:C:152:VAL:HG22 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:166:TYR:HB3  | 2:C:285:CYS:SG   | 2.59                     | 0.42              |
| 2:C:213:LYS:HG3  | 2:C:217:CYS:SG   | 2.60                     | 0.42              |
| 2:D:12:ASN:H     | 2:D:106:THR:HG1  | 1.67                     | 0.42              |
| 2:D:166:TYR:CG   | 2:D:289:ILE:HG23 | 2.55                     | 0.42              |
| 2:D:317:ILE:CB   | 2:D:327:ILE:HG21 | 2.50                     | 0.42              |
| 3:E:44:ASN:HB2   | 3:E:48:MET:HE2   | 2.00                     | 0.42              |
| 4:F:88:MET:HE3   | 4:F:88:MET:HB3   | 1.83                     | 0.42              |
| 1:A:4:LYS:HB2    | 1:A:10:GLU:HG3   | 2.02                     | 0.42              |
| 1:A:33:LYS:HD3   | 1:A:33:LYS:HA    | 1.79                     | 0.42              |
| 1:A:194:LEU:HD13 | 1:A:256:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:244:ASN:N    | 1:A:326:GLN:HE22 | 2.18                     | 0.42              |
| 1:A:275:SER:HB2  | 1:A:600:LYS:HB3  | 2.02                     | 0.42              |
| 1:A:535:PRO:HG2  | 1:A:543:GLU:HB2  | 2.01                     | 0.42              |
| 1:A:744:LYS:NZ   | 3:H:93:ARG:O     | 2.41                     | 0.42              |
| 1:A:769:ILE:HD13 | 1:A:769:ILE:HA   | 1.93                     | 0.42              |
| 1:B:18:ASN:O     | 1:B:82:LYS:HA    | 2.20                     | 0.42              |
| 1:B:34:LEU:HG    | 1:B:46:ALA:HB1   | 2.02                     | 0.42              |
| 1:B:170:ASP:HA   | 1:B:460:PHE:H    | 1.85                     | 0.42              |
| 1:B:385:GLN:CG   | 1:B:395:VAL:HG21 | 2.49                     | 0.42              |
| 1:B:782:ALA:HA   | 1:B:785:GLU:HG3  | 2.02                     | 0.42              |
| 2:C:137:GLN:HG3  | 2:C:339:VAL:HG11 | 2.02                     | 0.42              |
| 2:C:171:LEU:HD13 | 2:C:173:HIS:CE1  | 2.54                     | 0.42              |
| 2:C:205:GLU:HA   | 2:C:208:ILE:HB   | 2.02                     | 0.42              |
| 2:D:23:GLY:H     | 2:D:344:SER:C    | 2.27                     | 0.42              |
| 2:D:54:VAL:HG11  | 2:D:84:LYS:O     | 2.19                     | 0.42              |
| 2:D:193:LEU:HB3  | 2:D:200:PHE:HE2  | 1.85                     | 0.42              |
| 2:D:216:LEU:HA   | 2:D:238:LYS:NZ   | 2.35                     | 0.42              |
| 2:D:220:ALA:HB3  | 2:D:259:GLU:OE2  | 2.19                     | 0.42              |
| 2:D:222:ASP:OD1  | 2:D:226:GLU:HG3  | 2.20                     | 0.42              |
| 2:D:259:GLU:HB3  | 2:D:266:PHE:CE2  | 2.46                     | 0.42              |
| 3:E:58:GLU:HA    | 3:E:62:LYS:HB3   | 2.01                     | 0.42              |
| 3:E:66:PHE:HE2   | 3:E:69:PHE:HD2   | 1.66                     | 0.42              |
| 1:A:70:LEU:HD21  | 1:A:74:ASP:HB2   | 2.02                     | 0.42              |
| 1:A:132:ILE:C    | 1:A:137:ILE:HG13 | 2.45                     | 0.42              |
| 1:A:227:ALA:HB2  | 1:A:446:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:230:ILE:H    | 1:A:230:ILE:HG13 | 1.66                     | 0.42              |
| 1:A:292:TYR:HB3  | 1:A:332:PHE:CB   | 2.42                     | 0.42              |
| 1:A:294:ILE:HB   | 1:A:310:PHE:CD1  | 2.54                     | 0.42              |
| 1:A:315:PHE:HD2  | 1:A:359:VAL:HG12 | 1.84                     | 0.42              |
| 1:A:485:THR:CA   | 1:A:667:LEU:HD13 | 2.44                     | 0.42              |
| 1:A:494:ASN:ND2  | 1:A:716:ILE:HD11 | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:685:ILE:HG21 | 1:A:701:VAL:HG13 | 2.02                     | 0.42              |
| 1:A:696:LEU:HD23 | 1:A:697:ASP:C    | 2.44                     | 0.42              |
| 1:A:738:ALA:HB1  | 1:A:759:ALA:HB1  | 2.02                     | 0.42              |
| 1:B:68:VAL:HG12  | 1:B:69:THR:O     | 2.19                     | 0.42              |
| 1:B:88:ASP:HB3   | 1:B:91:GLU:HG3   | 2.02                     | 0.42              |
| 1:B:116:TYR:HD1  | 1:B:120:PHE:O    | 2.03                     | 0.42              |
| 1:B:119:LEU:HD13 | 1:B:500:LEU:CB   | 2.49                     | 0.42              |
| 1:B:528:ILE:CD1  | 1:B:583:ILE:HD13 | 2.50                     | 0.42              |
| 1:B:533:ASN:N    | 2:C:353:GLN:HE22 | 2.15                     | 0.42              |
| 1:B:661:GLN:HA   | 1:B:664:LYS:HD2  | 2.02                     | 0.42              |
| 1:B:804:ARG:HD2  | 3:E:43:THR:HA    | 2.00                     | 0.42              |
| 2:C:10:CYS:HB2   | 2:C:90:PHE:HZ    | 1.80                     | 0.42              |
| 2:C:31:PHE:CE2   | 2:C:85:ILE:HG23  | 2.55                     | 0.42              |
| 2:D:107:GLU:CD   | 2:D:116:ARG:HG2  | 2.45                     | 0.42              |
| 2:D:116:ARG:NH1  | 2:D:371:HIS:HA   | 2.32                     | 0.42              |
| 3:E:36:ARG:HG2   | 3:E:42:PRO:CD    | 2.49                     | 0.42              |
| 3:E:97:LYS:HD2   | 3:E:97:LYS:H     | 1.85                     | 0.42              |
| 3:E:128:VAL:O    | 3:E:132:GLU:N    | 2.53                     | 0.42              |
| 1:A:45:GLU:O     | 1:A:46:ALA:C     | 2.63                     | 0.41              |
| 1:A:55:ASP:CG    | 1:A:72:LYS:HG2   | 2.45                     | 0.41              |
| 1:A:108:TYR:HB3  | 1:A:696:LEU:CD1  | 2.48                     | 0.41              |
| 1:A:191:ILE:HG12 | 1:A:221:GLU:HB3  | 2.01                     | 0.41              |
| 1:A:275:SER:HB2  | 1:A:600:LYS:CB   | 2.50                     | 0.41              |
| 1:A:290:PHE:HB3  | 1:A:316:LEU:CD2  | 2.39                     | 0.41              |
| 1:A:293:LEU:HA   | 1:A:293:LEU:HD12 | 1.55                     | 0.41              |
| 1:A:294:ILE:CG1  | 1:A:307:LEU:HD22 | 2.35                     | 0.41              |
| 1:A:505:TYR:HB3  | 1:A:513:ASN:ND2  | 2.34                     | 0.41              |
| 1:A:569:PHE:HE2  | 1:A:581:PHE:CG   | 2.37                     | 0.41              |
| 1:A:656:PHE:HB3  | 1:A:657:ARG:H    | 1.61                     | 0.41              |
| 1:A:732:GLN:HG2  | 1:A:745:GLY:N    | 2.35                     | 0.41              |
| 1:A:736:ILE:HD11 | 1:A:795:VAL:HB   | 2.00                     | 0.41              |
| 1:B:12:PHE:HB2   | 1:B:132:ILE:HD13 | 2.02                     | 0.41              |
| 1:B:35:VAL:HG23  | 1:B:47:ALA:N     | 2.30                     | 0.41              |
| 1:B:170:ASP:O    | 1:B:677:THR:HB   | 2.20                     | 0.41              |
| 1:B:194:LEU:CD1  | 1:B:461:LEU:HD23 | 2.30                     | 0.41              |
| 1:B:475:ASN:HB3  | 1:B:592:TYR:CE1  | 2.54                     | 0.41              |
| 1:B:499:ILE:O    | 1:B:503:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:510:ILE:HG13 | 1:B:775:PHE:CG   | 2.55                     | 0.41              |
| 1:B:566:HIS:CB   | 1:B:569:PHE:HB2  | 2.48                     | 0.41              |
| 1:B:613:LEU:O    | 1:B:616:SER:OG   | 2.28                     | 0.41              |
| 2:C:35:VAL:HA    | 2:C:53:TYR:O     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:69:TYR:HD2   | 2:C:72:GLU:OE1   | 2.02                     | 0.41              |
| 2:C:70:PRO:HG2   | 2:C:85:ILE:HD12  | 2.01                     | 0.41              |
| 2:C:150:GLY:H    | 2:C:165:ILE:HB   | 1.85                     | 0.41              |
| 2:C:282:ILE:O    | 2:C:285:CYS:HB2  | 2.20                     | 0.41              |
| 2:C:317:ILE:HG23 | 2:C:317:ILE:HD12 | 1.70                     | 0.41              |
| 2:D:20:GLY:N     | 2:D:94:LEU:HD11  | 2.35                     | 0.41              |
| 2:D:35:VAL:HG12  | 2:D:68:LYS:HZ3   | 1.84                     | 0.41              |
| 3:E:35:MET:O     | 3:E:40:GLN:HB2   | 2.19                     | 0.41              |
| 1:A:145:LYS:HA   | 1:A:162:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:145:LYS:HD2  | 1:A:162:ARG:NH1  | 2.34                     | 0.41              |
| 1:A:152:HIS:C    | 1:A:154:TYR:N    | 2.78                     | 0.41              |
| 1:A:281:ALA:HB3  | 1:A:284:GLU:HB2  | 2.02                     | 0.41              |
| 1:A:293:LEU:HD12 | 1:A:297:ALA:HB2  | 2.01                     | 0.41              |
| 1:A:542:ASP:OD1  | 1:A:658:THR:OG1  | 2.33                     | 0.41              |
| 1:A:721:PHE:HE1  | 1:A:775:PHE:O    | 2.03                     | 0.41              |
| 1:A:767:TYR:CD1  | 1:A:780:VAL:HG11 | 2.55                     | 0.41              |
| 1:B:230:ILE:H    | 1:B:230:ILE:HG13 | 1.56                     | 0.41              |
| 1:B:248:PHE:CD2  | 1:B:248:PHE:C    | 2.98                     | 0.41              |
| 1:B:256:PHE:HA   | 1:B:261:TYR:O    | 2.20                     | 0.41              |
| 1:B:394:ASN:HB3  | 1:B:397:ASP:HB2  | 2.02                     | 0.41              |
| 1:B:498:PHE:HA   | 1:B:517:PHE:CD2  | 2.53                     | 0.41              |
| 1:B:532:THR:CA   | 1:B:535:PRO:HG3  | 2.41                     | 0.41              |
| 1:B:721:PHE:CD2  | 1:B:775:PHE:HB3  | 2.55                     | 0.41              |
| 1:B:763:ASP:C    | 1:B:767:TYR:CD1  | 2.98                     | 0.41              |
| 1:B:792:ILE:HG12 | 3:E:94:VAL:HG21  | 2.02                     | 0.41              |
| 1:B:799:PHE:CE2  | 3:E:112:LEU:HD21 | 2.55                     | 0.41              |
| 2:C:20:GLY:HA2   | 2:C:28:ARG:HB3   | 2.02                     | 0.41              |
| 2:C:94:LEU:HB3   | 2:C:96:VAL:CG2   | 2.45                     | 0.41              |
| 2:C:160:THR:HG22 | 2:C:176:MET:HE3  | 2.02                     | 0.41              |
| 2:C:188:TYR:HH   | 2:C:256:ARG:HH21 | 1.65                     | 0.41              |
| 2:C:218:TYR:O    | 2:C:258:PRO:HG2  | 2.20                     | 0.41              |
| 2:C:261:LEU:HG   | 2:C:274:ILE:CG2  | 2.50                     | 0.41              |
| 2:D:58:ALA:HB1   | 2:D:67:LEU:HD22  | 2.02                     | 0.41              |
| 2:D:75:ILE:HG23  | 2:D:115:ASN:OD1  | 2.20                     | 0.41              |
| 2:D:178:LEU:HD22 | 2:D:274:ILE:HA   | 2.02                     | 0.41              |
| 4:F:109:PHE:CZ   | 4:F:125:LEU:HD13 | 2.55                     | 0.41              |
| 3:H:80:LYS:HD2   | 3:H:82:GLN:OE1   | 2.20                     | 0.41              |
| 1:A:101:LEU:HA   | 1:A:101:LEU:HD23 | 1.84                     | 0.41              |
| 1:A:161:TYR:HA   | 1:A:256:PHE:CE2  | 2.52                     | 0.41              |
| 1:A:532:THR:OG1  | 2:D:3:ASP:O      | 2.31                     | 0.41              |
| 1:A:552:ASP:O    | 1:A:555:PHE:HB3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:802:GLN:OE1  | 3:H:83:GLY:HA2   | 2.20                     | 0.41              |
| 1:A:841:TRP:O    | 4:G:92:LYS:HE2   | 2.20                     | 0.41              |
| 1:B:52:GLU:OE2   | 1:B:72:LYS:NZ    | 2.36                     | 0.41              |
| 1:B:133:TYR:CB   | 1:B:189:LYS:HD3  | 2.46                     | 0.41              |
| 1:B:156:ILE:HG12 | 1:B:681:PHE:O    | 2.20                     | 0.41              |
| 1:B:231:LEU:HD11 | 1:B:267:ILE:CD1  | 2.49                     | 0.41              |
| 1:B:294:ILE:HB   | 1:B:310:PHE:CD1  | 2.55                     | 0.41              |
| 1:B:391:MET:CB   | 1:B:621:VAL:HG11 | 2.49                     | 0.41              |
| 1:B:571:LYS:HG2  | 1:B:577:ASP:HB2  | 2.02                     | 0.41              |
| 1:B:687:PRO:HB3  | 1:B:696:LEU:HD12 | 2.01                     | 0.41              |
| 1:B:718:ARG:HA   | 1:B:722:PRO:CG   | 2.50                     | 0.41              |
| 1:B:722:PRO:CG   | 1:B:778:THR:H    | 2.22                     | 0.41              |
| 1:B:755:LEU:HD23 | 1:B:755:LEU:HA   | 1.75                     | 0.41              |
| 2:C:38:PRO:HG2   | 2:C:41:GLN:HB3   | 2.02                     | 0.41              |
| 2:C:54:VAL:HG11  | 2:C:88:HIS:HB2   | 2.02                     | 0.41              |
| 2:C:118:LYS:O    | 2:C:122:ILE:HD12 | 2.21                     | 0.41              |
| 2:C:188:TYR:CE2  | 2:C:266:PHE:HD2  | 2.38                     | 0.41              |
| 2:C:261:LEU:HD23 | 2:C:262:PHE:CE1  | 2.56                     | 0.41              |
| 2:C:262:PHE:HB3  | 2:C:275:HIS:CE1  | 2.56                     | 0.41              |
| 2:D:2:GLU:O      | 2:D:3:ASP:C      | 2.64                     | 0.41              |
| 2:D:18:LYS:HB3   | 2:D:27:PRO:CB    | 2.49                     | 0.41              |
| 2:D:37:ARG:CD    | 2:D:51:ASP:HB3   | 2.50                     | 0.41              |
| 2:D:140:LEU:HD22 | 2:D:343:GLY:N    | 2.35                     | 0.41              |
| 2:D:145:SER:OG   | 2:D:333:PRO:HD2  | 2.20                     | 0.41              |
| 2:D:208:ILE:O    | 2:D:212:ILE:HG13 | 2.21                     | 0.41              |
| 3:E:112:LEU:HD13 | 3:E:127:LEU:CD2  | 2.50                     | 0.41              |
| 4:F:53:LEU:CD1   | 4:F:73:MET:HE3   | 2.50                     | 0.41              |
| 3:H:55:LYS:HG3   | 3:H:57:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:15:VAL:HG11  | 1:A:86:VAL:C     | 2.46                     | 0.41              |
| 1:A:15:VAL:HA    | 1:A:112:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:116:TYR:HA   | 1:A:116:TYR:HD1  | 1.77                     | 0.41              |
| 1:A:158:ASP:HA   | 1:A:193:TYR:CZ   | 2.55                     | 0.41              |
| 1:A:161:TYR:HE1  | 1:A:260:GLY:O    | 2.04                     | 0.41              |
| 1:A:232:GLU:HB3  | 1:A:244:ASN:OD1  | 2.20                     | 0.41              |
| 1:A:238:LYS:HE2  | 1:A:320:HIS:CG   | 2.55                     | 0.41              |
| 1:A:292:TYR:HA   | 1:A:328:ASP:HA   | 2.03                     | 0.41              |
| 1:A:294:ILE:HD13 | 1:A:309:GLY:C    | 2.45                     | 0.41              |
| 1:A:352:ILE:HG23 | 1:A:438:LEU:HD11 | 2.01                     | 0.41              |
| 1:B:9:ASP:HA     | 1:B:131:PRO:O    | 2.21                     | 0.41              |
| 1:B:271:LEU:H    | 1:B:666:GLN:CB   | 2.25                     | 0.41              |
| 1:B:393:ILE:CG2  | 1:B:613:LEU:HA   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:402:ILE:HG22 | 1:B:423:ALA:HB1  | 2.01                     | 0.41              |
| 1:B:785:GLU:OE1  | 1:B:788:ARG:NH1  | 2.32                     | 0.41              |
| 2:C:39:ARG:HH22  | 2:C:202:THR:HG21 | 1.85                     | 0.41              |
| 2:C:79:TRP:HB2   | 2:C:122:ILE:HD11 | 2.03                     | 0.41              |
| 2:C:229:THR:HG21 | 2:C:236:LEU:HD12 | 2.02                     | 0.41              |
| 2:D:17:VAL:HG21  | 2:D:85:ILE:HD12  | 2.02                     | 0.41              |
| 2:D:98:PRO:O     | 2:D:129:VAL:HA   | 2.20                     | 0.41              |
| 2:D:317:ILE:HG23 | 2:D:317:ILE:HD12 | 1.66                     | 0.41              |
| 3:E:57:ASP:O     | 3:E:61:LEU:N     | 2.48                     | 0.41              |
| 3:E:93:ARG:HD3   | 3:E:99:GLY:C     | 2.45                     | 0.41              |
| 4:F:123:ARG:O    | 4:F:126:LEU:HG   | 2.21                     | 0.41              |
| 1:A:35:VAL:HG21  | 1:A:47:ALA:HB3   | 2.02                     | 0.41              |
| 1:A:156:ILE:CG2  | 1:A:173:ILE:HG23 | 2.50                     | 0.41              |
| 1:A:173:ILE:HG12 | 1:A:461:LEU:CD2  | 2.47                     | 0.41              |
| 1:A:175:CYS:SG   | 1:A:187:THR:N    | 2.94                     | 0.41              |
| 1:A:310:PHE:CD2  | 1:A:321:VAL:HG22 | 2.56                     | 0.41              |
| 1:A:327:GLN:NE2  | 1:A:329:ASP:HB2  | 2.36                     | 0.41              |
| 1:A:327:GLN:O    | 1:A:331:MET:HB2  | 2.20                     | 0.41              |
| 1:A:844:PHE:N    | 4:G:92:LYS:HE3   | 2.34                     | 0.41              |
| 1:B:16:ASP:N     | 1:B:112:LEU:HD11 | 2.12                     | 0.41              |
| 1:B:82:LYS:HZ2   | 1:B:788:ARG:NH1  | 2.18                     | 0.41              |
| 1:B:310:PHE:HA   | 1:B:316:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:378:MET:HB3  | 1:B:403:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:619:LYS:HE2  | 1:B:619:LYS:HA   | 2.02                     | 0.41              |
| 1:B:693:ALA:C    | 1:B:695:LYS:H    | 2.28                     | 0.41              |
| 1:B:792:ILE:CG2  | 3:E:95:PHE:HB2   | 2.50                     | 0.41              |
| 1:B:831:ALA:O    | 4:F:96:THR:HG21  | 2.21                     | 0.41              |
| 2:C:8:LEU:HD23   | 2:C:21:PHE:HB3   | 2.02                     | 0.41              |
| 2:C:76:ILE:HG23  | 2:C:82:MET:CG    | 2.37                     | 0.41              |
| 2:D:302:GLY:CA   | 2:D:336:LYS:HG3  | 2.51                     | 0.41              |
| 3:E:46:GLU:HB2   | 3:E:49:LYS:HE3   | 2.03                     | 0.41              |
| 3:H:105:GLY:H    | 3:H:136:GLY:C    | 2.26                     | 0.41              |
| 1:A:271:LEU:H    | 1:A:666:GLN:CB   | 2.28                     | 0.41              |
| 1:A:275:SER:N    | 1:A:663:TYR:OH   | 2.32                     | 0.41              |
| 1:A:278:ILE:HB   | 1:A:315:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:324:PRO:C    | 1:A:326:GLN:H    | 2.29                     | 0.41              |
| 1:A:331:MET:O    | 1:A:334:GLU:HG2  | 2.19                     | 0.41              |
| 1:A:530:ARG:O    | 1:A:539:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:540:LEU:HD13 | 1:A:559:LEU:CA   | 2.51                     | 0.41              |
| 1:A:686:ILE:CB   | 1:A:704:GLN:HG3  | 2.41                     | 0.41              |
| 1:A:840:TRP:CZ2  | 4:G:92:LYS:HA    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:9:ASP:O      | 1:B:137:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:45:GLU:H     | 1:B:74:ASP:HB3   | 1.85                     | 0.41              |
| 1:B:157:ALA:CB   | 1:B:190:VAL:HG13 | 2.51                     | 0.41              |
| 1:B:299:GLU:HA   | 1:B:302:ARG:CB   | 2.34                     | 0.41              |
| 1:B:357:SER:O    | 1:B:360:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:362:LEU:HD11 | 1:B:430:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:381:ASN:HB3  | 1:B:399:THR:CG2  | 2.50                     | 0.41              |
| 1:B:390:LEU:C    | 1:B:391:MET:HE2  | 2.45                     | 0.41              |
| 1:B:474:ILE:O    | 1:B:479:GLN:HG2  | 2.20                     | 0.41              |
| 1:B:502:GLN:NE2  | 1:B:513:ASN:HB3  | 2.35                     | 0.41              |
| 1:B:662:LEU:O    | 1:B:665:GLU:HB3  | 2.21                     | 0.41              |
| 1:B:725:ILE:HD13 | 1:B:729:GLU:CD   | 2.45                     | 0.41              |
| 1:B:757:ILE:CD1  | 1:B:774:ILE:HD13 | 2.44                     | 0.41              |
| 1:B:768:ARG:HD2  | 1:B:768:ARG:HA   | 1.76                     | 0.41              |
| 1:B:851:LEU:HB2  | 4:F:164:HIS:NE2  | 2.36                     | 0.41              |
| 2:C:2:GLU:H      | 2:C:6:THR:HG21   | 1.85                     | 0.41              |
| 2:C:90:PHE:HZ    | 2:C:105:LEU:CD2  | 2.34                     | 0.41              |
| 2:C:105:LEU:HD21 | 2:C:123:MET:SD   | 2.61                     | 0.41              |
| 2:C:106:THR:HG21 | 2:C:339:VAL:HG12 | 2.02                     | 0.41              |
| 2:C:180:LEU:HA   | 2:C:184:ASP:OD2  | 2.21                     | 0.41              |
| 2:C:317:ILE:CG2  | 2:C:327:ILE:HG21 | 2.50                     | 0.41              |
| 2:D:16:LEU:CD1   | 2:D:336:LYS:HD3  | 2.50                     | 0.41              |
| 2:D:35:VAL:O     | 2:D:68:LYS:HG2   | 2.20                     | 0.41              |
| 2:D:86:TRP:CD2   | 2:D:123:MET:HE3  | 2.55                     | 0.41              |
| 2:D:107:GLU:OE1  | 2:D:116:ARG:HG2  | 2.19                     | 0.41              |
| 2:D:129:VAL:HG12 | 2:D:131:ALA:H    | 1.85                     | 0.41              |
| 3:E:120:THR:OG1  | 3:E:122:GLU:HG3  | 2.21                     | 0.41              |
| 4:F:57:LEU:HG    | 4:F:63:ASN:HA    | 2.01                     | 0.41              |
| 3:H:15:PHE:HA    | 3:H:34:VAL:HG11  | 2.02                     | 0.41              |
| 3:H:35:MET:HG2   | 3:H:69:PHE:CE1   | 2.56                     | 0.41              |
| 1:A:80:PRO:HD2   | 1:A:93:THR:OG1   | 2.21                     | 0.41              |
| 1:A:276:ARG:HH21 | 1:A:478:GLU:HB3  | 1.86                     | 0.41              |
| 1:A:336:LEU:HD23 | 1:A:339:MET:HE3  | 2.02                     | 0.41              |
| 1:A:362:LEU:HD21 | 1:A:398:PHE:CZ   | 2.49                     | 0.41              |
| 1:A:381:ASN:HB2  | 1:A:384:ALA:HB3  | 2.01                     | 0.41              |
| 1:A:391:MET:O    | 1:A:616:SER:HB3  | 2.21                     | 0.41              |
| 1:A:527:LEU:HA   | 1:A:530:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:563:GLN:HE22 | 1:A:571:LYS:CD   | 2.33                     | 0.41              |
| 1:A:712:GLU:CD   | 1:A:715:ARG:HH21 | 2.24                     | 0.41              |
| 1:A:807:LEU:HB3  | 3:H:123:GLU:HG2  | 2.03                     | 0.41              |
| 1:B:60:GLU:HG2   | 1:B:62:GLN:HG2   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:234:PHE:CE2  | 1:B:442:ILE:HD13 | 2.56                     | 0.41              |
| 1:B:306:LEU:O    | 1:B:313:TYR:OH   | 2.39                     | 0.41              |
| 1:B:362:LEU:HD13 | 1:B:431:ALA:N    | 2.35                     | 0.41              |
| 1:B:365:ILE:HG12 | 1:B:383:ALA:C    | 2.46                     | 0.41              |
| 1:B:368:LYS:HE2  | 1:B:378:MET:HG3  | 2.02                     | 0.41              |
| 1:B:425:PHE:HB3  | 1:B:604:PRO:CD   | 2.50                     | 0.41              |
| 1:B:541:LEU:HB2  | 1:B:555:PHE:CE2  | 2.55                     | 0.41              |
| 1:B:541:LEU:HD12 | 1:B:598:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:586:TYR:CE2  | 1:B:712:GLU:HG3  | 2.56                     | 0.41              |
| 1:B:613:LEU:O    | 1:B:622:ALA:HA   | 2.20                     | 0.41              |
| 1:B:797:ILE:HG12 | 3:E:116:GLY:CA   | 2.50                     | 0.41              |
| 1:B:829:CYS:O    | 1:B:833:LEU:HG   | 2.21                     | 0.41              |
| 2:C:4:GLU:HB2    | 2:C:6:THR:H      | 1.85                     | 0.41              |
| 2:C:53:TYR:C     | 2:C:57:GLU:HB2   | 2.46                     | 0.41              |
| 2:C:182:GLY:O    | 2:C:213:LYS:HE2  | 2.20                     | 0.41              |
| 2:C:217:CYS:HA   | 2:C:254:ARG:O    | 2.21                     | 0.41              |
| 2:C:251:GLY:C    | 2:C:253:GLU:N    | 2.76                     | 0.41              |
| 2:D:37:ARG:N     | 2:D:65:LEU:HD22  | 2.35                     | 0.41              |
| 2:D:80:ASP:O     | 2:D:83:GLU:HB2   | 2.21                     | 0.41              |
| 2:D:153:LEU:HD13 | 2:D:299:MET:SD   | 2.60                     | 0.41              |
| 2:D:275:HIS:CG   | 2:D:316:GLU:HB3  | 2.55                     | 0.41              |
| 2:D:315:LYS:HE3  | 2:D:315:LYS:HB3  | 1.88                     | 0.41              |
| 3:E:92:LEU:HA    | 3:E:95:PHE:HB3   | 2.02                     | 0.41              |
| 3:E:93:ARG:HA    | 3:E:93:ARG:CZ    | 2.49                     | 0.41              |
| 3:E:93:ARG:HD3   | 3:E:99:GLY:HA2   | 2.01                     | 0.41              |
| 3:E:139:ASN:OD1  | 3:E:142:GLU:N    | 2.31                     | 0.41              |
| 4:F:72:MET:HE3   | 4:F:88:MET:SD    | 2.61                     | 0.41              |
| 4:G:116:PHE:CD1  | 4:G:154:ASN:HB3  | 2.55                     | 0.41              |
| 1:A:10:GLU:OE2   | 1:A:137:ILE:HD13 | 2.20                     | 0.41              |
| 1:A:53:LYS:HB2   | 1:A:56:GLU:CB    | 2.49                     | 0.41              |
| 1:A:276:ARG:HA   | 1:A:279:ARG:O    | 2.20                     | 0.41              |
| 1:A:290:PHE:CE2  | 1:A:435:PHE:CG   | 3.08                     | 0.41              |
| 1:A:332:PHE:O    | 1:A:335:THR:HB   | 2.19                     | 0.41              |
| 1:A:435:PHE:HA   | 1:A:438:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:740:ASN:OD1  | 1:A:759:ALA:HB2  | 2.21                     | 0.41              |
| 1:B:325:ALA:O    | 1:B:326:GLN:HG2  | 2.21                     | 0.41              |
| 1:B:394:ASN:HD22 | 1:B:397:ASP:CG   | 2.28                     | 0.41              |
| 1:B:544:GLU:HG3  | 1:B:555:PHE:CA   | 2.50                     | 0.41              |
| 1:B:831:ALA:HA   | 1:B:834:LYS:HD2  | 2.03                     | 0.41              |
| 2:C:47:MET:HB3   | 2:C:64:ILE:HD12  | 2.02                     | 0.41              |
| 2:C:71:ILE:CD1   | 2:C:76:ILE:HG12  | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:90:PHE:CD2   | 2:C:98:PRO:HB3   | 2.56                     | 0.41              |
| 2:C:131:ALA:HB1  | 2:C:356:TRP:CD2  | 2.55                     | 0.41              |
| 2:C:180:LEU:CD2  | 2:C:264:PRO:HG3  | 2.50                     | 0.41              |
| 2:D:71:ILE:HG13  | 2:D:82:MET:SD    | 2.60                     | 0.41              |
| 2:D:108:ALA:CB   | 2:D:159:VAL:HG11 | 2.50                     | 0.41              |
| 2:D:132:MET:SD   | 2:D:357:ILE:HD13 | 2.61                     | 0.41              |
| 2:D:140:LEU:HB3  | 2:D:339:VAL:O    | 2.21                     | 0.41              |
| 2:D:156:GLY:C    | 2:D:158:GLY:N    | 2.76                     | 0.41              |
| 2:D:355:MET:HE3  | 2:D:355:MET:HB2  | 1.86                     | 0.41              |
| 3:E:15:PHE:CE2   | 3:E:26:ILE:HD13  | 2.55                     | 0.41              |
| 3:E:31:CYS:HA    | 3:E:34:VAL:HB    | 2.01                     | 0.41              |
| 4:F:37:PHE:HZ    | 4:F:46:GLY:H     | 1.68                     | 0.41              |
| 3:H:113:VAL:O    | 3:H:118:LYS:NZ   | 2.45                     | 0.41              |
| 1:A:120:PHE:CE2  | 1:A:713:GLY:C    | 2.99                     | 0.41              |
| 1:A:128:LYS:HE2  | 1:A:694:GLY:N    | 2.36                     | 0.41              |
| 1:A:161:TYR:CB   | 1:A:193:TYR:HE2  | 2.33                     | 0.41              |
| 1:A:163:SER:O    | 1:A:168:ARG:N    | 2.53                     | 0.41              |
| 1:A:163:SER:HB2  | 1:A:171:GLN:CG   | 2.50                     | 0.41              |
| 1:A:221:GLU:H    | 1:A:221:GLU:CD   | 2.29                     | 0.41              |
| 1:A:251:PHE:CE2  | 1:A:253:ARG:HB2  | 2.50                     | 0.41              |
| 1:A:279:ARG:HA   | 1:A:279:ARG:HD3  | 1.89                     | 0.41              |
| 1:A:358:SER:HB2  | 1:A:391:MET:HE3  | 2.02                     | 0.41              |
| 1:A:359:VAL:O    | 1:A:362:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:376:ALA:O    | 1:A:403:LEU:HD22 | 2.21                     | 0.41              |
| 1:A:398:PHE:O    | 1:A:402:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:528:ILE:CD1  | 1:A:583:ILE:HD13 | 2.50                     | 0.41              |
| 1:A:537:VAL:HG21 | 1:A:583:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:666:GLN:O    | 1:A:669:LYS:HB2  | 2.20                     | 0.41              |
| 1:A:696:LEU:CD1  | 1:A:701:VAL:HG21 | 2.49                     | 0.41              |
| 1:A:708:ASN:HB2  | 1:A:710:VAL:HG23 | 2.02                     | 0.41              |
| 1:A:728:GLN:HB2  | 1:A:731:ARG:HH21 | 1.84                     | 0.41              |
| 1:A:767:TYR:HD2  | 1:A:774:ILE:CG2  | 2.33                     | 0.41              |
| 1:A:819:LEU:HD11 | 3:H:13:GLU:C     | 2.46                     | 0.41              |
| 1:B:17:LYS:HE2   | 1:B:84:SER:O     | 2.21                     | 0.41              |
| 1:B:44:PHE:O     | 1:B:63:GLU:HG3   | 2.21                     | 0.41              |
| 1:B:45:GLU:O     | 1:B:47:ALA:N     | 2.54                     | 0.41              |
| 1:B:79:ASN:O     | 1:B:80:PRO:C     | 2.62                     | 0.41              |
| 1:B:133:TYR:HA   | 1:B:154:TYR:CE2  | 2.56                     | 0.41              |
| 1:B:173:ILE:HG22 | 1:B:175:CYS:SG   | 2.60                     | 0.41              |
| 1:B:178:GLU:HA   | 1:B:470:GLU:OE2  | 2.20                     | 0.41              |
| 1:B:293:LEU:HD12 | 1:B:293:LEU:HA   | 1.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:305:LEU:O    | 1:B:357:SER:OG   | 2.31                     | 0.41              |
| 1:B:352:ILE:O    | 1:B:355:VAL:HB   | 2.21                     | 0.41              |
| 1:B:446:VAL:HG13 | 1:B:450:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:541:LEU:HD22 | 1:B:597:TRP:HB3  | 2.03                     | 0.41              |
| 1:B:544:GLU:HG3  | 1:B:555:PHE:N    | 2.36                     | 0.41              |
| 1:B:559:LEU:HD13 | 1:B:581:PHE:CD1  | 2.56                     | 0.41              |
| 1:B:724:ARG:HG2  | 1:B:775:PHE:CG   | 2.56                     | 0.41              |
| 1:B:736:ILE:H    | 3:E:94:VAL:HG11  | 1.86                     | 0.41              |
| 1:B:789:ASP:HA   | 1:B:792:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:799:PHE:CD1  | 1:B:799:PHE:C    | 2.98                     | 0.41              |
| 1:B:807:LEU:CD1  | 3:E:123:GLU:HA   | 2.50                     | 0.41              |
| 2:C:20:GLY:O     | 2:C:94:LEU:HD11  | 2.20                     | 0.41              |
| 2:C:72:GLU:O     | 2:C:75:ILE:HB    | 2.21                     | 0.41              |
| 2:C:90:PHE:CZ    | 2:C:103:THR:HB   | 2.56                     | 0.41              |
| 2:C:107:GLU:O    | 2:C:137:GLN:HB2  | 2.21                     | 0.41              |
| 2:C:129:VAL:HG11 | 2:C:132:MET:HB2  | 2.03                     | 0.41              |
| 2:C:138:ALA:HB3  | 2:C:163:VAL:HG23 | 2.02                     | 0.41              |
| 2:C:164:PRO:HD2  | 2:C:175:ILE:HG12 | 2.03                     | 0.41              |
| 2:C:253:GLU:HA   | 2:C:256:ARG:HD3  | 2.02                     | 0.41              |
| 2:C:304:THR:HA   | 2:C:309:ILE:CG1  | 2.46                     | 0.41              |
| 2:D:83:GLU:O     | 2:D:127:PHE:CZ   | 2.68                     | 0.41              |
| 2:D:128:ASN:OD1  | 2:D:359:LYS:NZ   | 2.54                     | 0.41              |
| 2:D:143:TYR:CD2  | 2:D:346:LEU:HD21 | 2.55                     | 0.41              |
| 2:D:153:LEU:HD13 | 2:D:299:MET:CE   | 2.50                     | 0.41              |
| 2:D:188:TYR:O    | 2:D:192:ILE:HG12 | 2.21                     | 0.41              |
| 2:D:188:TYR:CD2  | 2:D:192:ILE:HD13 | 2.55                     | 0.41              |
| 3:E:93:ARG:NH2   | 3:E:102:THR:O    | 2.54                     | 0.41              |
| 3:E:104:MET:O    | 3:E:107:GLU:N    | 2.53                     | 0.41              |
| 4:F:123:ARG:HD2  | 4:F:123:ARG:HA   | 1.88                     | 0.41              |
| 4:F:123:ARG:NH2  | 4:F:132:ARG:HH12 | 2.19                     | 0.41              |
| 3:H:21:THR:OG1   | 3:H:23:ASP:OD1   | 2.39                     | 0.41              |
| 3:H:31:CYS:O     | 3:H:34:VAL:HB    | 2.19                     | 0.41              |
| 1:A:20:VAL:CG1   | 1:A:28:ASP:HB3   | 2.51                     | 0.41              |
| 1:A:86:VAL:HB    | 1:A:91:GLU:OE1   | 2.21                     | 0.41              |
| 1:A:93:THR:HA    | 1:A:782:ALA:HB3  | 2.02                     | 0.41              |
| 1:A:103:ASN:O    | 1:A:104:LEU:C    | 2.64                     | 0.41              |
| 1:A:120:PHE:N    | 1:A:120:PHE:CD1  | 2.87                     | 0.41              |
| 1:A:249:GLY:N    | 1:A:271:LEU:HB2  | 2.19                     | 0.41              |
| 1:A:326:GLN:HG2  | 1:A:331:MET:CE   | 2.49                     | 0.41              |
| 1:A:437:ARG:HH21 | 1:A:628:VAL:C    | 2.29                     | 0.41              |
| 1:A:686:ILE:H    | 1:A:704:GLN:HB2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:725:ILE:HB   | 1:A:776:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:799:PHE:HA   | 1:A:802:GLN:HG2  | 2.01                     | 0.41              |
| 1:A:807:LEU:O    | 1:A:811:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:840:TRP:HA   | 1:A:840:TRP:HE3  | 1.86                     | 0.41              |
| 1:B:24:LEU:HD12  | 1:B:24:LEU:HA    | 1.83                     | 0.41              |
| 1:B:77:LYS:HD2   | 1:B:94:CYS:SG    | 2.60                     | 0.41              |
| 1:B:78:MET:HE3   | 1:B:84:SER:HB3   | 2.02                     | 0.41              |
| 1:B:92:LEU:HD21  | 1:B:103:ASN:HD21 | 1.86                     | 0.41              |
| 1:B:220:LEU:CD2  | 1:B:452:LYS:HG3  | 2.43                     | 0.41              |
| 1:B:238:LYS:HB3  | 1:B:285:ARG:N    | 2.21                     | 0.41              |
| 1:B:291:TYR:CG   | 1:B:321:VAL:O    | 2.74                     | 0.41              |
| 1:B:367:PHE:CZ   | 1:B:399:THR:HA   | 2.56                     | 0.41              |
| 1:B:434:LYS:HA   | 1:B:625:TRP:NE1  | 2.35                     | 0.41              |
| 1:B:685:ILE:HD12 | 1:B:685:ILE:N    | 2.36                     | 0.41              |
| 1:B:734:TYR:CE2  | 1:B:737:LEU:HD12 | 2.56                     | 0.41              |
| 2:C:144:ALA:CB   | 2:C:341:ILE:HB   | 2.51                     | 0.41              |
| 2:C:252:ASN:ND2  | 2:C:256:ARG:HH11 | 2.19                     | 0.41              |
| 1:A:28:ASP:CB    | 1:A:81:PRO:HD2   | 2.51                     | 0.40              |
| 1:A:45:GLU:OE1   | 1:A:64:ASN:ND2   | 2.46                     | 0.40              |
| 1:A:46:ALA:O     | 1:A:62:GLN:HB2   | 2.21                     | 0.40              |
| 1:A:128:LYS:HE2  | 1:A:693:ALA:HB1  | 2.02                     | 0.40              |
| 1:A:278:ILE:HB   | 1:A:315:PHE:CE2  | 2.57                     | 0.40              |
| 1:A:344:PHE:CE2  | 1:A:442:ILE:HA   | 2.55                     | 0.40              |
| 1:A:569:PHE:HE2  | 1:A:581:PHE:CD2  | 2.39                     | 0.40              |
| 1:A:836:ARG:HG3  | 1:A:841:TRP:CE2  | 2.55                     | 0.40              |
| 1:A:836:ARG:HG3  | 1:A:841:TRP:CD2  | 2.56                     | 0.40              |
| 1:B:171:GLN:O    | 1:B:461:LEU:HA   | 2.22                     | 0.40              |
| 1:B:229:PRO:O    | 1:B:233:ALA:N    | 2.51                     | 0.40              |
| 1:B:280:GLN:HE22 | 1:B:315:PHE:HB3  | 1.86                     | 0.40              |
| 1:B:315:PHE:CD2  | 1:B:360:LEU:HA   | 2.55                     | 0.40              |
| 1:B:365:ILE:HG23 | 1:B:378:MET:HE1  | 2.03                     | 0.40              |
| 1:B:563:GLN:HB3  | 1:B:571:LYS:HB2  | 2.03                     | 0.40              |
| 1:B:612:LEU:O    | 1:B:616:SER:N    | 2.54                     | 0.40              |
| 1:B:614:ASN:C    | 1:B:616:SER:H    | 2.28                     | 0.40              |
| 1:B:757:ILE:HG21 | 1:B:767:TYR:CD1  | 2.56                     | 0.40              |
| 2:C:2:GLU:OE2    | 2:C:23:GLY:HA3   | 2.21                     | 0.40              |
| 2:C:153:LEU:CD2  | 2:C:155:SER:HB2  | 2.52                     | 0.40              |
| 2:C:192:ILE:HA   | 2:C:195:GLU:HB2  | 2.02                     | 0.40              |
| 2:D:5:THR:O      | 2:D:7:ALA:N      | 2.54                     | 0.40              |
| 2:D:11:ASP:HA    | 2:D:106:THR:HG21 | 2.04                     | 0.40              |
| 2:D:54:VAL:HG11  | 2:D:85:ILE:HA    | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:107:GLU:HG3  | 2:D:111:ASN:ND2  | 2.36                     | 0.40              |
| 2:D:192:ILE:HD12 | 2:D:256:ARG:CD   | 2.50                     | 0.40              |
| 2:D:216:LEU:HD22 | 2:D:250:ILE:HD13 | 2.03                     | 0.40              |
| 3:E:104:MET:HB2  | 3:E:107:GLU:H    | 1.86                     | 0.40              |
| 3:E:108:ILE:HG13 | 3:E:112:LEU:HD11 | 2.02                     | 0.40              |
| 4:G:99:GLU:OE1   | 4:G:163:LYS:HG2  | 2.21                     | 0.40              |
| 1:A:12:PHE:O     | 1:A:132:ILE:HD13 | 2.21                     | 0.40              |
| 1:A:278:ILE:HG22 | 1:A:359:VAL:HG13 | 2.02                     | 0.40              |
| 1:A:291:TYR:HB3  | 1:A:321:VAL:O    | 2.20                     | 0.40              |
| 1:A:302:ARG:HG2  | 1:A:307:LEU:CD1  | 2.50                     | 0.40              |
| 1:A:343:GLY:C    | 1:A:445:ARG:HD2  | 2.47                     | 0.40              |
| 1:A:348:GLU:HG3  | 1:A:620:PHE:CG   | 2.56                     | 0.40              |
| 1:A:351:SER:OG   | 1:A:621:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:378:MET:SD   | 1:A:381:ASN:HB3  | 2.61                     | 0.40              |
| 1:A:480:LEU:CD2  | 1:A:538:LEU:HD22 | 2.50                     | 0.40              |
| 1:A:532:THR:HG21 | 2:D:353:GLN:OE1  | 2.21                     | 0.40              |
| 1:A:764:PRO:CG   | 1:A:769:ILE:HG12 | 2.51                     | 0.40              |
| 1:A:823:LYS:HG2  | 3:H:10:GLU:CG    | 2.52                     | 0.40              |
| 1:B:111:GLY:O    | 1:B:113:ILE:HD12 | 2.20                     | 0.40              |
| 1:B:271:LEU:HD21 | 1:B:485:THR:OG1  | 2.21                     | 0.40              |
| 1:B:278:ILE:HD11 | 1:B:600:LYS:HA   | 2.03                     | 0.40              |
| 1:B:339:MET:HB3  | 1:B:344:PHE:CB   | 2.46                     | 0.40              |
| 1:B:473:GLU:H    | 1:B:473:GLU:CD   | 2.29                     | 0.40              |
| 1:B:510:ILE:C    | 1:B:512:TRP:H    | 2.29                     | 0.40              |
| 2:C:28:ARG:HD3   | 2:C:94:LEU:HD23  | 2.03                     | 0.40              |
| 2:C:42:GLY:H     | 2:C:47:MET:HE1   | 1.86                     | 0.40              |
| 2:C:54:VAL:CG2   | 2:C:84:LYS:HB3   | 2.49                     | 0.40              |
| 2:C:116:ARG:HB3  | 2:C:370:VAL:HB   | 2.03                     | 0.40              |
| 2:D:91:TYR:O     | 2:D:95:ARG:HA    | 2.21                     | 0.40              |
| 2:D:113:LYS:HG3  | 2:D:371:HIS:CE1  | 2.56                     | 0.40              |
| 3:E:103:VAL:HG22 | 3:E:140:TYR:HB3  | 2.03                     | 0.40              |
| 4:F:117:ILE:HD11 | 4:F:121:HIS:HB3  | 2.04                     | 0.40              |
| 1:A:13:LEU:HB2   | 1:A:132:ILE:CG2  | 2.51                     | 0.40              |
| 1:A:85:LYS:HB2   | 1:A:106:GLU:OE1  | 2.21                     | 0.40              |
| 1:A:173:ILE:N    | 1:A:461:LEU:HD21 | 2.36                     | 0.40              |
| 1:A:232:GLU:HA   | 1:A:236:ASN:OD1  | 2.22                     | 0.40              |
| 1:A:290:PHE:HA   | 1:A:356:VAL:HG11 | 2.04                     | 0.40              |
| 1:A:291:TYR:HD1  | 1:A:310:PHE:HD1  | 1.63                     | 0.40              |
| 1:A:347:GLU:HA   | 1:A:350:THR:HB   | 2.02                     | 0.40              |
| 1:A:517:PHE:HB3  | 1:A:715:ARG:NH1  | 2.35                     | 0.40              |
| 1:A:569:PHE:CE2  | 1:A:581:PHE:HB2  | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:809:ARG:NH2  | 3:H:148:LEU:HA   | 2.36                     | 0.40              |
| 1:B:49:ILE:HG12  | 1:B:75:ILE:CG2   | 2.52                     | 0.40              |
| 1:B:120:PHE:HE2  | 1:B:713:GLY:HA3  | 1.86                     | 0.40              |
| 1:B:165:LEU:HA   | 1:B:168:ARG:HH11 | 1.87                     | 0.40              |
| 1:B:292:TYR:HB3  | 1:B:332:PHE:CB   | 2.44                     | 0.40              |
| 1:B:294:ILE:HD12 | 1:B:310:PHE:CA   | 2.43                     | 0.40              |
| 1:B:359:VAL:O    | 1:B:362:LEU:HB2  | 2.22                     | 0.40              |
| 1:B:407:ILE:HG21 | 2:C:25:ASP:HB2   | 2.03                     | 0.40              |
| 1:B:497:MET:HE2  | 1:B:717:CYS:HB2  | 2.03                     | 0.40              |
| 1:B:610:THR:HG23 | 1:B:613:LEU:HD12 | 2.02                     | 0.40              |
| 1:B:657:ARG:NH2  | 1:B:662:LEU:HD23 | 2.36                     | 0.40              |
| 1:B:832:TYR:CD2  | 4:F:106:PHE:HZ   | 2.39                     | 0.40              |
| 2:C:20:GLY:CA    | 2:C:28:ARG:HB3   | 2.52                     | 0.40              |
| 2:C:99:GLU:CG    | 2:C:128:ASN:HB2  | 2.51                     | 0.40              |
| 2:C:151:ILE:HG13 | 2:C:293:LEU:O    | 2.21                     | 0.40              |
| 2:C:153:LEU:HD22 | 2:C:299:MET:SD   | 2.62                     | 0.40              |
| 2:C:200:PHE:HD1  | 2:C:205:GLU:HB3  | 1.87                     | 0.40              |
| 2:C:212:ILE:HG12 | 2:C:240:TYR:CB   | 2.51                     | 0.40              |
| 2:C:219:VAL:O    | 2:C:219:VAL:HG12 | 2.20                     | 0.40              |
| 2:C:236:LEU:HD23 | 2:C:254:ARG:NH1  | 2.35                     | 0.40              |
| 2:C:275:HIS:HD2  | 2:C:320:LEU:HD11 | 1.86                     | 0.40              |
| 2:C:356:TRP:C    | 2:C:373:LYS:HG2  | 2.46                     | 0.40              |
| 2:D:38:PRO:HG2   | 2:D:41:GLN:HG3   | 2.03                     | 0.40              |
| 2:D:189:LEU:HD11 | 2:D:250:ILE:CG2  | 2.51                     | 0.40              |
| 2:D:261:LEU:HD22 | 2:D:303:THR:O    | 2.21                     | 0.40              |
| 3:E:7:GLN:HG2    | 3:E:11:PHE:CE2   | 2.56                     | 0.40              |
| 3:E:18:PHE:O     | 3:E:30:GLN:NE2   | 2.54                     | 0.40              |
| 3:E:112:LEU:O    | 3:E:119:MET:HG3  | 2.22                     | 0.40              |
| 4:G:47:PHE:CE1   | 4:G:79:PRO:HB2   | 2.57                     | 0.40              |
| 3:H:109:ARG:HH11 | 3:H:128:VAL:HG21 | 1.87                     | 0.40              |
| 1:A:8:ASP:HA     | 1:A:11:LYS:CB    | 2.51                     | 0.40              |
| 1:A:114:TYR:C    | 1:A:151:PRO:HB2  | 2.46                     | 0.40              |
| 1:A:161:TYR:HD1  | 1:A:256:PHE:CE2  | 2.39                     | 0.40              |
| 1:A:245:SER:OG   | 1:A:247:ARG:NE   | 2.54                     | 0.40              |
| 1:A:327:GLN:HG2  | 1:A:328:ASP:N    | 2.37                     | 0.40              |
| 1:A:331:MET:HE3  | 1:A:331:MET:HB3  | 1.96                     | 0.40              |
| 1:A:434:LYS:HG2  | 1:A:613:LEU:HD13 | 2.04                     | 0.40              |
| 1:A:695:LYS:C    | 1:A:695:LYS:HD2  | 2.47                     | 0.40              |
| 1:A:730:PHE:CD1  | 1:A:734:TYR:HE1  | 2.39                     | 0.40              |
| 1:A:733:ARG:CB   | 1:A:788:ARG:HD3  | 2.52                     | 0.40              |
| 1:A:735:GLU:OE1  | 1:A:736:ILE:N    | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:76:GLN:OE1   | 1:B:96:ASN:HB3   | 2.21                     | 0.40              |
| 1:B:119:LEU:HB2  | 1:B:497:MET:SD   | 2.61                     | 0.40              |
| 1:B:293:LEU:HD23 | 1:B:357:SER:HB2  | 2.02                     | 0.40              |
| 1:B:322:PRO:HB3  | 1:B:327:GLN:OE1  | 2.21                     | 0.40              |
| 1:B:387:VAL:HG11 | 1:B:398:PHE:CZ   | 2.57                     | 0.40              |
| 1:B:485:THR:O    | 1:B:489:LEU:HG   | 2.21                     | 0.40              |
| 1:B:727:PHE:HD1  | 1:B:727:PHE:HA   | 1.75                     | 0.40              |
| 1:B:800:GLN:CG   | 3:E:112:LEU:HD23 | 2.49                     | 0.40              |
| 2:C:17:VAL:HG21  | 2:C:85:ILE:HD13  | 2.03                     | 0.40              |
| 2:C:92:ASN:HA    | 2:C:95:ARG:NH2   | 2.37                     | 0.40              |
| 2:C:217:CYS:HB3  | 2:C:306:TYR:CD1  | 2.57                     | 0.40              |
| 2:D:3:ASP:HA     | 2:D:353:GLN:OE1  | 2.22                     | 0.40              |
| 2:D:5:THR:HG1    | 2:D:347:ALA:C    | 2.25                     | 0.40              |
| 2:D:109:PRO:HG2  | 2:D:161:HIS:ND1  | 2.37                     | 0.40              |
| 2:D:238:LYS:HD3  | 2:D:254:ARG:HD2  | 2.02                     | 0.40              |
| 3:E:28:TYR:HE2   | 3:E:58:GLU:HG2   | 1.86                     | 0.40              |
| 4:F:96:THR:HG22  | 4:F:97:ASP:N     | 2.36                     | 0.40              |
| 1:A:4:LYS:HE3    | 1:A:140:MET:CG   | 2.51                     | 0.40              |
| 1:A:153:ILE:HD12 | 1:A:189:LYS:HG3  | 2.04                     | 0.40              |
| 1:A:234:PHE:CE1  | 1:A:289:ILE:HG21 | 2.57                     | 0.40              |
| 1:A:307:LEU:HD23 | 1:A:313:TYR:CE2  | 2.46                     | 0.40              |
| 1:A:332:PHE:CZ   | 1:A:336:LEU:HD11 | 2.56                     | 0.40              |
| 1:A:466:ILE:HG23 | 1:A:467:ALA:O    | 2.21                     | 0.40              |
| 1:A:469:PHE:HB2  | 1:A:707:CYS:C    | 2.46                     | 0.40              |
| 1:A:483:ASN:HD22 | 1:A:590:VAL:HG11 | 1.86                     | 0.40              |
| 1:A:510:ILE:CG1  | 1:A:768:ARG:HG2  | 2.32                     | 0.40              |
| 1:A:729:GLU:O    | 1:A:733:ARG:HB2  | 2.21                     | 0.40              |
| 1:A:754:ILE:HA   | 1:A:757:ILE:HB   | 2.02                     | 0.40              |
| 1:A:807:LEU:CD2  | 3:H:127:LEU:HB2  | 2.51                     | 0.40              |
| 1:A:836:ARG:O    | 1:A:842:ARG:NH1  | 2.52                     | 0.40              |
| 1:A:843:LEU:HG   | 4:F:63:ASN:O     | 2.21                     | 0.40              |
| 1:B:33:LYS:HG2   | 1:B:77:LYS:HG3   | 2.02                     | 0.40              |
| 1:B:258:VAL:H    | 1:B:456:GLN:HG2  | 1.87                     | 0.40              |
| 1:B:290:PHE:HB3  | 1:B:316:LEU:HD21 | 2.03                     | 0.40              |
| 1:B:337:GLU:O    | 1:B:341:ILE:HG13 | 2.21                     | 0.40              |
| 1:B:469:PHE:HZ   | 1:B:586:TYR:HB3  | 1.85                     | 0.40              |
| 1:B:560:ILE:HA   | 1:B:571:LYS:HG3  | 2.03                     | 0.40              |
| 1:B:685:ILE:HA   | 1:B:704:GLN:HB3  | 2.03                     | 0.40              |
| 1:B:702:LEU:HD21 | 1:B:711:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:764:PRO:HB3  | 1:B:768:ARG:NH1  | 2.35                     | 0.40              |
| 1:B:841:TRP:O    | 1:B:845:THR:HB   | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:104:LEU:HA   | 2:C:133:TYR:O    | 2.22                     | 0.40              |
| 2:C:150:GLY:O    | 2:C:152:VAL:HG23 | 2.22                     | 0.40              |
| 2:C:213:LYS:C    | 2:C:215:LYS:N    | 2.79                     | 0.40              |
| 2:C:287:ILE:HG21 | 2:D:244:ASP:HB2  | 2.04                     | 0.40              |
| 2:D:61:LYS:CG    | 2:D:64:ILE:HG12  | 2.49                     | 0.40              |
| 3:E:72:MET:O     | 3:E:72:MET:HG2   | 2.17                     | 0.40              |
| 3:E:119:MET:HB3  | 3:E:123:GLU:HB3  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 792/843 (94%)   | 655 (83%)  | 132 (17%) | 5 (1%)   | 21          | 59  |
| 1   | B     | 792/843 (94%)   | 653 (82%)  | 138 (17%) | 1 (0%)   | 48          | 83  |
| 2   | C     | 373/375 (100%)  | 319 (86%)  | 54 (14%)  | 0        | 100         | 100 |
| 2   | D     | 373/375 (100%)  | 313 (84%)  | 60 (16%)  | 0        | 100         | 100 |
| 3   | E     | 146/148 (99%)   | 120 (82%)  | 26 (18%)  | 0        | 100         | 100 |
| 3   | H     | 146/148 (99%)   | 129 (88%)  | 17 (12%)  | 0        | 100         | 100 |
| 4   | F     | 141/143 (99%)   | 133 (94%)  | 8 (6%)    | 0        | 100         | 100 |
| 4   | G     | 141/143 (99%)   | 128 (91%)  | 13 (9%)   | 0        | 100         | 100 |
| All | All   | 2904/3018 (96%) | 2450 (84%) | 448 (15%) | 6 (0%)   | 44          | 78  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 812 | PHE  |
| 1   | B     | 534 | PRO  |
| 1   | A     | 813 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 535 | PRO  |
| 1   | A     | 537 | VAL  |
| 1   | A     | 534 | PRO  |

### 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     | 703/741 (95%)   | 696 (99%)  | 7 (1%)   | 68          | 78  |
| 1   | B     | 703/741 (95%)   | 695 (99%)  | 8 (1%)   | 65          | 76  |
| 2   | C     | 318/318 (100%)  | 317 (100%) | 1 (0%)   | 86          | 86  |
| 2   | D     | 318/318 (100%)  | 315 (99%)  | 3 (1%)   | 70          | 79  |
| 3   | E     | 127/127 (100%)  | 126 (99%)  | 1 (1%)   | 73          | 80  |
| 3   | H     | 127/127 (100%)  | 125 (98%)  | 2 (2%)   | 55          | 70  |
| 4   | F     | 125/125 (100%)  | 125 (100%) | 0        | 100         | 100 |
| 4   | G     | 125/125 (100%)  | 125 (100%) | 0        | 100         | 100 |
| All | All   | 2546/2622 (97%) | 2524 (99%) | 22 (1%)  | 68          | 79  |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | VAL  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 230 | ILE  |
| 1   | A     | 256 | PHE  |
| 1   | A     | 352 | ILE  |
| 1   | A     | 404 | THR  |
| 1   | A     | 753 | CYS  |
| 1   | B     | 74  | ASP  |
| 1   | B     | 112 | LEU  |
| 1   | B     | 165 | LEU  |
| 1   | B     | 230 | ILE  |
| 1   | B     | 294 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 352 | ILE  |
| 1   | B     | 446 | VAL  |
| 1   | B     | 716 | ILE  |
| 2   | C     | 192 | ILE  |
| 2   | D     | 85  | ILE  |
| 2   | D     | 219 | VAL  |
| 2   | D     | 249 | THR  |
| 3   | E     | 147 | VAL  |
| 3   | H     | 123 | GLU  |
| 3   | H     | 133 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ASN  |
| 1   | A     | 62  | GLN  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 96  | ASN  |
| 1   | A     | 166 | GLN  |
| 1   | A     | 226 | GLN  |
| 1   | A     | 236 | ASN  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 288 | HIS  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 320 | HIS  |
| 1   | A     | 326 | GLN  |
| 1   | A     | 327 | GLN  |
| 1   | A     | 349 | GLN  |
| 1   | A     | 361 | GLN  |
| 1   | A     | 389 | HIS  |
| 1   | A     | 422 | GLN  |
| 1   | A     | 475 | ASN  |
| 1   | A     | 483 | ASN  |
| 1   | A     | 486 | ASN  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 513 | ASN  |
| 1   | A     | 563 | GLN  |
| 1   | A     | 566 | HIS  |
| 1   | A     | 606 | ASN  |
| 1   | A     | 661 | GLN  |
| 1   | A     | 728 | GLN  |
| 1   | A     | 751 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 765 | ASN  |
| 1   | A     | 771 | GLN  |
| 1   | A     | 828 | ASN  |
| 1   | B     | 3   | GLN  |
| 1   | B     | 18  | ASN  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 79  | ASN  |
| 1   | B     | 186 | ASN  |
| 1   | B     | 242 | ASN  |
| 1   | B     | 266 | ASN  |
| 1   | B     | 312 | ASN  |
| 1   | B     | 320 | HIS  |
| 1   | B     | 364 | ASN  |
| 1   | B     | 389 | HIS  |
| 1   | B     | 415 | GLN  |
| 1   | B     | 479 | GLN  |
| 1   | B     | 486 | ASN  |
| 1   | B     | 490 | GLN  |
| 1   | B     | 494 | ASN  |
| 1   | B     | 502 | GLN  |
| 1   | B     | 533 | ASN  |
| 1   | B     | 606 | ASN  |
| 1   | B     | 608 | ASN  |
| 1   | B     | 732 | GLN  |
| 1   | B     | 783 | HIS  |
| 1   | B     | 839 | GLN  |
| 2   | C     | 128 | ASN  |
| 2   | C     | 263 | GLN  |
| 2   | C     | 297 | ASN  |
| 2   | C     | 353 | GLN  |
| 2   | D     | 40  | HIS  |
| 2   | D     | 49  | GLN  |
| 2   | D     | 73  | HIS  |
| 2   | D     | 115 | ASN  |
| 2   | D     | 225 | ASN  |
| 2   | D     | 246 | GLN  |
| 2   | D     | 275 | HIS  |
| 2   | D     | 296 | ASN  |
| 2   | D     | 297 | ASN  |
| 3   | E     | 30  | GLN  |
| 3   | E     | 53  | ASN  |
| 3   | E     | 74  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 131 | HIS  |
| 4   | F     | 29  | GLN  |
| 4   | F     | 38  | ASN  |
| 4   | F     | 121 | HIS  |
| 4   | F     | 152 | ASN  |
| 4   | G     | 42  | GLN  |
| 4   | G     | 104 | ASN  |
| 3   | H     | 16  | GLN  |
| 3   | H     | 30  | GLN  |
| 3   | H     | 40  | GLN  |
| 3   | H     | 53  | ASN  |
| 3   | H     | 60  | ASN  |
| 3   | H     | 68  | GLN  |
| 3   | H     | 135 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

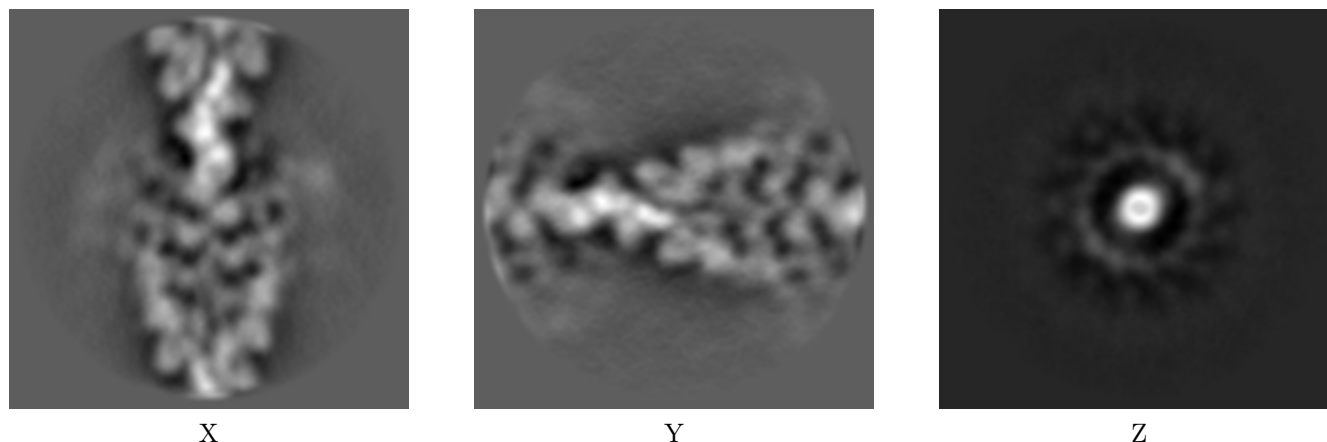
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29646. These allow visual inspection of the internal detail of the map and identification of artifacts.

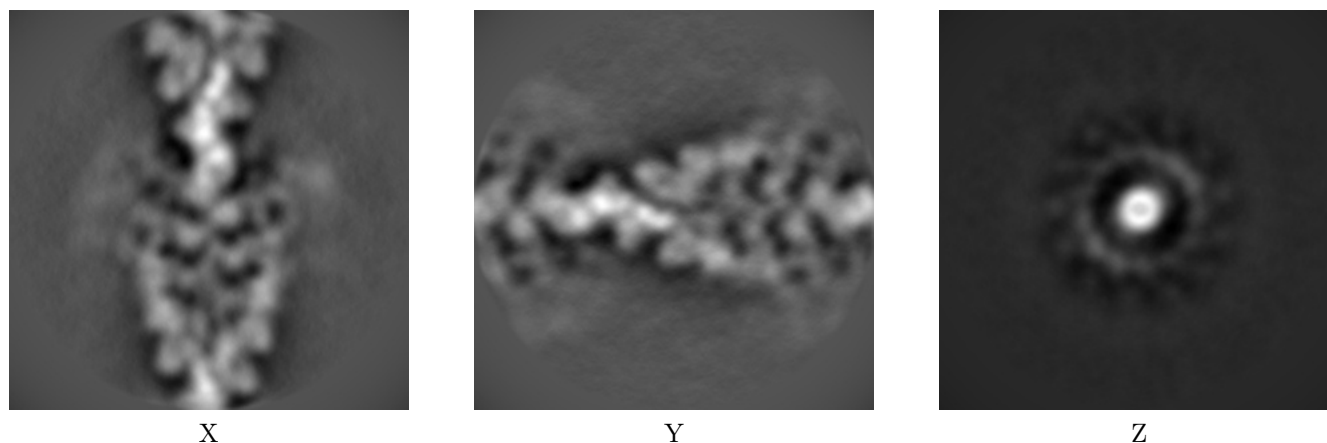
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map



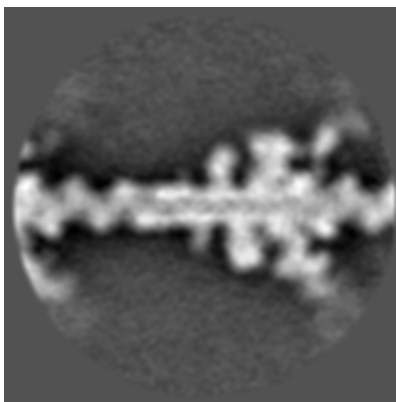
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

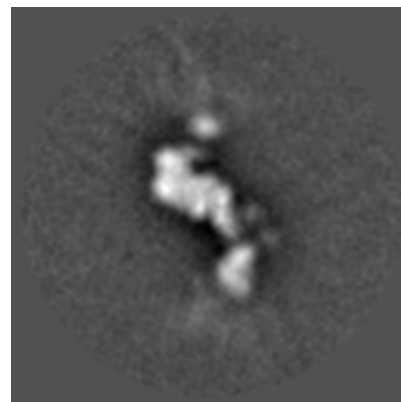
### 6.2.1 Primary map



X Index: 105

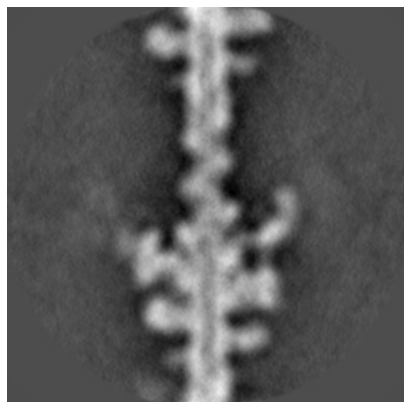


Y Index: 105

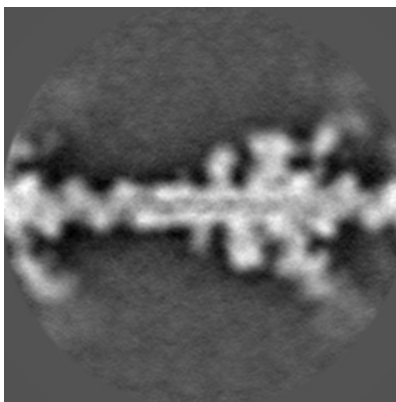


Z Index: 105

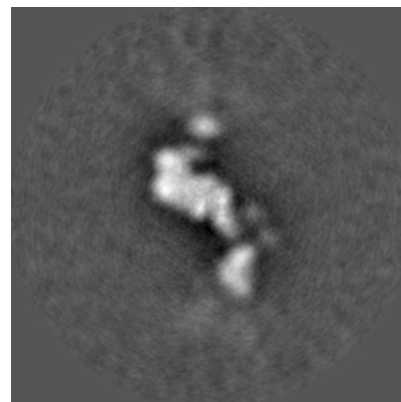
### 6.2.2 Raw map



X Index: 105



Y Index: 105



Z Index: 105

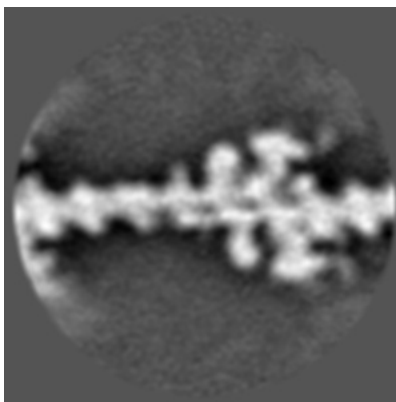
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

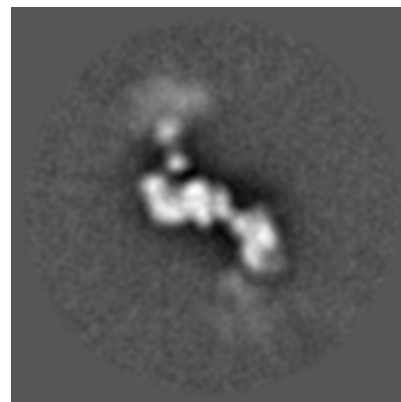
### 6.3.1 Primary map



X Index: 107

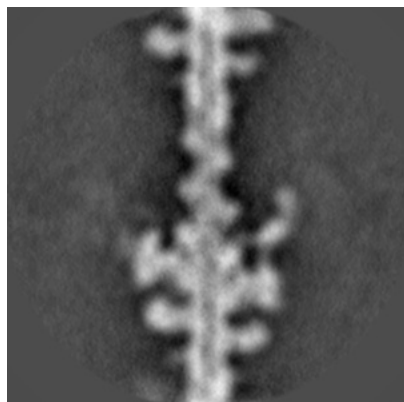


Y Index: 101

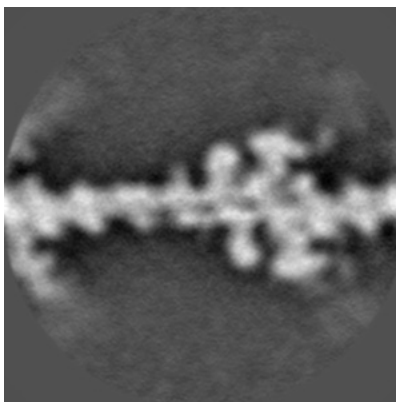


Z Index: 123

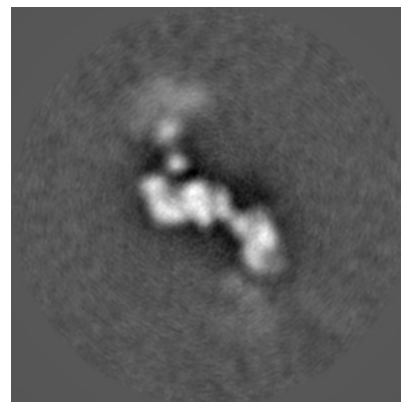
### 6.3.2 Raw map



X Index: 106



Y Index: 101

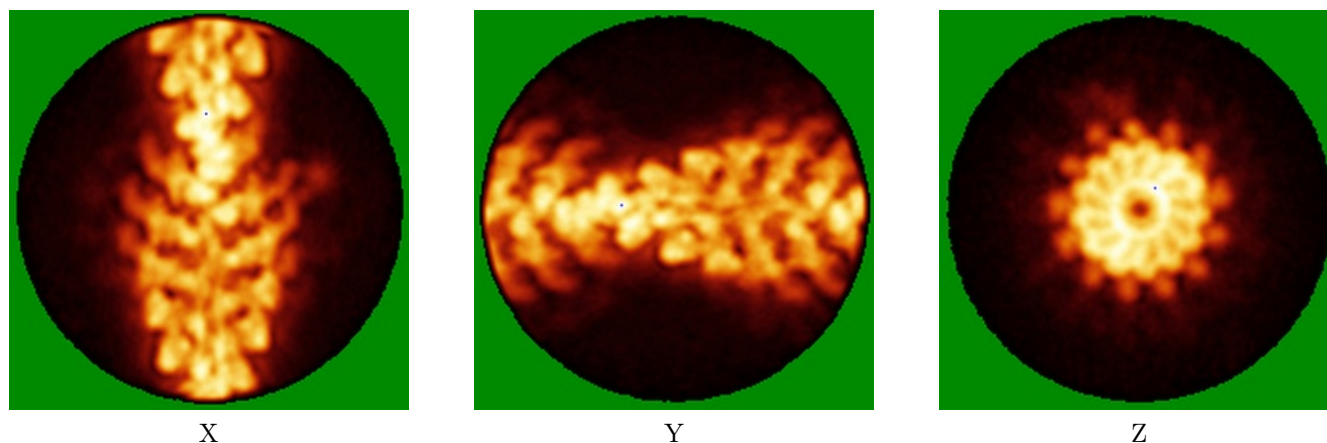


Z Index: 123

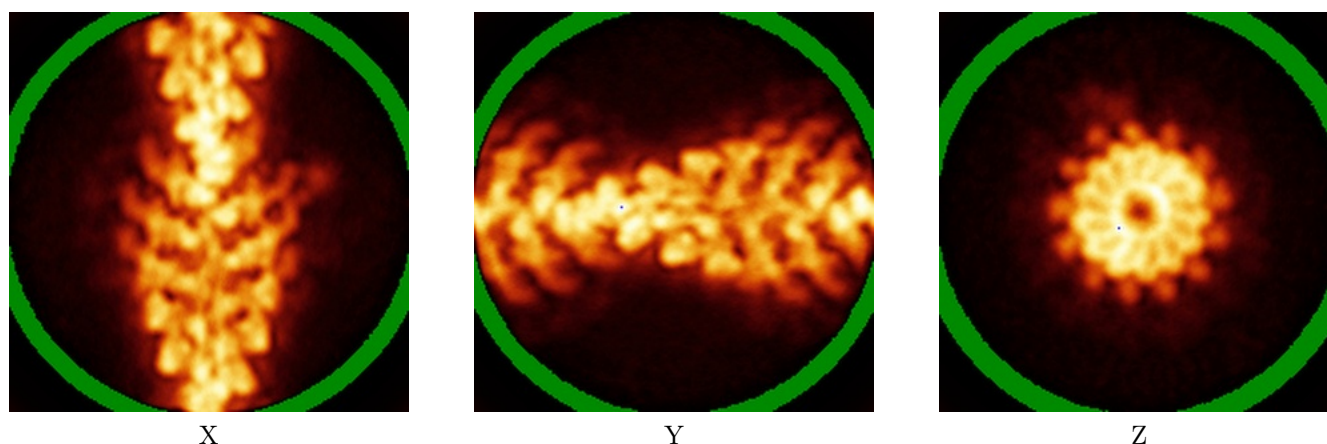
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

This section was not generated.

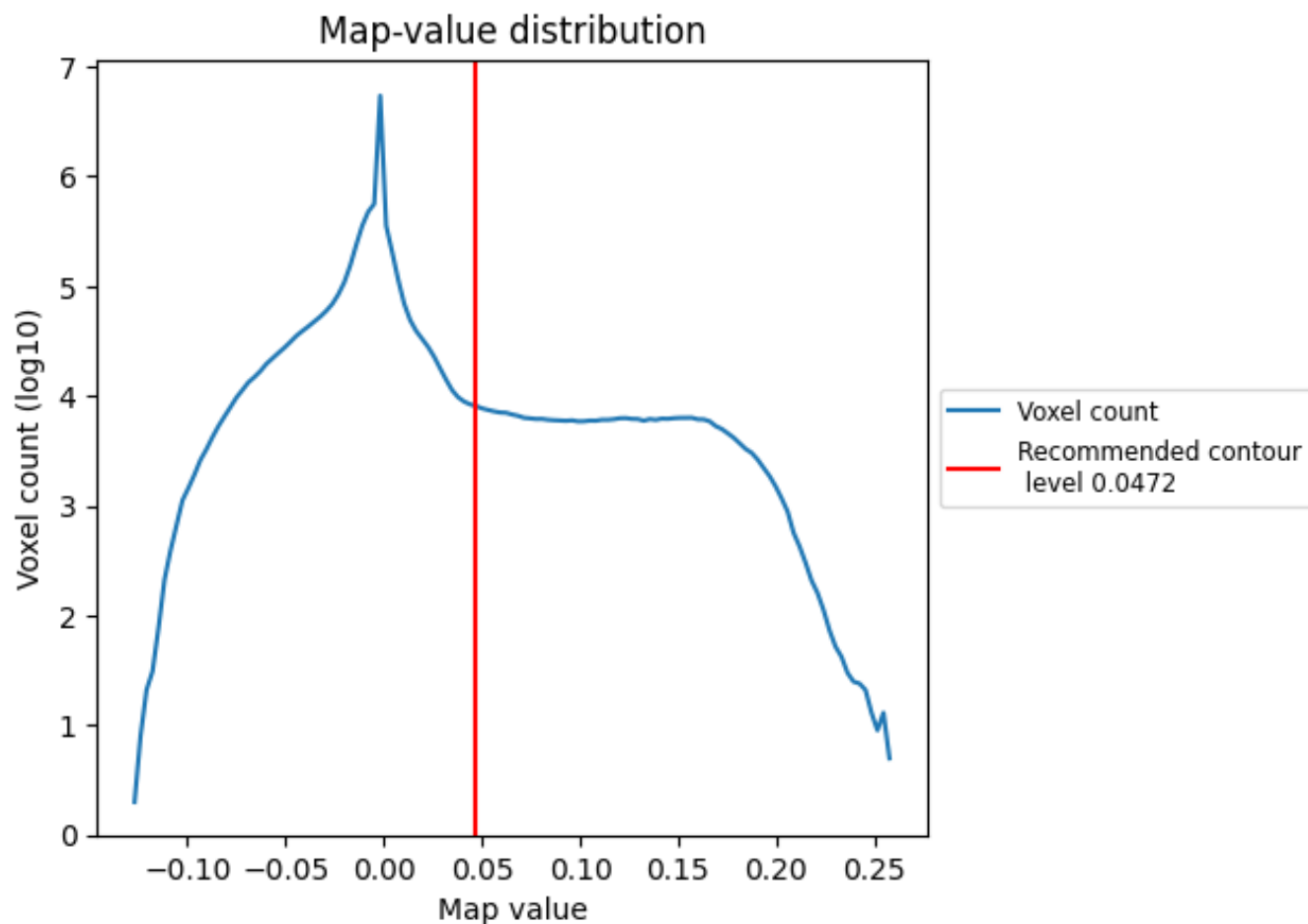
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

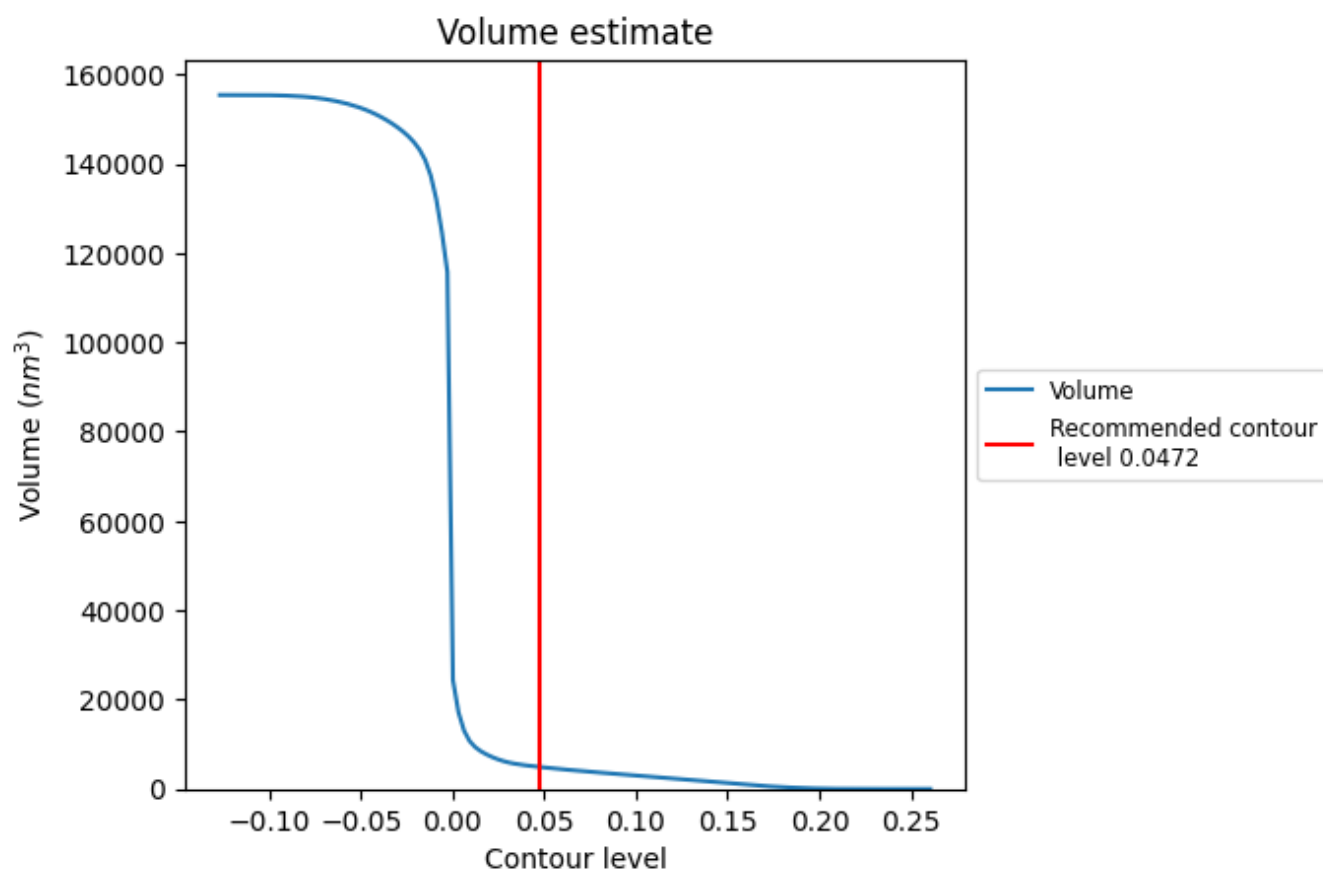
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

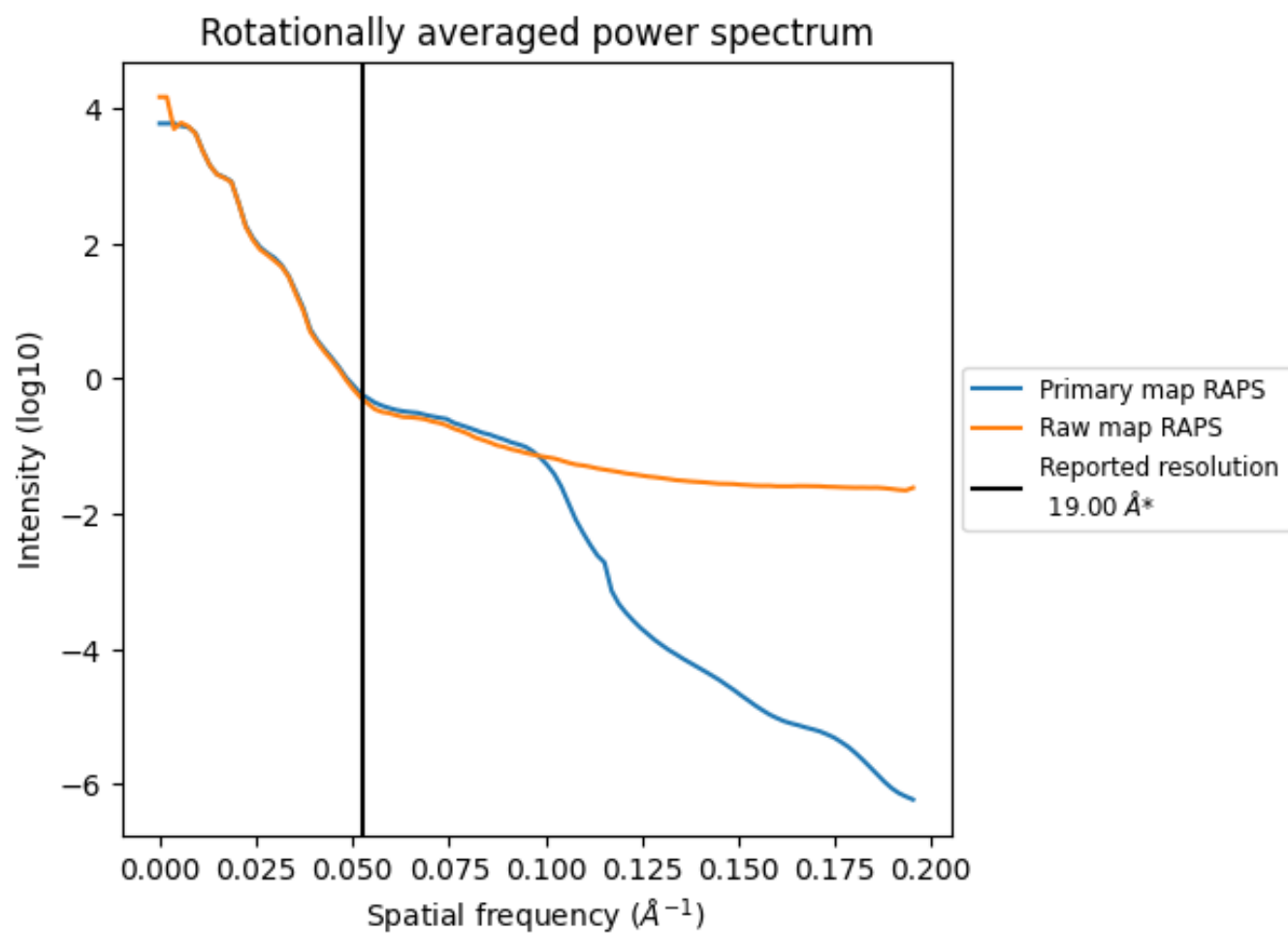
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4944  $\text{nm}^3$ ; this corresponds to an approximate mass of 4466 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

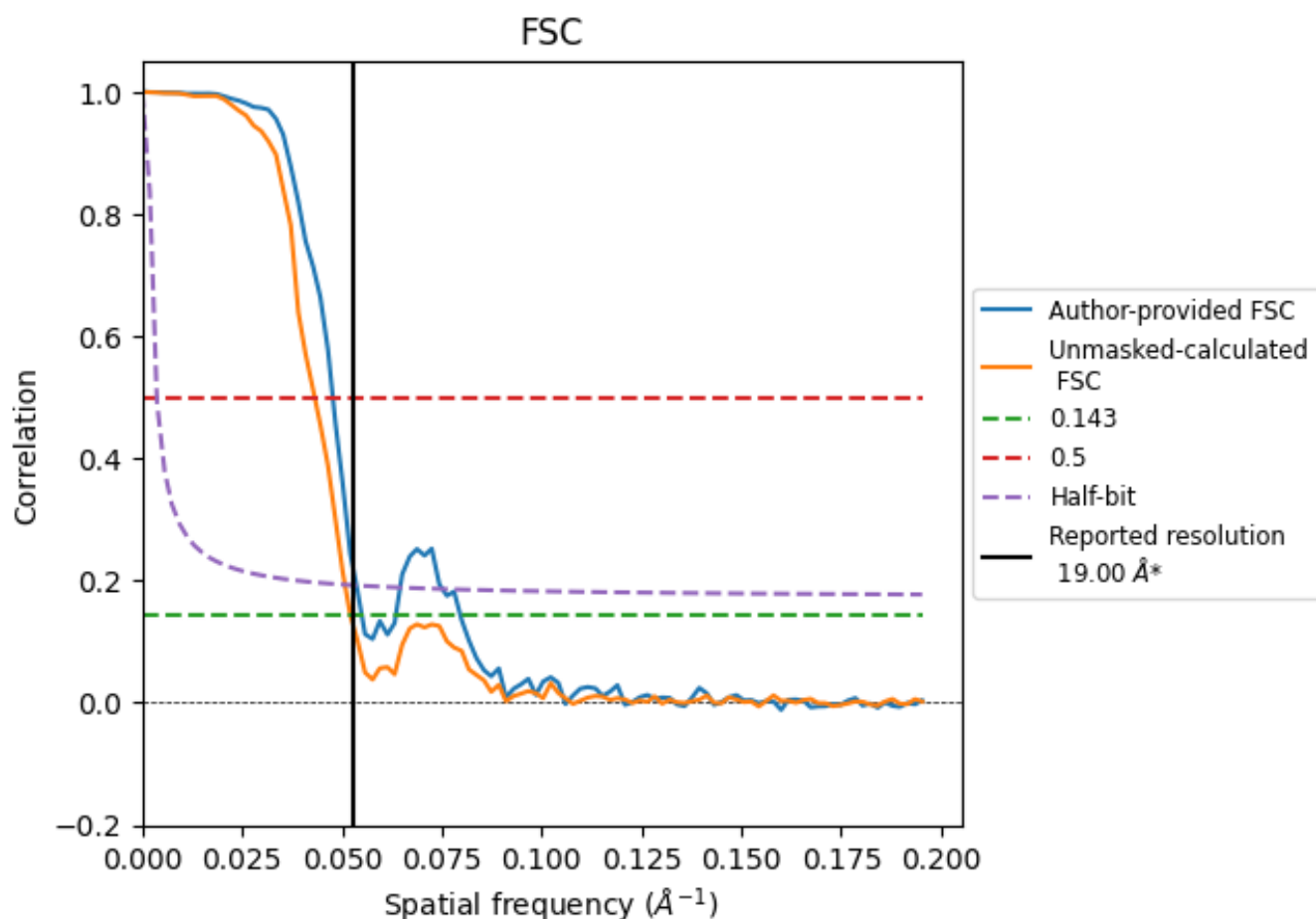


\*Reported resolution corresponds to spatial frequency of 0.053 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.053 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 19.00                              | -     | -        |
| Author-provided FSC curve | 18.18                              | 20.96 | 18.62    |
| Unmasked-calculated*      | 19.19                              | 23.15 | 19.69    |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

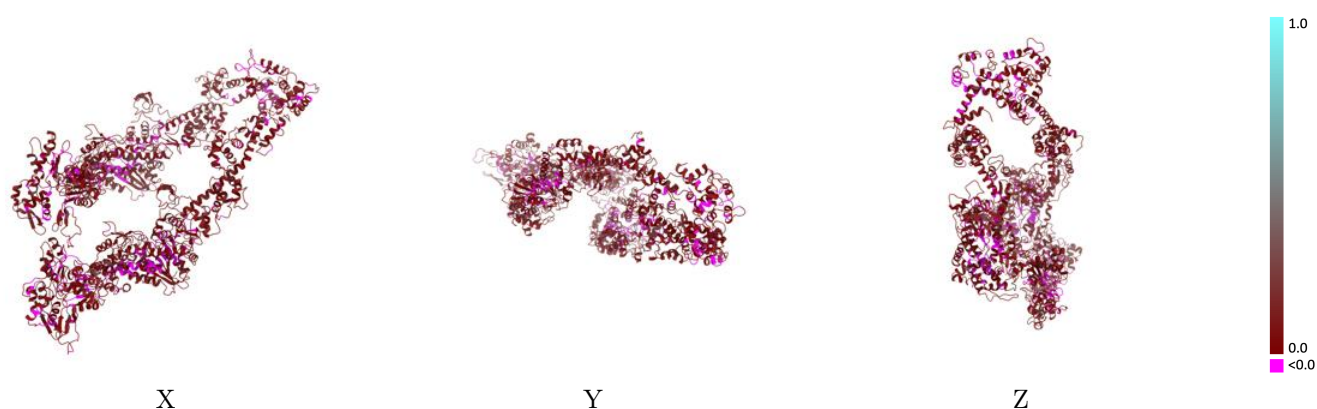
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29646 and PDB model 8SYF. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)

This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)

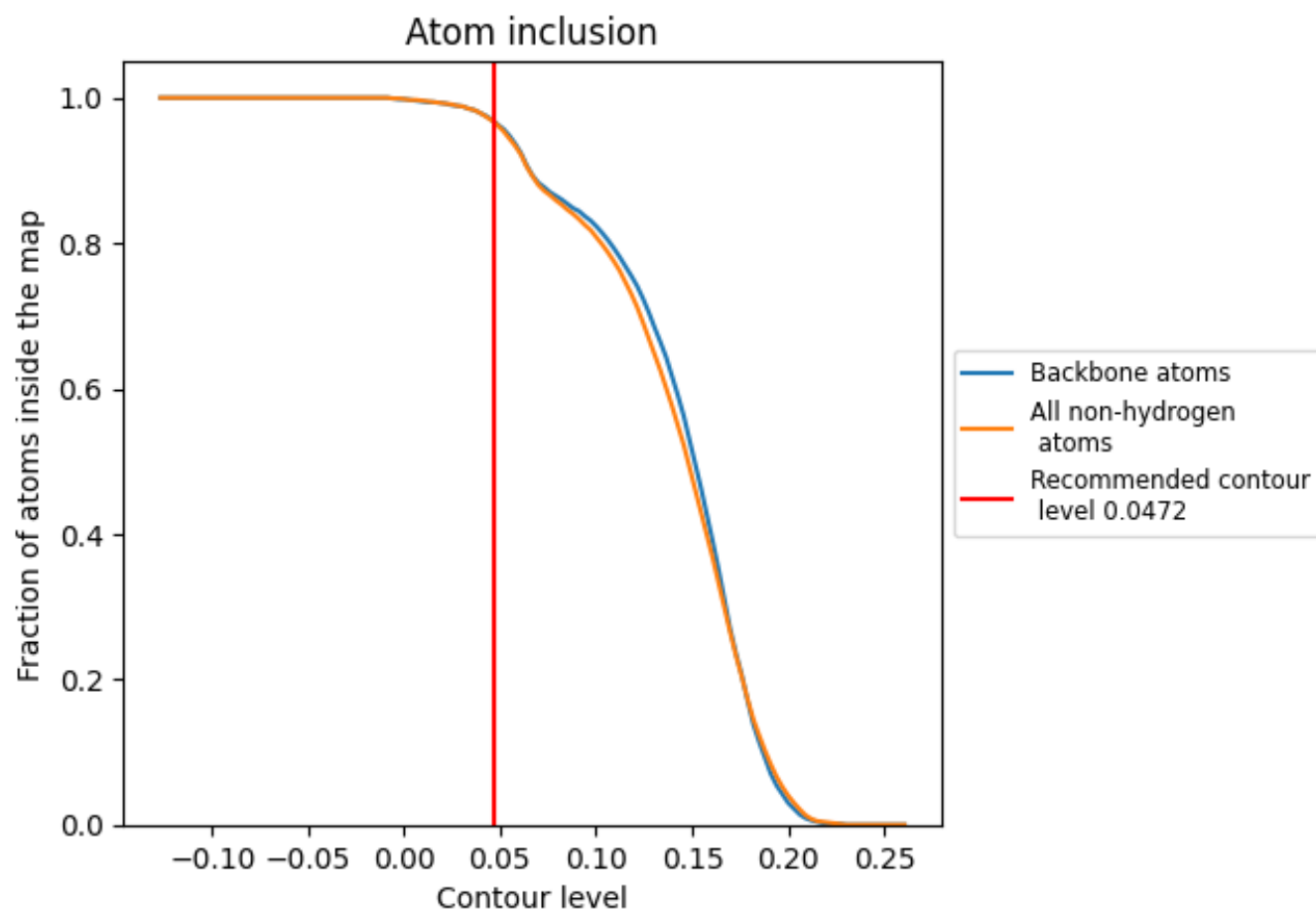


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0472) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9660 | <div></div> 0.0800 |
| A     | <div></div> 0.9950 | <div></div> 0.0810 |
| B     | <div></div> 1.0000 | <div></div> 0.0810 |
| C     | <div></div> 1.0000 | <div></div> 0.0740 |
| D     | <div></div> 1.0000 | <div></div> 0.0790 |
| E     | <div></div> 0.9800 | <div></div> 0.0890 |
| F     | <div></div> 0.9160 | <div></div> 0.0870 |
| G     | <div></div> 0.4470 | <div></div> 0.0570 |
| H     | <div></div> 0.9970 | <div></div> 0.1000 |

1.0

0.0

<0.0