



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 10:31 AM EDT

PDB ID : 5A20
EMDB ID: : EMD-2993
Title : Structure of bacteriophage SPP1 head-to-tail interface filled with DNA and tape measure protein
Authors : Chaban, Y.; Lurz, R.; Brasiles, S.; Cornilleau, C.; Karreman, M.; Zinn-Justin, S.; Tavares, P.; Orlova, E.V.
Deposited on : unknown
Resolution : 7.60 Å(reported)

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

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

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

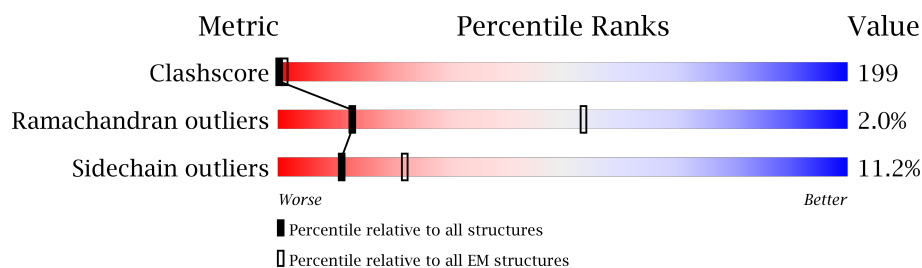
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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 (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 503 | |
| 1 | B | 503 | |
| 2 | C | 102 | |
| 2 | D | 102 | |
| 3 | E | 109 | |
| 3 | F | 109 | |
| 4 | G | 134 | |
| 5 | H | 177 | |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12799 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 PORTAL PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 440 | Total | C | N | O | S | 0 | 1 |
| | | | 3573 | 2259 | 589 | 711 | 14 | | |
| 1 | B | 440 | Total | C | N | O | S | 0 | 1 |
| | | | 3573 | 2259 | 589 | 711 | 14 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 365 | LYS | ASN | conflict | UNP P54309 |
| B | 365 | LYS | ASN | conflict | UNP P54309 |

- Molecule 2 is a protein called 15 PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | C | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 790 | 502 | 134 | 149 | 5 | | |
| 2 | D | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 790 | 502 | 134 | 149 | 5 | | |

- Molecule 3 is a protein called HEAD COMPLETION PROTEIN GP16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | E | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 891 | 569 | 145 | 175 | 2 | | |
| 3 | F | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 891 | 569 | 145 | 175 | 2 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| E | 6 | ARG | PRO | conflict | UNP O48446 |
| F | 6 | ARG | PRO | conflict | UNP O48446 |

- Molecule 4 is a protein called TAIL-TO-HEAD JOINING PROTEIN GP17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | G | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1047 | 667 | 172 | 204 | 4 | | |

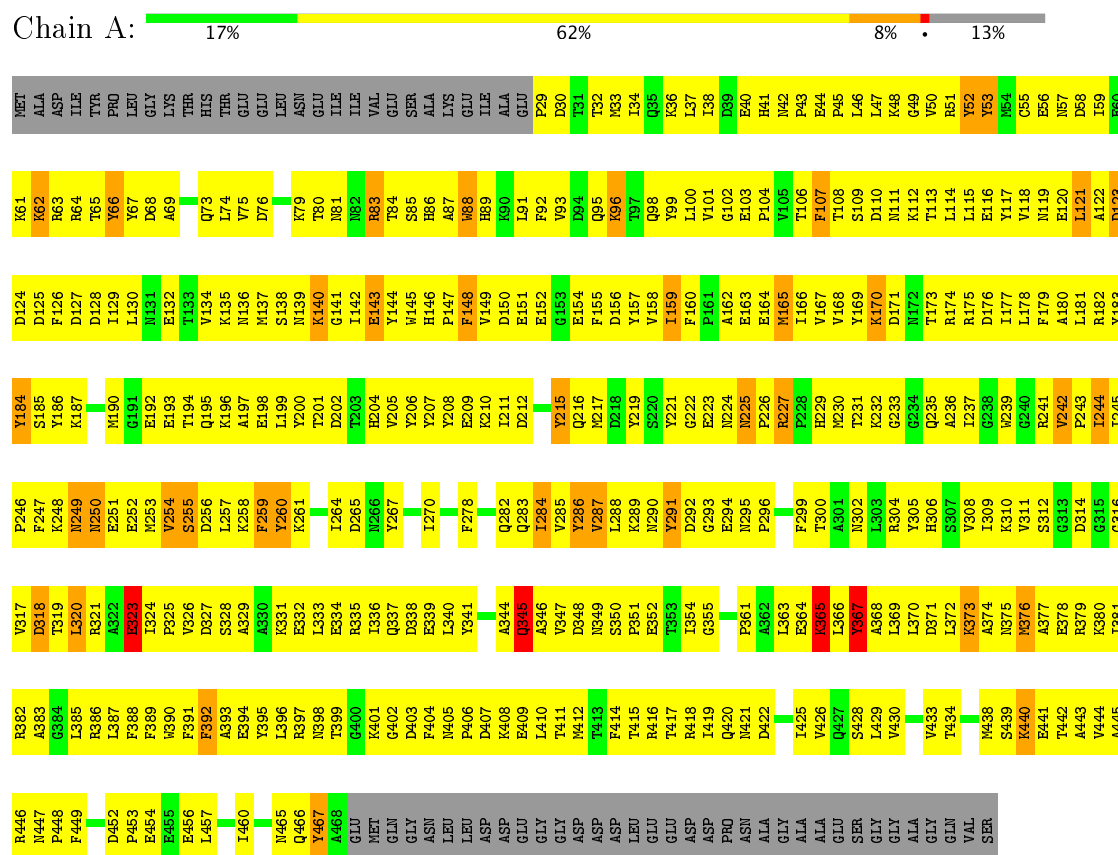
- Molecule 5 is a protein called MAJOR TAIL PROTEIN GP17.1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5 | H | 161 | Total | C | N | O | 0 | 0 |
| | | | 1244 | 776 | 205 | 263 | | |

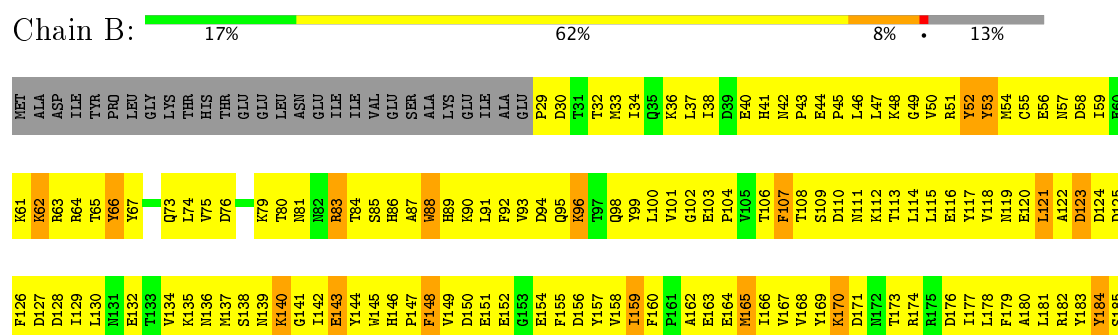
3 Residue-property plots

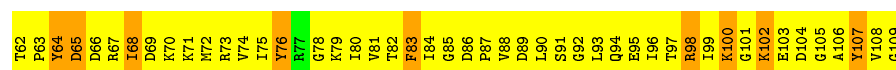
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: PORTAL PROTEIN

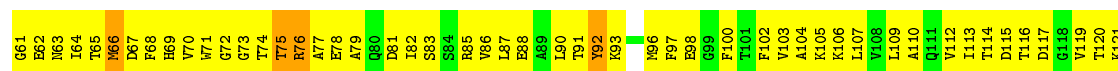


• Molecule 1: PORTAL PROTEIN

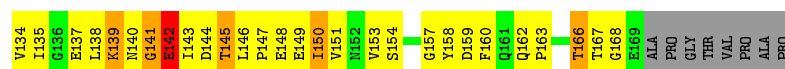
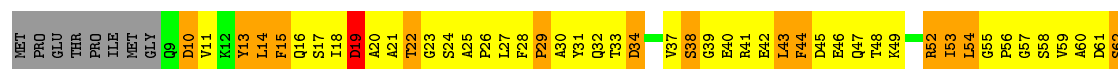




• Molecule 4: TAIL-TO-HEAD JOINING PROTEIN GP17



• Molecule 5: MAJOR TAIL PROTEIN GP17.1



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C6 | Depositor |
| Number of particles used | 14000 | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | EACH PARTICLE | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | 900 | Depositor |
| Maximum defocus (nm) | 3600 | Depositor |
| Magnification | 39000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.99 | 0/3651 | 1.07 | 0/4941 |
| 1 | B | 0.99 | 0/3651 | 1.07 | 0/4941 |
| 2 | C | 0.99 | 0/805 | 1.09 | 0/1085 |
| 2 | D | 0.99 | 0/805 | 1.09 | 0/1085 |
| 3 | E | 1.02 | 0/911 | 1.14 | 0/1229 |
| 3 | F | 1.02 | 0/911 | 1.11 | 0/1229 |
| 4 | G | 0.97 | 0/1069 | 1.11 | 1/1451 (0.1%) |
| 5 | H | 1.21 | 2/1264 (0.2%) | 1.36 | 3/1703 (0.2%) |
| All | All | 1.01 | 2/13067 (0.0%) | 1.11 | 4/17664 (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 | 6 |
| 1 | B | 0 | 6 |
| 2 | C | 0 | 4 |
| 2 | D | 0 | 4 |
| 3 | E | 0 | 2 |
| 3 | F | 0 | 2 |
| 4 | G | 0 | 3 |
| 5 | H | 0 | 5 |
| All | All | 0 | 32 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5 | H | 141 | GLY | C-N | 18.96 | 1.77 | 1.34 |
| 5 | H | 53 | ILE | C-N | 16.64 | 1.72 | 1.34 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|---------|--------|------------------------|---------------------|
| 5 | H | 141 | GLY | CA-C-N | -22.88 | 66.86 | 117.20 |
| 5 | H | 53 | ILE | O-C-N | -19.53 | 91.46 | 122.70 |
| 5 | H | 141 | GLY | C-N-CA | -11.11 | 93.92 | 121.70 |
| 4 | G | 44 | VAL | CB-CA-C | -5.01 | 101.89 | 111.40 |

There are no chirality outliers.

All (32) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 123 | ASP | Peptide |
| 1 | A | 255 | SER | Peptide |
| 1 | A | 282 | GLN | Peptide |
| 1 | A | 323 | GLU | Peptide |
| 1 | A | 365 | LYS | Peptide |
| 1 | A | 367 | TYR | Peptide |
| 1 | B | 123 | ASP | Peptide |
| 1 | B | 255 | SER | Peptide |
| 1 | B | 282 | GLN | Peptide |
| 1 | B | 323 | GLU | Peptide |
| 1 | B | 365 | LYS | Peptide |
| 1 | B | 367 | TYR | Peptide |
| 2 | C | 32 | ALA | Peptide |
| 2 | C | 38 | ASN | Peptide |
| 2 | C | 70 | LEU | Peptide |
| 2 | C | 87 | PRO | Peptide |
| 2 | D | 32 | ALA | Peptide |
| 2 | D | 38 | ASN | Peptide |
| 2 | D | 70 | LEU | Peptide |
| 2 | D | 87 | PRO | Peptide |
| 3 | E | 45 | GLU | Peptide |
| 3 | E | 6 | ARG | Peptide |
| 3 | F | 45 | GLU | Peptide |
| 3 | F | 54 | THR | Peptide |
| 4 | G | 28 | VAL | Peptide |
| 4 | G | 29 | ASN | Peptide |
| 4 | G | 75 | THR | Peptide |
| 5 | H | 113 | ILE | Peptide |
| 5 | H | 145 | THR | Peptide |
| 5 | H | 168 | GLY | Peptide |
| 5 | H | 29 | PRO | Peptide |
| 5 | H | 40 | 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 | 3573 | 0 | 3416 | 1326 | 0 |
| 1 | B | 3573 | 0 | 3414 | 1396 | 0 |
| 2 | C | 790 | 0 | 795 | 628 | 0 |
| 2 | D | 790 | 0 | 794 | 554 | 0 |
| 3 | E | 891 | 0 | 855 | 606 | 0 |
| 3 | F | 891 | 0 | 858 | 600 | 0 |
| 4 | G | 1047 | 0 | 1027 | 550 | 0 |
| 5 | H | 1244 | 0 | 1160 | 571 | 0 |
| All | All | 12799 | 0 | 12319 | 5006 | 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 199.

All (5006) 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:A:438:MET:SD | 1:B:434:THR:HA | 1.26 | 1.74 |
| 2:C:99:LYS:CA | 2:D:101:ALA:HA | 1.22 | 1.69 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:HB3 | 1.33 | 1.62 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:HD3 | 1.32 | 1.61 |
| 1:A:259:PHE:CE2 | 1:B:90:LYS:HD3 | 1.35 | 1.58 |
| 4:G:59:SER:CB | 5:H:138:LEU:HD12 | 1.11 | 1.58 |
| 2:C:94:LEU:HA | 2:D:97:TYR:CB | 1.27 | 1.57 |
| 2:C:66:THR:HG21 | 2:D:82:PHE:CE2 | 1.36 | 1.57 |
| 3:E:105:GLY:H | 4:G:119:VAL:CG2 | 1.06 | 1.57 |
| 2:C:66:THR:CG2 | 2:D:82:PHE:HE2 | 1.14 | 1.57 |
| 4:G:100:PHE:CE2 | 5:H:47:GLN:HA | 1.40 | 1.56 |
| 3:F:104:ASP:H | 4:G:31:VAL:CG2 | 1.05 | 1.56 |
| 4:G:100:PHE:HE1 | 5:H:45:ASP:CA | 1.15 | 1.55 |
| 2:C:98:ARG:HB2 | 2:D:97:TYR:CE2 | 1.07 | 1.55 |
| 2:C:99:LYS:CG | 2:D:101:ALA:HB1 | 1.31 | 1.55 |
| 4:G:100:PHE:CD2 | 5:H:47:GLN:HA | 1.04 | 1.54 |
| 4:G:59:SER:HB2 | 5:H:138:LEU:CD1 | 1.31 | 1.54 |
| 1:A:460:ILE:CG2 | 1:B:467:TYR:HB2 | 1.36 | 1.53 |
| 1:A:295:ASN:CB | 2:C:37:HIS:HE1 | 1.17 | 1.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:295:ASN:CA | 2:C:37:HIS:CE1 | 1.90 | 1.52 |
| 1:A:438:MET:CG | 1:B:434:THR:HA | 1.31 | 1.52 |
| 2:C:99:LYS:CA | 2:D:101:ALA:CA | 1.83 | 1.52 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:CB | 1.88 | 1.52 |
| 2:C:98:ARG:CB | 2:D:97:TYR:CE2 | 1.87 | 1.52 |
| 3:E:109:GLY:CA | 4:G:114:THR:H | 1.20 | 1.52 |
| 4:G:97:PHE:HA | 5:H:49:LYS:CE | 1.36 | 1.51 |
| 1:B:295:ASN:CA | 2:D:37:HIS:CE1 | 1.90 | 1.51 |
| 1:B:295:ASN:CB | 2:D:37:HIS:HE1 | 1.17 | 1.51 |
| 3:E:105:GLY:O | 4:G:41:TYR:CE2 | 1.64 | 1.49 |
| 2:C:99:LYS:CB | 2:D:101:ALA:HA | 1.37 | 1.49 |
| 2:C:4:GLN:CG | 3:E:1:MET:HE2 | 1.41 | 1.49 |
| 3:E:105:GLY:N | 4:G:119:VAL:HG21 | 1.28 | 1.48 |
| 2:C:4:GLN:CG | 3:E:1:MET:CE | 1.92 | 1.47 |
| 2:C:89:THR:HG23 | 2:D:92:LYS:CD | 1.44 | 1.47 |
| 4:G:59:SER:CB | 5:H:138:LEU:CD1 | 1.84 | 1.47 |
| 1:B:295:ASN:CB | 2:D:37:HIS:CE1 | 1.92 | 1.47 |
| 2:C:99:LYS:CB | 2:D:101:ALA:CB | 1.93 | 1.46 |
| 2:C:99:LYS:HB2 | 2:D:101:ALA:CA | 1.39 | 1.46 |
| 2:C:4:GLN:CD | 3:E:1:MET:CE | 1.79 | 1.46 |
| 1:A:295:ASN:CB | 2:C:37:HIS:CE1 | 1.92 | 1.46 |
| 2:C:99:LYS:CB | 2:D:101:ALA:CA | 1.88 | 1.45 |
| 2:D:4:GLN:HA | 3:F:1:MET:CB | 1.45 | 1.45 |
| 2:D:5:ARG:HA | 3:F:3:GLU:N | 1.21 | 1.45 |
| 3:F:104:ASP:N | 4:G:31:VAL:CG2 | 1.74 | 1.43 |
| 3:F:105:GLY:CA | 4:G:39:ASP:CG | 1.86 | 1.43 |
| 3:F:104:ASP:N | 4:G:31:VAL:HG21 | 1.29 | 1.43 |
| 1:B:295:ASN:CA | 2:D:37:HIS:HE1 | 1.09 | 1.42 |
| 2:C:4:GLN:NE2 | 3:E:1:MET:HE2 | 1.23 | 1.42 |
| 4:G:97:PHE:HA | 5:H:49:LYS:CD | 1.32 | 1.42 |
| 5:H:52:ARG:CD | 5:H:54:LEU:N | 1.80 | 1.42 |
| 4:G:100:PHE:CD2 | 5:H:47:GLN:CA | 1.97 | 1.42 |
| 5:H:53:ILE:C | 5:H:54:LEU:N | 1.72 | 1.42 |
| 1:A:295:ASN:CA | 2:C:37:HIS:HE1 | 1.09 | 1.41 |
| 5:H:141:GLY:CA | 5:H:142:GLU:N | 1.81 | 1.41 |
| 5:H:42:GLU:CG | 5:H:56:PRO:HG2 | 1.48 | 1.41 |
| 2:C:94:LEU:CA | 2:D:97:TYR:CG | 1.84 | 1.40 |
| 2:C:94:LEU:CA | 2:D:97:TYR:CB | 1.88 | 1.40 |
| 1:A:460:ILE:HG13 | 1:B:466:GLN:CG | 1.50 | 1.39 |
| 1:A:354:ILE:CD1 | 1:B:355:GLY:HA2 | 1.50 | 1.39 |
| 1:B:310:LYS:CB | 2:C:38:ASN:HD22 | 1.34 | 1.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:310:LYS:HB2 | 2:C:38:ASN:ND2 | 1.36 | 1.39 |
| 3:F:105:GLY:CA | 4:G:39:ASP:OD2 | 1.69 | 1.39 |
| 2:D:5:ARG:CA | 3:F:3:GLU:H | 1.36 | 1.38 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:CD | 2.04 | 1.38 |
| 5:H:141:GLY:C | 5:H:142:GLU:N | 1.77 | 1.38 |
| 1:A:438:MET:CG | 1:B:434:THR:CA | 2.00 | 1.38 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:C | 1.98 | 1.36 |
| 2:C:89:THR:CG2 | 2:D:92:LYS:CD | 2.01 | 1.36 |
| 3:E:105:GLY:O | 4:G:41:TYR:CZ | 1.77 | 1.35 |
| 1:A:295:ASN:HB2 | 2:C:37:HIS:CE1 | 1.50 | 1.35 |
| 2:C:4:GLN:NE2 | 3:E:1:MET:CE | 1.89 | 1.35 |
| 1:A:438:MET:SD | 1:B:434:THR:CA | 2.14 | 1.34 |
| 1:B:295:ASN:HB2 | 2:D:37:HIS:CE1 | 1.50 | 1.34 |
| 1:B:313:GLY:CA | 2:C:51:SER:OG | 1.76 | 1.34 |
| 1:A:460:ILE:CG2 | 1:B:467:TYR:CB | 2.06 | 1.33 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:H | 1.27 | 1.33 |
| 3:E:103:GLU:CG | 4:G:42:PRO:HD3 | 1.56 | 1.33 |
| 1:A:453:PRO:HB3 | 1:B:462:GLU:CG | 1.60 | 1.32 |
| 1:A:339:GLU:OE1 | 1:B:274:THR:CG2 | 1.77 | 1.32 |
| 1:A:460:ILE:HB | 1:B:467:TYR:CB | 1.59 | 1.31 |
| 2:C:89:THR:CG2 | 2:D:92:LYS:HG2 | 1.59 | 1.31 |
| 3:E:105:GLY:N | 4:G:119:VAL:CG2 | 1.78 | 1.31 |
| 5:H:42:GLU:OE2 | 5:H:56:PRO:CG | 1.77 | 1.31 |
| 3:E:109:GLY:CA | 4:G:114:THR:N | 1.92 | 1.30 |
| 3:F:105:GLY:N | 4:G:39:ASP:OD2 | 1.64 | 1.30 |
| 1:A:68:ASP:OD1 | 1:B:300:THR:HB | 1.18 | 1.30 |
| 2:C:99:LYS:CG | 2:D:101:ALA:CB | 2.09 | 1.30 |
| 2:C:89:THR:CG2 | 2:D:92:LYS:HD3 | 1.57 | 1.29 |
| 2:C:94:LEU:HA | 2:D:97:TYR:CD1 | 1.68 | 1.29 |
| 2:C:99:LYS:N | 2:D:101:ALA:HA | 1.45 | 1.29 |
| 5:H:52:ARG:HD2 | 5:H:54:LEU:N | 1.42 | 1.29 |
| 4:G:100:PHE:HE1 | 5:H:45:ASP:CB | 1.27 | 1.29 |
| 1:A:460:ILE:CB | 1:B:467:TYR:CB | 2.10 | 1.29 |
| 2:C:99:LYS:HA | 2:D:101:ALA:CB | 1.63 | 1.28 |
| 5:H:42:GLU:OE2 | 5:H:56:PRO:HG3 | 1.12 | 1.28 |
| 2:C:5:ARG:HB3 | 3:E:3:GLU:N | 1.48 | 1.28 |
| 1:A:296:PRO:CB | 2:C:36:CYS:O | 1.78 | 1.28 |
| 2:C:89:THR:OG1 | 2:D:88:SER:HB3 | 1.26 | 1.27 |
| 1:A:441:GLU:HG3 | 1:B:462:GLU:OE2 | 1.24 | 1.27 |
| 3:E:109:GLY:HA2 | 4:G:114:THR:N | 1.46 | 1.27 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:CA | 2.06 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:295:ASN:HA | 2:D:37:HIS:CE1 | 1.57 | 1.26 |
| 1:A:457:LEU:CG | 1:B:467:TYR:CD1 | 2.13 | 1.26 |
| 1:A:460:ILE:CB | 1:B:467:TYR:HB2 | 1.63 | 1.26 |
| 1:A:438:MET:CE | 1:B:433:VAL:HG22 | 1.63 | 1.26 |
| 1:A:453:PRO:HB3 | 1:B:462:GLU:CD | 1.56 | 1.26 |
| 2:C:71:THR:N | 3:E:92:GLY:CA | 1.95 | 1.26 |
| 3:E:103:GLU:OE2 | 4:G:42:PRO:CG | 1.84 | 1.26 |
| 3:F:104:ASP:CA | 4:G:31:VAL:HG23 | 1.62 | 1.26 |
| 2:C:99:LYS:HZ2 | 2:D:102:ARG:N | 1.30 | 1.25 |
| 2:C:89:THR:CG2 | 2:D:92:LYS:CG | 2.12 | 1.25 |
| 2:D:4:GLN:CA | 3:F:1:MET:HB3 | 1.65 | 1.25 |
| 5:H:42:GLU:HG3 | 5:H:56:PRO:CG | 1.66 | 1.25 |
| 2:C:100:MET:CE | 2:D:100:MET:HB2 | 1.67 | 1.24 |
| 4:G:132:ASN:HA | 5:H:54:LEU:O | 1.12 | 1.24 |
| 2:C:66:THR:CG2 | 2:D:82:PHE:CE2 | 2.00 | 1.24 |
| 1:B:292:ASP:OD1 | 2:D:33:LYS:C | 1.76 | 1.24 |
| 1:B:294:GLU:HG2 | 2:C:42:ASP:CA | 1.68 | 1.23 |
| 2:C:94:LEU:HA | 2:D:97:TYR:CG | 1.18 | 1.23 |
| 1:A:457:LEU:HG | 1:B:467:TYR:CD1 | 1.24 | 1.23 |
| 2:C:99:LYS:HG3 | 2:D:101:ALA:CB | 1.63 | 1.23 |
| 1:A:292:ASP:OD1 | 2:C:33:LYS:C | 1.76 | 1.22 |
| 2:C:7:LYS:HE2 | 3:E:4:GLU:CA | 1.67 | 1.22 |
| 1:A:438:MET:HG2 | 1:B:434:THR:C | 1.58 | 1.22 |
| 1:A:441:GLU:CG | 1:B:462:GLU:OE2 | 1.87 | 1.22 |
| 2:D:4:GLN:HG2 | 3:F:1:MET:SD | 1.78 | 1.22 |
| 2:C:98:ARG:CB | 2:D:97:TYR:HE2 | 1.36 | 1.21 |
| 1:A:460:ILE:CG1 | 1:B:467:TYR:CD2 | 2.24 | 1.20 |
| 3:E:19:ASN:ND2 | 4:G:77:ALA:HB1 | 1.56 | 1.20 |
| 1:A:438:MET:HG2 | 1:B:434:THR:CA | 1.66 | 1.20 |
| 2:D:69:GLY:O | 3:F:93:LEU:HD13 | 1.07 | 1.20 |
| 1:B:170:LYS:HB3 | 1:B:178:LEU:HD22 | 1.23 | 1.20 |
| 4:G:63:ASN:H | 5:H:139:LYS:HB3 | 1.07 | 1.20 |
| 1:B:296:PRO:CB | 2:D:36:CYS:O | 1.78 | 1.19 |
| 2:C:7:LYS:CD | 3:E:4:GLU:OE1 | 1.90 | 1.19 |
| 1:A:460:ILE:HG21 | 1:B:467:TYR:CB | 1.70 | 1.19 |
| 3:E:109:GLY:HA2 | 4:G:114:THR:CA | 1.56 | 1.19 |
| 4:G:132:ASN:CA | 5:H:54:LEU:O | 1.91 | 1.19 |
| 2:C:7:LYS:CE | 3:E:4:GLU:HA | 1.70 | 1.19 |
| 4:G:97:PHE:CA | 5:H:49:LYS:CE | 2.17 | 1.18 |
| 1:A:170:LYS:HB3 | 1:A:178:LEU:HD22 | 1.23 | 1.18 |
| 4:G:59:SER:CA | 5:H:138:LEU:HD12 | 1.72 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:53:GLN:HG3 | 4:G:40:PRO:HG3 | 1.21 | 1.18 |
| 5:H:42:GLU:CG | 5:H:56:PRO:CG | 2.18 | 1.18 |
| 2:C:99:LYS:CB | 2:D:101:ALA:HB1 | 1.62 | 1.18 |
| 1:A:295:ASN:HA | 2:C:37:HIS:CE1 | 1.56 | 1.18 |
| 2:D:69:GLY:O | 3:F:93:LEU:CD1 | 1.92 | 1.18 |
| 5:H:42:GLU:CD | 5:H:56:PRO:HG3 | 1.62 | 1.18 |
| 3:E:19:ASN:HD21 | 4:G:77:ALA:CB | 1.57 | 1.18 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:CB | 1.73 | 1.18 |
| 2:C:5:ARG:CB | 3:E:3:GLU:HA | 1.73 | 1.18 |
| 4:G:100:PHE:CZ | 5:H:46:GLU:N | 2.11 | 1.18 |
| 4:G:59:SER:OG | 5:H:138:LEU:HG | 1.41 | 1.18 |
| 2:C:71:THR:N | 3:E:92:GLY:HA2 | 1.11 | 1.17 |
| 4:G:100:PHE:CZ | 5:H:45:ASP:HB3 | 1.77 | 1.17 |
| 2:C:94:LEU:HA | 2:D:97:TYR:CA | 1.73 | 1.17 |
| 1:A:339:GLU:OE1 | 1:B:274:THR:HG23 | 1.00 | 1.17 |
| 4:G:134:ASN:HB3 | 5:H:59:VAL:CB | 1.37 | 1.17 |
| 5:H:52:ARG:NH2 | 5:H:54:LEU:CG | 1.98 | 1.17 |
| 4:G:134:ASN:CA | 5:H:59:VAL:HG23 | 1.29 | 1.16 |
| 1:A:367:TYR:HB3 | 1:A:369:LEU:HA | 1.20 | 1.16 |
| 1:A:354:ILE:HD12 | 1:B:355:GLY:CA | 1.76 | 1.16 |
| 2:C:94:LEU:N | 2:D:97:TYR:HB2 | 1.58 | 1.16 |
| 2:D:5:ARG:CA | 3:F:3:GLU:N | 1.99 | 1.16 |
| 4:G:64:ILE:HD12 | 5:H:140:ASN:ND2 | 1.60 | 1.16 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:N | 1.91 | 1.16 |
| 1:B:367:TYR:HB3 | 1:B:369:LEU:HA | 1.20 | 1.16 |
| 2:D:5:ARG:HA | 3:F:3:GLU:CA | 1.74 | 1.16 |
| 3:E:109:GLY:HA3 | 4:G:114:THR:H | 1.06 | 1.16 |
| 1:A:453:PRO:HB3 | 1:B:462:GLU:HG3 | 1.24 | 1.16 |
| 3:F:53:GLN:HG3 | 3:F:55:PRO:HD2 | 1.22 | 1.16 |
| 1:B:298:GLU:OE1 | 2:C:43:LYS:HG2 | 1.45 | 1.16 |
| 4:G:134:ASN:HB3 | 5:H:59:VAL:HB | 1.23 | 1.16 |
| 2:C:99:LYS:HA | 2:D:101:ALA:HB2 | 1.20 | 1.16 |
| 4:G:76:ARG:HG2 | 4:G:125:ILE:HD12 | 1.24 | 1.15 |
| 5:H:141:GLY:HA3 | 5:H:142:GLU:N | 1.51 | 1.15 |
| 3:F:105:GLY:HA3 | 4:G:39:ASP:N | 1.60 | 1.15 |
| 3:F:104:ASP:HA | 4:G:31:VAL:HG23 | 1.21 | 1.15 |
| 4:G:133:ASN:N | 5:H:55:GLY:HA2 | 1.60 | 1.15 |
| 3:E:75:ILE:HG13 | 3:E:80:ILE:HG22 | 1.29 | 1.15 |
| 2:C:66:THR:HG23 | 2:D:82:PHE:HE2 | 1.08 | 1.14 |
| 1:A:289:LYS:HG3 | 1:B:316:GLY:N | 1.61 | 1.14 |
| 1:B:144:TYR:HB3 | 1:B:244:ILE:HD11 | 1.28 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:44:GLU:HG2 | 3:F:46:TYR:H | 1.12 | 1.14 |
| 2:C:89:THR:HG23 | 2:D:92:LYS:CG | 1.74 | 1.14 |
| 1:B:37:LEU:HD22 | 1:B:168:VAL:HG11 | 1.16 | 1.14 |
| 2:C:89:THR:HG23 | 2:D:92:LYS:CE | 1.76 | 1.14 |
| 1:A:340:LEU:CD1 | 1:B:275:MET:CE | 2.26 | 1.14 |
| 2:C:5:ARG:CB | 3:E:3:GLU:CA | 2.25 | 1.14 |
| 3:F:105:GLY:HA3 | 4:G:39:ASP:CB | 1.77 | 1.14 |
| 3:F:6:ARG:HB2 | 3:F:8:VAL:HG12 | 1.16 | 1.14 |
| 1:A:460:ILE:HB | 1:B:467:TYR:CD2 | 1.81 | 1.13 |
| 1:A:460:ILE:CG1 | 1:B:466:GLN:HG3 | 1.76 | 1.13 |
| 1:A:251:GLU:HG3 | 1:B:54:MET:HA | 1.30 | 1.13 |
| 1:A:460:ILE:CG1 | 1:B:467:TYR:HD2 | 1.59 | 1.13 |
| 1:A:335:ARG:NH1 | 1:B:278:PHE:CE1 | 2.14 | 1.13 |
| 1:A:438:MET:HE1 | 1:B:433:VAL:HG22 | 1.28 | 1.13 |
| 2:C:99:LYS:HA | 2:D:101:ALA:CA | 1.64 | 1.13 |
| 3:F:102:LYS:HG3 | 4:G:39:ASP:OD1 | 1.49 | 1.13 |
| 1:A:37:LEU:HD22 | 1:A:168:VAL:HG11 | 1.16 | 1.13 |
| 1:A:460:ILE:HB | 1:B:467:TYR:CG | 1.82 | 1.13 |
| 1:A:295:ASN:HB2 | 2:C:37:HIS:NE2 | 1.62 | 1.13 |
| 2:C:7:LYS:HD3 | 3:E:4:GLU:OE1 | 0.95 | 1.12 |
| 5:H:49:LYS:HB2 | 5:H:52:ARG:HG2 | 1.16 | 1.12 |
| 1:A:110:ASP:HB3 | 1:A:396:LEU:HD13 | 1.31 | 1.12 |
| 1:A:144:TYR:HB3 | 1:A:244:ILE:HD11 | 1.28 | 1.12 |
| 1:B:295:ASN:HB2 | 2:D:37:HIS:NE2 | 1.62 | 1.12 |
| 3:E:109:GLY:CA | 4:G:113:ILE:HD12 | 1.77 | 1.12 |
| 4:G:97:PHE:CA | 5:H:49:LYS:CD | 2.22 | 1.12 |
| 2:C:98:ARG:HB2 | 2:D:97:TYR:CZ | 1.84 | 1.12 |
| 2:C:94:LEU:CA | 2:D:97:TYR:HB2 | 1.63 | 1.12 |
| 2:C:100:MET:HE2 | 2:D:100:MET:CB | 1.76 | 1.12 |
| 2:C:94:LEU:H | 2:D:97:TYR:N | 1.48 | 1.12 |
| 1:A:429:LEU:HD22 | 1:A:443:ALA:HB1 | 1.24 | 1.12 |
| 2:C:5:ARG:HB2 | 3:E:3:GLU:HA | 1.31 | 1.12 |
| 4:G:62:GLU:N | 5:H:139:LYS:N | 1.75 | 1.12 |
| 1:B:38:ILE:HG23 | 1:B:163:GLU:HG2 | 1.31 | 1.12 |
| 3:E:65:ASP:HB3 | 3:E:97:THR:HB | 1.31 | 1.12 |
| 3:E:103:GLU:OE2 | 4:G:42:PRO:HG3 | 1.47 | 1.12 |
| 4:G:59:SER:H | 5:H:138:LEU:HD11 | 0.99 | 1.12 |
| 1:B:110:ASP:HB3 | 1:B:396:LEU:HD13 | 1.31 | 1.11 |
| 3:E:79:LYS:HD3 | 3:F:70:LYS:H | 1.11 | 1.11 |
| 2:C:89:THR:HG21 | 2:D:92:LYS:HG2 | 1.12 | 1.11 |
| 3:F:55:PRO:HG3 | 3:F:102:LYS:HD3 | 1.30 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:99:LYS:CA | 2:D:101:ALA:CB | 2.14 | 1.11 |
| 3:E:103:GLU:HG3 | 4:G:42:PRO:CD | 1.80 | 1.11 |
| 5:H:42:GLU:CD | 5:H:56:PRO:CG | 2.18 | 1.11 |
| 1:A:438:MET:CG | 1:B:434:THR:O | 1.99 | 1.11 |
| 2:C:89:THR:HG21 | 2:D:88:SER:O | 1.48 | 1.11 |
| 1:A:167:VAL:HG13 | 1:A:177:ILE:HD12 | 1.30 | 1.11 |
| 5:H:60:ALA:HB3 | 5:H:134:VAL:HG11 | 1.22 | 1.11 |
| 1:A:38:ILE:HG23 | 1:A:163:GLU:HG2 | 1.31 | 1.10 |
| 4:G:100:PHE:HZ | 5:H:46:GLU:N | 1.45 | 1.10 |
| 1:B:167:VAL:HG13 | 1:B:177:ILE:HD12 | 1.30 | 1.10 |
| 1:B:63:ARG:HG2 | 1:B:79:LYS:HB2 | 1.30 | 1.10 |
| 1:B:40:GLU:HB2 | 1:B:166:ILE:HD11 | 1.12 | 1.10 |
| 1:B:310:LYS:CB | 2:C:38:ASN:HB2 | 1.81 | 1.10 |
| 3:F:105:GLY:CA | 4:G:39:ASP:H | 1.62 | 1.10 |
| 5:H:32:GLN:HG3 | 5:H:65:VAL:HG13 | 1.31 | 1.10 |
| 4:G:62:GLU:N | 5:H:139:LYS:HB2 | 1.50 | 1.10 |
| 1:A:453:PRO:CB | 1:B:462:GLU:HG3 | 1.80 | 1.10 |
| 2:C:4:GLN:CD | 3:E:1:MET:HE2 | 0.96 | 1.10 |
| 1:B:429:LEU:HD22 | 1:B:443:ALA:HB1 | 1.24 | 1.10 |
| 2:C:90:ILE:CD1 | 2:D:91:LEU:HG | 1.81 | 1.10 |
| 4:G:134:ASN:C | 5:H:59:VAL:HG23 | 1.69 | 1.10 |
| 1:B:306:HIS:HB3 | 1:B:308:VAL:HG12 | 1.31 | 1.10 |
| 2:D:70:LEU:O | 3:F:91:SER:HB2 | 1.52 | 1.10 |
| 3:F:105:GLY:HA2 | 4:G:39:ASP:OD2 | 1.41 | 1.10 |
| 1:A:252:GLU:HB3 | 1:A:254:VAL:HG13 | 1.30 | 1.09 |
| 1:A:40:GLU:HB2 | 1:A:166:ILE:HD11 | 1.12 | 1.09 |
| 1:A:438:MET:HG2 | 1:B:434:THR:O | 1.48 | 1.09 |
| 3:E:38:VAL:HG13 | 3:E:60:ILE:HG22 | 1.30 | 1.09 |
| 3:F:105:GLY:HA3 | 4:G:39:ASP:CG | 1.56 | 1.09 |
| 1:B:37:LEU:HD13 | 1:B:168:VAL:HG21 | 1.22 | 1.09 |
| 1:B:294:GLU:HG2 | 2:C:42:ASP:HA | 1.27 | 1.09 |
| 3:E:15:VAL:HG12 | 3:E:73:ARG:HE | 1.17 | 1.09 |
| 3:F:105:GLY:HA3 | 4:G:39:ASP:CA | 1.82 | 1.09 |
| 2:C:99:LYS:HZ1 | 2:D:102:ARG:HG3 | 1.16 | 1.09 |
| 3:E:105:GLY:N | 4:G:41:TYR:CD2 | 2.20 | 1.09 |
| 4:G:59:SER:H | 5:H:138:LEU:CD1 | 1.65 | 1.09 |
| 4:G:133:ASN:HB3 | 5:H:57:GLY:O | 1.51 | 1.09 |
| 1:A:66:TYR:HE1 | 1:A:74:LEU:HB3 | 1.14 | 1.09 |
| 1:B:306:HIS:NE2 | 2:C:39:PRO:HG3 | 1.65 | 1.09 |
| 2:C:4:GLN:HG3 | 3:E:1:MET:CE | 1.81 | 1.09 |
| 4:G:105:LYS:HG3 | 4:G:106:LYS:HG2 | 1.14 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:LEU:HD13 | 1:B:275:MET:CE | 1.82 | 1.09 |
| 1:B:313:GLY:HA3 | 2:C:51:SER:OG | 1.41 | 1.08 |
| 4:G:100:PHE:CZ | 5:H:45:ASP:C | 2.25 | 1.08 |
| 3:E:51:GLN:HG3 | 3:E:52:LEU:HD22 | 1.30 | 1.08 |
| 1:A:333:LEU:HD21 | 1:B:282:GLN:HE22 | 1.13 | 1.08 |
| 1:A:69:ALA:H | 1:B:300:THR:CG2 | 1.65 | 1.08 |
| 3:E:69:ASP:HB2 | 3:E:87:PRO:HG3 | 1.20 | 1.08 |
| 1:B:142:ILE:HG13 | 1:B:145:TRP:HB2 | 1.36 | 1.08 |
| 5:H:52:ARG:HD3 | 5:H:54:LEU:N | 1.64 | 1.08 |
| 4:G:21:TYR:HB3 | 4:G:24:LEU:HB2 | 1.08 | 1.08 |
| 1:A:142:ILE:HG13 | 1:A:145:TRP:HB2 | 1.36 | 1.08 |
| 1:A:306:HIS:HB3 | 1:A:308:VAL:HG12 | 1.31 | 1.07 |
| 1:A:37:LEU:HD13 | 1:A:168:VAL:HG21 | 1.22 | 1.07 |
| 1:A:259:PHE:CE2 | 1:B:90:LYS:CD | 2.30 | 1.07 |
| 1:A:63:ARG:HG2 | 1:A:79:LYS:HB2 | 1.30 | 1.07 |
| 1:B:66:TYR:HE1 | 1:B:74:LEU:HB3 | 1.14 | 1.07 |
| 3:E:77:ARG:HB3 | 3:F:66:ASP:HA | 1.13 | 1.07 |
| 3:F:88:VAL:HG22 | 3:F:98:ARG:HB2 | 1.34 | 1.07 |
| 2:C:85:GLU:HA | 2:D:86:ILE:HD12 | 1.34 | 1.07 |
| 3:F:102:LYS:HD2 | 4:G:39:ASP:OD1 | 1.53 | 1.07 |
| 2:C:90:ILE:HG12 | 2:D:91:LEU:CG | 1.85 | 1.07 |
| 4:G:59:SER:N | 5:H:138:LEU:HD11 | 1.70 | 1.07 |
| 3:E:103:GLU:OE2 | 4:G:42:PRO:CD | 2.03 | 1.07 |
| 1:A:69:ALA:H | 1:B:300:THR:HG21 | 0.94 | 1.06 |
| 1:A:252:GLU:OE2 | 1:B:53:TYR:O | 1.73 | 1.06 |
| 2:C:90:ILE:CG1 | 2:D:91:LEU:HG | 1.85 | 1.06 |
| 2:C:89:THR:HG22 | 2:D:92:LYS:HD3 | 1.12 | 1.06 |
| 1:A:68:ASP:OD1 | 1:B:300:THR:CB | 2.02 | 1.06 |
| 2:C:5:ARG:HB3 | 3:E:3:GLU:H | 1.00 | 1.06 |
| 2:C:5:ARG:HG3 | 2:C:8:ARG:H | 1.16 | 1.06 |
| 1:B:311:VAL:HG11 | 1:B:316:GLY:H | 1.17 | 1.06 |
| 3:E:108:VAL:HB | 4:G:43:TYR:OH | 1.54 | 1.06 |
| 1:A:292:ASP:OD1 | 2:C:34:ASP:N | 1.89 | 1.06 |
| 2:D:5:ARG:HB2 | 3:F:3:GLU:O | 1.52 | 1.06 |
| 2:D:69:GLY:HA3 | 2:D:73:ARG:HB3 | 1.37 | 1.06 |
| 4:G:133:ASN:CB | 5:H:57:GLY:O | 2.00 | 1.06 |
| 1:A:251:GLU:CG | 1:B:54:MET:CA | 2.32 | 1.06 |
| 2:C:98:ARG:HH12 | 2:D:102:ARG:HG2 | 1.15 | 1.06 |
| 3:F:43:GLN:HG2 | 3:F:53:GLN:H | 1.21 | 1.06 |
| 1:A:439:SER:OG | 1:B:459:ARG:HG3 | 1.54 | 1.06 |
| 2:C:74:SER:HB2 | 2:C:78:VAL:HG11 | 1.33 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:63:PRO:HB3 | 3:F:96:ILE:HG22 | 1.34 | 1.05 |
| 4:G:100:PHE:CE2 | 5:H:47:GLN:CA | 2.02 | 1.05 |
| 3:E:108:VAL:CB | 4:G:43:TYR:OH | 2.04 | 1.05 |
| 1:A:202:ASP:HB2 | 1:A:242:VAL:HB | 1.37 | 1.05 |
| 1:B:298:GLU:OE1 | 2:C:43:LYS:CG | 2.04 | 1.05 |
| 2:D:5:ARG:HG3 | 2:D:8:ARG:H | 1.16 | 1.05 |
| 4:G:63:ASN:H | 5:H:139:LYS:CB | 1.69 | 1.05 |
| 4:G:134:ASN:OD1 | 5:H:138:LEU:O | 1.65 | 1.05 |
| 2:C:87:PRO:HG3 | 2:C:90:ILE:HD12 | 1.35 | 1.05 |
| 2:C:99:LYS:HZ1 | 2:D:102:ARG:CG | 1.69 | 1.05 |
| 1:B:294:GLU:HG2 | 2:C:42:ASP:N | 1.71 | 1.05 |
| 3:F:63:PRO:HA | 3:F:96:ILE:HA | 1.32 | 1.05 |
| 1:B:252:GLU:HB3 | 1:B:254:VAL:HG13 | 1.30 | 1.05 |
| 2:C:100:MET:CE | 2:D:100:MET:CB | 2.31 | 1.05 |
| 1:B:202:ASP:HB2 | 1:B:242:VAL:HB | 1.37 | 1.04 |
| 3:E:40:PRO:HA | 3:F:100:LYS:HD2 | 1.40 | 1.04 |
| 1:A:311:VAL:HG11 | 1:A:316:GLY:H | 1.17 | 1.04 |
| 2:C:93:LYS:HG2 | 2:C:94:LEU:HD12 | 1.37 | 1.04 |
| 2:D:93:LYS:HG2 | 2:D:94:LEU:HD12 | 1.37 | 1.04 |
| 1:A:259:PHE:HZ | 1:B:90:LYS:CB | 1.69 | 1.04 |
| 1:A:252:GLU:OE2 | 1:B:53:TYR:CD1 | 2.11 | 1.04 |
| 4:G:117:ASP:HB3 | 4:G:119:VAL:HG23 | 1.38 | 1.04 |
| 4:G:97:PHE:HD2 | 5:H:47:GLN:HB3 | 1.19 | 1.04 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:OG | 1.43 | 1.04 |
| 1:B:292:ASP:OD1 | 2:D:34:ASP:N | 1.89 | 1.04 |
| 2:D:87:PRO:HG3 | 2:D:90:ILE:HD12 | 1.35 | 1.04 |
| 4:G:62:GLU:N | 5:H:139:LYS:CB | 1.93 | 1.04 |
| 3:E:40:PRO:HB2 | 3:E:42:SER:HB2 | 1.39 | 1.03 |
| 1:A:460:ILE:HG12 | 1:B:467:TYR:HD2 | 1.23 | 1.03 |
| 1:A:460:ILE:CB | 1:B:467:TYR:CD2 | 2.42 | 1.03 |
| 3:F:102:LYS:CG | 4:G:39:ASP:OD1 | 2.05 | 1.03 |
| 2:D:73:ARG:HG2 | 3:F:91:SER:CB | 1.88 | 1.03 |
| 4:G:97:PHE:CA | 5:H:49:LYS:HE2 | 1.63 | 1.03 |
| 2:D:74:SER:HB2 | 2:D:78:VAL:HG11 | 1.33 | 1.03 |
| 5:H:52:ARG:HH21 | 5:H:54:LEU:CD2 | 1.72 | 1.03 |
| 2:C:28:LEU:HD12 | 2:C:31:PHE:HZ | 1.24 | 1.03 |
| 2:C:69:GLY:HA3 | 2:C:73:ARG:HB3 | 1.37 | 1.03 |
| 2:C:99:LYS:HB2 | 2:D:101:ALA:C | 1.77 | 1.03 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:O | 1.90 | 1.03 |
| 1:A:371:ASP:OD1 | 1:B:363:LEU:C | 1.96 | 1.03 |
| 2:D:28:LEU:HD12 | 2:D:31:PHE:HZ | 1.24 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:5:ARG:HB2 | 3:E:3:GLU:CA | 1.88 | 1.03 |
| 4:G:100:PHE:CG | 5:H:47:GLN:HG2 | 1.93 | 1.02 |
| 5:H:52:ARG:NH2 | 5:H:54:LEU:CD2 | 2.22 | 1.02 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:HG2 | 1.74 | 1.02 |
| 3:F:85:GLY:HA3 | 3:F:99:ILE:HG23 | 1.37 | 1.02 |
| 4:G:133:ASN:HB2 | 5:H:56:PRO:N | 1.71 | 1.02 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:HB3 | 1.94 | 1.02 |
| 3:F:102:LYS:CD | 4:G:39:ASP:OD1 | 2.07 | 1.02 |
| 1:A:340:LEU:HD12 | 1:B:275:MET:HE1 | 1.41 | 1.02 |
| 1:B:306:HIS:CD2 | 2:C:39:PRO:HG3 | 1.94 | 1.02 |
| 2:C:90:ILE:HG12 | 2:D:91:LEU:CB | 1.90 | 1.02 |
| 5:H:111:ALA:HA | 5:H:132:LEU:HD13 | 1.41 | 1.02 |
| 2:C:99:LYS:HZ2 | 2:D:102:ARG:CA | 1.73 | 1.01 |
| 1:A:149:VAL:HB | 1:A:229:HIS:HA | 1.38 | 1.01 |
| 2:D:68:ALA:O | 3:E:1:MET:SD | 2.16 | 1.01 |
| 3:F:21:GLU:HA | 4:G:20:SER:HA | 1.42 | 1.01 |
| 1:A:259:PHE:HZ | 1:B:90:LYS:CD | 1.55 | 1.01 |
| 3:E:61:TYR:HB2 | 3:E:98:ARG:HG3 | 1.39 | 1.01 |
| 3:F:89:ASP:HB3 | 3:F:95:GLU:HB3 | 1.43 | 1.01 |
| 3:E:44:GLU:HG3 | 3:E:46:TYR:HB2 | 1.41 | 1.01 |
| 3:E:109:GLY:HA3 | 4:G:113:ILE:CD1 | 1.89 | 1.01 |
| 3:E:43:GLN:HG2 | 3:E:53:GLN:H | 1.22 | 1.01 |
| 1:B:313:GLY:CA | 2:C:51:SER:CB | 2.36 | 1.01 |
| 1:A:289:LYS:HG3 | 1:B:315:GLY:C | 1.80 | 1.01 |
| 1:B:376:MET:HE2 | 1:B:379:ARG:HH22 | 1.22 | 1.01 |
| 1:B:294:GLU:CD | 2:C:41:ILE:O | 1.99 | 1.01 |
| 1:A:367:TYR:HB3 | 1:A:368:ALA:HA | 1.42 | 1.01 |
| 1:A:376:MET:HE2 | 1:A:379:ARG:HH22 | 1.23 | 1.01 |
| 3:F:14:TYR:HB2 | 3:F:73:ARG:HD2 | 1.43 | 1.00 |
| 5:H:104:TYR:HE2 | 5:H:106:ALA:HB2 | 1.18 | 1.00 |
| 4:G:59:SER:N | 5:H:138:LEU:CD1 | 2.24 | 1.00 |
| 3:E:60:ILE:HG12 | 3:E:99:ILE:HG13 | 1.39 | 1.00 |
| 1:A:438:MET:HE3 | 1:B:433:VAL:HG22 | 1.42 | 1.00 |
| 1:B:149:VAL:HB | 1:B:229:HIS:HA | 1.38 | 1.00 |
| 3:F:65:ASP:HB3 | 3:F:68:ILE:HG23 | 1.43 | 1.00 |
| 4:G:59:SER:CB | 5:H:138:LEU:CG | 2.40 | 1.00 |
| 4:G:97:PHE:CA | 5:H:49:LYS:HD3 | 1.84 | 1.00 |
| 1:B:367:TYR:HB3 | 1:B:368:ALA:HA | 1.42 | 1.00 |
| 1:B:292:ASP:HB3 | 2:D:31:PHE:O | 1.58 | 1.00 |
| 1:B:395:TYR:HA | 1:B:398:ASN:HD22 | 1.26 | 1.00 |
| 5:H:137:GLU:O | 5:H:139:LYS:NZ | 1.92 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:103:GLU:CD | 4:G:42:PRO:HD3 | 1.82 | 1.00 |
| 4:G:59:SER:OG | 5:H:138:LEU:CG | 2.10 | 1.00 |
| 2:C:5:ARG:CB | 3:E:3:GLU:N | 2.25 | 1.00 |
| 1:A:395:TYR:HA | 1:A:398:ASN:HD22 | 1.26 | 0.99 |
| 1:A:336:ILE:O | 1:B:278:PHE:HE2 | 1.45 | 0.99 |
| 3:F:52:LEU:HB3 | 3:F:53:GLN:HA | 1.42 | 0.99 |
| 2:D:73:ARG:HG2 | 3:F:91:SER:HB2 | 1.04 | 0.99 |
| 1:A:145:TRP:HZ2 | 1:A:157:TYR:HB2 | 1.26 | 0.99 |
| 1:A:292:ASP:HB3 | 2:C:31:PHE:O | 1.58 | 0.99 |
| 2:D:76:ASP:OD2 | 3:E:39:GLN:NE2 | 1.72 | 0.99 |
| 5:H:141:GLY:C | 5:H:142:GLU:CB | 2.30 | 0.99 |
| 4:G:97:PHE:HD2 | 5:H:47:GLN:CB | 1.74 | 0.99 |
| 1:A:453:PRO:O | 1:B:467:TYR:OH | 1.79 | 0.99 |
| 3:E:58:TYR:HB3 | 3:F:100:LYS:HD3 | 1.44 | 0.99 |
| 1:A:111:ASN:HA | 1:A:401:LYS:HD3 | 1.41 | 0.99 |
| 1:A:335:ARG:HG3 | 1:B:333:LEU:HB2 | 1.45 | 0.99 |
| 4:G:61:GLY:C | 5:H:139:LYS:HB2 | 1.81 | 0.99 |
| 3:E:103:GLU:HG3 | 4:G:42:PRO:HD3 | 1.01 | 0.99 |
| 1:A:340:LEU:CD1 | 1:B:275:MET:HE1 | 1.89 | 0.98 |
| 1:B:382:ARG:HG3 | 1:B:383:ALA:HA | 1.45 | 0.98 |
| 2:D:4:GLN:CG | 3:F:1:MET:SD | 2.52 | 0.98 |
| 5:H:52:ARG:HD3 | 5:H:54:LEU:CA | 1.92 | 0.98 |
| 3:E:109:GLY:O | 4:G:114:THR:OG1 | 1.81 | 0.98 |
| 4:G:59:SER:HB2 | 5:H:138:LEU:CG | 1.91 | 0.98 |
| 4:G:62:GLU:HB3 | 5:H:138:LEU:O | 1.63 | 0.98 |
| 1:A:414:PHE:CD1 | 1:A:415:THR:HA | 1.99 | 0.98 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:CB | 2.27 | 0.98 |
| 2:C:70:LEU:H | 3:E:92:GLY:C | 1.66 | 0.98 |
| 2:C:70:LEU:HB2 | 3:E:92:GLY:O | 1.60 | 0.98 |
| 2:C:90:ILE:HG12 | 2:D:91:LEU:HG | 1.43 | 0.98 |
| 1:B:111:ASN:HA | 1:B:401:LYS:HD3 | 1.41 | 0.98 |
| 1:A:333:LEU:HD21 | 1:B:282:GLN:NE2 | 1.79 | 0.98 |
| 1:B:145:TRP:HZ2 | 1:B:157:TYR:HB2 | 1.26 | 0.97 |
| 1:A:336:ILE:O | 1:B:278:PHE:CE2 | 2.05 | 0.97 |
| 4:G:5:LEU:H | 4:G:5:LEU:HD13 | 1.27 | 0.97 |
| 5:H:21:ALA:HA | 5:H:90:LYS:HD3 | 1.45 | 0.97 |
| 1:A:382:ARG:HG3 | 1:A:383:ALA:HA | 1.45 | 0.97 |
| 2:C:98:ARG:HD3 | 2:D:97:TYR:CZ | 1.99 | 0.97 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:CB | 2.47 | 0.97 |
| 4:G:44:VAL:HG21 | 4:G:74:THR:H | 1.29 | 0.97 |
| 1:B:414:PHE:CD1 | 1:B:415:THR:HA | 1.99 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:5:ARG:HD3 | 2:C:7:LYS:HB2 | 1.45 | 0.97 |
| 5:H:42:GLU:OE2 | 5:H:56:PRO:CD | 2.11 | 0.97 |
| 1:A:96:LYS:HA | 1:A:373:LYS:HD3 | 1.47 | 0.97 |
| 4:G:132:ASN:O | 5:H:56:PRO:O | 1.83 | 0.97 |
| 2:D:70:LEU:N | 3:F:92:GLY:C | 1.87 | 0.97 |
| 1:B:96:LYS:HA | 1:B:373:LYS:HD3 | 1.47 | 0.97 |
| 4:G:44:VAL:HG11 | 4:G:74:THR:HG22 | 1.44 | 0.97 |
| 5:H:112:TYR:H | 5:H:132:LEU:HB3 | 1.29 | 0.97 |
| 1:A:175:ARG:NH2 | 1:B:156:ASP:OD2 | 1.97 | 0.97 |
| 1:A:460:ILE:HG12 | 1:B:467:TYR:CD2 | 1.95 | 0.97 |
| 1:B:310:LYS:HB2 | 2:C:38:ASN:HD22 | 0.88 | 0.97 |
| 3:E:70:LYS:HB3 | 3:E:84:ILE:HA | 1.43 | 0.97 |
| 2:C:98:ARG:CG | 2:D:97:TYR:CE2 | 2.47 | 0.97 |
| 5:H:90:LYS:HD3 | 5:H:150:ILE:HD11 | 1.45 | 0.97 |
| 2:D:5:ARG:HD3 | 2:D:7:LYS:HB2 | 1.45 | 0.96 |
| 3:E:105:GLY:H | 4:G:119:VAL:HG23 | 1.30 | 0.96 |
| 1:A:69:ALA:N | 1:B:300:THR:HG21 | 1.78 | 0.96 |
| 4:G:132:ASN:C | 5:H:55:GLY:HA2 | 1.85 | 0.96 |
| 4:G:42:PRO:HB3 | 4:G:72:GLY:HA3 | 1.44 | 0.96 |
| 2:C:4:GLN:HG3 | 3:E:1:MET:HE1 | 1.47 | 0.96 |
| 1:A:251:GLU:CG | 1:B:54:MET:HA | 1.91 | 0.96 |
| 2:D:28:LEU:HD12 | 2:D:31:PHE:CZ | 2.01 | 0.96 |
| 3:E:36:ALA:HB2 | 3:E:68:ILE:HD13 | 1.47 | 0.96 |
| 1:A:285:VAL:HG12 | 1:A:287:VAL:HG23 | 1.47 | 0.96 |
| 1:A:460:ILE:CB | 1:B:467:TYR:HD2 | 1.78 | 0.96 |
| 2:C:99:LYS:CE | 2:D:102:ARG:O | 2.14 | 0.96 |
| 1:A:460:ILE:HB | 1:B:467:TYR:HB3 | 1.48 | 0.96 |
| 2:D:4:GLN:HA | 3:F:1:MET:HB2 | 1.47 | 0.96 |
| 2:C:100:MET:HE2 | 2:D:100:MET:HB2 | 0.96 | 0.96 |
| 2:C:28:LEU:HD12 | 2:C:31:PHE:CZ | 2.01 | 0.96 |
| 3:E:19:ASN:HD21 | 4:G:77:ALA:HB1 | 0.79 | 0.96 |
| 3:E:43:GLN:HB2 | 3:E:47:TYR:HE1 | 1.29 | 0.96 |
| 3:F:105:GLY:HA3 | 4:G:39:ASP:H | 1.21 | 0.96 |
| 3:E:58:TYR:CD2 | 3:E:81:VAL:HG11 | 2.00 | 0.96 |
| 1:A:418:ARG:HB2 | 1:A:421:ASN:HB3 | 1.48 | 0.96 |
| 3:F:104:ASP:C | 4:G:39:ASP:OD2 | 2.04 | 0.95 |
| 5:H:52:ARG:HH21 | 5:H:54:LEU:HD21 | 1.28 | 0.95 |
| 1:B:140:LYS:HD3 | 1:B:261:LYS:HE3 | 1.48 | 0.95 |
| 1:B:410:LEU:HD22 | 1:B:412:MET:HE2 | 1.47 | 0.95 |
| 2:C:99:LYS:H | 2:D:101:ALA:N | 1.65 | 0.95 |
| 2:D:73:ARG:CG | 3:F:91:SER:HB2 | 1.97 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:141:GLY:C | 5:H:142:GLU:CA | 2.35 | 0.95 |
| 2:C:94:LEU:CA | 2:D:97:TYR:CD1 | 2.37 | 0.95 |
| 1:A:179:PHE:CD2 | 1:A:200:TYR:HB2 | 2.02 | 0.95 |
| 1:A:251:GLU:HG3 | 1:B:54:MET:CA | 1.81 | 0.95 |
| 1:B:310:LYS:HE3 | 2:C:36:CYS:HB2 | 1.49 | 0.95 |
| 2:C:94:LEU:H | 2:D:97:TYR:H | 1.06 | 0.95 |
| 1:B:285:VAL:HG12 | 1:B:287:VAL:HG23 | 1.47 | 0.95 |
| 3:E:108:VAL:CG1 | 4:G:43:TYR:OH | 2.15 | 0.95 |
| 4:G:64:ILE:CD1 | 5:H:140:ASN:ND2 | 2.30 | 0.95 |
| 2:C:99:LYS:HB2 | 2:D:102:ARG:N | 1.80 | 0.94 |
| 2:D:70:LEU:H | 3:F:92:GLY:C | 1.56 | 0.94 |
| 1:A:379:ARG:HD2 | 1:B:94:ASP:CB | 1.96 | 0.94 |
| 2:C:7:LYS:HD3 | 3:E:4:GLU:CD | 1.87 | 0.94 |
| 2:C:5:ARG:CB | 3:E:3:GLU:H | 1.80 | 0.94 |
| 5:H:52:ARG:CD | 5:H:54:LEU:CA | 2.44 | 0.94 |
| 2:C:98:ARG:HH12 | 2:D:102:ARG:CG | 1.80 | 0.94 |
| 4:G:113:ILE:HG21 | 4:G:121:LYS:HB3 | 1.47 | 0.94 |
| 4:G:100:PHE:CB | 5:H:47:GLN:HG2 | 1.95 | 0.94 |
| 1:A:140:LYS:HD3 | 1:A:261:LYS:HE3 | 1.48 | 0.94 |
| 1:A:259:PHE:HZ | 1:B:90:LYS:CG | 1.80 | 0.94 |
| 3:F:74:VAL:HB | 3:F:83:PHE:CZ | 2.02 | 0.94 |
| 3:E:36:ALA:HA | 3:E:62:THR:HG21 | 1.49 | 0.94 |
| 3:E:38:VAL:HB | 3:F:88:VAL:HG12 | 1.50 | 0.94 |
| 1:B:179:PHE:CD2 | 1:B:200:TYR:HB2 | 2.02 | 0.94 |
| 2:C:4:GLN:HA | 3:E:1:MET:HG2 | 1.49 | 0.94 |
| 5:H:21:ALA:HB2 | 5:H:150:ILE:HG12 | 1.50 | 0.94 |
| 2:C:63:PHE:CE2 | 2:C:86:ILE:HG23 | 2.03 | 0.94 |
| 2:C:94:LEU:N | 2:D:97:TYR:CB | 2.21 | 0.94 |
| 1:B:418:ARG:HB2 | 1:B:421:ASN:HB3 | 1.48 | 0.94 |
| 3:E:81:VAL:HG21 | 3:F:86:ASP:HB3 | 1.48 | 0.94 |
| 1:A:66:TYR:CE1 | 1:A:74:LEU:HB3 | 2.03 | 0.94 |
| 1:B:66:TYR:CE1 | 1:B:74:LEU:HB3 | 2.03 | 0.94 |
| 2:D:73:ARG:HE | 3:F:91:SER:HB3 | 1.31 | 0.94 |
| 4:G:64:ILE:HD12 | 5:H:140:ASN:HD21 | 1.24 | 0.94 |
| 1:A:340:LEU:CD1 | 1:B:275:MET:HE3 | 1.98 | 0.94 |
| 3:E:105:GLY:N | 4:G:119:VAL:HG23 | 1.79 | 0.94 |
| 1:A:328:SER:OG | 1:B:327:ASP:OD2 | 1.67 | 0.93 |
| 2:C:4:GLN:CG | 3:E:1:MET:HE1 | 1.97 | 0.93 |
| 2:C:99:LYS:HZ2 | 2:D:102:ARG:C | 1.72 | 0.93 |
| 4:G:59:SER:CA | 5:H:138:LEU:CD1 | 2.39 | 0.93 |
| 5:H:52:ARG:HD3 | 5:H:54:LEU:HA | 1.50 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:TRP:CZ2 | 1:A:157:TYR:HB2 | 2.03 | 0.93 |
| 1:B:145:TRP:CZ2 | 1:B:157:TYR:HB2 | 2.03 | 0.93 |
| 3:E:5:PHE:CD2 | 3:E:7:ASP:HB2 | 2.02 | 0.93 |
| 1:B:414:PHE:CE2 | 1:B:415:THR:HG22 | 2.03 | 0.93 |
| 2:D:63:PHE:CE2 | 2:D:86:ILE:HG23 | 2.03 | 0.93 |
| 3:F:59:ASN:HA | 3:F:99:ILE:HD12 | 1.51 | 0.93 |
| 5:H:59:VAL:HG11 | 5:H:137:GLU:HB3 | 1.48 | 0.93 |
| 5:H:46:GLU:HB2 | 5:H:151:VAL:HB | 1.50 | 0.93 |
| 1:A:142:ILE:CG1 | 1:A:145:TRP:HB2 | 1.99 | 0.93 |
| 1:B:123:ASP:HB3 | 1:B:127:ASP:H | 1.34 | 0.93 |
| 2:C:85:GLU:OE2 | 2:D:86:ILE:HG21 | 1.69 | 0.93 |
| 2:C:99:LYS:HZ3 | 2:D:102:ARG:H | 1.09 | 0.93 |
| 2:C:89:THR:OG1 | 2:D:88:SER:CB | 2.17 | 0.93 |
| 1:A:414:PHE:CE2 | 1:A:415:THR:HG22 | 2.03 | 0.93 |
| 2:C:99:LYS:CA | 2:D:101:ALA:HB2 | 1.88 | 0.93 |
| 3:E:56:ILE:HB | 3:E:103:GLU:HG3 | 1.47 | 0.93 |
| 3:F:104:ASP:H | 4:G:31:VAL:HG23 | 1.22 | 0.92 |
| 4:G:100:PHE:HD2 | 5:H:47:GLN:HA | 1.14 | 0.92 |
| 1:A:460:ILE:HG21 | 1:B:467:TYR:HB2 | 0.94 | 0.92 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:C | 2.23 | 0.92 |
| 2:C:94:LEU:CA | 2:D:97:TYR:CA | 2.41 | 0.92 |
| 3:E:84:ILE:CD1 | 3:E:103:GLU:HG2 | 1.98 | 0.92 |
| 1:B:148:PHE:HA | 1:B:205:VAL:HG23 | 1.51 | 0.92 |
| 1:A:438:MET:HE1 | 1:B:433:VAL:CG2 | 1.98 | 0.92 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:CA | 2.30 | 0.92 |
| 3:F:11:PHE:CE2 | 3:F:34:ALA:HB3 | 2.05 | 0.92 |
| 5:H:13:TYR:CD1 | 5:H:31:TYR:HB3 | 2.05 | 0.92 |
| 1:A:123:ASP:HB3 | 1:A:127:ASP:H | 1.34 | 0.92 |
| 1:B:289:LYS:CD | 1:B:319:THR:HG23 | 2.00 | 0.92 |
| 2:C:89:THR:HG23 | 2:D:92:LYS:HE3 | 1.51 | 0.92 |
| 3:E:38:VAL:CG1 | 3:E:60:ILE:HG22 | 1.99 | 0.92 |
| 3:E:58:TYR:CG | 3:F:100:LYS:HG2 | 2.04 | 0.92 |
| 5:H:37:VAL:HB | 5:H:64:GLU:HG2 | 1.49 | 0.92 |
| 1:A:289:LYS:CD | 1:A:319:THR:HG23 | 2.00 | 0.92 |
| 1:B:142:ILE:CG1 | 1:B:145:TRP:HB2 | 1.99 | 0.92 |
| 1:B:40:GLU:CB | 1:B:166:ILE:HD11 | 1.98 | 0.92 |
| 1:B:298:GLU:OE2 | 2:C:43:LYS:NZ | 2.03 | 0.92 |
| 3:F:88:VAL:CG2 | 3:F:98:ARG:HB2 | 1.99 | 0.92 |
| 5:H:94:VAL:HG21 | 5:H:160:PHE:CE2 | 2.04 | 0.92 |
| 1:A:62:LYS:CE | 1:A:63:ARG:HG3 | 1.99 | 0.92 |
| 1:B:62:LYS:CE | 1:B:63:ARG:HG3 | 1.99 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:382:ARG:HH22 | 1:A:385:LEU:HD23 | 1.34 | 0.92 |
| 2:D:59:LYS:HD3 | 2:D:90:ILE:HG21 | 1.50 | 0.92 |
| 3:E:43:GLN:HB2 | 3:E:47:TYR:CE1 | 2.04 | 0.92 |
| 4:G:32:THR:CG2 | 4:G:37:LYS:HA | 2.00 | 0.92 |
| 1:A:46:LEU:HB2 | 1:A:162:ALA:HB2 | 1.51 | 0.92 |
| 1:A:466:GLN:HA | 1:A:467:TYR:CD1 | 2.05 | 0.92 |
| 1:B:382:ARG:HH22 | 1:B:385:LEU:HD23 | 1.34 | 0.92 |
| 1:B:429:LEU:CD2 | 1:B:443:ALA:HB1 | 2.00 | 0.92 |
| 2:D:5:ARG:CB | 3:F:3:GLU:O | 2.18 | 0.92 |
| 3:E:47:TYR:HB3 | 3:E:50:GLN:CB | 2.00 | 0.92 |
| 2:D:5:ARG:HB2 | 3:F:3:GLU:C | 1.91 | 0.92 |
| 5:H:104:TYR:CE2 | 5:H:106:ALA:HB2 | 2.04 | 0.92 |
| 1:A:92:PHE:CE1 | 1:A:369:LEU:HD22 | 2.05 | 0.91 |
| 1:B:466:GLN:HA | 1:B:467:TYR:CD1 | 2.05 | 0.91 |
| 1:A:429:LEU:CD2 | 1:A:443:ALA:HB1 | 2.00 | 0.91 |
| 1:A:296:PRO:HB3 | 2:C:36:CYS:O | 0.96 | 0.91 |
| 3:F:105:GLY:HA2 | 4:G:39:ASP:CG | 1.70 | 0.91 |
| 1:A:40:GLU:CB | 1:A:166:ILE:HD11 | 1.98 | 0.91 |
| 1:A:338:ASP:OD2 | 1:B:337:GLN:OE1 | 1.87 | 0.91 |
| 3:F:46:TYR:HB3 | 3:F:48:LYS:HE2 | 1.50 | 0.91 |
| 4:G:27:MET:HG2 | 4:G:31:VAL:CG1 | 2.00 | 0.91 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:CG | 2.33 | 0.91 |
| 2:D:75:MET:HE3 | 3:F:90:LEU:HD21 | 1.52 | 0.91 |
| 3:E:105:GLY:CA | 4:G:119:VAL:HG23 | 1.99 | 0.91 |
| 3:F:105:GLY:C | 4:G:39:ASP:H | 1.73 | 0.91 |
| 4:G:97:PHE:CD2 | 5:H:47:GLN:HB3 | 2.05 | 0.91 |
| 1:B:146:HIS:HD2 | 1:B:205:VAL:HG22 | 1.34 | 0.91 |
| 3:F:11:PHE:CD2 | 3:F:34:ALA:HB3 | 2.06 | 0.91 |
| 4:G:32:THR:HG21 | 4:G:43:TYR:HB2 | 1.51 | 0.91 |
| 5:H:22:THR:HB | 5:H:108:PHE:CE2 | 2.06 | 0.91 |
| 5:H:146:LEU:HB2 | 5:H:147:PRO:HD3 | 1.53 | 0.91 |
| 1:A:34:ILE:HG22 | 1:A:181:LEU:HD13 | 1.51 | 0.91 |
| 2:C:90:ILE:HD11 | 2:D:91:LEU:HG | 1.49 | 0.91 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:N | 2.38 | 0.91 |
| 1:A:444:VAL:CG1 | 1:A:449:PHE:HB2 | 2.01 | 0.91 |
| 1:B:310:LYS:HB2 | 2:C:38:ASN:CG | 1.91 | 0.91 |
| 2:C:59:LYS:HD3 | 2:C:90:ILE:HG21 | 1.50 | 0.91 |
| 3:E:46:TYR:HB3 | 3:E:48:LYS:HE2 | 1.51 | 0.91 |
| 3:F:12:GLN:HG2 | 3:F:75:ILE:HG12 | 1.50 | 0.91 |
| 1:A:252:GLU:HB2 | 1:A:254:VAL:HG22 | 1.53 | 0.91 |
| 1:B:92:PHE:CE1 | 1:B:369:LEU:HD22 | 2.05 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:59:VAL:CG1 | 5:H:137:GLU:HB3 | 1.99 | 0.91 |
| 1:A:146:HIS:HD2 | 1:A:205:VAL:HG22 | 1.34 | 0.91 |
| 1:A:148:PHE:HA | 1:A:205:VAL:HG23 | 1.51 | 0.91 |
| 1:A:289:LYS:HG3 | 1:B:315:GLY:CA | 2.00 | 0.91 |
| 1:B:252:GLU:HB2 | 1:B:254:VAL:HG22 | 1.53 | 0.91 |
| 2:C:99:LYS:HE3 | 2:D:102:ARG:O | 1.70 | 0.91 |
| 4:G:132:ASN:HA | 5:H:54:LEU:C | 1.90 | 0.91 |
| 3:E:36:ALA:CB | 3:E:68:ILE:HD13 | 2.00 | 0.90 |
| 5:H:41:ARG:HG3 | 5:H:42:GLU:H | 1.34 | 0.90 |
| 5:H:104:TYR:CE1 | 5:H:159:ASP:HB3 | 2.07 | 0.90 |
| 1:B:146:HIS:CD2 | 1:B:205:VAL:HG22 | 2.07 | 0.90 |
| 2:C:73:ARG:HH21 | 3:E:90:LEU:HD11 | 1.35 | 0.90 |
| 1:A:108:THR:HG23 | 1:A:412:MET:HE1 | 1.53 | 0.90 |
| 1:B:32:THR:CG2 | 1:B:36:LYS:HE2 | 2.02 | 0.90 |
| 3:E:60:ILE:HD13 | 3:E:83:PHE:CE2 | 2.06 | 0.90 |
| 1:B:46:LEU:HB2 | 1:B:162:ALA:HB2 | 1.51 | 0.90 |
| 2:C:99:LYS:N | 2:D:101:ALA:CA | 2.16 | 0.90 |
| 3:F:44:GLU:HG2 | 3:F:46:TYR:N | 1.86 | 0.90 |
| 1:A:410:LEU:HD22 | 1:A:412:MET:HE2 | 1.52 | 0.90 |
| 3:F:43:GLN:H | 3:F:53:GLN:HB2 | 1.37 | 0.90 |
| 1:A:335:ARG:NH1 | 1:B:278:PHE:CZ | 2.39 | 0.90 |
| 2:C:75:MET:HB2 | 2:C:78:VAL:HB | 1.54 | 0.90 |
| 2:D:25:VAL:HG13 | 2:D:53:VAL:HG11 | 1.54 | 0.90 |
| 3:F:6:ARG:CB | 3:F:8:VAL:HG12 | 1.99 | 0.90 |
| 1:A:289:LYS:CG | 1:B:316:GLY:N | 2.29 | 0.90 |
| 1:B:444:VAL:CG1 | 1:B:449:PHE:HB2 | 2.01 | 0.90 |
| 2:C:25:VAL:HG13 | 2:C:53:VAL:HG11 | 1.54 | 0.90 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:CG | 2.34 | 0.90 |
| 1:B:37:LEU:CD1 | 1:B:168:VAL:HG21 | 2.02 | 0.89 |
| 3:E:79:LYS:HD3 | 3:F:70:LYS:N | 1.86 | 0.89 |
| 4:G:133:ASN:CB | 5:H:56:PRO:N | 2.31 | 0.89 |
| 1:A:438:MET:CG | 1:B:434:THR:C | 2.27 | 0.89 |
| 2:D:75:MET:HB2 | 2:D:78:VAL:HB | 1.54 | 0.89 |
| 2:C:4:GLN:NE2 | 3:E:1:MET:HE3 | 1.87 | 0.89 |
| 1:B:445:ALA:HA | 1:B:448:PRO:HB3 | 1.54 | 0.89 |
| 3:E:109:GLY:HA3 | 4:G:114:THR:N | 1.71 | 0.89 |
| 3:F:102:LYS:HG3 | 4:G:39:ASP:CG | 1.93 | 0.89 |
| 1:A:96:LYS:HE3 | 1:A:377:ALA:HA | 1.55 | 0.89 |
| 1:B:96:LYS:HE3 | 1:B:377:ALA:HA | 1.55 | 0.89 |
| 3:E:29:VAL:HG11 | 3:E:72:MET:HA | 1.54 | 0.89 |
| 1:A:146:HIS:CD2 | 1:A:205:VAL:HG22 | 2.07 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:289:LYS:HD3 | 1:A:319:THR:HG23 | 1.53 | 0.89 |
| 1:A:32:THR:CG2 | 1:A:36:LYS:HE2 | 2.02 | 0.89 |
| 1:B:34:ILE:HG22 | 1:B:181:LEU:HD13 | 1.51 | 0.89 |
| 2:C:94:LEU:N | 2:D:97:TYR:N | 2.20 | 0.89 |
| 3:F:43:GLN:HG2 | 3:F:53:GLN:N | 1.88 | 0.89 |
| 5:H:22:THR:HB | 5:H:108:PHE:CD2 | 2.08 | 0.89 |
| 1:A:43:PRO:HA | 1:A:164:GLU:H | 1.37 | 0.89 |
| 1:B:187:LYS:HG2 | 1:B:193:GLU:HA | 1.55 | 0.89 |
| 3:E:108:VAL:HG11 | 4:G:43:TYR:OH | 1.73 | 0.89 |
| 3:E:38:VAL:HB | 3:F:88:VAL:CG1 | 2.01 | 0.89 |
| 5:H:42:GLU:HG3 | 5:H:56:PRO:HG2 | 0.89 | 0.89 |
| 1:A:259:PHE:HE2 | 1:B:90:LYS:HD3 | 1.34 | 0.89 |
| 2:D:5:ARG:CB | 3:F:3:GLU:N | 2.35 | 0.89 |
| 1:A:37:LEU:CD1 | 1:A:168:VAL:HG21 | 2.02 | 0.89 |
| 1:A:251:GLU:HG2 | 1:B:54:MET:N | 1.87 | 0.89 |
| 2:C:94:LEU:CB | 2:D:97:TYR:CD1 | 2.56 | 0.89 |
| 3:F:20:GLY:O | 4:G:20:SER:O | 1.89 | 0.89 |
| 4:G:64:ILE:CD1 | 5:H:140:ASN:CG | 2.41 | 0.89 |
| 1:A:373:LYS:HE3 | 1:A:374:ALA:HB2 | 1.56 | 0.88 |
| 4:G:133:ASN:CG | 5:H:57:GLY:O | 2.12 | 0.88 |
| 2:C:5:ARG:CA | 3:E:3:GLU:HA | 2.02 | 0.88 |
| 1:B:295:ASN:HA | 2:D:37:HIS:ND1 | 1.86 | 0.88 |
| 2:D:63:PHE:HE2 | 2:D:86:ILE:HG23 | 1.35 | 0.88 |
| 3:F:104:ASP:N | 4:G:31:VAL:HG23 | 1.58 | 0.88 |
| 4:G:113:ILE:HG12 | 4:G:121:LYS:CA | 2.03 | 0.88 |
| 1:A:167:VAL:HG13 | 1:A:177:ILE:CD1 | 2.03 | 0.88 |
| 1:A:354:ILE:HD12 | 1:B:355:GLY:HA2 | 0.89 | 0.88 |
| 3:E:77:ARG:HB3 | 3:F:66:ASP:CA | 2.00 | 0.88 |
| 4:G:61:GLY:CA | 5:H:139:LYS:HE2 | 2.03 | 0.88 |
| 1:B:289:LYS:HD3 | 1:B:319:THR:HG23 | 1.53 | 0.88 |
| 1:A:181:LEU:H | 1:A:181:LEU:HD23 | 1.38 | 0.88 |
| 1:A:204:HIS:HE1 | 1:A:221:TYR:HB3 | 1.38 | 0.88 |
| 1:B:43:PRO:HA | 1:B:164:GLU:H | 1.38 | 0.88 |
| 1:A:187:LYS:HG2 | 1:A:193:GLU:HA | 1.55 | 0.88 |
| 1:A:339:GLU:CB | 1:B:274:THR:HG21 | 2.04 | 0.88 |
| 2:C:4:GLN:C | 3:E:1:MET:H3 | 1.76 | 0.88 |
| 2:C:74:SER:HB2 | 2:C:78:VAL:CG1 | 2.03 | 0.88 |
| 3:F:28:TRP:CZ3 | 3:F:80:ILE:HG21 | 2.08 | 0.88 |
| 1:A:142:ILE:HG21 | 1:A:145:TRP:CA | 2.03 | 0.88 |
| 1:B:108:THR:HG23 | 1:B:412:MET:HE1 | 1.55 | 0.88 |
| 1:B:181:LEU:HD23 | 1:B:181:LEU:H | 1.38 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:31:GLU:HB2 | 3:E:72:MET:HB2 | 1.55 | 0.88 |
| 1:B:142:ILE:HG21 | 1:B:145:TRP:CA | 2.03 | 0.88 |
| 4:G:133:ASN:OD1 | 5:H:57:GLY:O | 1.90 | 0.88 |
| 3:E:109:GLY:HA3 | 4:G:113:ILE:HD12 | 0.93 | 0.88 |
| 3:E:70:LYS:CB | 3:E:84:ILE:HA | 2.04 | 0.88 |
| 2:C:71:THR:CA | 3:E:92:GLY:HA2 | 2.04 | 0.88 |
| 1:A:37:LEU:CD2 | 1:A:168:VAL:HG11 | 2.05 | 0.87 |
| 1:B:163:GLU:HB2 | 1:B:182:ARG:HG3 | 1.55 | 0.87 |
| 1:B:167:VAL:HG13 | 1:B:177:ILE:CD1 | 2.03 | 0.87 |
| 1:A:460:ILE:HG13 | 1:B:466:GLN:CD | 1.92 | 0.87 |
| 2:C:94:LEU:N | 2:D:97:TYR:CA | 2.36 | 0.87 |
| 3:F:21:GLU:OE1 | 4:G:16:GLU:HG3 | 1.72 | 0.87 |
| 1:A:445:ALA:HA | 1:A:448:PRO:HB3 | 1.54 | 0.87 |
| 2:D:74:SER:HB2 | 2:D:78:VAL:CG1 | 2.03 | 0.87 |
| 3:E:8:VAL:HG22 | 3:E:34:ALA:HA | 1.55 | 0.87 |
| 5:H:137:GLU:C | 5:H:138:LEU:HA | 1.94 | 0.87 |
| 1:A:381:ILE:HG23 | 1:A:385:LEU:HD13 | 1.57 | 0.87 |
| 2:D:4:GLN:OE1 | 3:F:2:TYR:N | 2.07 | 0.87 |
| 5:H:143:ILE:HG12 | 5:H:147:PRO:HG2 | 1.55 | 0.87 |
| 1:A:163:GLU:HB2 | 1:A:182:ARG:HG3 | 1.55 | 0.87 |
| 1:B:294:GLU:HB3 | 2:C:42:ASP:OD2 | 1.74 | 0.87 |
| 1:B:114:LEU:HD21 | 1:B:392:PHE:CE1 | 2.09 | 0.87 |
| 2:C:63:PHE:HE2 | 2:C:86:ILE:HG23 | 1.35 | 0.87 |
| 3:E:40:PRO:HA | 3:F:100:LYS:CD | 2.04 | 0.87 |
| 5:H:112:TYR:N | 5:H:132:LEU:HB3 | 1.89 | 0.87 |
| 1:A:354:ILE:HD11 | 1:B:354:ILE:O | 1.75 | 0.87 |
| 1:A:44:GLU:HB3 | 1:A:45:PRO:HD3 | 1.54 | 0.87 |
| 2:D:93:LYS:HG2 | 2:D:94:LEU:CD1 | 2.04 | 0.87 |
| 3:E:50:GLN:HE21 | 3:F:52:LEU:HB2 | 1.39 | 0.87 |
| 1:B:323:GLU:HG3 | 1:B:325:PRO:HD2 | 1.55 | 0.87 |
| 1:A:460:ILE:CG1 | 1:B:466:GLN:CG | 2.41 | 0.87 |
| 5:H:16:GLN:HB3 | 5:H:27:LEU:H | 1.39 | 0.87 |
| 1:A:292:ASP:OD1 | 2:C:34:ASP:C | 2.14 | 0.87 |
| 1:A:114:LEU:HD21 | 1:A:392:PHE:CE1 | 2.09 | 0.87 |
| 1:B:255:SER:HB2 | 1:B:256:ASP:HA | 1.56 | 0.87 |
| 1:B:381:ILE:HG23 | 1:B:385:LEU:HD13 | 1.57 | 0.87 |
| 2:C:54:LEU:HD11 | 2:D:28:LEU:HD21 | 1.55 | 0.87 |
| 3:F:28:TRP:HH2 | 3:F:80:ILE:HD13 | 1.39 | 0.87 |
| 5:H:90:LYS:HZ1 | 5:H:146:LEU:HD13 | 1.38 | 0.87 |
| 1:A:88:TRP:HA | 1:A:88:TRP:HE3 | 1.40 | 0.86 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:HB3 | 1.90 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:32:PHE:CD2 | 3:F:67:ARG:HD2 | 2.10 | 0.86 |
| 3:E:105:GLY:HA3 | 4:G:119:VAL:HG23 | 1.56 | 0.86 |
| 5:H:60:ALA:HB3 | 5:H:134:VAL:CG1 | 2.04 | 0.86 |
| 4:G:64:ILE:HD12 | 5:H:140:ASN:CG | 1.94 | 0.86 |
| 1:B:367:TYR:CB | 1:B:369:LEU:HA | 2.04 | 0.86 |
| 1:B:373:LYS:HE3 | 1:B:374:ALA:HB2 | 1.56 | 0.86 |
| 1:B:44:GLU:HB3 | 1:B:45:PRO:HD3 | 1.54 | 0.86 |
| 2:D:70:LEU:O | 3:F:91:SER:CB | 2.23 | 0.86 |
| 3:E:81:VAL:CG2 | 3:F:86:ASP:HB3 | 2.05 | 0.86 |
| 4:G:44:VAL:HG13 | 4:G:70:VAL:HA | 1.57 | 0.86 |
| 1:B:96:LYS:CG | 1:B:373:LYS:HB2 | 2.05 | 0.86 |
| 1:A:255:SER:HB2 | 1:A:256:ASP:HA | 1.56 | 0.86 |
| 1:A:96:LYS:CG | 1:A:373:LYS:HB2 | 2.05 | 0.86 |
| 1:B:296:PRO:HB3 | 2:D:36:CYS:O | 0.96 | 0.86 |
| 1:A:379:ARG:HD2 | 1:B:94:ASP:OD2 | 1.76 | 0.86 |
| 4:G:113:ILE:HG21 | 4:G:121:LYS:HD3 | 1.57 | 0.86 |
| 1:A:323:GLU:HG3 | 1:A:325:PRO:HD2 | 1.55 | 0.86 |
| 1:A:367:TYR:CB | 1:A:369:LEU:HA | 2.04 | 0.86 |
| 2:D:5:ARG:HB3 | 3:F:2:TYR:CB | 2.04 | 0.86 |
| 3:E:43:GLN:HG2 | 3:E:53:GLN:N | 1.90 | 0.86 |
| 3:E:79:LYS:CD | 3:F:70:LYS:HB3 | 2.05 | 0.86 |
| 3:F:104:ASP:CA | 4:G:31:VAL:CG2 | 2.37 | 0.86 |
| 3:E:105:GLY:O | 4:G:41:TYR:CD2 | 2.29 | 0.86 |
| 5:H:42:GLU:OE2 | 5:H:56:PRO:HD3 | 1.76 | 0.86 |
| 1:B:225:ASN:HB2 | 1:B:226:PRO:HA | 1.56 | 0.86 |
| 1:A:460:ILE:CG2 | 1:B:467:TYR:HB3 | 2.03 | 0.86 |
| 2:C:94:LEU:H | 2:D:97:TYR:CA | 1.87 | 0.86 |
| 2:D:4:GLN:HA | 3:F:1:MET:HB3 | 0.87 | 0.86 |
| 1:B:204:HIS:HE1 | 1:B:221:TYR:HB3 | 1.38 | 0.86 |
| 1:B:292:ASP:OD1 | 2:D:34:ASP:C | 2.14 | 0.86 |
| 1:A:466:GLN:HG3 | 1:A:467:TYR:CG | 2.11 | 0.86 |
| 2:C:5:ARG:HB3 | 3:E:3:GLU:CA | 2.00 | 0.86 |
| 3:E:89:ASP:HA | 3:E:97:THR:HA | 1.57 | 0.86 |
| 3:F:22:GLY:H | 4:G:19:GLU:HG3 | 1.38 | 0.86 |
| 1:B:179:PHE:HE1 | 1:B:244:ILE:HD13 | 1.40 | 0.86 |
| 2:C:93:LYS:HG2 | 2:C:94:LEU:CD1 | 2.04 | 0.86 |
| 5:H:91:PHE:CE2 | 5:H:111:ALA:HB1 | 2.11 | 0.86 |
| 4:G:59:SER:OG | 5:H:138:LEU:CD1 | 2.19 | 0.86 |
| 5:H:37:VAL:CB | 5:H:64:GLU:HG2 | 2.05 | 0.86 |
| 1:B:142:ILE:HG21 | 1:B:145:TRP:HA | 1.58 | 0.85 |
| 1:B:367:TYR:HD2 | 1:B:369:LEU:HD23 | 1.40 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:5:ARG:HG3 | 2:D:8:ARG:N | 1.91 | 0.85 |
| 2:C:90:ILE:HG12 | 2:D:91:LEU:HB3 | 1.57 | 0.85 |
| 1:A:37:LEU:HD13 | 1:A:168:VAL:CG2 | 2.06 | 0.85 |
| 1:A:86:HIS:CE1 | 1:A:88:TRP:HB2 | 2.11 | 0.85 |
| 1:B:324:ILE:HB | 1:B:325:PRO:HD3 | 1.58 | 0.85 |
| 2:C:34:ASP:HB3 | 2:C:36:CYS:H | 1.38 | 0.85 |
| 1:A:179:PHE:HE1 | 1:A:244:ILE:HD13 | 1.40 | 0.85 |
| 3:F:32:PHE:CZ | 3:F:67:ARG:HB2 | 2.11 | 0.85 |
| 1:A:114:LEU:HD21 | 1:A:392:PHE:CZ | 2.12 | 0.85 |
| 3:E:29:VAL:HB | 3:E:73:ARG:H | 1.38 | 0.85 |
| 5:H:90:LYS:CD | 5:H:150:ILE:HD11 | 2.06 | 0.85 |
| 2:C:73:ARG:HH21 | 3:E:90:LEU:CD1 | 1.90 | 0.85 |
| 1:A:225:ASN:HB2 | 1:A:226:PRO:HA | 1.56 | 0.85 |
| 1:B:114:LEU:HD21 | 1:B:392:PHE:CZ | 2.12 | 0.85 |
| 2:C:5:ARG:HG3 | 2:C:8:ARG:N | 1.92 | 0.85 |
| 2:D:63:PHE:CE2 | 2:D:85:GLU:HB3 | 2.12 | 0.85 |
| 1:A:100:LEU:HG | 1:A:377:ALA:HB1 | 1.59 | 0.85 |
| 1:A:289:LYS:CG | 1:B:315:GLY:C | 2.44 | 0.85 |
| 1:A:460:ILE:HG13 | 1:B:466:GLN:HG3 | 0.87 | 0.85 |
| 2:C:63:PHE:CE2 | 2:C:85:GLU:HB3 | 2.12 | 0.85 |
| 3:F:105:GLY:C | 4:G:38:ASP:N | 2.27 | 0.85 |
| 1:A:335:ARG:HD3 | 1:B:333:LEU:HB3 | 1.57 | 0.85 |
| 1:B:466:GLN:HG3 | 1:B:467:TYR:CG | 2.10 | 0.85 |
| 2:C:93:LYS:NZ | 2:D:96:PRO:O | 2.10 | 0.85 |
| 1:A:336:ILE:HD13 | 1:B:278:PHE:HA | 1.57 | 0.85 |
| 1:B:310:LYS:CA | 2:C:38:ASN:HD22 | 1.89 | 0.85 |
| 2:D:34:ASP:HB3 | 2:D:36:CYS:H | 1.38 | 0.85 |
| 3:E:1:MET:HG3 | 3:E:2:TYR:H | 1.40 | 0.85 |
| 1:B:292:ASP:CB | 2:D:31:PHE:O | 2.25 | 0.85 |
| 1:A:295:ASN:HA | 2:C:37:HIS:ND1 | 1.86 | 0.84 |
| 1:B:100:LEU:HG | 1:B:377:ALA:HB1 | 1.59 | 0.84 |
| 2:C:4:GLN:HG2 | 3:E:1:MET:SD | 2.16 | 0.84 |
| 3:E:65:ASP:CB | 3:E:97:THR:HB | 2.07 | 0.84 |
| 4:G:102:PHE:HD1 | 5:H:56:PRO:HD3 | 1.40 | 0.84 |
| 1:A:34:ILE:HG22 | 1:A:181:LEU:CD1 | 2.07 | 0.84 |
| 2:C:84:THR:OG1 | 2:D:83:ALA:HA | 1.77 | 0.84 |
| 3:E:56:ILE:HD13 | 4:G:40:PRO:O | 1.77 | 0.84 |
| 5:H:91:PHE:CZ | 5:H:111:ALA:HB1 | 2.12 | 0.84 |
| 1:A:142:ILE:HG21 | 1:A:145:TRP:HA | 1.59 | 0.84 |
| 1:B:170:LYS:HB3 | 1:B:178:LEU:CD2 | 2.06 | 0.84 |
| 2:C:89:THR:CB | 2:D:88:SER:HB3 | 2.06 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:E:91:SER:O | 3:E:96:ILE:HG12 | 1.78 | 0.84 |
| 5:H:162:GLN:HB2 | 5:H:163:PRO:HD3 | 1.56 | 0.84 |
| 1:A:292:ASP:CB | 2:C:31:PHE:O | 2.25 | 0.84 |
| 1:B:140:LYS:HB2 | 1:B:257:LEU:HD23 | 1.59 | 0.84 |
| 1:B:310:LYS:HB3 | 2:C:38:ASN:HB2 | 1.59 | 0.84 |
| 3:F:47:TYR:HB3 | 3:F:50:GLN:HB3 | 1.58 | 0.84 |
| 4:G:63:ASN:N | 5:H:139:LYS:HB3 | 1.92 | 0.84 |
| 1:A:140:LYS:HB2 | 1:A:257:LEU:HD23 | 1.59 | 0.84 |
| 1:A:367:TYR:HD2 | 1:A:369:LEU:HD23 | 1.40 | 0.84 |
| 1:A:371:ASP:C | 1:B:363:LEU:HD21 | 1.90 | 0.84 |
| 4:G:44:VAL:HG21 | 4:G:74:THR:N | 1.93 | 0.84 |
| 5:H:60:ALA:CB | 5:H:134:VAL:HG11 | 2.07 | 0.84 |
| 4:G:62:GLU:N | 5:H:139:LYS:H | 1.73 | 0.84 |
| 1:B:381:ILE:CG2 | 1:B:385:LEU:HD13 | 2.08 | 0.84 |
| 1:A:460:ILE:CB | 1:B:467:TYR:HB3 | 2.06 | 0.84 |
| 3:E:47:TYR:HB3 | 3:E:50:GLN:HB2 | 1.57 | 0.84 |
| 3:E:103:GLU:OE2 | 4:G:42:PRO:HD3 | 1.67 | 0.84 |
| 1:A:324:ILE:HB | 1:A:325:PRO:HD3 | 1.58 | 0.84 |
| 1:A:333:LEU:CD2 | 1:B:282:GLN:NE2 | 2.39 | 0.84 |
| 1:B:310:LYS:CB | 2:C:38:ASN:ND2 | 2.11 | 0.84 |
| 2:C:94:LEU:H | 2:D:97:TYR:HB2 | 1.42 | 0.84 |
| 2:C:4:GLN:HG2 | 3:E:1:MET:CE | 2.03 | 0.84 |
| 1:B:170:LYS:CB | 1:B:178:LEU:HD22 | 2.08 | 0.84 |
| 3:E:36:ALA:HA | 3:E:62:THR:CG2 | 2.08 | 0.84 |
| 3:F:64:TYR:CE1 | 3:F:95:GLU:HB2 | 2.12 | 0.84 |
| 1:B:86:HIS:CE1 | 1:B:88:TRP:HB2 | 2.11 | 0.84 |
| 2:C:99:LYS:HG3 | 2:D:101:ALA:HB1 | 0.84 | 0.84 |
| 3:E:15:VAL:HG12 | 3:E:73:ARG:NE | 1.92 | 0.84 |
| 2:D:5:ARG:CA | 3:F:3:GLU:CA | 2.49 | 0.84 |
| 1:B:34:ILE:HG22 | 1:B:181:LEU:CD1 | 2.07 | 0.83 |
| 1:B:88:TRP:HA | 1:B:88:TRP:HE3 | 1.40 | 0.83 |
| 1:B:310:LYS:CB | 2:C:38:ASN:CB | 2.56 | 0.83 |
| 2:D:25:VAL:HB | 2:D:26:PRO:HD3 | 1.58 | 0.83 |
| 1:B:292:ASP:OD1 | 2:D:35:GLU:N | 2.12 | 0.83 |
| 2:D:41:ILE:CG2 | 2:D:45:GLY:HA2 | 2.08 | 0.83 |
| 4:G:102:PHE:CD1 | 5:H:56:PRO:HD3 | 2.13 | 0.83 |
| 1:B:46:LEU:CB | 1:B:162:ALA:HB2 | 2.08 | 0.83 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:N | 2.26 | 0.83 |
| 5:H:149:GLU:O | 5:H:153:VAL:HG12 | 1.79 | 0.83 |
| 1:A:171:ASP:CB | 1:A:178:LEU:HD11 | 2.08 | 0.83 |
| 1:A:416:ARG:HB2 | 1:A:417:THR:O | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:LEU:CD2 | 1:B:282:GLN:HE22 | 1.91 | 0.83 |
| 1:A:292:ASP:OD1 | 2:C:35:GLU:N | 2.12 | 0.83 |
| 3:E:52:LEU:HB3 | 3:E:53:GLN:HB2 | 1.58 | 0.83 |
| 3:F:16:GLU:O | 3:F:26:TYR:HA | 1.79 | 0.83 |
| 1:A:381:ILE:CG2 | 1:A:385:LEU:HD13 | 2.08 | 0.83 |
| 2:C:7:LYS:NZ | 3:E:4:GLU:OE2 | 2.10 | 0.83 |
| 3:F:40:PRO:HB2 | 3:F:42:SER:HB3 | 1.58 | 0.83 |
| 4:G:113:ILE:HG12 | 4:G:121:LYS:HA | 1.61 | 0.83 |
| 1:B:171:ASP:CB | 1:B:178:LEU:HD11 | 2.08 | 0.83 |
| 3:F:45:GLU:HA | 3:F:47:TYR:CE1 | 2.13 | 0.83 |
| 5:H:141:GLY:C | 5:H:142:GLU:HB3 | 1.98 | 0.83 |
| 5:H:46:GLU:N | 5:H:151:VAL:HG21 | 1.94 | 0.83 |
| 1:A:46:LEU:CG | 1:A:162:ALA:HB2 | 2.07 | 0.83 |
| 1:B:376:MET:HE2 | 1:B:379:ARG:NH2 | 1.94 | 0.83 |
| 2:D:20:TYR:O | 2:D:24:MET:HG3 | 1.79 | 0.83 |
| 3:E:65:ASP:HB3 | 3:E:97:THR:CB | 2.07 | 0.83 |
| 1:B:144:TYR:CZ | 1:B:246:PRO:HB3 | 2.13 | 0.83 |
| 1:B:46:LEU:CG | 1:B:162:ALA:HB2 | 2.07 | 0.83 |
| 2:C:25:VAL:HB | 2:C:26:PRO:HD3 | 1.58 | 0.83 |
| 2:C:4:GLN:HE21 | 3:E:1:MET:CE | 1.89 | 0.83 |
| 3:F:60:ILE:HD12 | 3:F:83:PHE:CD2 | 2.14 | 0.83 |
| 1:A:46:LEU:CB | 1:A:162:ALA:HB2 | 2.08 | 0.83 |
| 1:A:64:ARG:HH21 | 1:B:284:ILE:CB | 1.91 | 0.83 |
| 1:B:367:TYR:CB | 1:B:368:ALA:HA | 2.05 | 0.83 |
| 2:C:20:TYR:O | 2:C:24:MET:HG3 | 1.79 | 0.83 |
| 2:C:63:PHE:CZ | 2:C:85:GLU:HB3 | 2.14 | 0.83 |
| 1:A:248:LYS:O | 1:A:253:MET:HG2 | 1.79 | 0.83 |
| 1:B:121:LEU:HB3 | 1:B:124:ASP:N | 1.94 | 0.83 |
| 2:D:70:LEU:N | 3:F:93:LEU:N | 2.25 | 0.83 |
| 3:E:44:GLU:HG2 | 3:E:47:TYR:H | 1.42 | 0.83 |
| 3:E:73:ARG:NH1 | 3:E:80:ILE:HD12 | 1.92 | 0.83 |
| 5:H:143:ILE:HG12 | 5:H:147:PRO:CG | 2.09 | 0.83 |
| 1:A:170:LYS:HB3 | 1:A:178:LEU:CD2 | 2.06 | 0.82 |
| 1:B:441:GLU:HG3 | 1:B:453:PRO:HA | 1.61 | 0.82 |
| 1:A:379:ARG:HD2 | 1:B:94:ASP:HB2 | 1.58 | 0.82 |
| 1:B:294:GLU:CG | 2:C:41:ILE:C | 2.47 | 0.82 |
| 3:E:21:GLU:HG3 | 3:E:22:GLY:H | 1.44 | 0.82 |
| 1:A:144:TYR:CZ | 1:A:246:PRO:HB3 | 2.13 | 0.82 |
| 1:A:38:ILE:HG21 | 1:A:183:TYR:CE2 | 2.15 | 0.82 |
| 1:A:209:GLU:HG3 | 1:A:211:ILE:HG12 | 1.60 | 0.82 |
| 1:A:202:ASP:HA | 1:A:242:VAL:HG23 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:202:ASP:HA | 1:B:242:VAL:HG23 | 1.61 | 0.82 |
| 2:C:92:LYS:HB2 | 2:D:92:LYS:HE2 | 1.60 | 0.82 |
| 2:D:75:MET:CE | 3:F:90:LEU:HD21 | 2.09 | 0.82 |
| 1:A:115:LEU:HG | 1:A:119:ASN:HD21 | 1.44 | 0.82 |
| 3:E:69:ASP:CB | 3:E:87:PRO:HG3 | 2.07 | 0.82 |
| 3:F:12:GLN:HG2 | 3:F:75:ILE:CG1 | 2.08 | 0.82 |
| 1:A:121:LEU:HB3 | 1:A:124:ASP:N | 1.94 | 0.82 |
| 1:A:121:LEU:O | 1:A:124:ASP:HB2 | 1.79 | 0.82 |
| 2:C:41:ILE:CG2 | 2:C:45:GLY:HA2 | 2.08 | 0.82 |
| 3:E:12:GLN:HB2 | 3:E:28:TRP:CE3 | 2.14 | 0.82 |
| 1:B:115:LEU:HG | 1:B:119:ASN:HD21 | 1.44 | 0.82 |
| 1:B:37:LEU:HD13 | 1:B:168:VAL:CG2 | 2.06 | 0.82 |
| 2:D:63:PHE:CZ | 2:D:85:GLU:HB3 | 2.14 | 0.82 |
| 3:E:51:GLN:HG3 | 3:E:52:LEU:CD2 | 2.08 | 0.82 |
| 1:A:114:LEU:O | 1:A:118:VAL:HG23 | 1.79 | 0.82 |
| 1:A:169:TYR:CG | 1:A:174:ARG:HA | 2.15 | 0.82 |
| 1:B:209:GLU:HG3 | 1:B:211:ILE:HG12 | 1.60 | 0.82 |
| 2:C:94:LEU:HA | 2:D:97:TYR:HA | 1.58 | 0.82 |
| 2:D:55:ILE:HD11 | 2:D:94:LEU:HD21 | 1.61 | 0.82 |
| 1:A:376:MET:HE2 | 1:A:379:ARG:NH2 | 1.94 | 0.82 |
| 2:C:73:ARG:NE | 3:E:91:SER:HB3 | 1.94 | 0.82 |
| 4:G:21:TYR:HB3 | 4:G:24:LEU:CB | 2.02 | 0.82 |
| 4:G:62:GLU:H | 5:H:139:LYS:H | 1.26 | 0.82 |
| 4:G:49:GLN:HG2 | 4:G:67:ASP:OD2 | 1.80 | 0.82 |
| 4:G:76:ARG:HG2 | 4:G:125:ILE:CD1 | 2.10 | 0.82 |
| 1:B:248:LYS:O | 1:B:253:MET:HG2 | 1.79 | 0.82 |
| 2:C:89:THR:HG1 | 2:D:88:SER:HB3 | 1.45 | 0.82 |
| 3:F:21:GLU:CG | 4:G:19:GLU:OE2 | 2.19 | 0.82 |
| 3:F:43:GLN:HB2 | 3:F:47:TYR:HE1 | 1.45 | 0.82 |
| 1:B:114:LEU:O | 1:B:118:VAL:HG23 | 1.79 | 0.82 |
| 1:B:169:TYR:CG | 1:B:174:ARG:HA | 2.15 | 0.82 |
| 1:A:251:GLU:HG2 | 1:B:54:MET:CA | 2.05 | 0.82 |
| 2:C:71:THR:H | 3:E:92:GLY:HA2 | 1.03 | 0.82 |
| 3:F:89:ASP:CB | 3:F:95:GLU:HB3 | 2.10 | 0.82 |
| 3:F:90:LEU:HB2 | 3:F:98:ARG:HD3 | 1.60 | 0.82 |
| 1:A:354:ILE:CD1 | 1:B:355:GLY:CA | 2.45 | 0.82 |
| 3:E:47:TYR:HB3 | 3:E:50:GLN:CG | 2.09 | 0.82 |
| 1:A:232:LYS:HB2 | 1:A:237:ILE:HB | 1.61 | 0.81 |
| 1:A:370:LEU:O | 1:A:373:LYS:HG3 | 1.80 | 0.81 |
| 1:B:416:ARG:HB2 | 1:B:417:THR:O | 1.78 | 0.81 |
| 2:C:99:LYS:HB2 | 2:D:101:ALA:CB | 1.78 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:C:30:GLU:O | 2:C:35:GLU:HG3 | 1.80 | 0.81 |
| 1:A:38:ILE:HD11 | 1:A:181:LEU:HD12 | 1.61 | 0.81 |
| 1:B:121:LEU:O | 1:B:124:ASP:HB2 | 1.79 | 0.81 |
| 1:B:37:LEU:CD2 | 1:B:168:VAL:HG11 | 2.05 | 0.81 |
| 1:B:370:LEU:O | 1:B:373:LYS:HG3 | 1.80 | 0.81 |
| 3:F:104:ASP:H | 4:G:31:VAL:HG21 | 0.65 | 0.81 |
| 1:A:460:ILE:CD1 | 1:B:466:GLN:CD | 2.49 | 0.81 |
| 2:D:41:ILE:HG22 | 2:D:42:ASP:O | 1.81 | 0.81 |
| 4:G:100:PHE:HE1 | 5:H:45:ASP:N | 1.73 | 0.81 |
| 2:C:63:PHE:CZ | 2:C:82:PHE:HA | 2.15 | 0.81 |
| 2:D:69:GLY:HA2 | 2:D:72:GLY:C | 2.00 | 0.81 |
| 1:B:171:ASP:HB2 | 1:B:178:LEU:HD11 | 1.60 | 0.81 |
| 1:B:96:LYS:CB | 1:B:373:LYS:HB2 | 2.10 | 0.81 |
| 1:B:38:ILE:HG21 | 1:B:183:TYR:CE2 | 2.15 | 0.81 |
| 2:C:55:ILE:HD11 | 2:C:94:LEU:HD21 | 1.61 | 0.81 |
| 2:D:30:GLU:O | 2:D:35:GLU:HG3 | 1.80 | 0.81 |
| 3:E:60:ILE:HG12 | 3:E:99:ILE:CG1 | 2.10 | 0.81 |
| 2:D:6:VAL:H | 3:F:3:GLU:HA | 1.45 | 0.81 |
| 1:A:96:LYS:CB | 1:A:373:LYS:HB2 | 2.10 | 0.81 |
| 1:A:382:ARG:NH2 | 1:A:385:LEU:HD23 | 1.95 | 0.81 |
| 1:B:241:ARG:NH2 | 1:B:245:ILE:HG12 | 1.96 | 0.81 |
| 2:C:94:LEU:C | 2:D:97:TYR:HB2 | 2.01 | 0.81 |
| 2:C:89:THR:CG2 | 2:D:88:SER:O | 2.28 | 0.81 |
| 3:E:40:PRO:CB | 3:E:42:SER:HB2 | 2.11 | 0.81 |
| 3:F:63:PRO:CB | 3:F:96:ILE:HG22 | 2.11 | 0.81 |
| 1:A:241:ARG:NH2 | 1:A:245:ILE:HG12 | 1.96 | 0.81 |
| 1:A:69:ALA:N | 1:B:300:THR:CG2 | 2.38 | 0.81 |
| 1:B:298:GLU:HG3 | 2:C:42:ASP:HB3 | 1.62 | 0.81 |
| 1:A:352:GLU:HG3 | 1:A:354:ILE:H | 1.45 | 0.81 |
| 1:B:38:ILE:HD11 | 1:B:181:LEU:HD12 | 1.61 | 0.81 |
| 1:B:62:LYS:HE2 | 1:B:63:ARG:HG3 | 1.61 | 0.81 |
| 2:C:4:GLN:HE21 | 3:E:1:MET:HE2 | 1.42 | 0.81 |
| 4:G:31:VAL:CG2 | 4:G:32:THR:HA | 2.10 | 0.81 |
| 4:G:34:SER:O | 4:G:37:LYS:HD2 | 1.80 | 0.81 |
| 3:E:75:ILE:CG1 | 3:E:80:ILE:HG22 | 2.11 | 0.81 |
| 1:A:441:GLU:HG3 | 1:A:453:PRO:HA | 1.61 | 0.80 |
| 1:A:62:LYS:HE3 | 1:A:81:ASN:CA | 2.12 | 0.80 |
| 2:D:63:PHE:CZ | 2:D:82:PHE:HA | 2.15 | 0.80 |
| 2:C:85:GLU:CA | 2:D:86:ILE:HD12 | 2.08 | 0.80 |
| 4:G:16:GLU:O | 4:G:19:GLU:HG2 | 1.80 | 0.80 |
| 4:G:22:GLN:O | 4:G:25:MET:HG2 | 1.81 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CD1 | 2.16 | 0.80 |
| 1:A:171:ASP:H | 1:A:178:LEU:HD13 | 1.46 | 0.80 |
| 1:B:171:ASP:H | 1:B:178:LEU:HD13 | 1.46 | 0.80 |
| 1:B:187:LYS:HD3 | 1:B:193:GLU:HB3 | 1.63 | 0.80 |
| 1:B:88:TRP:HA | 1:B:88:TRP:CE3 | 2.11 | 0.80 |
| 2:C:41:ILE:HG22 | 2:C:42:ASP:O | 1.81 | 0.80 |
| 2:C:66:THR:HG21 | 2:D:82:PHE:CD2 | 2.13 | 0.80 |
| 2:C:69:GLY:HA2 | 2:C:72:GLY:C | 2.00 | 0.80 |
| 3:E:84:ILE:HD12 | 3:E:103:GLU:HG2 | 1.61 | 0.80 |
| 5:H:111:ALA:HA | 5:H:132:LEU:CD1 | 2.10 | 0.80 |
| 1:A:252:GLU:CB | 1:A:254:VAL:HG13 | 2.11 | 0.80 |
| 3:E:44:GLU:CG | 3:E:46:TYR:HB2 | 2.11 | 0.80 |
| 3:F:45:GLU:HA | 3:F:47:TYR:CD1 | 2.16 | 0.80 |
| 4:G:86:VAL:O | 4:G:90:LEU:HD13 | 1.81 | 0.80 |
| 1:A:187:LYS:HD3 | 1:A:193:GLU:HB3 | 1.64 | 0.80 |
| 1:A:59:ILE:H | 1:A:59:ILE:HD12 | 1.46 | 0.80 |
| 1:A:88:TRP:HA | 1:A:88:TRP:CE3 | 2.11 | 0.80 |
| 1:B:310:LYS:HB2 | 2:C:38:ASN:CB | 2.11 | 0.80 |
| 2:D:50:PRO:HG2 | 2:D:53:VAL:HG21 | 1.62 | 0.80 |
| 1:B:58:ASP:HB3 | 1:B:81:ASN:HD21 | 1.44 | 0.80 |
| 2:C:54:LEU:CD1 | 2:D:28:LEU:HD21 | 2.10 | 0.80 |
| 3:F:104:ASP:HB2 | 4:G:31:VAL:HB | 1.62 | 0.80 |
| 1:B:62:LYS:HE3 | 1:B:81:ASN:CA | 2.12 | 0.80 |
| 2:C:99:LYS:N | 2:D:101:ALA:N | 2.26 | 0.80 |
| 3:F:17:GLN:HB3 | 3:F:19:ASN:HD21 | 1.46 | 0.80 |
| 4:G:41:TYR:HD2 | 4:G:119:VAL:HG21 | 1.45 | 0.80 |
| 1:A:58:ASP:HB3 | 1:A:81:ASN:HD21 | 1.44 | 0.80 |
| 1:B:96:LYS:HB2 | 1:B:373:LYS:HB2 | 1.63 | 0.80 |
| 1:B:382:ARG:NH2 | 1:B:385:LEU:HD23 | 1.95 | 0.80 |
| 2:C:50:PRO:HG2 | 2:C:53:VAL:HG21 | 1.62 | 0.80 |
| 5:H:46:GLU:CB | 5:H:151:VAL:HB | 2.12 | 0.80 |
| 1:A:171:ASP:HB2 | 1:A:178:LEU:HD11 | 1.60 | 0.80 |
| 1:A:38:ILE:HG12 | 1:A:181:LEU:HG | 1.64 | 0.80 |
| 1:A:299:PHE:HA | 1:A:302:ASN:HD21 | 1.44 | 0.80 |
| 1:A:367:TYR:HB3 | 1:A:369:LEU:CA | 2.08 | 0.80 |
| 1:A:408:LYS:O | 1:A:411:THR:HG22 | 1.81 | 0.80 |
| 1:A:62:LYS:HE2 | 1:A:63:ARG:HG3 | 1.61 | 0.80 |
| 1:B:200:TYR:CD1 | 1:B:205:VAL:HG13 | 2.17 | 0.80 |
| 3:E:37:HIS:CD2 | 3:F:88:VAL:HB | 2.16 | 0.80 |
| 3:E:84:ILE:H | 3:E:84:ILE:HD13 | 1.47 | 0.80 |
| 3:F:28:TRP:CH2 | 3:F:80:ILE:HD13 | 2.16 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CG | 2.17 | 0.80 |
| 1:A:200:TYR:CD1 | 1:A:205:VAL:HG13 | 2.17 | 0.80 |
| 1:A:367:TYR:CB | 1:A:368:ALA:HA | 2.05 | 0.80 |
| 1:A:96:LYS:HG2 | 1:A:373:LYS:CD | 2.12 | 0.80 |
| 1:A:96:LYS:HB2 | 1:A:373:LYS:HB2 | 1.63 | 0.80 |
| 1:B:38:ILE:HG12 | 1:B:181:LEU:HG | 1.64 | 0.80 |
| 1:B:252:GLU:CB | 1:B:254:VAL:HG13 | 2.11 | 0.80 |
| 1:B:408:LYS:O | 1:B:411:THR:HG22 | 1.81 | 0.80 |
| 1:B:46:LEU:HD22 | 1:B:162:ALA:HB2 | 1.64 | 0.80 |
| 1:B:59:ILE:HD12 | 1:B:59:ILE:H | 1.46 | 0.80 |
| 2:D:70:LEU:H | 3:F:93:LEU:N | 1.78 | 0.80 |
| 3:E:66:ASP:HA | 3:E:87:PRO:CB | 2.11 | 0.80 |
| 3:E:86:ASP:OD1 | 3:E:100:LYS:HB3 | 1.82 | 0.80 |
| 3:F:61:TYR:HB2 | 3:F:98:ARG:HG3 | 1.64 | 0.80 |
| 4:G:63:ASN:N | 5:H:139:LYS:CB | 2.44 | 0.80 |
| 5:H:143:ILE:HG21 | 5:H:147:PRO:HD3 | 1.64 | 0.80 |
| 1:A:320:LEU:HB2 | 1:A:321:ARG:O | 1.83 | 0.79 |
| 1:B:367:TYR:CD2 | 1:B:369:LEU:HB3 | 2.16 | 0.79 |
| 1:B:55:CYS:SG | 1:B:83:ARG:HB2 | 2.21 | 0.79 |
| 2:C:98:ARG:CA | 2:D:97:TYR:CE2 | 2.64 | 0.79 |
| 3:F:24:LYS:HG2 | 3:F:25:THR:H | 1.45 | 0.79 |
| 1:B:232:LYS:HB2 | 1:B:237:ILE:HB | 1.61 | 0.79 |
| 1:B:352:GLU:HG3 | 1:B:354:ILE:H | 1.45 | 0.79 |
| 3:F:12:GLN:HG2 | 3:F:75:ILE:CD1 | 2.11 | 0.79 |
| 5:H:143:ILE:H | 5:H:143:ILE:HD12 | 1.46 | 0.79 |
| 1:A:170:LYS:CB | 1:A:178:LEU:HD22 | 2.08 | 0.79 |
| 1:A:260:TYR:O | 1:A:264:ILE:HG13 | 1.82 | 0.79 |
| 1:A:76:ASP:OD2 | 1:A:79:LYS:HG2 | 1.82 | 0.79 |
| 1:B:96:LYS:HG2 | 1:B:373:LYS:HD2 | 1.65 | 0.79 |
| 1:B:417:THR:HB | 1:B:418:ARG:HA | 1.64 | 0.79 |
| 3:E:79:LYS:CE | 3:F:69:ASP:HB3 | 2.12 | 0.79 |
| 1:B:299:PHE:HA | 1:B:302:ASN:HD21 | 1.44 | 0.79 |
| 3:F:105:GLY:CA | 4:G:39:ASP:CB | 2.46 | 0.79 |
| 3:E:77:ARG:HH12 | 3:F:64:TYR:HA | 1.47 | 0.79 |
| 4:G:44:VAL:CG1 | 4:G:70:VAL:HG12 | 2.13 | 0.79 |
| 1:A:440:LYS:HD3 | 1:A:440:LYS:O | 1.82 | 0.79 |
| 1:A:96:LYS:HG2 | 1:A:373:LYS:HD2 | 1.65 | 0.79 |
| 1:B:260:TYR:O | 1:B:264:ILE:HG13 | 1.82 | 0.79 |
| 1:B:62:LYS:HE3 | 1:B:81:ASN:HB2 | 1.65 | 0.79 |
| 1:B:96:LYS:HG2 | 1:B:373:LYS:CD | 2.12 | 0.79 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:H | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:53:ILE:O | 5:H:54:LEU:N | 2.14 | 0.79 |
| 1:A:367:TYR:CD2 | 1:A:369:LEU:HB3 | 2.16 | 0.79 |
| 1:A:417:THR:HB | 1:A:418:ARG:HA | 1.64 | 0.79 |
| 4:G:27:MET:HG2 | 4:G:31:VAL:HG13 | 1.64 | 0.79 |
| 1:A:410:LEU:CD2 | 1:A:412:MET:HG2 | 2.13 | 0.79 |
| 1:A:55:CYS:SG | 1:A:83:ARG:HB2 | 2.21 | 0.79 |
| 1:A:254:VAL:CG1 | 1:B:85:SER:OG | 2.31 | 0.79 |
| 1:B:99:TYR:HB2 | 1:B:370:LEU:HD12 | 1.65 | 0.79 |
| 2:D:82:PHE:O | 2:D:86:ILE:HG12 | 1.83 | 0.79 |
| 3:E:53:GLN:HG3 | 4:G:40:PRO:CG | 2.10 | 0.79 |
| 1:A:331:LYS:O | 1:A:334:GLU:HG2 | 1.83 | 0.79 |
| 1:A:382:ARG:CG | 1:A:383:ALA:HA | 2.12 | 0.79 |
| 1:A:460:ILE:HG13 | 1:B:467:TYR:CD2 | 2.14 | 0.79 |
| 1:B:310:LYS:CG | 2:C:38:ASN:HB2 | 2.13 | 0.79 |
| 2:D:34:ASP:HB3 | 2:D:36:CYS:N | 1.97 | 0.79 |
| 3:E:77:ARG:HA | 3:F:66:ASP:OD2 | 1.83 | 0.79 |
| 3:F:51:GLN:HG3 | 3:F:52:LEU:HD22 | 1.65 | 0.79 |
| 3:E:77:ARG:CB | 3:F:66:ASP:HA | 2.05 | 0.79 |
| 5:H:139:LYS:N | 5:H:139:LYS:HD3 | 1.96 | 0.79 |
| 1:A:62:LYS:HE3 | 1:A:81:ASN:HB2 | 1.65 | 0.79 |
| 1:B:76:ASP:OD2 | 1:B:79:LYS:HG2 | 1.83 | 0.79 |
| 3:E:108:VAL:HG11 | 4:G:43:TYR:HH | 1.45 | 0.79 |
| 3:E:85:GLY:HA3 | 3:E:99:ILE:HG23 | 1.63 | 0.79 |
| 1:A:130:LEU:HD22 | 1:A:388:PHE:CE2 | 2.18 | 0.79 |
| 1:A:395:TYR:HA | 1:A:398:ASN:ND2 | 1.97 | 0.79 |
| 1:B:179:PHE:CE2 | 1:B:200:TYR:HB2 | 2.17 | 0.79 |
| 1:B:410:LEU:CD2 | 1:B:412:MET:HG2 | 2.13 | 0.79 |
| 1:B:59:ILE:HG23 | 1:B:62:LYS:NZ | 1.98 | 0.79 |
| 2:C:63:PHE:HZ | 2:C:82:PHE:HA | 1.48 | 0.79 |
| 2:D:4:GLN:HG2 | 3:F:1:MET:CE | 2.13 | 0.79 |
| 3:E:52:LEU:HD12 | 3:E:53:GLN:CD | 2.03 | 0.79 |
| 1:A:128:ASP:O | 1:A:132:GLU:HG2 | 1.83 | 0.78 |
| 1:B:367:TYR:HB3 | 1:B:369:LEU:CA | 2.08 | 0.78 |
| 2:C:4:GLN:HB2 | 2:C:8:ARG:CZ | 2.13 | 0.78 |
| 2:D:4:GLN:HB2 | 2:D:8:ARG:CZ | 2.13 | 0.78 |
| 2:D:70:LEU:HD21 | 3:F:90:LEU:O | 1.82 | 0.78 |
| 1:A:367:TYR:OH | 1:A:372:LEU:HB2 | 1.84 | 0.78 |
| 1:B:239:TRP:CZ3 | 1:B:243:PRO:HG3 | 2.18 | 0.78 |
| 1:B:331:LYS:O | 1:B:334:GLU:HG2 | 1.83 | 0.78 |
| 2:D:63:PHE:HZ | 2:D:82:PHE:HA | 1.48 | 0.78 |
| 4:G:128:ARG:HD2 | 4:G:128:ARG:H | 1.48 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:21:TYR:CD1 | 4:G:23:PRO:HD2 | 2.18 | 0.78 |
| 1:B:204:HIS:CE1 | 1:B:221:TYR:HB3 | 2.18 | 0.78 |
| 1:B:367:TYR:OH | 1:B:372:LEU:HB2 | 1.84 | 0.78 |
| 1:B:416:ARG:O | 1:B:418:ARG:HG2 | 1.84 | 0.78 |
| 1:B:395:TYR:HA | 1:B:398:ASN:ND2 | 1.97 | 0.78 |
| 2:C:34:ASP:HB3 | 2:C:36:CYS:N | 1.97 | 0.78 |
| 2:C:82:PHE:O | 2:C:86:ILE:HG12 | 1.83 | 0.78 |
| 2:C:94:LEU:H | 2:D:97:TYR:CB | 1.91 | 0.78 |
| 2:D:87:PRO:O | 2:D:91:LEU:HD23 | 1.83 | 0.78 |
| 4:G:63:ASN:CA | 5:H:140:ASN:ND2 | 2.45 | 0.78 |
| 1:A:179:PHE:CE2 | 1:A:200:TYR:HB2 | 2.17 | 0.78 |
| 1:A:99:TYR:HB2 | 1:A:370:LEU:HD12 | 1.65 | 0.78 |
| 1:B:382:ARG:CG | 1:B:383:ALA:HA | 2.12 | 0.78 |
| 2:C:93:LYS:HZ2 | 2:C:94:LEU:HD11 | 1.46 | 0.78 |
| 3:E:62:THR:HB | 3:E:68:ILE:HD12 | 1.65 | 0.78 |
| 1:A:204:HIS:CE1 | 1:A:221:TYR:HB3 | 2.18 | 0.78 |
| 1:B:37:LEU:HD22 | 1:B:168:VAL:CG1 | 2.08 | 0.78 |
| 1:A:416:ARG:O | 1:A:418:ARG:HG2 | 1.84 | 0.78 |
| 1:B:128:ASP:O | 1:B:132:GLU:HG2 | 1.83 | 0.78 |
| 1:B:144:TYR:HB3 | 1:B:244:ILE:CD1 | 2.10 | 0.78 |
| 1:B:163:GLU:CB | 1:B:182:ARG:HG3 | 2.14 | 0.78 |
| 1:B:320:LEU:HB2 | 1:B:321:ARG:O | 1.83 | 0.78 |
| 2:D:95:ASN:HB3 | 2:D:97:TYR:N | 1.99 | 0.78 |
| 5:H:111:ALA:CA | 5:H:132:LEU:HD13 | 2.12 | 0.78 |
| 5:H:16:GLN:HB2 | 5:H:25:ALA:O | 1.83 | 0.78 |
| 1:B:130:LEU:HD22 | 1:B:388:PHE:CE2 | 2.18 | 0.78 |
| 1:B:294:GLU:HG2 | 2:C:41:ILE:C | 2.04 | 0.78 |
| 2:D:87:PRO:HB3 | 2:D:90:ILE:H | 1.47 | 0.78 |
| 3:E:13:SER:HB2 | 3:E:75:ILE:HD13 | 1.66 | 0.78 |
| 3:E:84:ILE:HG21 | 3:E:103:GLU:OE1 | 1.84 | 0.78 |
| 5:H:17:SER:HA | 5:H:23:GLY:HA3 | 1.63 | 0.78 |
| 1:A:144:TYR:HB3 | 1:A:244:ILE:CD1 | 2.10 | 0.78 |
| 1:B:202:ASP:HB2 | 1:B:242:VAL:CB | 2.13 | 0.78 |
| 1:B:256:ASP:O | 1:B:259:PHE:HB2 | 1.84 | 0.78 |
| 2:C:87:PRO:HB3 | 2:C:90:ILE:H | 1.47 | 0.78 |
| 2:D:5:ARG:HA | 3:F:3:GLU:HA | 1.63 | 0.78 |
| 4:G:61:GLY:HA2 | 5:H:139:LYS:HE2 | 1.63 | 0.78 |
| 1:A:59:ILE:HG23 | 1:A:62:LYS:NZ | 1.98 | 0.78 |
| 1:B:190:MET:HB3 | 1:B:192:GLU:OE1 | 1.84 | 0.78 |
| 1:B:440:LYS:O | 1:B:440:LYS:HD3 | 1.82 | 0.78 |
| 1:B:59:ILE:HA | 1:B:62:LYS:HD2 | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:87:PRO:O | 2:C:91:LEU:HD23 | 1.84 | 0.78 |
| 3:E:50:GLN:HG2 | 3:F:52:LEU:HD23 | 1.66 | 0.78 |
| 5:H:88:GLN:C | 5:H:89:ILE:HD13 | 2.04 | 0.78 |
| 1:A:30:ASP:O | 1:A:34:ILE:HG13 | 1.84 | 0.77 |
| 1:A:96:LYS:HE3 | 1:A:377:ALA:CA | 2.12 | 0.77 |
| 1:A:340:LEU:HD13 | 1:B:275:MET:SD | 2.24 | 0.77 |
| 1:B:38:ILE:CG1 | 1:B:181:LEU:HG | 2.14 | 0.77 |
| 5:H:13:TYR:CE1 | 5:H:31:TYR:HB3 | 2.18 | 0.77 |
| 1:B:294:GLU:CG | 2:C:42:ASP:N | 2.47 | 0.77 |
| 1:B:96:LYS:HE3 | 1:B:377:ALA:CA | 2.12 | 0.77 |
| 3:E:79:LYS:HD2 | 3:F:70:LYS:HB3 | 1.64 | 0.77 |
| 5:H:121:GLY:HA2 | 5:H:126:VAL:HA | 1.66 | 0.77 |
| 5:H:16:GLN:HB3 | 5:H:27:LEU:N | 1.99 | 0.77 |
| 1:A:239:TRP:CZ3 | 1:A:243:PRO:HG3 | 2.18 | 0.77 |
| 1:A:418:ARG:HH12 | 1:B:426:VAL:HG21 | 1.48 | 0.77 |
| 2:C:54:LEU:HD11 | 2:D:28:LEU:CD2 | 2.12 | 0.77 |
| 1:A:163:GLU:CB | 1:A:182:ARG:HG3 | 2.14 | 0.77 |
| 1:A:190:MET:HB3 | 1:A:192:GLU:OE1 | 1.84 | 0.77 |
| 1:A:224:ASN:ND2 | 1:A:225:ASN:HA | 1.99 | 0.77 |
| 1:A:146:HIS:ND1 | 1:A:243:PRO:HB2 | 1.99 | 0.77 |
| 3:E:45:GLU:HA | 3:E:47:TYR:CE1 | 2.20 | 0.77 |
| 3:E:41:ILE:H | 3:F:100:LYS:HE2 | 1.49 | 0.77 |
| 3:F:51:GLN:HG3 | 3:F:52:LEU:CD2 | 2.14 | 0.77 |
| 4:G:100:PHE:CG | 5:H:47:GLN:CG | 2.68 | 0.77 |
| 1:B:100:LEU:CG | 1:B:377:ALA:HB1 | 2.15 | 0.77 |
| 1:B:291:TYR:HB3 | 1:B:312:SER:HB2 | 1.67 | 0.77 |
| 1:B:30:ASP:O | 1:B:34:ILE:HG13 | 1.84 | 0.77 |
| 3:F:44:GLU:CG | 3:F:46:TYR:HB2 | 2.14 | 0.77 |
| 3:F:73:ARG:HH11 | 3:F:80:ILE:HB | 1.49 | 0.77 |
| 1:A:202:ASP:HB2 | 1:A:242:VAL:CB | 2.13 | 0.77 |
| 1:A:291:TYR:HB3 | 1:A:312:SER:HB2 | 1.67 | 0.77 |
| 1:B:121:LEU:HD12 | 1:B:124:ASP:H | 1.48 | 0.77 |
| 3:E:8:VAL:CG2 | 3:E:34:ALA:HA | 2.14 | 0.77 |
| 1:A:100:LEU:CG | 1:A:377:ALA:HB1 | 2.15 | 0.77 |
| 1:A:59:ILE:HA | 1:A:62:LYS:HD2 | 1.65 | 0.77 |
| 1:B:146:HIS:ND1 | 1:B:243:PRO:HB2 | 1.99 | 0.77 |
| 1:B:112:LYS:HG2 | 1:B:401:LYS:HZ2 | 1.50 | 0.77 |
| 3:E:53:GLN:HG3 | 3:E:55:PRO:HD3 | 1.65 | 0.77 |
| 3:E:13:SER:OG | 3:E:73:ARG:HD2 | 1.84 | 0.77 |
| 3:E:79:LYS:HE2 | 3:F:69:ASP:HB3 | 1.65 | 0.77 |
| 4:G:21:TYR:CB | 4:G:24:LEU:HB2 | 2.04 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:38:ILE:CG1 | 1:A:181:LEU:HG | 2.14 | 0.77 |
| 1:B:418:ARG:HB2 | 1:B:421:ASN:CB | 2.14 | 0.77 |
| 2:D:4:GLN:CA | 3:F:1:MET:CB | 2.39 | 0.77 |
| 4:G:113:ILE:HG21 | 4:G:121:LYS:CB | 2.15 | 0.77 |
| 1:B:64:ARG:HD3 | 1:B:79:LYS:NZ | 2.00 | 0.77 |
| 2:C:55:ILE:HD12 | 2:C:94:LEU:HD11 | 1.66 | 0.77 |
| 3:F:41:ILE:HG23 | 3:F:42:SER:H | 1.48 | 0.77 |
| 3:F:85:GLY:CA | 3:F:99:ILE:HG23 | 2.14 | 0.77 |
| 1:A:254:VAL:HB | 1:A:259:PHE:CE1 | 2.20 | 0.77 |
| 1:A:261:LYS:HG2 | 1:A:265:ASP:OD2 | 1.85 | 0.77 |
| 1:B:184:TYR:O | 1:B:196:LYS:HB2 | 1.85 | 0.77 |
| 1:B:224:ASN:ND2 | 1:B:225:ASN:HA | 1.99 | 0.77 |
| 2:C:95:ASN:HB3 | 2:C:97:TYR:N | 1.99 | 0.77 |
| 2:D:5:ARG:HA | 3:F:3:GLU:H | 0.69 | 0.77 |
| 1:A:256:ASP:O | 1:A:259:PHE:HB2 | 1.84 | 0.76 |
| 1:A:418:ARG:HB2 | 1:A:421:ASN:CB | 2.14 | 0.76 |
| 1:B:261:LYS:HG2 | 1:B:265:ASP:OD2 | 1.85 | 0.76 |
| 2:C:14:ASN:HD21 | 2:C:21:LEU:HG | 1.50 | 0.76 |
| 1:B:298:GLU:CG | 2:C:42:ASP:HB3 | 2.14 | 0.76 |
| 2:D:7:LYS:HE2 | 3:F:5:PHE:H | 1.49 | 0.76 |
| 1:A:37:LEU:HD22 | 1:A:168:VAL:CG1 | 2.08 | 0.76 |
| 1:A:43:PRO:O | 1:A:47:LEU:HG | 1.85 | 0.76 |
| 1:A:64:ARG:HD3 | 1:A:79:LYS:NZ | 2.00 | 0.76 |
| 1:B:444:VAL:HG13 | 1:B:449:PHE:HB2 | 1.66 | 0.76 |
| 1:B:64:ARG:HD3 | 1:B:79:LYS:HZ2 | 1.50 | 0.76 |
| 3:E:85:GLY:HA3 | 3:E:99:ILE:CG2 | 2.15 | 0.76 |
| 4:G:113:ILE:HG12 | 4:G:121:LYS:CB | 2.15 | 0.76 |
| 5:H:143:ILE:HB | 5:H:144:ASP:C | 2.05 | 0.76 |
| 1:A:182:ARG:CZ | 1:A:184:TYR:HB3 | 2.16 | 0.76 |
| 1:A:149:VAL:HG21 | 1:A:227:ARG:HD2 | 1.67 | 0.76 |
| 1:B:149:VAL:HG21 | 1:B:227:ARG:HD2 | 1.67 | 0.76 |
| 1:B:254:VAL:HB | 1:B:259:PHE:CE1 | 2.20 | 0.76 |
| 1:B:285:VAL:CG1 | 1:B:287:VAL:HG23 | 2.16 | 0.76 |
| 1:A:46:LEU:HD22 | 1:A:162:ALA:HB2 | 1.64 | 0.76 |
| 1:A:140:LYS:CD | 1:A:261:LYS:HE3 | 2.15 | 0.76 |
| 1:A:32:THR:O | 1:A:36:LYS:HG2 | 1.86 | 0.76 |
| 1:A:34:ILE:HG22 | 1:A:181:LEU:HD22 | 1.68 | 0.76 |
| 1:A:438:MET:HG3 | 1:B:434:THR:O | 1.83 | 0.76 |
| 2:C:29:VAL:HG13 | 2:C:50:PRO:HG3 | 1.67 | 0.76 |
| 2:D:14:ASN:HD21 | 2:D:21:LEU:HG | 1.50 | 0.76 |
| 2:D:69:GLY:HA2 | 2:D:72:GLY:O | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:ASP:HB3 | 1:A:396:LEU:CD1 | 2.14 | 0.76 |
| 1:A:121:LEU:HD12 | 1:A:124:ASP:H | 1.48 | 0.76 |
| 1:A:439:SER:OG | 1:B:459:ARG:CG | 2.32 | 0.76 |
| 1:B:167:VAL:CG1 | 1:B:177:ILE:HD12 | 2.12 | 0.76 |
| 1:A:453:PRO:CB | 1:B:462:GLU:CD | 2.48 | 0.76 |
| 1:A:460:ILE:CG1 | 1:B:466:GLN:CD | 2.54 | 0.76 |
| 2:C:99:LYS:CA | 2:D:101:ALA:N | 2.49 | 0.76 |
| 2:D:29:VAL:HG13 | 2:D:50:PRO:HG3 | 1.67 | 0.76 |
| 1:A:444:VAL:HG13 | 1:A:449:PHE:HB2 | 1.66 | 0.76 |
| 1:B:140:LYS:CD | 1:B:261:LYS:HE3 | 2.15 | 0.76 |
| 3:F:84:ILE:HD12 | 3:F:103:GLU:OE2 | 1.86 | 0.76 |
| 3:E:105:GLY:CA | 4:G:119:VAL:CG2 | 2.57 | 0.76 |
| 1:A:460:ILE:CD1 | 1:B:466:GLN:NE2 | 2.49 | 0.76 |
| 1:B:32:THR:O | 1:B:36:LYS:HG2 | 1.86 | 0.76 |
| 2:C:4:GLN:CG | 3:E:1:MET:SD | 2.68 | 0.76 |
| 3:F:44:GLU:HG3 | 3:F:46:TYR:HB2 | 1.65 | 0.76 |
| 3:F:52:LEU:CD1 | 3:F:54:THR:H | 1.98 | 0.76 |
| 3:F:52:LEU:CB | 3:F:53:GLN:HA | 2.11 | 0.76 |
| 1:B:364:GLU:O | 1:B:368:ALA:HB3 | 1.84 | 0.76 |
| 2:D:55:ILE:HD12 | 2:D:94:LEU:HD11 | 1.66 | 0.76 |
| 4:G:32:THR:CG2 | 4:G:43:TYR:HB2 | 2.15 | 0.76 |
| 1:A:364:GLU:O | 1:A:368:ALA:HB3 | 1.84 | 0.76 |
| 1:B:178:LEU:HA | 1:B:242:VAL:HG13 | 1.66 | 0.76 |
| 1:B:376:MET:HB2 | 1:B:379:ARG:NH2 | 2.01 | 0.76 |
| 2:D:6:VAL:N | 3:F:3:GLU:HA | 2.01 | 0.76 |
| 3:F:70:LYS:HZ3 | 3:F:71:LYS:HB2 | 1.49 | 0.76 |
| 1:B:182:ARG:CZ | 1:B:184:TYR:HB3 | 2.16 | 0.76 |
| 2:D:25:VAL:CG1 | 2:D:53:VAL:HG11 | 2.16 | 0.75 |
| 3:F:103:GLU:HB3 | 4:G:31:VAL:HG11 | 1.69 | 0.75 |
| 4:G:134:ASN:CG | 5:H:138:LEU:O | 2.22 | 0.75 |
| 5:H:14:LEU:HB2 | 5:H:27:LEU:O | 1.85 | 0.75 |
| 1:A:130:LEU:HD13 | 1:A:388:PHE:CE2 | 2.22 | 0.75 |
| 1:A:376:MET:HB2 | 1:A:379:ARG:CZ | 2.16 | 0.75 |
| 1:B:99:TYR:CD2 | 1:B:370:LEU:HD12 | 2.20 | 0.75 |
| 1:B:313:GLY:C | 2:C:51:SER:HB2 | 2.06 | 0.75 |
| 1:A:147:PRO:HG2 | 1:A:239:TRP:HH2 | 1.51 | 0.75 |
| 1:A:99:TYR:CD2 | 1:A:370:LEU:HD12 | 2.20 | 0.75 |
| 1:A:376:MET:HB2 | 1:A:379:ARG:NH2 | 2.01 | 0.75 |
| 1:B:147:PRO:HG2 | 1:B:239:TRP:HH2 | 1.51 | 0.75 |
| 3:F:32:PHE:CE1 | 3:F:67:ARG:HB2 | 2.21 | 0.75 |
| 4:G:63:ASN:OD1 | 5:H:139:LYS:HB3 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:LYS:HG2 | 1:A:401:LYS:HZ2 | 1.50 | 0.75 |
| 1:A:178:LEU:HA | 1:A:242:VAL:HG13 | 1.66 | 0.75 |
| 1:A:252:GLU:OE1 | 1:B:53:TYR:CE1 | 2.39 | 0.75 |
| 1:A:285:VAL:CG1 | 1:A:287:VAL:HG23 | 2.16 | 0.75 |
| 1:B:110:ASP:HB3 | 1:B:396:LEU:CD1 | 2.14 | 0.75 |
| 3:F:21:GLU:OE1 | 4:G:16:GLU:CG | 2.34 | 0.75 |
| 3:E:48:LYS:HD3 | 3:F:48:LYS:HG3 | 1.69 | 0.75 |
| 4:G:31:VAL:HG23 | 4:G:32:THR:HA | 1.69 | 0.75 |
| 1:A:167:VAL:CG1 | 1:A:177:ILE:HD12 | 2.12 | 0.75 |
| 2:C:56:PHE:HA | 2:C:59:LYS:NZ | 2.02 | 0.75 |
| 2:C:70:LEU:O | 3:E:91:SER:OG | 2.05 | 0.75 |
| 1:B:294:GLU:HB3 | 2:C:42:ASP:CG | 2.06 | 0.75 |
| 1:B:376:MET:HB2 | 1:B:379:ARG:CZ | 2.16 | 0.75 |
| 1:B:43:PRO:O | 1:B:47:LEU:HG | 1.85 | 0.75 |
| 1:B:63:ARG:NE | 1:B:75:VAL:HG11 | 2.01 | 0.75 |
| 4:G:45:VAL:HG22 | 4:G:71:TRP:HZ3 | 1.51 | 0.75 |
| 5:H:17:SER:HB2 | 5:H:91:PHE:HA | 1.69 | 0.75 |
| 1:A:144:TYR:CE1 | 1:A:246:PRO:HB3 | 2.21 | 0.75 |
| 1:B:130:LEU:HD13 | 1:B:388:PHE:CE2 | 2.22 | 0.75 |
| 1:B:168:VAL:O | 1:B:177:ILE:HG13 | 1.87 | 0.75 |
| 1:B:144:TYR:CE1 | 1:B:246:PRO:HB3 | 2.21 | 0.75 |
| 1:B:410:LEU:HB3 | 1:B:411:THR:C | 2.07 | 0.75 |
| 2:C:100:MET:HE1 | 2:D:100:MET:CB | 2.17 | 0.75 |
| 2:D:70:LEU:H | 3:F:93:LEU:CA | 1.98 | 0.75 |
| 1:A:45:PRO:O | 1:A:48:LYS:HG2 | 1.87 | 0.75 |
| 1:B:111:ASN:HD21 | 1:B:113:THR:HB | 1.52 | 0.75 |
| 1:B:99:TYR:CB | 1:B:370:LEU:HD12 | 2.17 | 0.75 |
| 1:B:40:GLU:HB2 | 1:B:166:ILE:CD1 | 2.07 | 0.75 |
| 1:B:45:PRO:O | 1:B:48:LYS:HG2 | 1.87 | 0.75 |
| 2:C:69:GLY:HA2 | 2:C:72:GLY:O | 1.85 | 0.75 |
| 3:F:21:GLU:CA | 4:G:20:SER:HA | 2.17 | 0.75 |
| 4:G:97:PHE:CD2 | 5:H:47:GLN:CB | 2.66 | 0.75 |
| 1:A:184:TYR:O | 1:A:196:LYS:HB2 | 1.85 | 0.75 |
| 1:B:248:LYS:HB2 | 1:B:249:ASN:C | 2.06 | 0.75 |
| 1:B:52:TYR:HB3 | 1:B:261:LYS:HD3 | 1.69 | 0.75 |
| 2:C:74:SER:CB | 2:C:78:VAL:HG11 | 2.14 | 0.75 |
| 2:D:56:PHE:CD1 | 2:D:59:LYS:HE2 | 2.21 | 0.75 |
| 2:D:59:LYS:O | 2:D:62:GLN:HG2 | 1.87 | 0.75 |
| 2:D:70:LEU:HB2 | 3:E:2:TYR:CE1 | 2.22 | 0.75 |
| 3:E:61:TYR:CE1 | 3:E:96:ILE:HB | 2.21 | 0.75 |
| 4:G:105:LYS:HG3 | 4:G:106:LYS:CG | 2.08 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:63:ASN:HA | 5:H:140:ASN:ND2 | 2.02 | 0.75 |
| 1:A:248:LYS:HB2 | 1:A:249:ASN:C | 2.06 | 0.74 |
| 1:A:52:TYR:HB3 | 1:A:261:LYS:HD3 | 1.69 | 0.74 |
| 2:C:98:ARG:CD | 2:D:97:TYR:CZ | 2.70 | 0.74 |
| 5:H:99:ASN:HB2 | 5:H:104:TYR:HB2 | 1.67 | 0.74 |
| 5:H:21:ALA:CB | 5:H:150:ILE:HG12 | 2.16 | 0.74 |
| 1:A:453:PRO:HB3 | 1:B:462:GLU:OE2 | 1.87 | 0.74 |
| 4:G:113:ILE:CG2 | 4:G:121:LYS:HB3 | 2.17 | 0.74 |
| 1:A:99:TYR:CB | 1:A:370:LEU:HD12 | 2.17 | 0.74 |
| 1:B:34:ILE:HG22 | 1:B:181:LEU:HD22 | 1.68 | 0.74 |
| 1:A:378:GLU:CD | 1:B:98:GLN:NE2 | 2.40 | 0.74 |
| 2:C:56:PHE:CD1 | 2:C:59:LYS:HE2 | 2.22 | 0.74 |
| 4:G:134:ASN:CB | 5:H:138:LEU:O | 2.35 | 0.74 |
| 1:A:168:VAL:O | 1:A:177:ILE:HG13 | 1.87 | 0.74 |
| 1:A:46:LEU:HD22 | 1:A:162:ALA:CB | 2.18 | 0.74 |
| 1:A:64:ARG:HH21 | 1:B:284:ILE:CG2 | 1.99 | 0.74 |
| 1:B:298:GLU:OE1 | 2:C:43:LYS:HG3 | 1.87 | 0.74 |
| 2:D:28:LEU:HA | 2:D:31:PHE:CE1 | 2.23 | 0.74 |
| 3:E:70:LYS:HG2 | 3:E:85:GLY:O | 1.87 | 0.74 |
| 3:F:87:PRO:HB3 | 3:F:97:THR:HG23 | 1.67 | 0.74 |
| 1:A:335:ARG:CG | 1:B:333:LEU:HB2 | 2.17 | 0.74 |
| 1:A:438:MET:SD | 1:B:434:THR:CB | 2.75 | 0.74 |
| 1:A:111:ASN:HD21 | 1:A:113:THR:HB | 1.52 | 0.74 |
| 1:A:202:ASP:OD1 | 1:A:242:VAL:HA | 1.87 | 0.74 |
| 1:B:202:ASP:OD1 | 1:B:242:VAL:HA | 1.87 | 0.74 |
| 1:B:46:LEU:HB2 | 1:B:162:ALA:CB | 2.18 | 0.74 |
| 1:A:379:ARG:HD2 | 1:B:94:ASP:CG | 2.07 | 0.74 |
| 3:E:59:ASN:H | 3:F:100:LYS:HE3 | 1.52 | 0.74 |
| 1:A:48:LYS:HA | 1:A:51:ARG:HH12 | 1.53 | 0.74 |
| 1:A:64:ARG:HH21 | 1:B:284:ILE:HG21 | 1.51 | 0.74 |
| 1:B:299:PHE:HD2 | 2:D:35:GLU:O | 1.71 | 0.74 |
| 1:B:34:ILE:HG22 | 1:B:181:LEU:CD2 | 2.18 | 0.74 |
| 1:A:63:ARG:NE | 1:A:75:VAL:HG11 | 2.01 | 0.74 |
| 2:C:25:VAL:CG1 | 2:C:53:VAL:HG11 | 2.16 | 0.74 |
| 2:C:88:SER:O | 2:C:92:LYS:HG2 | 1.87 | 0.74 |
| 3:E:12:GLN:O | 3:E:30:ASP:HB2 | 1.86 | 0.74 |
| 5:H:90:LYS:HD3 | 5:H:150:ILE:CD1 | 2.18 | 0.74 |
| 1:B:99:TYR:CD2 | 1:B:370:LEU:HB3 | 2.23 | 0.74 |
| 1:B:48:LYS:HA | 1:B:51:ARG:HH12 | 1.53 | 0.74 |
| 3:E:73:ARG:HH12 | 3:E:80:ILE:HD12 | 1.50 | 0.74 |
| 4:G:100:PHE:CD2 | 5:H:47:GLN:CB | 2.71 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:438:MET:HE3 | 1:B:433:VAL:O | 1.88 | 0.74 |
| 1:B:313:GLY:CA | 2:C:51:SER:HB2 | 2.16 | 0.74 |
| 1:A:299:PHE:HD2 | 2:C:35:GLU:O | 1.71 | 0.74 |
| 2:C:4:GLN:C | 3:E:1:MET:N | 2.41 | 0.74 |
| 2:D:56:PHE:HA | 2:D:59:LYS:NZ | 2.02 | 0.74 |
| 3:F:7:ASP:HB3 | 3:F:9:ILE:N | 2.02 | 0.74 |
| 3:F:86:ASP:OD1 | 3:F:100:LYS:HB3 | 1.88 | 0.74 |
| 4:G:113:ILE:CD1 | 4:G:122:HIS:H | 2.00 | 0.74 |
| 1:A:426:VAL:HA | 1:A:429:LEU:HD12 | 1.70 | 0.73 |
| 1:B:441:GLU:HG2 | 1:B:456:GLU:HB2 | 1.70 | 0.73 |
| 2:C:28:LEU:HA | 2:C:31:PHE:CE1 | 2.23 | 0.73 |
| 4:G:64:ILE:HD11 | 5:H:140:ASN:CG | 2.09 | 0.73 |
| 1:A:38:ILE:CG2 | 1:A:163:GLU:HG2 | 2.15 | 0.73 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:HD2 | 2.22 | 0.73 |
| 1:A:46:LEU:HB2 | 1:A:162:ALA:CB | 2.18 | 0.73 |
| 1:B:179:PHE:CE1 | 1:B:244:ILE:HD13 | 2.23 | 0.73 |
| 2:C:4:GLN:CA | 3:E:1:MET:HG2 | 2.18 | 0.73 |
| 2:D:6:VAL:HG23 | 3:F:3:GLU:HG3 | 1.70 | 0.73 |
| 4:G:33:GLU:CD | 4:G:46:ILE:HB | 2.09 | 0.73 |
| 5:H:147:PRO:HA | 5:H:150:ILE:HG13 | 1.69 | 0.73 |
| 1:A:163:GLU:HB2 | 1:A:182:ARG:CG | 2.18 | 0.73 |
| 1:A:441:GLU:HG2 | 1:A:456:GLU:HB2 | 1.70 | 0.73 |
| 1:B:46:LEU:CD2 | 1:B:162:ALA:HB2 | 2.18 | 0.73 |
| 3:F:105:GLY:CA | 4:G:39:ASP:N | 2.31 | 0.73 |
| 3:F:7:ASP:N | 3:F:8:VAL:HA | 2.03 | 0.73 |
| 5:H:94:VAL:HG21 | 5:H:160:PHE:CZ | 2.22 | 0.73 |
| 1:A:410:LEU:HB3 | 1:A:411:THR:C | 2.07 | 0.73 |
| 1:A:457:LEU:HG | 1:B:467:TYR:CG | 2.14 | 0.73 |
| 1:B:241:ARG:HH21 | 1:B:245:ILE:HG12 | 1.53 | 0.73 |
| 1:B:308:VAL:HG11 | 2:C:36:CYS:SG | 2.29 | 0.73 |
| 1:B:335:ARG:NH1 | 1:B:336:ILE:HA | 2.03 | 0.73 |
| 2:C:59:LYS:O | 2:C:62:GLN:HG2 | 1.87 | 0.73 |
| 2:D:55:ILE:HD12 | 2:D:93:LYS:HZ2 | 1.54 | 0.73 |
| 3:E:47:TYR:HB2 | 3:F:44:GLU:OE2 | 1.88 | 0.73 |
| 1:B:163:GLU:HB2 | 1:B:182:ARG:CG | 2.18 | 0.73 |
| 1:B:46:LEU:HD22 | 1:B:162:ALA:CB | 2.18 | 0.73 |
| 3:E:38:VAL:HG22 | 3:E:60:ILE:CG2 | 2.17 | 0.73 |
| 4:G:73:GLY:HA2 | 4:G:76:ARG:HH21 | 1.53 | 0.73 |
| 1:B:426:VAL:HA | 1:B:429:LEU:HD12 | 1.70 | 0.73 |
| 2:C:78:VAL:HG13 | 2:C:79:SER:O | 1.89 | 0.73 |
| 2:D:88:SER:O | 2:D:92:LYS:HG2 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:62:THR:O | 3:E:65:ASP:HB2 | 1.88 | 0.73 |
| 2:D:4:GLN:CD | 3:F:1:MET:SD | 2.66 | 0.73 |
| 5:H:160:PHE:HB3 | 5:H:163:PRO:HG2 | 1.70 | 0.73 |
| 1:A:241:ARG:HH21 | 1:A:245:ILE:HG12 | 1.53 | 0.73 |
| 2:C:39:PRO:O | 2:C:41:ILE:HG13 | 1.89 | 0.73 |
| 2:D:39:PRO:O | 2:D:41:ILE:HG13 | 1.89 | 0.73 |
| 2:D:78:VAL:HG13 | 2:D:79:SER:O | 1.89 | 0.73 |
| 4:G:41:TYR:CD2 | 4:G:119:VAL:HG21 | 2.23 | 0.73 |
| 5:H:49:LYS:CB | 5:H:52:ARG:HG2 | 2.08 | 0.73 |
| 1:A:453:PRO:CB | 1:B:462:GLU:CG | 2.46 | 0.73 |
| 2:C:63:PHE:CG | 2:C:85:GLU:HG2 | 2.24 | 0.73 |
| 3:F:63:PRO:HA | 3:F:96:ILE:CA | 2.15 | 0.73 |
| 3:F:85:GLY:HA3 | 3:F:99:ILE:CG2 | 2.16 | 0.73 |
| 4:G:28:VAL:HG13 | 4:G:29:ASN:H | 1.54 | 0.73 |
| 1:A:34:ILE:HG22 | 1:A:181:LEU:CD2 | 2.18 | 0.73 |
| 1:A:46:LEU:CD2 | 1:A:162:ALA:HB2 | 2.18 | 0.73 |
| 1:A:99:TYR:CD2 | 1:A:370:LEU:HB3 | 2.23 | 0.73 |
| 2:C:73:ARG:NH2 | 3:E:90:LEU:HD11 | 2.04 | 0.73 |
| 4:G:133:ASN:HB2 | 5:H:55:GLY:C | 2.08 | 0.73 |
| 1:A:259:PHE:CZ | 1:B:90:LYS:CG | 2.61 | 0.73 |
| 1:A:439:SER:HB3 | 1:A:440:LYS:C | 2.10 | 0.73 |
| 1:B:163:GLU:HB3 | 1:B:164:GLU:C | 2.10 | 0.73 |
| 4:G:32:THR:HG23 | 4:G:37:LYS:HA | 1.70 | 0.73 |
| 5:H:21:ALA:HA | 5:H:90:LYS:CD | 2.17 | 0.73 |
| 1:A:335:ARG:NH1 | 1:A:336:ILE:HA | 2.03 | 0.72 |
| 1:A:416:ARG:HB2 | 1:A:417:THR:C | 2.09 | 0.72 |
| 1:A:58:ASP:HB3 | 1:A:81:ASN:ND2 | 2.04 | 0.72 |
| 1:B:209:GLU:CG | 1:B:211:ILE:HG12 | 2.19 | 0.72 |
| 1:B:294:GLU:CG | 2:C:42:ASP:HA | 2.15 | 0.72 |
| 2:D:36:CYS:HB3 | 2:D:37:HIS:C | 2.09 | 0.72 |
| 2:C:98:ARG:CA | 2:D:97:TYR:HE2 | 2.02 | 0.72 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:N | 2.03 | 0.72 |
| 2:C:89:THR:HG21 | 2:D:88:SER:C | 2.09 | 0.72 |
| 3:E:44:GLU:HG2 | 3:E:46:TYR:N | 2.04 | 0.72 |
| 5:H:39:GLY:C | 5:H:43:LEU:HB3 | 2.10 | 0.72 |
| 5:H:75:GLY:O | 5:H:79:ILE:HG13 | 1.89 | 0.72 |
| 1:A:171:ASP:H | 1:A:178:LEU:CD1 | 2.02 | 0.72 |
| 1:A:209:GLU:CG | 1:A:211:ILE:HG12 | 2.19 | 0.72 |
| 1:A:460:ILE:HD11 | 1:B:466:GLN:NE2 | 2.04 | 0.72 |
| 1:B:145:TRP:N | 1:B:244:ILE:HD12 | 2.04 | 0.72 |
| 2:C:36:CYS:HB3 | 2:C:37:HIS:C | 2.09 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:92:LYS:CB | 2:D:92:LYS:HE2 | 2.19 | 0.72 |
| 2:C:99:LYS:HB2 | 2:D:102:ARG:H | 1.54 | 0.72 |
| 2:D:74:SER:CB | 2:D:78:VAL:HG11 | 2.14 | 0.72 |
| 2:D:63:PHE:CD2 | 2:D:85:GLU:HB3 | 2.24 | 0.72 |
| 2:D:63:PHE:CG | 2:D:85:GLU:HG2 | 2.23 | 0.72 |
| 2:D:95:ASN:HB3 | 2:D:96:PRO:C | 2.09 | 0.72 |
| 3:E:2:TYR:CZ | 3:F:95:GLU:HG2 | 2.24 | 0.72 |
| 4:G:70:VAL:O | 4:G:122:HIS:HB2 | 1.89 | 0.72 |
| 1:A:163:GLU:HB3 | 1:A:164:GLU:C | 2.09 | 0.72 |
| 1:A:34:ILE:O | 1:A:181:LEU:HD21 | 1.90 | 0.72 |
| 1:A:179:PHE:CE1 | 1:A:244:ILE:HD13 | 2.23 | 0.72 |
| 1:A:295:ASN:HB2 | 2:C:37:HIS:HE2 | 1.54 | 0.72 |
| 1:B:34:ILE:O | 1:B:181:LEU:HD21 | 1.90 | 0.72 |
| 1:B:429:LEU:HD22 | 1:B:443:ALA:CB | 2.14 | 0.72 |
| 2:C:98:ARG:HD3 | 2:D:97:TYR:OH | 1.89 | 0.72 |
| 4:G:113:ILE:HG12 | 4:G:121:LYS:HB3 | 1.70 | 0.72 |
| 4:G:4:LYS:CG | 4:G:5:LEU:HD13 | 2.20 | 0.72 |
| 5:H:13:TYR:HD1 | 5:H:31:TYR:HB3 | 1.54 | 0.72 |
| 1:A:145:TRP:N | 1:A:244:ILE:HD12 | 2.04 | 0.72 |
| 1:B:38:ILE:CG2 | 1:B:163:GLU:HG2 | 2.15 | 0.72 |
| 1:B:58:ASP:HB3 | 1:B:81:ASN:ND2 | 2.04 | 0.72 |
| 2:C:69:GLY:O | 3:E:93:LEU:HD13 | 1.88 | 0.72 |
| 3:E:29:VAL:HG12 | 3:E:72:MET:CE | 2.19 | 0.72 |
| 2:D:5:ARG:HB3 | 3:F:2:TYR:HB2 | 1.71 | 0.72 |
| 1:A:183:TYR:HB2 | 1:A:196:LYS:O | 1.90 | 0.72 |
| 2:C:95:ASN:HB3 | 2:C:96:PRO:C | 2.09 | 0.72 |
| 3:E:55:PRO:HB2 | 3:E:57:GLY:O | 1.89 | 0.72 |
| 1:A:410:LEU:CB | 1:A:412:MET:HG3 | 2.20 | 0.72 |
| 1:B:100:LEU:HB2 | 1:B:377:ALA:HB1 | 1.72 | 0.72 |
| 1:B:81:ASN:HD22 | 1:B:83:ARG:HH11 | 1.38 | 0.72 |
| 2:C:99:LYS:HA | 2:D:101:ALA:N | 2.03 | 0.72 |
| 4:G:66:MET:HB3 | 4:G:68:PHE:HE1 | 1.54 | 0.72 |
| 5:H:58:SER:HB3 | 5:H:143:ILE:HG13 | 1.71 | 0.72 |
| 4:G:132:ASN:N | 5:H:54:LEU:O | 2.23 | 0.72 |
| 1:A:444:VAL:O | 1:A:448:PRO:HA | 1.90 | 0.72 |
| 1:B:183:TYR:HB2 | 1:B:196:LYS:O | 1.90 | 0.72 |
| 1:B:44:GLU:OE2 | 1:B:48:LYS:HB3 | 1.90 | 0.72 |
| 1:A:332:GLU:OE2 | 1:B:326:VAL:O | 2.08 | 0.72 |
| 1:A:34:ILE:CG2 | 1:A:181:LEU:HD13 | 2.20 | 0.72 |
| 1:B:439:SER:HB3 | 1:B:440:LYS:C | 2.10 | 0.72 |
| 2:D:59:LYS:HG3 | 2:D:60:ALA:N | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:38:VAL:HG13 | 3:E:60:ILE:CG2 | 2.17 | 0.72 |
| 3:F:53:GLN:CG | 3:F:55:PRO:HD2 | 2.13 | 0.72 |
| 4:G:97:PHE:HA | 5:H:49:LYS:HD3 | 1.20 | 0.72 |
| 1:A:165:MET:SD | 1:A:182:ARG:HB2 | 2.30 | 0.72 |
| 1:A:323:GLU:HG3 | 1:A:325:PRO:CD | 2.20 | 0.72 |
| 1:A:81:ASN:HD22 | 1:A:83:ARG:HH11 | 1.38 | 0.72 |
| 1:B:34:ILE:CG2 | 1:B:181:LEU:HD13 | 2.20 | 0.72 |
| 1:B:295:ASN:HB2 | 2:D:37:HIS:HE2 | 1.53 | 0.72 |
| 1:B:416:ARG:HB2 | 1:B:417:THR:C | 2.09 | 0.72 |
| 1:A:457:LEU:O | 1:B:467:TYR:CD2 | 2.42 | 0.72 |
| 3:F:11:PHE:HB2 | 3:F:32:PHE:O | 1.88 | 0.72 |
| 3:F:49:ALA:O | 3:F:50:GLN:HG2 | 1.89 | 0.72 |
| 4:G:68:PHE:O | 4:G:124:ILE:HG12 | 1.89 | 0.72 |
| 5:H:30:ALA:HB3 | 5:H:67:TYR:CD2 | 2.25 | 0.72 |
| 1:A:100:LEU:HB2 | 1:A:377:ALA:HB1 | 1.72 | 0.71 |
| 1:B:84:THR:HG22 | 1:B:85:SER:O | 1.90 | 0.71 |
| 4:G:21:TYR:HD2 | 4:G:24:LEU:HD12 | 1.55 | 0.71 |
| 1:A:142:ILE:HB | 1:A:143:GLU:C | 2.11 | 0.71 |
| 1:A:414:PHE:CG | 1:A:415:THR:HA | 2.25 | 0.71 |
| 1:A:99:TYR:CG | 1:A:370:LEU:HD12 | 2.25 | 0.71 |
| 2:C:63:PHE:CD2 | 2:C:85:GLU:HB3 | 2.24 | 0.71 |
| 2:D:9:LEU:O | 2:D:15:ASP:HB3 | 1.90 | 0.71 |
| 2:D:50:PRO:HG2 | 2:D:53:VAL:CG2 | 2.20 | 0.71 |
| 3:E:105:GLY:H | 4:G:119:VAL:HG21 | 0.55 | 0.71 |
| 3:F:100:LYS:HG3 | 3:F:101:GLY:N | 2.05 | 0.71 |
| 3:F:9:ILE:HG13 | 3:F:11:PHE:CE1 | 2.24 | 0.71 |
| 1:B:171:ASP:H | 1:B:178:LEU:CD1 | 2.02 | 0.71 |
| 1:A:339:GLU:HB3 | 1:B:274:THR:HG21 | 1.71 | 0.71 |
| 1:B:410:LEU:CB | 1:B:412:MET:HG3 | 2.20 | 0.71 |
| 1:A:460:ILE:HD11 | 1:B:466:GLN:CD | 2.09 | 0.71 |
| 2:C:50:PRO:HG2 | 2:C:53:VAL:CG2 | 2.20 | 0.71 |
| 2:C:5:ARG:HA | 3:E:3:GLU:HA | 1.71 | 0.71 |
| 2:D:75:MET:CE | 3:F:90:LEU:CD2 | 2.68 | 0.71 |
| 5:H:37:VAL:CG1 | 5:H:63:GLY:HA2 | 2.20 | 0.71 |
| 1:A:147:PRO:HG2 | 1:A:239:TRP:CH2 | 2.26 | 0.71 |
| 1:A:422:ASP:O | 1:A:426:VAL:HG23 | 1.89 | 0.71 |
| 1:A:62:LYS:HE3 | 1:A:81:ASN:CB | 2.19 | 0.71 |
| 3:F:65:ASP:CB | 3:F:68:ILE:HD12 | 2.20 | 0.71 |
| 3:F:74:VAL:HB | 3:F:83:PHE:CE2 | 2.25 | 0.71 |
| 4:G:63:ASN:CA | 5:H:140:ASN:HD21 | 2.03 | 0.71 |
| 1:A:252:GLU:OE2 | 1:B:53:TYR:HD1 | 1.68 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:136:ASN:HA | 1:B:139:ASN:OD1 | 1.91 | 0.71 |
| 1:B:296:PRO:O | 1:B:300:THR:HG23 | 1.91 | 0.71 |
| 1:B:422:ASP:O | 1:B:426:VAL:HG23 | 1.89 | 0.71 |
| 2:C:9:LEU:O | 2:C:15:ASP:HB3 | 1.90 | 0.71 |
| 1:B:294:GLU:HA | 2:D:31:PHE:HB2 | 1.71 | 0.71 |
| 3:E:74:VAL:HB | 3:E:83:PHE:CZ | 2.25 | 0.71 |
| 4:G:32:THR:HB | 4:G:44:VAL:N | 2.06 | 0.71 |
| 4:G:64:ILE:CD1 | 5:H:140:ASN:OD1 | 2.38 | 0.71 |
| 5:H:49:LYS:HB2 | 5:H:52:ARG:CG | 2.09 | 0.71 |
| 1:A:202:ASP:CB | 1:A:242:VAL:HB | 2.20 | 0.71 |
| 1:B:414:PHE:CZ | 1:B:415:THR:HG22 | 2.25 | 0.71 |
| 3:E:40:PRO:HG3 | 3:F:100:LYS:HB2 | 1.72 | 0.71 |
| 3:E:58:TYR:H | 3:E:83:PHE:HB3 | 1.56 | 0.71 |
| 5:H:43:LEU:O | 5:H:43:LEU:HD13 | 1.91 | 0.71 |
| 1:A:136:ASN:HA | 1:A:139:ASN:OD1 | 1.91 | 0.71 |
| 1:A:44:GLU:OE2 | 1:A:48:LYS:HB3 | 1.90 | 0.71 |
| 1:B:165:MET:SD | 1:B:182:ARG:HB2 | 2.30 | 0.71 |
| 1:A:64:ARG:NH2 | 1:B:284:ILE:HB | 2.05 | 0.71 |
| 1:B:311:VAL:HG11 | 1:B:316:GLY:N | 2.02 | 0.71 |
| 1:B:444:VAL:O | 1:B:448:PRO:HA | 1.90 | 0.71 |
| 1:B:62:LYS:HE3 | 1:B:81:ASN:CB | 2.19 | 0.71 |
| 2:C:59:LYS:HD2 | 2:C:87:PRO:HG2 | 1.73 | 0.71 |
| 3:E:80:ILE:HG12 | 3:F:70:LYS:NZ | 2.06 | 0.71 |
| 3:E:58:TYR:HB3 | 3:F:100:LYS:CD | 2.19 | 0.71 |
| 3:E:79:LYS:HG2 | 3:F:87:PRO:HD3 | 1.71 | 0.71 |
| 1:A:179:PHE:HE1 | 1:A:244:ILE:CD1 | 2.03 | 0.71 |
| 1:A:288:LEU:HD23 | 1:A:288:LEU:H | 1.56 | 0.71 |
| 1:A:294:GLU:HA | 2:C:31:PHE:HB2 | 1.71 | 0.71 |
| 1:A:84:THR:HG22 | 1:A:85:SER:O | 1.90 | 0.71 |
| 1:A:88:TRP:CZ2 | 1:A:369:LEU:HD21 | 2.25 | 0.71 |
| 1:B:310:LYS:HG3 | 2:C:38:ASN:HB2 | 1.72 | 0.71 |
| 1:B:414:PHE:CG | 1:B:415:THR:HA | 2.25 | 0.71 |
| 4:G:43:TYR:O | 4:G:71:TRP:HB2 | 1.91 | 0.71 |
| 5:H:100:GLU:O | 5:H:104:TYR:HB3 | 1.91 | 0.71 |
| 1:A:159:ILE:HD13 | 1:A:160:PHE:N | 2.06 | 0.71 |
| 1:A:29:PRO:CG | 1:A:170:LYS:HD3 | 2.21 | 0.71 |
| 1:B:29:PRO:CG | 1:B:170:LYS:HD3 | 2.21 | 0.71 |
| 3:E:44:GLU:HG2 | 3:E:46:TYR:H | 1.56 | 0.71 |
| 4:G:27:MET:HB3 | 4:G:29:ASN:C | 2.11 | 0.71 |
| 4:G:75:THR:OG1 | 4:G:78:GLU:HB2 | 1.90 | 0.71 |
| 1:A:162:ALA:HB1 | 1:A:164:GLU:HB2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:179:PHE:CE1 | 1:A:244:ILE:HG23 | 2.26 | 0.71 |
| 1:A:419:ILE:HA | 1:A:422:ASP:OD2 | 1.91 | 0.71 |
| 1:B:288:LEU:HD23 | 1:B:288:LEU:H | 1.56 | 0.71 |
| 1:B:419:ILE:HA | 1:B:422:ASP:OD2 | 1.91 | 0.71 |
| 3:E:38:VAL:O | 3:E:40:PRO:HD3 | 1.91 | 0.71 |
| 3:F:103:GLU:C | 4:G:31:VAL:HG21 | 2.10 | 0.71 |
| 1:B:159:ILE:HD13 | 1:B:160:PHE:N | 2.06 | 0.70 |
| 1:B:179:PHE:HE1 | 1:B:244:ILE:CD1 | 2.03 | 0.70 |
| 3:E:31:GLU:HB2 | 3:E:72:MET:CB | 2.20 | 0.70 |
| 3:F:20:GLY:O | 4:G:20:SER:C | 2.29 | 0.70 |
| 4:G:33:GLU:CA | 4:G:45:VAL:HA | 2.20 | 0.70 |
| 1:A:96:LYS:HA | 1:A:373:LYS:CD | 2.21 | 0.70 |
| 1:A:414:PHE:CZ | 1:A:415:THR:HG22 | 2.25 | 0.70 |
| 1:B:109:SER:OG | 1:B:118:VAL:HG21 | 1.92 | 0.70 |
| 1:B:323:GLU:HG3 | 1:B:325:PRO:CD | 2.20 | 0.70 |
| 1:B:88:TRP:CZ2 | 1:B:369:LEU:HD21 | 2.25 | 0.70 |
| 1:B:112:LYS:HG2 | 1:B:401:LYS:NZ | 2.06 | 0.70 |
| 2:C:55:ILE:CD1 | 2:C:94:LEU:HD11 | 2.22 | 0.70 |
| 2:D:59:LYS:HD2 | 2:D:87:PRO:HG2 | 1.73 | 0.70 |
| 3:E:97:THR:C | 3:E:98:ARG:HD2 | 2.11 | 0.70 |
| 3:E:41:ILE:N | 3:F:100:LYS:HE2 | 2.06 | 0.70 |
| 1:A:422:ASP:HA | 1:A:425:ILE:CG2 | 2.21 | 0.70 |
| 1:A:429:LEU:HD22 | 1:A:443:ALA:CB | 2.14 | 0.70 |
| 1:B:202:ASP:CB | 1:B:242:VAL:HB | 2.20 | 0.70 |
| 1:B:255:SER:HB3 | 1:B:259:PHE:CE2 | 2.26 | 0.70 |
| 1:B:256:ASP:CG | 1:B:380:LYS:HE3 | 2.11 | 0.70 |
| 1:B:62:LYS:CE | 1:B:81:ASN:HB2 | 2.21 | 0.70 |
| 2:C:87:PRO:HB2 | 2:C:91:LEU:HD23 | 1.73 | 0.70 |
| 2:D:87:PRO:HB2 | 2:D:91:LEU:HD23 | 1.73 | 0.70 |
| 3:E:65:ASP:HA | 3:E:68:ILE:HD12 | 1.74 | 0.70 |
| 4:G:27:MET:HG2 | 4:G:31:VAL:HG12 | 1.71 | 0.70 |
| 4:G:5:LEU:HD22 | 4:G:6:ALA:N | 2.05 | 0.70 |
| 1:A:109:SER:OG | 1:A:118:VAL:HG21 | 1.91 | 0.70 |
| 1:A:100:LEU:HD11 | 1:A:381:ILE:CG1 | 2.21 | 0.70 |
| 1:B:147:PRO:HG2 | 1:B:239:TRP:CH2 | 2.26 | 0.70 |
| 3:E:77:ARG:HD2 | 3:F:87:PRO:HB3 | 1.74 | 0.70 |
| 1:A:242:VAL:HG22 | 1:A:243:PRO:O | 1.91 | 0.70 |
| 1:A:296:PRO:O | 1:A:300:THR:HG23 | 1.91 | 0.70 |
| 1:A:256:ASP:CG | 1:A:380:LYS:HE3 | 2.11 | 0.70 |
| 1:A:64:ARG:HD3 | 1:A:79:LYS:HZ2 | 1.55 | 0.70 |
| 1:B:142:ILE:HB | 1:B:143:GLU:C | 2.11 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:422:ASP:HA | 1:B:425:ILE:CG2 | 2.21 | 0.70 |
| 1:B:310:LYS:C | 2:C:38:ASN:HD22 | 1.94 | 0.70 |
| 3:E:61:TYR:HE1 | 3:E:96:ILE:HB | 1.57 | 0.70 |
| 3:F:12:GLN:O | 3:F:75:ILE:HD13 | 1.91 | 0.70 |
| 4:G:32:THR:HG21 | 4:G:43:TYR:CD2 | 2.26 | 0.70 |
| 1:A:112:LYS:HG2 | 1:A:401:LYS:NZ | 2.06 | 0.70 |
| 1:A:466:GLN:HG3 | 1:A:467:TYR:CB | 2.22 | 0.70 |
| 1:B:242:VAL:HG22 | 1:B:243:PRO:O | 1.91 | 0.70 |
| 1:B:179:PHE:CE1 | 1:B:244:ILE:HG23 | 2.26 | 0.70 |
| 1:B:410:LEU:HD23 | 1:B:412:MET:HG2 | 1.73 | 0.70 |
| 1:B:99:TYR:CG | 1:B:370:LEU:HD12 | 2.25 | 0.70 |
| 3:E:109:GLY:HA2 | 4:G:114:THR:CB | 2.19 | 0.70 |
| 3:E:53:GLN:HG2 | 3:E:55:PRO:HG3 | 1.73 | 0.70 |
| 3:F:55:PRO:HG3 | 3:F:102:LYS:CD | 2.16 | 0.70 |
| 4:G:59:SER:CB | 5:H:138:LEU:HG | 2.17 | 0.70 |
| 1:A:144:TYR:CB | 1:A:244:ILE:HD11 | 2.15 | 0.70 |
| 1:A:62:LYS:CE | 1:A:81:ASN:HB2 | 2.21 | 0.70 |
| 1:B:149:VAL:HG21 | 1:B:227:ARG:CD | 2.22 | 0.70 |
| 1:B:440:LYS:HE2 | 1:B:444:VAL:CG2 | 2.22 | 0.70 |
| 2:C:70:LEU:O | 2:C:73:ARG:HG2 | 1.91 | 0.70 |
| 3:E:66:ASP:HA | 3:E:87:PRO:HB3 | 1.74 | 0.70 |
| 5:H:16:GLN:HG3 | 5:H:92:TRP:CD1 | 2.26 | 0.70 |
| 1:A:254:VAL:O | 1:A:258:LYS:HB3 | 1.92 | 0.70 |
| 1:A:410:LEU:HD23 | 1:A:412:MET:HG2 | 1.73 | 0.70 |
| 1:A:466:GLN:HG3 | 1:A:467:TYR:HB2 | 1.74 | 0.70 |
| 1:B:422:ASP:HA | 1:B:425:ILE:HG22 | 1.74 | 0.70 |
| 1:B:63:ARG:HB3 | 1:B:75:VAL:HG13 | 1.73 | 0.70 |
| 3:E:58:TYR:CB | 3:F:100:LYS:HD3 | 2.20 | 0.70 |
| 1:B:111:ASN:ND2 | 1:B:113:THR:HB | 2.06 | 0.70 |
| 1:B:138:SER:O | 1:B:256:ASP:HB2 | 1.91 | 0.70 |
| 2:C:26:PRO:O | 2:C:30:GLU:HG3 | 1.92 | 0.70 |
| 2:C:70:LEU:CA | 3:E:91:SER:HB2 | 2.18 | 0.70 |
| 2:C:66:THR:HG23 | 2:D:82:PHE:CE2 | 1.94 | 0.70 |
| 1:A:149:VAL:HG21 | 1:A:227:ARG:CD | 2.22 | 0.70 |
| 1:B:111:ASN:H | 1:B:396:LEU:HD22 | 1.57 | 0.70 |
| 1:B:299:PHE:HA | 1:B:302:ASN:ND2 | 2.07 | 0.70 |
| 1:B:100:LEU:HD11 | 1:B:381:ILE:CG1 | 2.21 | 0.70 |
| 1:B:466:GLN:HG3 | 1:B:467:TYR:CB | 2.22 | 0.70 |
| 1:B:74:LEU:HD23 | 1:B:75:VAL:N | 2.07 | 0.70 |
| 3:F:65:ASP:CB | 3:F:68:ILE:HG23 | 2.20 | 0.70 |
| 4:G:22:GLN:HG3 | 4:G:23:PRO:HD3 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ASN:ND2 | 1:A:113:THR:HB | 2.06 | 0.69 |
| 1:A:29:PRO:HG3 | 1:A:170:LYS:NZ | 2.07 | 0.69 |
| 2:C:49:ILE:HD11 | 2:C:54:LEU:CD1 | 2.22 | 0.69 |
| 2:C:59:LYS:HG3 | 2:C:60:ALA:N | 2.04 | 0.69 |
| 2:D:49:ILE:HD11 | 2:D:54:LEU:CD1 | 2.22 | 0.69 |
| 3:F:60:ILE:HG13 | 3:F:83:PHE:CE2 | 2.27 | 0.69 |
| 3:F:87:PRO:HB3 | 3:F:97:THR:CG2 | 2.21 | 0.69 |
| 5:H:143:ILE:HG21 | 5:H:147:PRO:CD | 2.20 | 0.69 |
| 5:H:15:PHE:O | 5:H:27:LEU:HB2 | 1.91 | 0.69 |
| 1:A:111:ASN:H | 1:A:396:LEU:HD22 | 1.57 | 0.69 |
| 1:A:422:ASP:HA | 1:A:425:ILE:HG22 | 1.74 | 0.69 |
| 1:A:440:LYS:HE2 | 1:A:444:VAL:CG2 | 2.22 | 0.69 |
| 1:B:130:LEU:HD22 | 1:B:388:PHE:HE2 | 1.55 | 0.69 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:CA | 2.22 | 0.69 |
| 2:C:94:LEU:C | 2:D:97:TYR:CB | 2.48 | 0.69 |
| 2:C:73:ARG:CD | 3:E:91:SER:HB3 | 2.21 | 0.69 |
| 4:G:113:ILE:CG2 | 4:G:121:LYS:HD3 | 2.21 | 0.69 |
| 4:G:44:VAL:HG11 | 4:G:74:THR:CG2 | 2.19 | 0.69 |
| 4:G:83:SER:O | 4:G:87:LEU:HD13 | 1.91 | 0.69 |
| 1:A:41:HIS:HB3 | 1:A:164:GLU:O | 1.93 | 0.69 |
| 1:A:456:GLU:OE2 | 1:B:466:GLN:OE1 | 2.10 | 0.69 |
| 1:B:162:ALA:HB1 | 1:B:164:GLU:HB2 | 1.72 | 0.69 |
| 2:C:98:ARG:HH12 | 2:D:102:ARG:N | 1.90 | 0.69 |
| 2:D:26:PRO:O | 2:D:30:GLU:HG3 | 1.92 | 0.69 |
| 3:E:69:ASP:CG | 3:E:99:ILE:HG12 | 2.13 | 0.69 |
| 1:A:74:LEU:HD23 | 1:A:75:VAL:N | 2.07 | 0.69 |
| 1:B:198:GLU:HB3 | 1:B:206:TYR:O | 1.92 | 0.69 |
| 1:B:466:GLN:HG3 | 1:B:467:TYR:HB2 | 1.74 | 0.69 |
| 3:E:41:ILE:HG23 | 3:E:42:SER:H | 1.58 | 0.69 |
| 3:F:12:GLN:HE21 | 3:F:80:ILE:HG22 | 1.57 | 0.69 |
| 1:A:198:GLU:HB3 | 1:A:206:TYR:O | 1.92 | 0.69 |
| 1:A:288:LEU:HD11 | 2:C:34:ASP:O | 1.93 | 0.69 |
| 1:A:43:PRO:HB2 | 1:A:47:LEU:CD1 | 2.22 | 0.69 |
| 2:C:63:PHE:CE1 | 2:C:85:GLU:HB3 | 2.28 | 0.69 |
| 2:D:70:LEU:O | 2:D:73:ARG:HG2 | 1.91 | 0.69 |
| 3:F:12:GLN:CG | 3:F:75:ILE:HG12 | 2.22 | 0.69 |
| 4:G:63:ASN:HB2 | 4:G:129:PHE:O | 1.93 | 0.69 |
| 1:A:255:SER:HB3 | 1:A:259:PHE:CE2 | 2.26 | 0.69 |
| 1:A:138:SER:O | 1:A:256:ASP:HB2 | 1.91 | 0.69 |
| 1:A:130:LEU:HD22 | 1:A:388:PHE:HE2 | 1.55 | 0.69 |
| 1:B:34:ILE:CG2 | 1:B:181:LEU:HD22 | 2.21 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:VAL:O | 1:B:258:LYS:HB3 | 1.92 | 0.69 |
| 1:B:341:TYR:HA | 1:B:344:ALA:HB2 | 1.74 | 0.69 |
| 1:B:41:HIS:HB3 | 1:B:164:GLU:O | 1.93 | 0.69 |
| 1:A:379:ARG:CD | 1:B:94:ASP:HB2 | 2.22 | 0.69 |
| 2:C:29:VAL:HG22 | 2:C:50:PRO:HG2 | 1.74 | 0.69 |
| 2:D:29:VAL:HG22 | 2:D:50:PRO:HG2 | 1.74 | 0.69 |
| 2:D:55:ILE:CD1 | 2:D:94:LEU:HD11 | 2.22 | 0.69 |
| 3:E:29:VAL:HG12 | 3:E:72:MET:HE2 | 1.75 | 0.69 |
| 4:G:70:VAL:HG21 | 4:G:76:ARG:NH2 | 2.06 | 0.69 |
| 5:H:58:SER:HB3 | 5:H:143:ILE:CD1 | 2.22 | 0.69 |
| 5:H:68:TYR:OH | 5:H:125:ALA:HB3 | 1.91 | 0.69 |
| 1:B:29:PRO:HG3 | 1:B:170:LYS:NZ | 2.07 | 0.69 |
| 1:B:144:TYR:CB | 1:B:244:ILE:HD11 | 2.15 | 0.69 |
| 2:D:89:THR:O | 2:D:92:LYS:HB2 | 1.92 | 0.69 |
| 1:A:334:GLU:O | 1:A:337:GLN:HG2 | 1.92 | 0.69 |
| 1:A:63:ARG:HB3 | 1:A:75:VAL:HG13 | 1.73 | 0.69 |
| 1:A:340:LEU:HD12 | 1:B:275:MET:CE | 2.05 | 0.69 |
| 1:A:367:TYR:O | 1:B:363:LEU:HD12 | 1.93 | 0.69 |
| 1:B:96:LYS:CA | 1:B:373:LYS:HD3 | 2.20 | 0.69 |
| 2:C:98:ARG:CG | 2:D:97:TYR:CZ | 2.75 | 0.69 |
| 3:E:79:LYS:CG | 3:F:87:PRO:HD3 | 2.22 | 0.69 |
| 1:A:34:ILE:CG2 | 1:A:181:LEU:HD22 | 2.21 | 0.69 |
| 1:A:439:SER:HA | 1:B:459:ARG:HD2 | 1.75 | 0.69 |
| 4:G:32:THR:HG21 | 4:G:43:TYR:HD2 | 1.57 | 0.69 |
| 1:A:163:GLU:HB2 | 1:A:182:ARG:CB | 2.23 | 0.69 |
| 1:A:378:GLU:CD | 1:B:98:GLN:HE22 | 1.97 | 0.69 |
| 2:C:89:THR:O | 2:C:92:LYS:HB2 | 1.92 | 0.69 |
| 1:A:441:GLU:HG2 | 1:A:456:GLU:OE1 | 1.93 | 0.69 |
| 1:B:422:ASP:CA | 1:B:425:ILE:HG22 | 2.23 | 0.69 |
| 1:B:59:ILE:HG23 | 1:B:62:LYS:HZ2 | 1.56 | 0.69 |
| 2:C:53:VAL:O | 2:C:57:VAL:HG22 | 1.93 | 0.69 |
| 1:B:288:LEU:HD11 | 2:D:34:ASP:O | 1.93 | 0.69 |
| 2:D:63:PHE:CE1 | 2:D:85:GLU:HB3 | 2.28 | 0.69 |
| 3:E:93:LEU:H | 3:E:93:LEU:HD22 | 1.58 | 0.69 |
| 3:E:38:VAL:HG21 | 3:F:86:ASP:OD2 | 1.93 | 0.69 |
| 4:G:61:GLY:HA2 | 5:H:139:LYS:CE | 2.21 | 0.69 |
| 5:H:18:ILE:HG12 | 5:H:23:GLY:O | 1.93 | 0.69 |
| 1:A:299:PHE:HA | 1:A:302:ASN:ND2 | 2.07 | 0.68 |
| 1:A:311:VAL:HG11 | 1:A:316:GLY:N | 2.02 | 0.68 |
| 3:E:57:GLY:HA3 | 3:E:83:PHE:HA | 1.75 | 0.68 |
| 3:E:104:ASP:C | 4:G:119:VAL:HG21 | 2.11 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:466:GLN:HG3 | 1:B:467:TYR:CD2 | 2.27 | 0.68 |
| 2:C:29:VAL:HG22 | 2:C:53:VAL:HG21 | 1.75 | 0.68 |
| 2:D:29:VAL:HG22 | 2:D:53:VAL:HG21 | 1.75 | 0.68 |
| 5:H:141:GLY:O | 5:H:142:GLU:HB2 | 1.93 | 0.68 |
| 5:H:22:THR:HG23 | 5:H:92:TRP:NE1 | 2.07 | 0.68 |
| 1:A:38:ILE:HG21 | 1:A:183:TYR:CD2 | 2.28 | 0.68 |
| 1:A:466:GLN:HG3 | 1:A:467:TYR:CD2 | 2.27 | 0.68 |
| 1:A:438:MET:HG3 | 1:B:434:THR:CA | 2.16 | 0.68 |
| 2:D:53:VAL:O | 2:D:57:VAL:HG22 | 1.93 | 0.68 |
| 3:E:52:LEU:HB3 | 3:E:53:GLN:CB | 2.24 | 0.68 |
| 3:E:74:VAL:HG11 | 3:E:83:PHE:CE2 | 2.28 | 0.68 |
| 3:F:74:VAL:C | 3:F:75:ILE:HD12 | 2.13 | 0.68 |
| 4:G:30:GLN:O | 4:G:33:GLU:HB3 | 1.93 | 0.68 |
| 4:G:63:ASN:OD1 | 5:H:139:LYS:CB | 2.40 | 0.68 |
| 4:G:48:ASP:HA | 4:G:67:ASP:HB2 | 1.75 | 0.68 |
| 1:A:252:GLU:CG | 1:B:85:SER:HB2 | 2.22 | 0.68 |
| 1:A:339:GLU:HB2 | 1:B:274:THR:HG21 | 1.75 | 0.68 |
| 1:A:422:ASP:CA | 1:A:425:ILE:HG22 | 2.23 | 0.68 |
| 1:B:163:GLU:HB2 | 1:B:182:ARG:CB | 2.23 | 0.68 |
| 1:B:38:ILE:HG21 | 1:B:183:TYR:CD2 | 2.28 | 0.68 |
| 1:B:405:ASN:ND2 | 1:B:406:PRO:HD2 | 2.09 | 0.68 |
| 2:C:34:ASP:N | 2:C:35:GLU:HA | 2.08 | 0.68 |
| 3:F:96:ILE:HD11 | 3:F:98:ARG:HH21 | 1.58 | 0.68 |
| 4:G:62:GLU:OE1 | 5:H:139:LYS:HD3 | 1.94 | 0.68 |
| 1:A:341:TYR:HA | 1:A:344:ALA:HB2 | 1.74 | 0.68 |
| 1:A:43:PRO:HB2 | 1:A:47:LEU:HD11 | 1.76 | 0.68 |
| 1:B:167:VAL:CG1 | 1:B:177:ILE:HB | 2.23 | 0.68 |
| 2:C:94:LEU:HG | 2:D:97:TYR:CD1 | 2.29 | 0.68 |
| 3:E:44:GLU:CG | 3:E:47:TYR:H | 2.07 | 0.68 |
| 1:A:167:VAL:CG1 | 1:A:177:ILE:HB | 2.23 | 0.68 |
| 1:A:405:ASN:ND2 | 1:A:406:PRO:HD2 | 2.09 | 0.68 |
| 1:B:123:ASP:HB2 | 1:B:124:ASP:CA | 2.24 | 0.68 |
| 1:B:163:GLU:N | 1:B:164:GLU:HA | 2.08 | 0.68 |
| 1:B:179:PHE:HD1 | 1:B:244:ILE:H | 1.41 | 0.68 |
| 1:B:294:GLU:CD | 2:C:41:ILE:C | 2.51 | 0.68 |
| 1:B:43:PRO:HB2 | 1:B:47:LEU:HD11 | 1.76 | 0.68 |
| 3:E:52:LEU:HD12 | 3:E:53:GLN:OE1 | 1.92 | 0.68 |
| 3:E:29:VAL:HG12 | 3:E:72:MET:CB | 2.24 | 0.68 |
| 2:C:70:LEU:N | 3:E:92:GLY:C | 2.34 | 0.68 |
| 3:F:60:ILE:CD1 | 3:F:99:ILE:HD11 | 2.23 | 0.68 |
| 3:E:79:LYS:HB3 | 3:F:87:PRO:CD | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:58:SER:CB | 5:H:143:ILE:HG13 | 2.23 | 0.68 |
| 5:H:37:VAL:HG11 | 5:H:62:SER:C | 2.14 | 0.68 |
| 1:A:179:PHE:HD1 | 1:A:244:ILE:H | 1.41 | 0.68 |
| 1:A:453:PRO:HB2 | 1:B:462:GLU:HG3 | 1.75 | 0.68 |
| 5:H:41:ARG:HG3 | 5:H:42:GLU:N | 2.07 | 0.68 |
| 5:H:44:PHE:CZ | 5:H:60:ALA:HB2 | 2.28 | 0.68 |
| 1:A:457:LEU:O | 1:A:457:LEU:HD23 | 1.94 | 0.68 |
| 1:B:248:LYS:HB2 | 1:B:249:ASN:O | 1.94 | 0.68 |
| 1:B:334:GLU:O | 1:B:337:GLN:HG2 | 1.92 | 0.68 |
| 1:B:447:ASN:HB2 | 1:B:448:PRO:C | 2.14 | 0.68 |
| 2:D:34:ASP:N | 2:D:35:GLU:HA | 2.08 | 0.68 |
| 3:E:62:THR:CB | 3:E:68:ILE:HD12 | 2.24 | 0.68 |
| 3:F:60:ILE:H | 3:F:60:ILE:HD13 | 1.56 | 0.68 |
| 2:D:75:MET:HE1 | 3:F:90:LEU:CD2 | 2.24 | 0.68 |
| 4:G:61:GLY:CA | 5:H:139:LYS:HB2 | 2.24 | 0.68 |
| 4:G:62:GLU:HG2 | 4:G:63:ASN:N | 2.09 | 0.68 |
| 1:A:248:LYS:HB2 | 1:A:249:ASN:O | 1.94 | 0.68 |
| 3:E:103:GLU:HG3 | 4:G:41:TYR:O | 1.92 | 0.68 |
| 3:E:40:PRO:HB2 | 3:E:42:SER:CB | 2.21 | 0.68 |
| 3:F:52:LEU:HD13 | 3:F:54:THR:H | 1.57 | 0.68 |
| 3:F:106:ALA:N | 4:G:39:ASP:N | 2.41 | 0.68 |
| 5:H:33:THR:HG22 | 5:H:34:ASP:OD2 | 1.94 | 0.68 |
| 1:A:231:THR:CA | 1:A:237:ILE:HG22 | 2.24 | 0.68 |
| 1:A:241:ARG:HE | 1:A:245:ILE:HD11 | 1.58 | 0.68 |
| 1:A:457:LEU:HD12 | 1:B:467:TYR:HE1 | 1.58 | 0.68 |
| 1:A:96:LYS:CA | 1:A:373:LYS:HD3 | 2.20 | 0.68 |
| 1:B:43:PRO:HB2 | 1:B:47:LEU:CD1 | 2.23 | 0.68 |
| 2:D:4:GLN:OE1 | 3:F:1:MET:CG | 2.42 | 0.68 |
| 3:E:50:GLN:HE21 | 3:F:52:LEU:CB | 2.07 | 0.68 |
| 3:F:32:PHE:CZ | 3:F:34:ALA:HB2 | 2.29 | 0.68 |
| 3:E:79:LYS:NZ | 3:F:99:ILE:HG12 | 2.08 | 0.68 |
| 5:H:15:PHE:HD1 | 5:H:16:GLN:N | 1.91 | 0.68 |
| 1:A:163:GLU:N | 1:A:164:GLU:HA | 2.08 | 0.67 |
| 1:B:171:ASP:HB2 | 1:B:178:LEU:HD21 | 1.77 | 0.67 |
| 2:C:25:VAL:HG12 | 2:C:29:VAL:CG2 | 2.24 | 0.67 |
| 1:B:310:LYS:C | 2:C:38:ASN:ND2 | 2.46 | 0.67 |
| 3:E:3:GLU:HG2 | 3:E:4:GLU:H | 1.59 | 0.67 |
| 3:E:70:LYS:CG | 3:E:85:GLY:H | 2.06 | 0.67 |
| 3:F:102:LYS:HB3 | 3:F:102:LYS:HZ3 | 1.58 | 0.67 |
| 5:H:143:ILE:HG12 | 5:H:147:PRO:CD | 2.23 | 0.67 |
| 1:B:414:PHE:CD2 | 1:B:415:THR:HG22 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:425:ILE:O | 1:B:429:LEU:HG | 1.95 | 0.67 |
| 1:B:457:LEU:HD23 | 1:B:457:LEU:O | 1.94 | 0.67 |
| 2:C:89:THR:HG22 | 2:D:92:LYS:CD | 1.91 | 0.67 |
| 3:E:56:ILE:N | 4:G:41:TYR:O | 2.27 | 0.67 |
| 5:H:139:LYS:H | 5:H:139:LYS:HD3 | 1.58 | 0.67 |
| 5:H:32:GLN:HE22 | 5:H:93:ARG:HD2 | 1.60 | 0.67 |
| 5:H:42:GLU:OE1 | 5:H:42:GLU:HA | 1.93 | 0.67 |
| 1:A:123:ASP:HB2 | 1:A:124:ASP:CA | 2.24 | 0.67 |
| 1:A:142:ILE:HG13 | 1:A:145:TRP:CB | 2.21 | 0.67 |
| 1:A:447:ASN:HB2 | 1:A:448:PRO:C | 2.14 | 0.67 |
| 1:B:284:ILE:HD11 | 1:B:321:ARG:HH12 | 1.58 | 0.67 |
| 1:A:418:ARG:HH22 | 1:B:426:VAL:CG1 | 2.07 | 0.67 |
| 2:C:70:LEU:O | 3:E:91:SER:CB | 2.43 | 0.67 |
| 2:C:4:GLN:CA | 3:E:1:MET:H3 | 2.07 | 0.67 |
| 5:H:112:TYR:CD2 | 5:H:114:GLU:HG2 | 2.29 | 0.67 |
| 1:A:195:GLN:HB2 | 1:A:210:LYS:HG3 | 1.75 | 0.67 |
| 1:A:200:TYR:CE1 | 1:A:205:VAL:HG13 | 2.28 | 0.67 |
| 1:A:425:ILE:O | 1:A:429:LEU:HG | 1.95 | 0.67 |
| 3:F:28:TRP:CH2 | 3:F:80:ILE:HG21 | 2.29 | 0.67 |
| 4:G:49:GLN:HB3 | 4:G:69:HIS:HE1 | 1.57 | 0.67 |
| 5:H:42:GLU:HG3 | 5:H:56:PRO:CD | 2.23 | 0.67 |
| 1:A:410:LEU:HD22 | 1:A:412:MET:CE | 2.25 | 0.67 |
| 2:D:70:LEU:H | 3:F:93:LEU:HA | 1.60 | 0.67 |
| 1:A:100:LEU:CB | 1:A:377:ALA:HB1 | 2.25 | 0.67 |
| 1:A:148:PHE:HA | 1:A:205:VAL:CG2 | 2.24 | 0.67 |
| 1:A:460:ILE:CB | 1:B:467:TYR:CG | 2.60 | 0.67 |
| 1:B:241:ARG:HE | 1:B:245:ILE:HD11 | 1.58 | 0.67 |
| 1:B:332:GLU:O | 1:B:336:ILE:HG13 | 1.95 | 0.67 |
| 1:B:441:GLU:HG2 | 1:B:456:GLU:OE1 | 1.93 | 0.67 |
| 2:C:56:PHE:HA | 2:C:59:LYS:HZ3 | 1.58 | 0.67 |
| 3:E:53:GLN:HG3 | 3:E:55:PRO:CD | 2.24 | 0.67 |
| 3:E:70:LYS:HB3 | 3:E:84:ILE:CA | 2.22 | 0.67 |
| 3:F:76:TYR:CD2 | 3:F:79:LYS:HB3 | 2.28 | 0.67 |
| 5:H:16:GLN:CD | 5:H:26:PRO:HA | 2.14 | 0.67 |
| 1:A:410:LEU:HB2 | 1:A:412:MET:HG3 | 1.77 | 0.67 |
| 1:B:38:ILE:HD11 | 1:B:181:LEU:CD1 | 2.25 | 0.67 |
| 1:B:42:ASN:ND2 | 1:B:43:PRO:HD2 | 2.10 | 0.67 |
| 3:F:74:VAL:O | 3:F:75:ILE:HD12 | 1.95 | 0.67 |
| 4:G:59:SER:HG | 5:H:138:LEU:HG | 1.56 | 0.67 |
| 5:H:32:GLN:HA | 5:H:67:TYR:CD1 | 2.30 | 0.67 |
| 1:A:183:TYR:CB | 1:A:197:ALA:HA | 2.25 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:148:PHE:HA | 1:B:205:VAL:CG2 | 2.24 | 0.67 |
| 2:D:4:GLN:OE1 | 3:F:1:MET:HB3 | 1.93 | 0.67 |
| 4:G:62:GLU:HB3 | 5:H:138:LEU:C | 2.14 | 0.67 |
| 1:A:142:ILE:HG21 | 1:A:145:TRP:CB | 2.25 | 0.67 |
| 1:A:40:GLU:HB2 | 1:A:166:ILE:CD1 | 2.07 | 0.67 |
| 1:B:142:ILE:HG21 | 1:B:145:TRP:CB | 2.25 | 0.67 |
| 1:B:46:LEU:HG | 1:B:143:GLU:OE1 | 1.94 | 0.67 |
| 2:C:99:LYS:CG | 2:D:101:ALA:HB2 | 2.22 | 0.67 |
| 3:E:46:TYR:CB | 3:E:48:LYS:HE2 | 2.24 | 0.67 |
| 3:F:35:ALA:O | 3:F:62:THR:HG23 | 1.95 | 0.67 |
| 4:G:33:GLU:HB2 | 4:G:46:ILE:N | 2.09 | 0.67 |
| 4:G:98:GLU:HG2 | 5:H:48:THR:O | 1.95 | 0.67 |
| 1:A:123:ASP:HB2 | 1:A:124:ASP:O | 1.95 | 0.67 |
| 1:A:171:ASP:HB2 | 1:A:178:LEU:HD21 | 1.77 | 0.67 |
| 1:A:38:ILE:HD11 | 1:A:181:LEU:CD1 | 2.25 | 0.67 |
| 1:A:414:PHE:CD2 | 1:A:415:THR:HG22 | 2.29 | 0.67 |
| 1:A:46:LEU:HG | 1:A:143:GLU:OE1 | 1.94 | 0.67 |
| 1:B:123:ASP:HB2 | 1:B:124:ASP:O | 1.95 | 0.67 |
| 1:B:200:TYR:CE1 | 1:B:205:VAL:HG13 | 2.28 | 0.67 |
| 3:E:29:VAL:CG1 | 3:E:72:MET:HA | 2.25 | 0.67 |
| 1:A:284:ILE:HD11 | 1:A:321:ARG:HH12 | 1.58 | 0.66 |
| 1:A:332:GLU:O | 1:A:336:ILE:HG13 | 1.95 | 0.66 |
| 1:B:381:ILE:HG22 | 1:B:385:LEU:HB2 | 1.76 | 0.66 |
| 1:B:410:LEU:HD22 | 1:B:412:MET:CE | 2.25 | 0.66 |
| 1:B:86:HIS:CD2 | 1:B:264:ILE:HG23 | 2.30 | 0.66 |
| 2:D:25:VAL:HG12 | 2:D:29:VAL:CG2 | 2.24 | 0.66 |
| 1:A:86:HIS:CD2 | 1:A:264:ILE:HG23 | 2.30 | 0.66 |
| 1:A:42:ASN:ND2 | 1:A:43:PRO:HD2 | 2.10 | 0.66 |
| 1:A:441:GLU:CG | 1:A:456:GLU:HB2 | 2.26 | 0.66 |
| 1:A:46:LEU:HA | 1:A:143:GLU:OE1 | 1.95 | 0.66 |
| 1:B:62:LYS:HE3 | 1:B:81:ASN:N | 2.11 | 0.66 |
| 2:C:59:LYS:HD3 | 2:C:90:ILE:CD1 | 2.25 | 0.66 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:HG2 | 2.09 | 0.66 |
| 2:D:87:PRO:HB3 | 2:D:90:ILE:N | 2.10 | 0.66 |
| 4:G:100:PHE:CE1 | 5:H:45:ASP:O | 2.47 | 0.66 |
| 1:A:381:ILE:HG22 | 1:A:385:LEU:HB2 | 1.76 | 0.66 |
| 1:B:110:ASP:HA | 1:B:409:GLU:OE1 | 1.95 | 0.66 |
| 1:B:231:THR:CA | 1:B:237:ILE:HG22 | 2.24 | 0.66 |
| 1:B:66:TYR:HD1 | 1:B:66:TYR:H | 1.44 | 0.66 |
| 2:D:59:LYS:HD3 | 2:D:90:ILE:CD1 | 2.25 | 0.66 |
| 2:D:77:THR:HG21 | 3:E:46:TYR:OH | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:58:TYR:O | 3:E:99:ILE:HD12 | 1.96 | 0.66 |
| 2:C:11:SER:O | 3:E:93:LEU:HB3 | 1.96 | 0.66 |
| 4:G:62:GLU:OE1 | 5:H:139:LYS:CD | 2.37 | 0.66 |
| 1:A:62:LYS:HD3 | 1:A:63:ARG:N | 2.11 | 0.66 |
| 1:A:64:ARG:NH2 | 1:B:284:ILE:CB | 2.57 | 0.66 |
| 1:A:441:GLU:HB2 | 1:B:462:GLU:OE1 | 1.95 | 0.66 |
| 2:C:98:ARG:HH12 | 2:C:99:LYS:HZ3 | 1.43 | 0.66 |
| 5:H:39:GLY:HA2 | 5:H:43:LEU:CB | 2.26 | 0.66 |
| 1:A:148:PHE:HB3 | 1:A:205:VAL:HG21 | 1.78 | 0.66 |
| 1:B:335:ARG:NH1 | 1:B:336:ILE:HG12 | 2.11 | 0.66 |
| 1:B:96:LYS:HA | 1:B:373:LYS:CD | 2.21 | 0.66 |
| 1:B:389:PHE:HB3 | 1:B:405:ASN:HD21 | 1.61 | 0.66 |
| 2:C:33:LYS:HB2 | 2:C:35:GLU:OE2 | 1.96 | 0.66 |
| 2:C:62:GLN:O | 2:C:65:MET:HG2 | 1.95 | 0.66 |
| 2:D:5:ARG:CB | 3:F:3:GLU:C | 2.64 | 0.66 |
| 3:F:73:ARG:HG3 | 3:F:81:VAL:O | 1.96 | 0.66 |
| 5:H:90:LYS:NZ | 5:H:146:LEU:HD13 | 2.09 | 0.66 |
| 1:A:110:ASP:HA | 1:A:409:GLU:OE1 | 1.95 | 0.66 |
| 1:A:390:TRP:CH2 | 1:B:125:ASP:OD2 | 2.49 | 0.66 |
| 1:B:195:GLN:HB2 | 1:B:210:LYS:HG3 | 1.75 | 0.66 |
| 4:G:100:PHE:HB3 | 5:H:47:GLN:HG2 | 1.76 | 0.66 |
| 1:A:318:ASP:O | 1:A:321:ARG:HA | 1.95 | 0.66 |
| 1:A:389:PHE:HB3 | 1:A:405:ASN:HD21 | 1.61 | 0.66 |
| 2:C:98:ARG:CZ | 2:D:102:ARG:HG2 | 2.25 | 0.66 |
| 4:G:18:LEU:HB3 | 4:G:24:LEU:CD2 | 2.26 | 0.66 |
| 5:H:122:VAL:HG13 | 5:H:125:ALA:H | 1.60 | 0.66 |
| 5:H:37:VAL:HG21 | 5:H:62:SER:OG | 1.96 | 0.66 |
| 1:A:62:LYS:HE3 | 1:A:81:ASN:N | 2.11 | 0.66 |
| 1:B:183:TYR:CB | 1:B:197:ALA:HA | 2.25 | 0.66 |
| 1:B:99:TYR:HB3 | 1:B:373:LYS:NZ | 2.11 | 0.66 |
| 3:E:62:THR:HG22 | 3:E:63:PRO:HD2 | 1.78 | 0.66 |
| 3:F:20:GLY:O | 4:G:20:SER:HA | 1.95 | 0.66 |
| 1:B:169:TYR:CE1 | 1:B:174:ARG:HG3 | 2.31 | 0.66 |
| 1:B:169:TYR:HB3 | 1:B:176:ASP:O | 1.96 | 0.66 |
| 1:B:204:HIS:HE2 | 1:B:226:PRO:HG2 | 1.60 | 0.66 |
| 1:B:100:LEU:CB | 1:B:377:ALA:HB1 | 2.25 | 0.66 |
| 1:B:43:PRO:HA | 1:B:164:GLU:N | 2.09 | 0.66 |
| 2:C:87:PRO:HB3 | 2:C:90:ILE:N | 2.10 | 0.66 |
| 3:E:96:ILE:HD12 | 3:E:98:ARG:HH21 | 1.61 | 0.66 |
| 4:G:113:ILE:HG21 | 4:G:121:LYS:CD | 2.26 | 0.66 |
| 5:H:141:GLY:O | 5:H:142:GLU:CB | 2.43 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:204:HIS:HE2 | 1:A:226:PRO:HG2 | 1.61 | 0.66 |
| 1:A:66:TYR:H | 1:A:66:TYR:HD1 | 1.44 | 0.66 |
| 1:A:438:MET:HG3 | 1:B:434:THR:CG2 | 2.25 | 0.66 |
| 2:C:98:ARG:HG3 | 2:D:97:TYR:CE2 | 2.30 | 0.66 |
| 3:F:46:TYR:CB | 3:F:48:LYS:HE2 | 2.24 | 0.66 |
| 4:G:4:LYS:HG2 | 4:G:5:LEU:HD13 | 1.78 | 0.66 |
| 1:A:169:TYR:CE1 | 1:A:174:ARG:HG3 | 2.31 | 0.65 |
| 1:A:99:TYR:HB3 | 1:A:373:LYS:NZ | 2.11 | 0.65 |
| 1:B:352:GLU:HG3 | 1:B:354:ILE:N | 2.11 | 0.65 |
| 1:B:294:GLU:OE1 | 2:C:41:ILE:O | 2.14 | 0.65 |
| 2:C:5:ARG:CG | 2:C:8:ARG:HB2 | 2.26 | 0.65 |
| 2:C:94:LEU:CA | 2:D:97:TYR:HA | 2.20 | 0.65 |
| 2:D:59:LYS:HD3 | 2:D:90:ILE:HD13 | 1.77 | 0.65 |
| 2:D:98:ARG:HH12 | 2:D:99:LYS:HZ3 | 1.44 | 0.65 |
| 5:H:32:GLN:HB2 | 5:H:67:TYR:HE1 | 1.59 | 0.65 |
| 5:H:42:GLU:N | 5:H:43:LEU:HA | 2.10 | 0.65 |
| 2:D:5:ARG:CG | 2:D:8:ARG:HB2 | 2.26 | 0.65 |
| 3:E:76:TYR:O | 3:F:87:PRO:HG2 | 1.95 | 0.65 |
| 3:E:88:VAL:C | 3:E:97:THR:HG23 | 2.16 | 0.65 |
| 3:F:28:TRP:HZ3 | 3:F:80:ILE:HG21 | 1.58 | 0.65 |
| 3:F:47:TYR:HB3 | 3:F:50:GLN:CB | 2.26 | 0.65 |
| 4:G:33:GLU:HG3 | 4:G:46:ILE:H | 1.60 | 0.65 |
| 1:B:62:LYS:HD3 | 1:B:63:ARG:N | 2.11 | 0.65 |
| 2:C:4:GLN:HA | 3:E:1:MET:N | 2.11 | 0.65 |
| 2:C:52:GLY:O | 2:C:55:ILE:HG12 | 1.95 | 0.65 |
| 2:C:7:LYS:HZ3 | 3:E:4:GLU:CD | 2.00 | 0.65 |
| 2:C:9:LEU:CD1 | 2:D:20:TYR:HE2 | 2.10 | 0.65 |
| 1:A:125:ASP:O | 1:A:129:ILE:HG12 | 1.97 | 0.65 |
| 1:A:290:ASN:HB2 | 1:A:291:TYR:CB | 2.27 | 0.65 |
| 1:A:335:ARG:CZ | 1:B:278:PHE:CE1 | 2.78 | 0.65 |
| 1:B:187:LYS:CD | 1:B:193:GLU:HB3 | 2.26 | 0.65 |
| 1:B:111:ASN:CB | 1:B:396:LEU:HD22 | 2.26 | 0.65 |
| 2:D:33:LYS:HB2 | 2:D:35:GLU:OE2 | 1.96 | 0.65 |
| 3:E:79:LYS:HZ1 | 3:F:99:ILE:HG12 | 1.59 | 0.65 |
| 4:G:21:TYR:CE1 | 4:G:23:PRO:HD2 | 2.32 | 0.65 |
| 4:G:44:VAL:CG1 | 4:G:74:THR:HG22 | 2.25 | 0.65 |
| 1:A:121:LEU:HB3 | 1:A:124:ASP:H | 1.60 | 0.65 |
| 1:A:169:TYR:HB3 | 1:A:176:ASP:O | 1.96 | 0.65 |
| 1:A:373:LYS:HE3 | 1:A:374:ALA:CB | 2.26 | 0.65 |
| 1:A:339:GLU:CD | 1:B:274:THR:CG2 | 2.65 | 0.65 |
| 1:B:318:ASP:O | 1:B:321:ARG:HA | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:373:LYS:HE3 | 1:B:374:ALA:CB | 2.26 | 0.65 |
| 1:B:53:TYR:HB2 | 1:B:140:LYS:HE3 | 1.79 | 0.65 |
| 1:B:298:GLU:HG3 | 2:C:42:ASP:OD2 | 1.97 | 0.65 |
| 2:C:85:GLU:OE2 | 2:D:86:ILE:CG2 | 2.42 | 0.65 |
| 2:C:87:PRO:HG3 | 2:C:90:ILE:CD1 | 2.22 | 0.65 |
| 2:D:62:GLN:O | 2:D:65:MET:HG2 | 1.95 | 0.65 |
| 2:C:12:ILE:HA | 3:E:93:LEU:HG | 1.78 | 0.65 |
| 4:G:88:GLU:O | 4:G:91:THR:HG22 | 1.96 | 0.65 |
| 1:B:148:PHE:HB3 | 1:B:205:VAL:HG21 | 1.78 | 0.65 |
| 1:B:306:HIS:CE1 | 2:C:39:PRO:HG3 | 2.30 | 0.65 |
| 1:B:410:LEU:HB2 | 1:B:412:MET:HG3 | 1.77 | 0.65 |
| 1:B:441:GLU:CG | 1:B:456:GLU:HB2 | 2.25 | 0.65 |
| 1:B:46:LEU:HA | 1:B:143:GLU:OE1 | 1.95 | 0.65 |
| 2:C:90:ILE:O | 2:C:93:LYS:HB3 | 1.96 | 0.65 |
| 2:D:10:LEU:O | 2:D:16:LYS:HB2 | 1.97 | 0.65 |
| 2:D:56:PHE:HA | 2:D:59:LYS:HZ3 | 1.58 | 0.65 |
| 4:G:44:VAL:HG13 | 4:G:70:VAL:HG12 | 1.78 | 0.65 |
| 1:A:187:LYS:CD | 1:A:193:GLU:HB3 | 2.26 | 0.65 |
| 1:A:371:ASP:C | 1:B:363:LEU:CD2 | 2.52 | 0.65 |
| 1:B:125:ASP:O | 1:B:129:ILE:HG12 | 1.97 | 0.65 |
| 3:E:57:GLY:HA2 | 3:E:82:THR:O | 1.97 | 0.65 |
| 4:G:33:GLU:CG | 4:G:46:ILE:H | 2.10 | 0.65 |
| 1:A:53:TYR:HB2 | 1:A:140:LYS:HE3 | 1.79 | 0.65 |
| 1:A:59:ILE:HG23 | 1:A:62:LYS:HZ2 | 1.59 | 0.65 |
| 1:B:121:LEU:HB3 | 1:B:124:ASP:H | 1.60 | 0.65 |
| 1:B:199:LEU:O | 1:B:206:TYR:HB2 | 1.96 | 0.65 |
| 1:B:433:VAL:HB | 1:B:440:LYS:HG3 | 1.78 | 0.65 |
| 3:E:57:GLY:CA | 3:E:83:PHE:HA | 2.26 | 0.65 |
| 3:E:30:ASP:HA | 3:E:73:ARG:O | 1.97 | 0.65 |
| 2:C:71:THR:CA | 3:E:92:GLY:CA | 2.70 | 0.65 |
| 3:F:43:GLN:HB2 | 3:F:47:TYR:CE1 | 2.31 | 0.65 |
| 5:H:58:SER:HB3 | 5:H:143:ILE:CG1 | 2.26 | 0.65 |
| 1:A:43:PRO:HA | 1:A:164:GLU:N | 2.09 | 0.65 |
| 1:B:126:PHE:HE2 | 1:B:392:PHE:CZ | 2.15 | 0.65 |
| 1:A:456:GLU:HG2 | 1:B:466:GLN:OE1 | 1.97 | 0.65 |
| 1:A:460:ILE:CG1 | 1:B:467:TYR:HB2 | 2.27 | 0.65 |
| 3:E:104:ASP:HB2 | 4:G:119:VAL:HG21 | 1.78 | 0.65 |
| 4:G:61:GLY:HA3 | 5:H:139:LYS:HE2 | 1.79 | 0.65 |
| 1:A:126:PHE:HE2 | 1:A:392:PHE:CZ | 2.15 | 0.65 |
| 2:C:98:ARG:CB | 2:D:97:TYR:CZ | 2.59 | 0.65 |
| 2:D:59:LYS:HD3 | 2:D:90:ILE:CG2 | 2.24 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:105:GLY:C | 4:G:39:ASP:N | 2.47 | 0.65 |
| 2:D:73:ARG:NE | 3:F:91:SER:HB3 | 2.07 | 0.65 |
| 4:G:65:THR:HG23 | 4:G:127:VAL:O | 1.97 | 0.65 |
| 4:G:74:THR:HG23 | 4:G:75:THR:HG22 | 1.77 | 0.65 |
| 5:H:143:ILE:N | 5:H:144:ASP:HA | 2.12 | 0.65 |
| 1:A:123:ASP:HB2 | 1:A:124:ASP:C | 2.17 | 0.64 |
| 1:A:140:LYS:HG2 | 1:A:141:GLY:N | 2.11 | 0.64 |
| 1:A:457:LEU:HD12 | 1:B:467:TYR:CE1 | 2.31 | 0.64 |
| 2:C:59:LYS:HD3 | 2:C:90:ILE:HD13 | 1.77 | 0.64 |
| 4:G:76:ARG:CD | 4:G:125:ILE:HG13 | 2.26 | 0.64 |
| 1:A:199:LEU:O | 1:A:206:TYR:HB2 | 1.96 | 0.64 |
| 1:A:433:VAL:HB | 1:A:440:LYS:HG3 | 1.78 | 0.64 |
| 2:C:10:LEU:O | 2:C:16:LYS:HB2 | 1.97 | 0.64 |
| 2:D:52:GLY:O | 2:D:55:ILE:HG12 | 1.95 | 0.64 |
| 2:D:75:MET:CB | 2:D:78:VAL:HB | 2.27 | 0.64 |
| 3:F:75:ILE:HG23 | 3:F:79:LYS:O | 1.97 | 0.64 |
| 4:G:100:PHE:HZ | 5:H:46:GLU:CA | 1.90 | 0.64 |
| 5:H:44:PHE:H | 5:H:44:PHE:HD1 | 1.44 | 0.64 |
| 1:A:457:LEU:CD1 | 1:B:467:TYR:CE1 | 2.60 | 0.64 |
| 1:A:289:LYS:CG | 1:B:315:GLY:CA | 2.73 | 0.64 |
| 1:A:453:PRO:HA | 1:B:462:GLU:OE2 | 1.98 | 0.64 |
| 2:C:75:MET:CB | 2:C:78:VAL:HB | 2.27 | 0.64 |
| 2:C:90:ILE:HG23 | 2:D:96:PRO:HG2 | 1.78 | 0.64 |
| 3:E:62:THR:HG21 | 3:E:68:ILE:CD1 | 2.27 | 0.64 |
| 1:A:396:LEU:O | 1:A:399:THR:HB | 1.98 | 0.64 |
| 1:B:41:HIS:HD2 | 1:B:164:GLU:HB3 | 1.63 | 0.64 |
| 1:B:183:TYR:HB3 | 1:B:197:ALA:CB | 2.27 | 0.64 |
| 2:D:90:ILE:O | 2:D:93:LYS:HB3 | 1.96 | 0.64 |
| 3:E:56:ILE:CD1 | 4:G:40:PRO:O | 2.45 | 0.64 |
| 4:G:113:ILE:HD13 | 4:G:122:HIS:ND1 | 2.11 | 0.64 |
| 1:A:120:GLU:HG3 | 1:A:121:LEU:HD22 | 1.80 | 0.64 |
| 1:A:165:MET:CG | 1:A:182:ARG:HB2 | 2.28 | 0.64 |
| 1:A:352:GLU:HG3 | 1:A:354:ILE:N | 2.11 | 0.64 |
| 2:C:11:SER:C | 3:E:93:LEU:HB3 | 2.17 | 0.64 |
| 2:D:16:LYS:HD3 | 3:E:3:GLU:OE1 | 1.97 | 0.64 |
| 3:E:102:LYS:HG2 | 3:E:102:LYS:O | 1.98 | 0.64 |
| 3:E:88:VAL:N | 3:E:97:THR:HG23 | 2.12 | 0.64 |
| 2:C:73:ARG:NH2 | 3:E:90:LEU:CD1 | 2.60 | 0.64 |
| 3:F:69:ASP:CB | 3:F:87:PRO:HG3 | 2.27 | 0.64 |
| 4:G:97:PHE:HA | 5:H:49:LYS:CG | 2.21 | 0.64 |
| 1:A:183:TYR:HB3 | 1:A:197:ALA:CB | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:354:ILE:HG22 | 1:A:355:GLY:O | 1.97 | 0.64 |
| 1:B:221:TYR:N | 1:B:222:GLY:HA3 | 2.12 | 0.64 |
| 1:B:294:GLU:OE2 | 2:C:41:ILE:N | 2.30 | 0.64 |
| 2:C:87:PRO:CB | 2:C:90:ILE:HB | 2.28 | 0.64 |
| 2:C:94:LEU:CD1 | 2:D:96:PRO:HB2 | 2.28 | 0.64 |
| 5:H:53:ILE:C | 5:H:54:LEU:O | 2.36 | 0.64 |
| 1:A:117:TYR:O | 1:A:120:GLU:HG2 | 1.97 | 0.64 |
| 1:A:291:TYR:CE1 | 2:C:33:LYS:HA | 2.32 | 0.64 |
| 1:A:410:LEU:N | 1:A:411:THR:HA | 2.12 | 0.64 |
| 1:B:290:ASN:HB2 | 1:B:291:TYR:CB | 2.27 | 0.64 |
| 1:B:410:LEU:N | 1:B:411:THR:HA | 2.12 | 0.64 |
| 1:B:89:HIS:CE1 | 1:B:257:LEU:HG | 2.32 | 0.64 |
| 2:C:59:LYS:HD3 | 2:C:90:ILE:CG2 | 2.24 | 0.64 |
| 3:E:3:GLU:HG2 | 3:E:4:GLU:N | 2.13 | 0.64 |
| 3:E:61:TYR:CE1 | 3:E:96:ILE:HD12 | 2.33 | 0.64 |
| 3:E:70:LYS:CD | 3:E:85:GLY:H | 2.10 | 0.64 |
| 4:G:14:THR:HA | 4:G:17:ASN:OD1 | 1.97 | 0.64 |
| 4:G:63:ASN:HA | 5:H:140:ASN:HD21 | 1.62 | 0.64 |
| 5:H:91:PHE:HE2 | 5:H:132:LEU:HD22 | 1.62 | 0.64 |
| 1:A:163:GLU:CA | 1:A:182:ARG:HG3 | 2.28 | 0.64 |
| 1:A:41:HIS:HD2 | 1:A:164:GLU:HB3 | 1.63 | 0.64 |
| 1:A:111:ASN:CB | 1:A:396:LEU:HD22 | 2.26 | 0.64 |
| 1:A:59:ILE:HA | 1:A:81:ASN:OD1 | 1.98 | 0.64 |
| 1:B:123:ASP:HB2 | 1:B:124:ASP:C | 2.17 | 0.64 |
| 1:B:96:LYS:CD | 1:B:377:ALA:HB2 | 2.27 | 0.64 |
| 3:F:20:GLY:O | 4:G:20:SER:CA | 2.46 | 0.64 |
| 4:G:70:VAL:HG11 | 4:G:76:ARG:NH1 | 2.13 | 0.64 |
| 1:A:221:TYR:HB2 | 1:A:222:GLY:CA | 2.28 | 0.64 |
| 1:A:96:LYS:CD | 1:A:377:ALA:HB2 | 2.27 | 0.64 |
| 1:B:117:TYR:O | 1:B:120:GLU:HG2 | 1.97 | 0.64 |
| 1:B:239:TRP:CH2 | 1:B:243:PRO:HG3 | 2.33 | 0.64 |
| 2:D:49:ILE:HD11 | 2:D:54:LEU:HD12 | 1.80 | 0.64 |
| 3:E:60:ILE:HG13 | 3:E:65:ASP:OD2 | 1.97 | 0.64 |
| 3:F:76:TYR:CE2 | 3:F:79:LYS:HB3 | 2.33 | 0.64 |
| 3:F:74:VAL:CG1 | 3:F:81:VAL:HG13 | 2.28 | 0.64 |
| 4:G:113:ILE:HD13 | 4:G:122:HIS:H | 1.61 | 0.64 |
| 4:G:70:VAL:HG21 | 4:G:76:ARG:CZ | 2.27 | 0.64 |
| 5:H:90:LYS:HE2 | 5:H:146:LEU:HB3 | 1.80 | 0.64 |
| 5:H:14:LEU:HD22 | 5:H:163:PRO:HG3 | 1.80 | 0.64 |
| 5:H:37:VAL:HG11 | 5:H:62:SER:O | 1.97 | 0.64 |
| 1:A:239:TRP:CH2 | 1:A:243:PRO:HG3 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:HIS:CE1 | 1:A:257:LEU:HG | 2.32 | 0.64 |
| 1:B:221:TYR:HB2 | 1:B:222:GLY:CA | 2.28 | 0.64 |
| 3:E:54:THR:HG23 | 3:F:102:LYS:O | 1.98 | 0.64 |
| 4:G:33:GLU:HA | 4:G:45:VAL:HA | 1.80 | 0.64 |
| 5:H:137:GLU:C | 5:H:138:LEU:CA | 2.66 | 0.64 |
| 1:B:120:GLU:HG3 | 1:B:121:LEU:HD22 | 1.80 | 0.63 |
| 1:B:140:LYS:HG2 | 1:B:141:GLY:N | 2.11 | 0.63 |
| 1:A:68:ASP:CG | 1:B:300:THR:HB | 2.14 | 0.63 |
| 1:B:396:LEU:O | 1:B:399:THR:HB | 1.98 | 0.63 |
| 1:B:291:TYR:CE1 | 2:D:33:LYS:HA | 2.32 | 0.63 |
| 2:D:87:PRO:HB2 | 2:D:91:LEU:CD2 | 2.28 | 0.63 |
| 2:D:87:PRO:CB | 2:D:90:ILE:HB | 2.28 | 0.63 |
| 1:B:433:VAL:CB | 1:B:440:LYS:HG3 | 2.28 | 0.63 |
| 2:C:34:ASP:HB3 | 2:C:35:GLU:HA | 1.80 | 0.63 |
| 2:D:5:ARG:HG2 | 2:D:8:ARG:HB2 | 1.79 | 0.63 |
| 3:E:12:GLN:HB2 | 3:E:28:TRP:HE3 | 1.61 | 0.63 |
| 3:E:29:VAL:O | 3:E:73:ARG:HB3 | 1.98 | 0.63 |
| 2:D:4:GLN:C | 3:F:1:MET:HB3 | 2.17 | 0.63 |
| 3:F:65:ASP:HB3 | 3:F:68:ILE:HD12 | 1.80 | 0.63 |
| 1:A:338:ASP:OD2 | 1:B:337:GLN:CD | 2.36 | 0.63 |
| 1:A:99:TYR:HB3 | 1:A:373:LYS:CE | 2.28 | 0.63 |
| 1:B:165:MET:CG | 1:B:182:ARG:HB2 | 2.28 | 0.63 |
| 1:B:99:TYR:HB3 | 1:B:373:LYS:CE | 2.28 | 0.63 |
| 1:A:418:ARG:HH22 | 1:B:426:VAL:HG11 | 1.63 | 0.63 |
| 1:B:87:ALA:O | 1:B:91:LEU:HD13 | 1.98 | 0.63 |
| 3:E:12:GLN:HB3 | 3:E:28:TRP:HB3 | 1.81 | 0.63 |
| 3:F:41:ILE:CG2 | 3:F:53:GLN:HG2 | 2.28 | 0.63 |
| 5:H:52:ARG:NE | 5:H:54:LEU:CA | 2.61 | 0.63 |
| 5:H:17:SER:HB3 | 5:H:89:ILE:HG22 | 1.80 | 0.63 |
| 2:C:5:ARG:HG2 | 2:C:8:ARG:HB2 | 1.79 | 0.63 |
| 2:D:25:VAL:HG13 | 2:D:53:VAL:CG1 | 2.28 | 0.63 |
| 2:D:77:THR:CG2 | 3:E:46:TYR:OH | 2.47 | 0.63 |
| 3:F:37:HIS:HB3 | 3:F:61:TYR:CE2 | 2.34 | 0.63 |
| 4:G:34:SER:HB3 | 4:G:35:PRO:HD2 | 1.80 | 0.63 |
| 1:A:29:PRO:HG3 | 1:A:170:LYS:HD3 | 1.80 | 0.63 |
| 1:A:363:LEU:O | 1:A:363:LEU:HD23 | 1.99 | 0.63 |
| 1:A:387:LEU:HD11 | 1:A:391:PHE:CE1 | 2.33 | 0.63 |
| 1:B:163:GLU:CA | 1:B:182:ARG:HG3 | 2.28 | 0.63 |
| 1:B:363:LEU:HD23 | 1:B:363:LEU:O | 1.99 | 0.63 |
| 1:B:32:THR:HG23 | 1:B:36:LYS:HE2 | 1.81 | 0.63 |
| 1:B:99:TYR:HD2 | 1:B:373:LYS:HE2 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:49:ILE:HD11 | 2:C:54:LEU:HD12 | 1.80 | 0.63 |
| 2:C:94:LEU:HB3 | 2:D:97:TYR:CD1 | 2.33 | 0.63 |
| 3:E:87:PRO:HB3 | 3:E:97:THR:HG21 | 1.81 | 0.63 |
| 5:H:10:ASP:OD1 | 5:H:167:THR:HG21 | 1.99 | 0.63 |
| 5:H:41:ARG:HE | 5:H:61:ASP:HB2 | 1.62 | 0.63 |
| 1:A:292:ASP:OD1 | 2:C:34:ASP:CA | 2.46 | 0.63 |
| 1:A:32:THR:HG23 | 1:A:36:LYS:HE2 | 1.81 | 0.63 |
| 1:B:46:LEU:HD13 | 1:B:162:ALA:CB | 2.29 | 0.63 |
| 2:C:87:PRO:HB3 | 2:C:90:ILE:HB | 1.80 | 0.63 |
| 2:D:34:ASP:HB3 | 2:D:35:GLU:HA | 1.80 | 0.63 |
| 3:E:83:PHE:CD2 | 3:E:99:ILE:HD11 | 2.34 | 0.63 |
| 3:F:7:ASP:N | 3:F:35:ALA:HB2 | 2.13 | 0.63 |
| 3:E:79:LYS:HB3 | 3:F:87:PRO:CG | 2.28 | 0.63 |
| 4:G:3:TRP:CH2 | 5:H:52:ARG:NH2 | 2.67 | 0.63 |
| 1:A:252:GLU:HG2 | 1:B:85:SER:HB2 | 1.80 | 0.63 |
| 1:A:433:VAL:CB | 1:A:440:LYS:HG3 | 2.28 | 0.63 |
| 1:B:442:THR:O | 1:B:445:ALA:HB3 | 1.99 | 0.63 |
| 2:D:54:LEU:O | 2:D:54:LEU:HD23 | 1.99 | 0.63 |
| 2:D:78:VAL:HG22 | 2:D:79:SER:N | 2.14 | 0.63 |
| 3:E:41:ILE:H | 3:F:100:LYS:CE | 2.11 | 0.63 |
| 3:E:46:TYR:HB3 | 3:E:48:LYS:CE | 2.27 | 0.63 |
| 3:F:105:GLY:N | 4:G:39:ASP:CB | 2.62 | 0.63 |
| 4:G:59:SER:CB | 5:H:138:LEU:HD11 | 2.18 | 0.63 |
| 4:G:5:LEU:HD22 | 4:G:6:ALA:H | 1.62 | 0.63 |
| 5:H:94:VAL:HG22 | 5:H:104:TYR:CE2 | 2.33 | 0.63 |
| 1:A:221:TYR:N | 1:A:222:GLY:HA3 | 2.12 | 0.63 |
| 1:A:149:VAL:CB | 1:A:229:HIS:HA | 2.21 | 0.63 |
| 1:A:335:ARG:CZ | 1:A:336:ILE:HG12 | 2.29 | 0.63 |
| 1:A:378:GLU:OE2 | 1:B:98:GLN:CD | 2.37 | 0.63 |
| 1:A:108:THR:CG2 | 1:A:412:MET:HE1 | 2.25 | 0.63 |
| 1:A:87:ALA:O | 1:A:91:LEU:HD13 | 1.98 | 0.63 |
| 1:B:179:PHE:CD1 | 1:B:244:ILE:HG23 | 2.34 | 0.63 |
| 1:B:292:ASP:OD1 | 2:D:34:ASP:CA | 2.46 | 0.63 |
| 1:B:320:LEU:N | 1:B:321:ARG:HA | 2.14 | 0.63 |
| 1:B:335:ARG:CZ | 1:B:336:ILE:HG12 | 2.29 | 0.63 |
| 1:B:354:ILE:HG22 | 1:B:355:GLY:O | 1.97 | 0.63 |
| 1:B:418:ARG:NE | 1:B:421:ASN:HB2 | 2.13 | 0.63 |
| 1:B:310:LYS:CE | 2:C:36:CYS:HB2 | 2.27 | 0.63 |
| 2:C:90:ILE:CD1 | 2:D:91:LEU:CG | 2.70 | 0.63 |
| 2:C:84:THR:HG23 | 2:D:86:ILE:HD11 | 1.80 | 0.63 |
| 3:E:53:GLN:C | 3:E:55:PRO:HD3 | 2.18 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:5:ARG:HB3 | 3:F:3:GLU:N | 2.12 | 0.63 |
| 4:G:33:GLU:OE1 | 4:G:46:ILE:HB | 1.99 | 0.63 |
| 5:H:10:ASP:HB3 | 5:H:167:THR:HB | 1.81 | 0.63 |
| 1:A:111:ASN:HD22 | 1:A:114:LEU:H | 1.46 | 0.63 |
| 1:A:46:LEU:HD13 | 1:A:162:ALA:CB | 2.29 | 0.63 |
| 1:A:378:GLU:CG | 1:B:98:GLN:OE1 | 2.47 | 0.63 |
| 1:A:442:THR:O | 1:A:445:ALA:HB3 | 1.99 | 0.63 |
| 1:B:291:TYR:HB3 | 1:B:312:SER:CB | 2.29 | 0.63 |
| 1:B:387:LEU:HD11 | 1:B:391:PHE:CE1 | 2.33 | 0.63 |
| 1:B:80:THR:HG22 | 1:B:81:ASN:N | 2.14 | 0.63 |
| 1:B:59:ILE:HA | 1:B:81:ASN:OD1 | 1.98 | 0.63 |
| 2:C:87:PRO:HB2 | 2:C:91:LEU:CD2 | 2.28 | 0.63 |
| 3:E:44:GLU:OE2 | 3:E:47:TYR:HA | 1.98 | 0.63 |
| 4:G:97:PHE:HB2 | 4:G:102:PHE:HE2 | 1.63 | 0.63 |
| 4:G:97:PHE:HD2 | 5:H:47:GLN:CA | 2.00 | 0.63 |
| 1:A:146:HIS:CA | 1:A:244:ILE:HG21 | 2.29 | 0.62 |
| 1:A:99:TYR:HD2 | 1:A:373:LYS:HE2 | 1.64 | 0.62 |
| 1:B:298:GLU:HG3 | 2:C:42:ASP:CB | 2.28 | 0.62 |
| 1:B:441:GLU:OE2 | 1:B:456:GLU:HB2 | 1.98 | 0.62 |
| 1:A:252:GLU:OE2 | 1:B:53:TYR:CE1 | 2.50 | 0.62 |
| 2:C:54:LEU:HD23 | 2:C:54:LEU:O | 1.99 | 0.62 |
| 3:E:66:ASP:OD1 | 3:E:87:PRO:HB2 | 1.98 | 0.62 |
| 5:H:122:VAL:HG22 | 5:H:123:GLU:N | 2.14 | 0.62 |
| 5:H:91:PHE:CE2 | 5:H:132:LEU:HD22 | 2.33 | 0.62 |
| 1:A:109:SER:HB3 | 1:A:114:LEU:HD23 | 1.81 | 0.62 |
| 1:B:146:HIS:CA | 1:B:244:ILE:HG21 | 2.29 | 0.62 |
| 2:C:25:VAL:HG13 | 2:C:53:VAL:CG1 | 2.28 | 0.62 |
| 5:H:114:GLU:HG3 | 5:H:115:SER:N | 2.14 | 0.62 |
| 1:A:226:PRO:HB3 | 1:A:227:ARG:HH21 | 1.63 | 0.62 |
| 1:A:284:ILE:CD1 | 1:A:321:ARG:HH12 | 2.11 | 0.62 |
| 1:B:115:LEU:HG | 1:B:119:ASN:ND2 | 2.14 | 0.62 |
| 1:B:88:TRP:NE1 | 1:B:92:PHE:HZ | 1.97 | 0.62 |
| 3:E:41:ILE:HG23 | 3:E:42:SER:N | 2.14 | 0.62 |
| 1:A:179:PHE:CD1 | 1:A:244:ILE:HG23 | 2.34 | 0.62 |
| 1:A:418:ARG:NE | 1:A:421:ASN:HB2 | 2.13 | 0.62 |
| 1:B:29:PRO:HG3 | 1:B:170:LYS:HD3 | 1.80 | 0.62 |
| 1:A:371:ASP:OD1 | 1:B:363:LEU:O | 2.16 | 0.62 |
| 2:D:87:PRO:HB3 | 2:D:90:ILE:HB | 1.80 | 0.62 |
| 3:F:22:GLY:O | 4:G:19:GLU:HB2 | 1.98 | 0.62 |
| 1:A:101:VAL:HG23 | 1:A:102:GLY:N | 2.15 | 0.62 |
| 1:A:447:ASN:HB2 | 1:A:449:PHE:N | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:SER:HB3 | 1:B:114:LEU:HD23 | 1.81 | 0.62 |
| 1:B:178:LEU:HA | 1:B:242:VAL:CG1 | 2.29 | 0.62 |
| 1:B:284:ILE:CD1 | 1:B:321:ARG:HH12 | 2.11 | 0.62 |
| 2:C:63:PHE:HZ | 2:C:82:PHE:CA | 2.12 | 0.62 |
| 3:E:9:ILE:HG13 | 3:E:11:PHE:CZ | 2.35 | 0.62 |
| 4:G:105:LYS:CG | 4:G:106:LYS:HG2 | 2.09 | 0.62 |
| 4:G:28:VAL:HG13 | 4:G:29:ASN:N | 2.13 | 0.62 |
| 4:G:44:VAL:HG21 | 4:G:74:THR:CB | 2.29 | 0.62 |
| 1:A:162:ALA:HB1 | 1:A:164:GLU:CB | 2.29 | 0.62 |
| 1:A:296:PRO:HA | 1:A:299:PHE:HB3 | 1.82 | 0.62 |
| 1:A:320:LEU:N | 1:A:321:ARG:HA | 2.14 | 0.62 |
| 1:A:441:GLU:OE2 | 1:A:456:GLU:HB2 | 1.98 | 0.62 |
| 1:A:80:THR:HG22 | 1:A:81:ASN:N | 2.14 | 0.62 |
| 2:D:93:LYS:HZ2 | 2:D:94:LEU:HD11 | 1.64 | 0.62 |
| 2:C:94:LEU:N | 2:D:97:TYR:H | 1.87 | 0.62 |
| 3:F:36:ALA:HB1 | 3:F:61:TYR:O | 2.00 | 0.62 |
| 3:F:73:ARG:HG2 | 3:F:75:ILE:CD1 | 2.30 | 0.62 |
| 4:G:97:PHE:CD2 | 5:H:47:GLN:CA | 2.72 | 0.62 |
| 5:H:16:GLN:HG3 | 5:H:92:TRP:HD1 | 1.64 | 0.62 |
| 1:A:74:LEU:HD23 | 1:A:75:VAL:H | 1.64 | 0.62 |
| 1:A:88:TRP:CZ3 | 1:A:91:LEU:HD22 | 2.35 | 0.62 |
| 1:B:111:ASN:HD22 | 1:B:114:LEU:H | 1.46 | 0.62 |
| 1:B:74:LEU:HD23 | 1:B:75:VAL:H | 1.64 | 0.62 |
| 2:C:84:THR:HG23 | 2:C:85:GLU:N | 2.14 | 0.62 |
| 3:E:88:VAL:O | 3:E:97:THR:HA | 2.00 | 0.62 |
| 3:F:14:TYR:HB2 | 3:F:73:ARG:CD | 2.25 | 0.62 |
| 3:F:3:GLU:HG2 | 3:F:4:GLU:N | 2.14 | 0.62 |
| 1:A:291:TYR:O | 1:A:312:SER:HB2 | 2.00 | 0.62 |
| 1:B:148:PHE:H | 1:B:148:PHE:HD1 | 1.46 | 0.62 |
| 1:B:46:LEU:HD13 | 1:B:162:ALA:HB2 | 1.81 | 0.62 |
| 1:B:417:THR:HB | 1:B:419:ILE:H | 1.64 | 0.62 |
| 1:B:447:ASN:HB2 | 1:B:449:PHE:N | 2.14 | 0.62 |
| 2:D:8:ARG:HD2 | 2:D:8:ARG:O | 2.00 | 0.62 |
| 2:D:5:ARG:HB3 | 3:F:2:TYR:HB3 | 1.81 | 0.62 |
| 3:F:61:TYR:CE1 | 3:F:96:ILE:HD12 | 2.35 | 0.62 |
| 1:A:146:HIS:HA | 1:A:244:ILE:CG2 | 2.30 | 0.62 |
| 1:A:341:TYR:HA | 1:A:344:ALA:CB | 2.28 | 0.62 |
| 1:B:425:ILE:HG12 | 1:B:429:LEU:HD21 | 1.82 | 0.62 |
| 2:D:87:PRO:HB3 | 2:D:90:ILE:CB | 2.30 | 0.62 |
| 5:H:99:ASN:HB2 | 5:H:104:TYR:CB | 2.29 | 0.62 |
| 1:A:335:ARG:HD3 | 1:B:333:LEU:CB | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:THR:HB | 1:A:418:ARG:CA | 2.29 | 0.62 |
| 1:A:46:LEU:HD13 | 1:A:162:ALA:HB2 | 1.81 | 0.62 |
| 1:B:142:ILE:HG13 | 1:B:145:TRP:CB | 2.21 | 0.62 |
| 2:C:98:ARG:HA | 2:D:97:TYR:CD2 | 2.35 | 0.62 |
| 3:E:77:ARG:HB2 | 3:F:87:PRO:HG2 | 1.81 | 0.62 |
| 5:H:21:ALA:O | 5:H:22:THR:HG22 | 1.99 | 0.62 |
| 1:B:296:PRO:HA | 1:B:299:PHE:HB3 | 1.82 | 0.61 |
| 1:B:108:THR:CG2 | 1:B:412:MET:HE1 | 2.28 | 0.61 |
| 1:B:438:MET:HB2 | 1:B:439:SER:HA | 1.82 | 0.61 |
| 1:A:252:GLU:CD | 1:B:53:TYR:CE1 | 2.74 | 0.61 |
| 2:C:78:VAL:HG22 | 2:C:79:SER:N | 2.14 | 0.61 |
| 2:D:84:THR:HG23 | 2:D:85:GLU:N | 2.14 | 0.61 |
| 3:E:62:THR:CG2 | 3:E:63:PRO:HD2 | 2.29 | 0.61 |
| 4:G:44:VAL:HG11 | 4:G:70:VAL:HG12 | 1.81 | 0.61 |
| 5:H:108:PHE:CD2 | 5:H:150:ILE:HG23 | 2.35 | 0.61 |
| 1:A:148:PHE:HD1 | 1:A:148:PHE:H | 1.46 | 0.61 |
| 1:A:152:GLU:HB3 | 1:A:154:GLU:OE1 | 2.00 | 0.61 |
| 1:A:88:TRP:NE1 | 1:A:92:PHE:HZ | 1.97 | 0.61 |
| 1:B:162:ALA:HB1 | 1:B:164:GLU:CB | 2.29 | 0.61 |
| 1:B:149:VAL:CB | 1:B:229:HIS:HA | 2.21 | 0.61 |
| 1:A:68:ASP:CG | 1:B:300:THR:HG21 | 2.21 | 0.61 |
| 1:B:291:TYR:O | 1:B:312:SER:HB2 | 2.00 | 0.61 |
| 2:D:6:VAL:H | 3:F:3:GLU:CA | 2.13 | 0.61 |
| 3:E:1:MET:HB2 | 3:F:93:LEU:HA | 1.82 | 0.61 |
| 5:H:111:ALA:CB | 5:H:132:LEU:HD13 | 2.30 | 0.61 |
| 5:H:122:VAL:HG12 | 5:H:125:ALA:O | 2.01 | 0.61 |
| 4:G:59:SER:HB2 | 5:H:138:LEU:HD12 | 0.62 | 0.61 |
| 4:G:60:PHE:O | 5:H:139:LYS:HE2 | 2.00 | 0.61 |
| 1:A:335:ARG:NH1 | 1:A:336:ILE:HG12 | 2.11 | 0.61 |
| 1:A:438:MET:HG3 | 1:B:434:THR:HG23 | 1.82 | 0.61 |
| 1:B:226:PRO:HB3 | 1:B:227:ARG:HH21 | 1.63 | 0.61 |
| 1:B:340:LEU:O | 1:B:344:ALA:HB2 | 2.00 | 0.61 |
| 1:B:88:TRP:CZ3 | 1:B:91:LEU:HD22 | 2.35 | 0.61 |
| 2:C:49:ILE:CD1 | 2:C:54:LEU:HG | 2.30 | 0.61 |
| 5:H:39:GLY:CA | 5:H:43:LEU:HG | 2.30 | 0.61 |
| 1:A:205:VAL:C | 1:A:206:TYR:HD1 | 2.04 | 0.61 |
| 1:A:211:ILE:HG13 | 1:A:212:ASP:N | 2.15 | 0.61 |
| 1:A:340:LEU:O | 1:A:344:ALA:HB2 | 2.00 | 0.61 |
| 1:A:425:ILE:HG12 | 1:A:429:LEU:HD21 | 1.82 | 0.61 |
| 1:B:101:VAL:HG23 | 1:B:102:GLY:N | 2.15 | 0.61 |
| 1:B:211:ILE:HG13 | 1:B:212:ASP:N | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:HIS:ND1 | 1:B:230:MET:HG3 | 2.15 | 0.61 |
| 1:B:341:TYR:HA | 1:B:344:ALA:CB | 2.28 | 0.61 |
| 1:A:442:THR:OG1 | 1:B:459:ARG:HB2 | 2.00 | 0.61 |
| 2:D:13:THR:HB | 3:E:1:MET:H2 | 1.65 | 0.61 |
| 3:E:40:PRO:CG | 3:F:100:LYS:HB2 | 2.30 | 0.61 |
| 3:E:66:ASP:HA | 3:E:87:PRO:HB2 | 1.82 | 0.61 |
| 3:F:55:PRO:HB3 | 3:F:102:LYS:HB2 | 1.82 | 0.61 |
| 3:F:76:TYR:HE1 | 3:F:81:VAL:CG1 | 2.13 | 0.61 |
| 5:H:122:VAL:HG22 | 5:H:123:GLU:H | 1.64 | 0.61 |
| 1:A:121:LEU:HB3 | 1:A:123:ASP:C | 2.21 | 0.61 |
| 1:A:291:TYR:HB3 | 1:A:312:SER:CB | 2.29 | 0.61 |
| 1:A:438:MET:HB2 | 1:A:439:SER:HA | 1.82 | 0.61 |
| 1:B:146:HIS:HA | 1:B:244:ILE:CG2 | 2.30 | 0.61 |
| 1:B:205:VAL:C | 1:B:206:TYR:HD1 | 2.04 | 0.61 |
| 1:B:267:TYR:CD2 | 1:B:345:GLN:HG3 | 2.36 | 0.61 |
| 1:B:416:ARG:N | 1:B:417:THR:HA | 2.15 | 0.61 |
| 1:B:417:THR:HB | 1:B:418:ARG:CA | 2.29 | 0.61 |
| 2:C:25:VAL:HG12 | 2:C:29:VAL:HG21 | 1.81 | 0.61 |
| 4:G:54:PHE:CD2 | 4:G:55:GLU:HG2 | 2.35 | 0.61 |
| 4:G:74:THR:HG23 | 4:G:75:THR:N | 2.16 | 0.61 |
| 5:H:37:VAL:HG13 | 5:H:38:SER:N | 2.15 | 0.61 |
| 1:A:267:TYR:CD2 | 1:A:345:GLN:HG3 | 2.36 | 0.61 |
| 1:B:152:GLU:HB3 | 1:B:154:GLU:OE1 | 2.00 | 0.61 |
| 2:C:4:GLN:HG3 | 3:E:1:MET:HE2 | 1.51 | 0.61 |
| 3:E:40:PRO:HA | 3:F:100:LYS:CE | 2.31 | 0.61 |
| 3:F:53:GLN:HG3 | 3:F:55:PRO:CD | 2.15 | 0.61 |
| 3:F:105:GLY:N | 4:G:39:ASP:HB2 | 2.15 | 0.61 |
| 4:G:64:ILE:N | 4:G:64:ILE:HD12 | 2.16 | 0.61 |
| 5:H:92:TRP:CZ3 | 5:H:106:ALA:HB3 | 2.36 | 0.61 |
| 1:A:178:LEU:HG | 1:A:242:VAL:HG11 | 1.82 | 0.61 |
| 1:A:229:HIS:ND1 | 1:A:230:MET:HG3 | 2.15 | 0.61 |
| 1:A:252:GLU:OE1 | 1:B:53:TYR:HE1 | 1.83 | 0.61 |
| 1:A:428:SER:OG | 1:B:430:VAL:HG11 | 2.00 | 0.61 |
| 1:A:64:ARG:HE | 1:B:283:GLN:NE2 | 1.98 | 0.61 |
| 2:C:69:GLY:O | 3:E:93:LEU:CD1 | 2.49 | 0.61 |
| 2:C:8:ARG:HD2 | 2:C:8:ARG:O | 2.00 | 0.61 |
| 2:D:49:ILE:CD1 | 2:D:54:LEU:HG | 2.30 | 0.61 |
| 2:D:49:ILE:HD12 | 2:D:54:LEU:HG | 1.83 | 0.61 |
| 2:D:63:PHE:HZ | 2:D:82:PHE:CA | 2.12 | 0.61 |
| 3:E:75:ILE:HG23 | 3:E:79:LYS:O | 2.01 | 0.61 |
| 3:E:77:ARG:HG3 | 3:F:87:PRO:HB2 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:133:ASN:N | 5:H:55:GLY:CA | 2.50 | 0.61 |
| 5:H:59:VAL:HG13 | 5:H:137:GLU:HB3 | 1.83 | 0.61 |
| 5:H:14:LEU:H | 5:H:14:LEU:HD23 | 1.65 | 0.61 |
| 5:H:18:ILE:HG13 | 5:H:19:ASP:N | 2.14 | 0.61 |
| 1:A:115:LEU:HG | 1:A:119:ASN:ND2 | 2.14 | 0.61 |
| 1:A:210:LYS:O | 1:A:210:LYS:HD3 | 2.01 | 0.61 |
| 1:A:439:SER:N | 1:A:440:LYS:HA | 2.16 | 0.61 |
| 1:A:46:LEU:CD1 | 1:A:162:ALA:HB2 | 2.31 | 0.61 |
| 1:A:96:LYS:HD3 | 1:A:377:ALA:HB2 | 1.82 | 0.61 |
| 2:C:73:ARG:CD | 3:E:91:SER:CB | 2.79 | 0.61 |
| 2:D:25:VAL:HG12 | 2:D:29:VAL:HG21 | 1.81 | 0.61 |
| 3:F:69:ASP:OD2 | 3:F:97:THR:HG21 | 2.00 | 0.61 |
| 4:G:64:ILE:HD12 | 5:H:140:ASN:OD1 | 2.00 | 0.61 |
| 5:H:53:ILE:O | 5:H:54:LEU:O | 2.19 | 0.61 |
| 1:A:167:VAL:HA | 1:A:177:ILE:HD12 | 1.83 | 0.61 |
| 1:A:46:LEU:H | 1:A:46:LEU:HD12 | 1.66 | 0.61 |
| 1:B:121:LEU:HB3 | 1:B:123:ASP:C | 2.21 | 0.61 |
| 2:C:49:ILE:HD12 | 2:C:54:LEU:HG | 1.83 | 0.61 |
| 2:C:5:ARG:HB2 | 3:E:3:GLU:C | 2.21 | 0.61 |
| 2:C:4:GLN:CA | 3:E:1:MET:N | 2.63 | 0.61 |
| 3:E:70:LYS:HG2 | 3:E:85:GLY:H | 1.66 | 0.61 |
| 3:F:3:GLU:HG2 | 3:F:4:GLU:H | 1.66 | 0.61 |
| 5:H:166:THR:O | 5:H:167:THR:HG22 | 2.00 | 0.61 |
| 1:A:204:HIS:CD2 | 1:A:226:PRO:HB2 | 2.36 | 0.61 |
| 2:C:87:PRO:HB3 | 2:C:90:ILE:CB | 2.30 | 0.61 |
| 3:E:2:TYR:CE1 | 3:F:95:GLU:HA | 2.35 | 0.61 |
| 3:E:71:LYS:HG2 | 3:E:71:LYS:O | 2.00 | 0.61 |
| 3:F:52:LEU:HB3 | 3:F:53:GLN:NE2 | 2.16 | 0.61 |
| 3:E:79:LYS:HE3 | 3:F:86:ASP:N | 2.16 | 0.61 |
| 4:G:63:ASN:C | 5:H:140:ASN:HD21 | 2.04 | 0.61 |
| 1:A:178:LEU:HA | 1:A:242:VAL:CG1 | 2.29 | 0.60 |
| 1:B:46:LEU:HD21 | 1:B:164:GLU:OE2 | 2.01 | 0.60 |
| 1:B:204:HIS:CD2 | 1:B:226:PRO:HB2 | 2.36 | 0.60 |
| 1:B:96:LYS:HD3 | 1:B:377:ALA:HB2 | 1.82 | 0.60 |
| 5:H:30:ALA:HB1 | 5:H:68:TYR:O | 2.01 | 0.60 |
| 1:A:118:VAL:O | 1:A:122:ALA:HA | 2.01 | 0.60 |
| 2:D:59:LYS:HD2 | 2:D:87:PRO:CG | 2.31 | 0.60 |
| 3:E:2:TYR:CE2 | 3:F:95:GLU:HG2 | 2.35 | 0.60 |
| 4:G:124:ILE:HD13 | 4:G:125:ILE:N | 2.15 | 0.60 |
| 5:H:145:THR:HG23 | 5:H:146:LEU:N | 2.16 | 0.60 |
| 5:H:17:SER:CB | 5:H:89:ILE:HG22 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:335:ARG:CD | 1:B:333:LEU:CB | 2.79 | 0.60 |
| 1:B:99:TYR:CD2 | 1:B:373:LYS:HE2 | 2.36 | 0.60 |
| 2:D:26:PRO:HA | 2:D:29:VAL:HB | 1.84 | 0.60 |
| 2:D:28:LEU:HA | 2:D:31:PHE:HE1 | 1.64 | 0.60 |
| 2:C:70:LEU:O | 3:E:91:SER:HB2 | 1.99 | 0.60 |
| 3:F:73:ARG:NH1 | 3:F:80:ILE:HD12 | 2.16 | 0.60 |
| 5:H:32:GLN:HG3 | 5:H:65:VAL:CG1 | 2.20 | 0.60 |
| 1:B:41:HIS:HB2 | 1:B:166:ILE:CG1 | 2.32 | 0.60 |
| 1:B:167:VAL:HA | 1:B:177:ILE:HD12 | 1.83 | 0.60 |
| 1:B:417:THR:N | 1:B:418:ARG:HA | 2.16 | 0.60 |
| 1:B:46:LEU:HG | 1:B:143:GLU:H | 1.67 | 0.60 |
| 1:B:63:ARG:HB3 | 1:B:75:VAL:CG1 | 2.31 | 0.60 |
| 2:C:26:PRO:HA | 2:C:29:VAL:HB | 1.84 | 0.60 |
| 3:E:31:GLU:HA | 3:E:72:MET:SD | 2.41 | 0.60 |
| 3:F:32:PHE:CE2 | 3:F:34:ALA:HB2 | 2.37 | 0.60 |
| 3:F:64:TYR:HE1 | 3:F:95:GLU:HB2 | 1.66 | 0.60 |
| 4:G:54:PHE:HD2 | 4:G:55:GLU:HG2 | 1.67 | 0.60 |
| 1:A:63:ARG:HB3 | 1:A:75:VAL:CG1 | 2.31 | 0.60 |
| 1:B:118:VAL:O | 1:B:122:ALA:HA | 2.02 | 0.60 |
| 1:A:378:GLU:OE2 | 1:B:98:GLN:NE2 | 2.34 | 0.60 |
| 2:C:100:MET:HE2 | 2:D:100:MET:CG | 2.32 | 0.60 |
| 2:C:56:PHE:CE1 | 2:C:59:LYS:HE2 | 2.35 | 0.60 |
| 2:D:56:PHE:CE1 | 2:D:59:LYS:HE2 | 2.35 | 0.60 |
| 3:E:109:GLY:CA | 4:G:113:ILE:CD1 | 2.66 | 0.60 |
| 3:E:84:ILE:HD11 | 3:E:103:GLU:H | 1.65 | 0.60 |
| 3:E:93:LEU:HD22 | 3:E:93:LEU:N | 2.16 | 0.60 |
| 3:F:6:ARG:HH11 | 3:F:33:THR:CG2 | 2.13 | 0.60 |
| 4:G:33:GLU:HA | 4:G:45:VAL:HG12 | 1.84 | 0.60 |
| 4:G:70:VAL:HG11 | 4:G:76:ARG:CZ | 2.31 | 0.60 |
| 5:H:14:LEU:HD11 | 5:H:16:GLN:HE21 | 1.66 | 0.60 |
| 5:H:44:PHE:CE1 | 5:H:60:ALA:HA | 2.36 | 0.60 |
| 1:A:417:THR:N | 1:A:418:ARG:HA | 2.16 | 0.60 |
| 1:A:46:LEU:HD12 | 1:A:46:LEU:N | 2.17 | 0.60 |
| 1:B:148:PHE:CE1 | 1:B:158:VAL:HG23 | 2.37 | 0.60 |
| 1:B:210:LYS:HD3 | 1:B:210:LYS:O | 2.01 | 0.60 |
| 1:B:439:SER:N | 1:B:440:LYS:HA | 2.16 | 0.60 |
| 1:B:93:VAL:HG21 | 1:B:257:LEU:HD11 | 1.84 | 0.60 |
| 2:C:59:LYS:HD2 | 2:C:87:PRO:CG | 2.31 | 0.60 |
| 2:D:54:LEU:HA | 2:D:57:VAL:HG22 | 1.84 | 0.60 |
| 2:C:94:LEU:HD12 | 2:D:97:TYR:N | 2.17 | 0.60 |
| 5:H:15:PHE:HZ | 5:H:91:PHE:CE2 | 2.20 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:HIS:HB2 | 1:A:166:ILE:CG1 | 2.32 | 0.60 |
| 1:A:416:ARG:N | 1:A:417:THR:HA | 2.15 | 0.60 |
| 1:A:46:LEU:HG | 1:A:143:GLU:H | 1.67 | 0.60 |
| 1:A:93:VAL:HG21 | 1:A:257:LEU:HD11 | 1.84 | 0.60 |
| 1:B:140:LYS:HD3 | 1:B:261:LYS:CE | 2.30 | 0.60 |
| 1:B:313:GLY:HA2 | 2:C:51:SER:HB2 | 1.77 | 0.60 |
| 1:B:376:MET:HA | 1:B:379:ARG:HG3 | 1.83 | 0.60 |
| 1:B:385:LEU:HD11 | 1:B:389:PHE:CZ | 2.36 | 0.60 |
| 2:C:57:VAL:HG23 | 2:C:58:ALA:N | 2.16 | 0.60 |
| 4:G:113:ILE:CG1 | 4:G:121:LYS:HB3 | 2.32 | 0.60 |
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CE1 | 2.36 | 0.60 |
| 1:A:339:GLU:OE1 | 1:B:274:THR:HG21 | 1.92 | 0.60 |
| 1:A:376:MET:HA | 1:A:379:ARG:HG3 | 1.84 | 0.60 |
| 1:A:46:LEU:HD22 | 1:A:162:ALA:CA | 2.32 | 0.60 |
| 1:A:68:ASP:OD1 | 1:B:300:THR:CG2 | 2.50 | 0.60 |
| 1:B:46:LEU:CD1 | 1:B:162:ALA:HB2 | 2.31 | 0.60 |
| 2:C:13:THR:HG23 | 2:C:14:ASN:N | 2.17 | 0.60 |
| 2:D:54:LEU:HA | 2:D:57:VAL:CG2 | 2.31 | 0.60 |
| 3:F:41:ILE:HG23 | 3:F:42:SER:N | 2.15 | 0.60 |
| 4:G:97:PHE:HB2 | 4:G:102:PHE:CE2 | 2.37 | 0.60 |
| 1:A:283:GLN:OE1 | 1:A:284:ILE:HG22 | 2.02 | 0.60 |
| 1:A:440:LYS:HE2 | 1:A:444:VAL:HG22 | 1.84 | 0.60 |
| 1:B:46:LEU:HD22 | 1:B:162:ALA:CA | 2.32 | 0.60 |
| 1:B:393:ALA:HA | 1:B:396:LEU:HD12 | 1.82 | 0.60 |
| 1:B:440:LYS:HE2 | 1:B:444:VAL:HG22 | 1.84 | 0.60 |
| 1:B:46:LEU:H | 1:B:46:LEU:HD12 | 1.66 | 0.60 |
| 1:B:46:LEU:N | 1:B:46:LEU:HD12 | 2.17 | 0.60 |
| 1:B:62:LYS:NZ | 1:B:63:ARG:HG3 | 2.17 | 0.60 |
| 1:B:314:ASP:N | 2:C:51:SER:HB2 | 2.17 | 0.60 |
| 2:C:99:LYS:HZ1 | 2:D:102:ARG:C | 2.05 | 0.60 |
| 2:C:99:LYS:HB2 | 2:D:101:ALA:HB1 | 1.56 | 0.60 |
| 2:C:7:LYS:CE | 3:E:4:GLU:CD | 2.70 | 0.60 |
| 3:E:50:GLN:O | 3:F:52:LEU:HD23 | 2.01 | 0.60 |
| 3:E:87:PRO:CB | 3:E:97:THR:HG21 | 2.32 | 0.60 |
| 3:F:65:ASP:HB2 | 3:F:68:ILE:HD12 | 1.84 | 0.60 |
| 4:G:70:VAL:HG11 | 4:G:76:ARG:NH2 | 2.15 | 0.60 |
| 1:A:46:LEU:HD21 | 1:A:164:GLU:OE2 | 2.02 | 0.60 |
| 1:A:100:LEU:HB2 | 1:A:377:ALA:CB | 2.32 | 0.60 |
| 1:A:417:THR:HB | 1:A:419:ILE:H | 1.64 | 0.60 |
| 1:B:181:LEU:CD2 | 1:B:181:LEU:H | 2.14 | 0.60 |
| 2:C:54:LEU:HA | 2:C:57:VAL:HG22 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:32:GLN:HB2 | 5:H:67:TYR:CE1 | 2.36 | 0.60 |
| 1:B:178:LEU:HG | 1:B:242:VAL:HG11 | 1.82 | 0.59 |
| 1:A:460:ILE:HG22 | 1:B:467:TYR:CB | 2.26 | 0.59 |
| 2:C:63:PHE:CD1 | 2:C:85:GLU:HB3 | 2.37 | 0.59 |
| 2:D:59:LYS:HA | 2:D:62:GLN:OE1 | 2.02 | 0.59 |
| 4:G:109:LEU:HD13 | 4:G:110:ALA:N | 2.17 | 0.59 |
| 4:G:134:ASN:HA | 5:H:138:LEU:O | 2.02 | 0.59 |
| 5:H:43:LEU:HD22 | 5:H:44:PHE:C | 2.23 | 0.59 |
| 1:A:367:TYR:CD2 | 1:A:369:LEU:HD23 | 2.31 | 0.59 |
| 2:C:28:LEU:HA | 2:C:31:PHE:HE1 | 1.64 | 0.59 |
| 2:C:59:LYS:HA | 2:C:62:GLN:OE1 | 2.02 | 0.59 |
| 2:D:33:LYS:HD3 | 2:D:50:PRO:HB3 | 1.84 | 0.59 |
| 3:E:13:SER:HB2 | 3:E:75:ILE:CD1 | 2.33 | 0.59 |
| 3:F:90:LEU:HB3 | 3:F:98:ARG:NE | 2.17 | 0.59 |
| 4:G:59:SER:HB2 | 5:H:138:LEU:CB | 2.32 | 0.59 |
| 1:A:199:LEU:O | 1:A:200:TYR:HD1 | 1.84 | 0.59 |
| 2:C:54:LEU:HA | 2:C:57:VAL:CG2 | 2.31 | 0.59 |
| 2:C:55:ILE:HG13 | 2:C:56:PHE:N | 2.17 | 0.59 |
| 3:E:74:VAL:HG11 | 3:E:76:TYR:HE1 | 1.67 | 0.59 |
| 4:G:119:VAL:HG12 | 4:G:120:THR:N | 2.17 | 0.59 |
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CD2 | 2.37 | 0.59 |
| 1:A:46:LEU:CD2 | 1:A:143:GLU:H | 2.16 | 0.59 |
| 1:A:224:ASN:ND2 | 1:A:227:ARG:HA | 2.17 | 0.59 |
| 1:A:270:ILE:HD11 | 1:B:275:MET:SD | 2.43 | 0.59 |
| 1:A:426:VAL:HA | 1:A:429:LEU:CD1 | 2.32 | 0.59 |
| 1:A:433:VAL:HG13 | 1:A:434:THR:N | 2.18 | 0.59 |
| 1:B:174:ARG:HG2 | 1:B:174:ARG:HH11 | 1.67 | 0.59 |
| 1:B:248:LYS:N | 1:B:249:ASN:HA | 2.17 | 0.59 |
| 1:A:68:ASP:CG | 1:B:300:THR:CG2 | 2.70 | 0.59 |
| 1:B:38:ILE:HG23 | 1:B:163:GLU:CG | 2.21 | 0.59 |
| 1:B:433:VAL:HG13 | 1:B:434:THR:N | 2.18 | 0.59 |
| 2:D:57:VAL:HG23 | 2:D:58:ALA:N | 2.16 | 0.59 |
| 2:D:59:LYS:CD | 2:D:90:ILE:HG21 | 2.28 | 0.59 |
| 3:E:29:VAL:CG1 | 3:E:72:MET:HG2 | 2.32 | 0.59 |
| 3:F:52:LEU:HB3 | 3:F:53:GLN:CA | 2.26 | 0.59 |
| 3:E:38:VAL:HB | 3:F:88:VAL:HG11 | 1.83 | 0.59 |
| 5:H:91:PHE:CG | 5:H:111:ALA:HB2 | 2.38 | 0.59 |
| 5:H:32:GLN:HA | 5:H:67:TYR:CE1 | 2.37 | 0.59 |
| 5:H:32:GLN:HE22 | 5:H:93:ARG:CG | 2.15 | 0.59 |
| 5:H:96:THR:HG23 | 5:H:97:VAL:N | 2.18 | 0.59 |
| 1:A:148:PHE:CE1 | 1:A:158:VAL:HG23 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:385:LEU:HD11 | 1:A:389:PHE:CZ | 2.36 | 0.59 |
| 1:A:393:ALA:HA | 1:A:396:LEU:HD12 | 1.82 | 0.59 |
| 1:A:62:LYS:NZ | 1:A:63:ARG:HG3 | 2.17 | 0.59 |
| 1:B:100:LEU:HB2 | 1:B:377:ALA:CB | 2.32 | 0.59 |
| 1:B:106:THR:HG22 | 1:B:107:PHE:N | 2.17 | 0.59 |
| 2:C:63:PHE:CG | 2:C:85:GLU:HB3 | 2.37 | 0.59 |
| 2:D:63:PHE:CD1 | 2:D:85:GLU:HB3 | 2.37 | 0.59 |
| 3:E:29:VAL:HG12 | 3:E:72:MET:HB3 | 1.85 | 0.59 |
| 3:E:51:GLN:HA | 3:F:51:GLN:OE1 | 2.03 | 0.59 |
| 1:B:169:TYR:HD2 | 1:B:171:ASP:O | 1.84 | 0.59 |
| 1:B:179:PHE:HB2 | 1:B:243:PRO:O | 2.03 | 0.59 |
| 1:B:283:GLN:OE1 | 1:B:284:ILE:HG22 | 2.02 | 0.59 |
| 1:B:419:ILE:HG23 | 1:B:420:GLN:N | 2.18 | 0.59 |
| 2:C:59:LYS:CD | 2:C:90:ILE:HG21 | 2.28 | 0.59 |
| 2:C:93:LYS:HZ2 | 2:C:94:LEU:CD1 | 2.15 | 0.59 |
| 2:D:63:PHE:CG | 2:D:85:GLU:HB3 | 2.37 | 0.59 |
| 2:D:98:ARG:HH12 | 2:D:99:LYS:NZ | 2.00 | 0.59 |
| 3:E:79:LYS:HE3 | 3:F:85:GLY:C | 2.23 | 0.59 |
| 1:A:106:THR:HG22 | 1:A:107:PHE:N | 2.17 | 0.59 |
| 1:A:290:ASN:HB2 | 1:A:291:TYR:CA | 2.32 | 0.59 |
| 1:A:99:TYR:CD2 | 1:A:373:LYS:HE2 | 2.36 | 0.59 |
| 1:B:224:ASN:ND2 | 1:B:227:ARG:HA | 2.17 | 0.59 |
| 1:B:65:THR:HG21 | 1:B:73:GLN:OE1 | 2.03 | 0.59 |
| 2:D:70:LEU:HD23 | 2:D:70:LEU:O | 2.00 | 0.59 |
| 4:G:44:VAL:HG13 | 4:G:70:VAL:CA | 2.29 | 0.59 |
| 5:H:44:PHE:HZ | 5:H:60:ALA:HB2 | 1.66 | 0.59 |
| 1:A:184:TYR:HD1 | 1:A:184:TYR:H | 1.51 | 0.59 |
| 1:A:179:PHE:HB2 | 1:A:243:PRO:O | 2.03 | 0.59 |
| 1:B:46:LEU:CD2 | 1:B:143:GLU:H | 2.16 | 0.59 |
| 1:B:199:LEU:O | 1:B:200:TYR:HD1 | 1.84 | 0.59 |
| 2:C:14:ASN:ND2 | 2:C:21:LEU:HG | 2.18 | 0.59 |
| 2:D:13:THR:HG23 | 2:D:14:ASN:N | 2.17 | 0.59 |
| 2:D:55:ILE:HG13 | 2:D:56:PHE:N | 2.17 | 0.59 |
| 3:E:52:LEU:HB3 | 3:E:53:GLN:CA | 2.32 | 0.59 |
| 3:F:98:ARG:HG2 | 3:F:98:ARG:NH1 | 2.16 | 0.59 |
| 1:A:46:LEU:HD11 | 1:A:164:GLU:OE2 | 2.02 | 0.59 |
| 1:A:174:ARG:HH11 | 1:A:174:ARG:HG2 | 1.67 | 0.59 |
| 1:A:248:LYS:N | 1:A:249:ASN:HA | 2.17 | 0.59 |
| 1:A:419:ILE:HG23 | 1:A:420:GLN:N | 2.18 | 0.59 |
| 1:A:99:TYR:HB3 | 1:A:373:LYS:HE2 | 1.84 | 0.59 |
| 1:A:175:ARG:NH2 | 1:B:148:PHE:HZ | 2.00 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:438:MET:HE3 | 1:B:433:VAL:C | 2.23 | 0.59 |
| 2:D:33:LYS:HE2 | 2:D:50:PRO:HB3 | 1.84 | 0.59 |
| 2:C:94:LEU:HG | 2:D:97:TYR:HD1 | 1.67 | 0.59 |
| 3:E:61:TYR:CB | 3:E:98:ARG:HG3 | 2.23 | 0.59 |
| 3:E:50:GLN:NE2 | 3:F:52:LEU:HB2 | 2.14 | 0.59 |
| 3:F:61:TYR:HB2 | 3:F:97:THR:O | 2.03 | 0.59 |
| 3:F:62:THR:HG21 | 3:F:68:ILE:HG21 | 1.85 | 0.59 |
| 3:F:81:VAL:HG22 | 3:F:82:THR:N | 2.18 | 0.59 |
| 4:G:82:ILE:HG13 | 4:G:83:SER:N | 2.17 | 0.59 |
| 5:H:92:TRP:CE3 | 5:H:106:ALA:HB3 | 2.37 | 0.59 |
| 5:H:30:ALA:HB3 | 5:H:67:TYR:HD2 | 1.67 | 0.59 |
| 1:A:169:TYR:CD2 | 1:A:174:ARG:HA | 2.37 | 0.59 |
| 1:A:403:ASP:O | 1:A:404:PHE:HD1 | 1.86 | 0.59 |
| 1:A:410:LEU:HD22 | 1:A:412:MET:HG2 | 1.84 | 0.59 |
| 1:B:181:LEU:HD23 | 1:B:181:LEU:N | 2.15 | 0.59 |
| 1:B:290:ASN:HB2 | 1:B:291:TYR:CA | 2.32 | 0.59 |
| 1:B:291:TYR:C | 1:B:312:SER:HB2 | 2.23 | 0.59 |
| 1:B:286:TYR:CD1 | 1:B:321:ARG:HD2 | 2.37 | 0.59 |
| 1:B:59:ILE:HD12 | 1:B:59:ILE:N | 2.15 | 0.59 |
| 2:C:84:THR:OG1 | 2:D:83:ALA:CA | 2.47 | 0.59 |
| 3:E:106:ALA:O | 4:G:41:TYR:OH | 2.19 | 0.59 |
| 3:E:80:ILE:HG12 | 3:F:70:LYS:HZ2 | 1.66 | 0.59 |
| 1:A:442:THR:HA | 1:A:445:ALA:CB | 2.32 | 0.58 |
| 1:B:134:VAL:HG23 | 1:B:135:LYS:N | 2.18 | 0.58 |
| 1:B:46:LEU:HD11 | 1:B:164:GLU:OE2 | 2.02 | 0.58 |
| 1:B:169:TYR:CD2 | 1:B:174:ARG:HA | 2.37 | 0.58 |
| 1:B:206:TYR:O | 1:B:207:TYR:HD1 | 1.84 | 0.58 |
| 1:B:59:ILE:CD1 | 1:B:59:ILE:H | 2.16 | 0.58 |
| 2:C:98:ARG:HH12 | 2:C:99:LYS:NZ | 2.00 | 0.58 |
| 2:D:69:GLY:CA | 2:D:73:ARG:HB3 | 2.25 | 0.58 |
| 2:C:93:LYS:NZ | 2:D:96:PRO:C | 2.54 | 0.58 |
| 3:E:74:VAL:HG21 | 3:E:76:TYR:CZ | 2.38 | 0.58 |
| 3:E:83:PHE:HD1 | 3:E:83:PHE:O | 1.85 | 0.58 |
| 4:G:133:ASN:O | 5:H:58:SER:N | 2.36 | 0.58 |
| 4:G:5:LEU:H | 4:G:5:LEU:CD1 | 2.06 | 0.58 |
| 5:H:37:VAL:HG11 | 5:H:63:GLY:HA2 | 1.83 | 0.58 |
| 5:H:86:GLY:O | 5:H:87:LYS:HG2 | 2.03 | 0.58 |
| 1:A:59:ILE:H | 1:A:59:ILE:CD1 | 2.16 | 0.58 |
| 1:A:65:THR:HG21 | 1:A:73:GLN:OE1 | 2.03 | 0.58 |
| 1:B:167:VAL:HG13 | 1:B:177:ILE:HB | 1.84 | 0.58 |
| 1:B:184:TYR:H | 1:B:184:TYR:HD1 | 1.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:206:TYR:HD2 | 1:B:208:TYR:OH | 1.86 | 0.58 |
| 1:B:232:LYS:CB | 1:B:237:ILE:HB | 2.31 | 0.58 |
| 1:B:53:TYR:HA | 1:B:261:LYS:NZ | 2.18 | 0.58 |
| 1:B:403:ASP:O | 1:B:404:PHE:HD1 | 1.86 | 0.58 |
| 1:B:294:GLU:CG | 2:C:41:ILE:O | 2.50 | 0.58 |
| 3:E:59:ASN:N | 3:F:100:LYS:HE3 | 2.19 | 0.58 |
| 3:F:36:ALA:HB2 | 3:F:62:THR:OG1 | 2.03 | 0.58 |
| 3:F:7:ASP:OD2 | 3:F:9:ILE:HG23 | 2.04 | 0.58 |
| 3:F:96:ILE:HG13 | 3:F:98:ARG:HE | 1.68 | 0.58 |
| 3:F:97:THR:HG22 | 3:F:98:ARG:N | 2.19 | 0.58 |
| 4:G:4:LYS:HB3 | 4:G:5:LEU:HD13 | 1.85 | 0.58 |
| 4:G:86:VAL:HG13 | 4:G:87:LEU:N | 2.17 | 0.58 |
| 5:H:55:GLY:HA2 | 5:H:56:PRO:C | 2.22 | 0.58 |
| 1:A:181:LEU:CD2 | 1:A:181:LEU:H | 2.14 | 0.58 |
| 1:A:206:TYR:HD2 | 1:A:208:TYR:OH | 1.86 | 0.58 |
| 1:B:111:ASN:HB2 | 1:B:396:LEU:HD22 | 1.85 | 0.58 |
| 1:B:99:TYR:HB3 | 1:B:373:LYS:HE2 | 1.84 | 0.58 |
| 2:C:33:LYS:HD3 | 2:C:50:PRO:HB3 | 1.84 | 0.58 |
| 3:E:70:LYS:HD3 | 3:E:84:ILE:HB | 1.86 | 0.58 |
| 3:F:103:GLU:HB3 | 4:G:31:VAL:HG21 | 1.85 | 0.58 |
| 1:A:169:TYR:HD2 | 1:A:171:ASP:O | 1.84 | 0.58 |
| 1:A:187:LYS:HE2 | 1:A:193:GLU:HB2 | 1.86 | 0.58 |
| 1:A:232:LYS:CB | 1:A:237:ILE:HB | 2.31 | 0.58 |
| 1:A:416:ARG:C | 1:A:418:ARG:HG2 | 2.23 | 0.58 |
| 1:B:426:VAL:HA | 1:B:429:LEU:CD1 | 2.32 | 0.58 |
| 2:C:33:LYS:HE2 | 2:C:50:PRO:HB3 | 1.85 | 0.58 |
| 1:A:286:TYR:HA | 1:A:321:ARG:HD2 | 1.85 | 0.58 |
| 1:A:46:LEU:O | 1:A:50:VAL:HG23 | 2.03 | 0.58 |
| 1:A:371:ASP:O | 1:B:363:LEU:HD21 | 2.03 | 0.58 |
| 3:E:58:TYR:CB | 3:F:100:LYS:HG2 | 2.34 | 0.58 |
| 2:D:5:ARG:NH2 | 3:F:2:TYR:CD2 | 2.72 | 0.58 |
| 3:F:70:LYS:NZ | 3:F:71:LYS:HB2 | 2.18 | 0.58 |
| 3:F:73:ARG:HD3 | 3:F:80:ILE:HB | 1.85 | 0.58 |
| 3:F:98:ARG:HG2 | 3:F:98:ARG:HH11 | 1.66 | 0.58 |
| 4:G:116:THR:HG23 | 4:G:117:ASP:N | 2.18 | 0.58 |
| 4:G:134:ASN:CG | 5:H:58:SER:O | 2.42 | 0.58 |
| 1:A:286:TYR:CD1 | 1:A:321:ARG:HD2 | 2.37 | 0.58 |
| 1:B:365:LYS:HD3 | 1:B:365:LYS:C | 2.24 | 0.58 |
| 1:B:410:LEU:HD22 | 1:B:412:MET:HG2 | 1.84 | 0.58 |
| 1:B:442:THR:HA | 1:B:445:ALA:CB | 2.32 | 0.58 |
| 3:E:79:LYS:CE | 3:F:87:PRO:HD3 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:49:GLN:HG3 | 4:G:49:GLN:O | 2.04 | 0.58 |
| 5:H:101:ASN:OD1 | 5:H:163:PRO:HB2 | 2.03 | 0.58 |
| 1:A:167:VAL:HG13 | 1:A:177:ILE:HB | 1.84 | 0.58 |
| 1:A:254:VAL:HG13 | 1:B:85:SER:OG | 2.04 | 0.58 |
| 1:A:53:TYR:HA | 1:A:261:LYS:NZ | 2.18 | 0.58 |
| 1:A:291:TYR:C | 1:A:312:SER:HB2 | 2.23 | 0.58 |
| 1:A:365:LYS:C | 1:A:365:LYS:HD3 | 2.24 | 0.58 |
| 1:A:407:ASP:O | 1:A:411:THR:HB | 2.03 | 0.58 |
| 1:B:187:LYS:HE2 | 1:B:193:GLU:HB2 | 1.86 | 0.58 |
| 3:E:29:VAL:HG12 | 3:E:72:MET:CG | 2.33 | 0.58 |
| 3:E:37:HIS:HE1 | 3:E:39:GLN:HB2 | 1.69 | 0.58 |
| 2:C:11:SER:HB3 | 3:E:94:GLN:N | 2.18 | 0.58 |
| 3:F:52:LEU:HD12 | 3:F:54:THR:H | 1.69 | 0.58 |
| 3:F:14:TYR:CB | 3:F:73:ARG:HD2 | 2.27 | 0.58 |
| 4:G:52:THR:HG23 | 4:G:53:PRO:HD2 | 1.85 | 0.58 |
| 4:G:63:ASN:OD1 | 5:H:139:LYS:CG | 2.51 | 0.58 |
| 1:A:206:TYR:O | 1:A:207:TYR:HD1 | 1.84 | 0.58 |
| 1:A:59:ILE:HD12 | 1:A:59:ILE:N | 2.15 | 0.58 |
| 1:B:286:TYR:HA | 1:B:321:ARG:HD2 | 1.85 | 0.58 |
| 1:B:407:ASP:O | 1:B:411:THR:HB | 2.03 | 0.58 |
| 2:C:94:LEU:CG | 2:D:97:TYR:CD1 | 2.86 | 0.58 |
| 3:E:98:ARG:HG2 | 3:E:98:ARG:HH11 | 1.67 | 0.58 |
| 3:F:108:VAL:HG22 | 3:F:109:GLY:N | 2.17 | 0.58 |
| 3:F:13:SER:HB2 | 3:F:29:VAL:CG2 | 2.33 | 0.58 |
| 3:E:109:GLY:C | 4:G:114:THR:H | 2.03 | 0.58 |
| 5:H:39:GLY:O | 5:H:43:LEU:HD12 | 2.03 | 0.58 |
| 5:H:41:ARG:HE | 5:H:61:ASP:CB | 2.17 | 0.58 |
| 1:A:165:MET:HB2 | 1:A:180:ALA:HB3 | 1.86 | 0.58 |
| 1:A:111:ASN:HB2 | 1:A:396:LEU:HD22 | 1.85 | 0.58 |
| 1:B:201:THR:HG22 | 1:B:202:ASP:N | 2.18 | 0.58 |
| 1:B:202:ASP:CA | 1:B:242:VAL:HG23 | 2.32 | 0.58 |
| 1:B:326:VAL:HG12 | 1:B:327:ASP:N | 2.17 | 0.58 |
| 3:E:53:GLN:CG | 3:E:55:PRO:HG3 | 2.34 | 0.58 |
| 3:E:61:TYR:HB2 | 3:E:98:ARG:CG | 2.25 | 0.58 |
| 3:E:61:TYR:HE1 | 3:E:96:ILE:CB | 2.15 | 0.58 |
| 2:D:5:ARG:N | 3:F:3:GLU:H | 1.97 | 0.58 |
| 5:H:104:TYR:CD1 | 5:H:159:ASP:HB3 | 2.39 | 0.58 |
| 5:H:37:VAL:CG2 | 5:H:64:GLU:HG2 | 2.33 | 0.58 |
| 5:H:96:THR:HG23 | 5:H:97:VAL:H | 1.68 | 0.58 |
| 1:B:88:TRP:HZ3 | 1:B:91:LEU:HD22 | 1.68 | 0.58 |
| 2:D:14:ASN:ND2 | 2:D:21:LEU:HG | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:40:PHE:O | 2:D:48:SER:HB3 | 2.04 | 0.58 |
| 3:F:7:ASP:HB2 | 3:F:35:ALA:HA | 1.86 | 0.58 |
| 5:H:100:GLU:HB3 | 5:H:103:LYS:HB3 | 1.86 | 0.58 |
| 5:H:32:GLN:HE22 | 5:H:93:ARG:CD | 2.16 | 0.58 |
| 1:A:134:VAL:HG23 | 1:A:135:LYS:N | 2.18 | 0.57 |
| 1:A:181:LEU:N | 1:A:181:LEU:HD23 | 2.15 | 0.57 |
| 1:A:183:TYR:HB2 | 1:A:197:ALA:HA | 1.85 | 0.57 |
| 1:B:163:GLU:HA | 1:B:182:ARG:HG3 | 1.85 | 0.57 |
| 1:B:416:ARG:C | 1:B:418:ARG:HG2 | 2.23 | 0.57 |
| 3:E:38:VAL:HA | 3:E:60:ILE:HB | 1.84 | 0.57 |
| 3:E:79:LYS:HD3 | 3:F:70:LYS:HB3 | 1.85 | 0.57 |
| 4:G:18:LEU:HB3 | 4:G:24:LEU:HD22 | 1.86 | 0.57 |
| 5:H:113:ILE:HG23 | 5:H:114:GLU:N | 2.18 | 0.57 |
| 5:H:138:LEU:HD22 | 5:H:138:LEU:N | 2.19 | 0.57 |
| 5:H:53:ILE:O | 5:H:54:LEU:C | 2.42 | 0.57 |
| 1:A:109:SER:H | 1:A:115:LEU:HD13 | 1.68 | 0.57 |
| 1:B:148:PHE:CZ | 1:B:158:VAL:HG23 | 2.39 | 0.57 |
| 1:B:165:MET:HB2 | 1:B:180:ALA:HB3 | 1.86 | 0.57 |
| 1:B:387:LEU:HD11 | 1:B:391:PHE:CZ | 2.40 | 0.57 |
| 2:C:85:GLU:HA | 2:D:86:ILE:CD1 | 2.24 | 0.57 |
| 3:E:54:THR:OG1 | 3:F:105:GLY:HA3 | 2.02 | 0.57 |
| 2:D:7:LYS:HD3 | 3:F:4:GLU:OE1 | 2.04 | 0.57 |
| 3:F:32:PHE:CE2 | 3:F:67:ARG:HD2 | 2.38 | 0.57 |
| 4:G:31:VAL:HG22 | 4:G:32:THR:HA | 1.87 | 0.57 |
| 1:A:148:PHE:CZ | 1:A:158:VAL:HG23 | 2.39 | 0.57 |
| 1:A:182:ARG:HG2 | 1:A:183:TYR:N | 2.19 | 0.57 |
| 1:A:187:LYS:CE | 1:A:193:GLU:HB3 | 2.35 | 0.57 |
| 1:A:326:VAL:HG12 | 1:A:327:ASP:N | 2.17 | 0.57 |
| 1:B:162:ALA:HB1 | 1:B:164:GLU:CA | 2.35 | 0.57 |
| 1:B:415:THR:HB | 1:B:417:THR:OG1 | 2.04 | 0.57 |
| 1:A:441:GLU:CB | 1:B:462:GLU:OE2 | 2.52 | 0.57 |
| 2:D:4:GLN:OE1 | 3:F:1:MET:CB | 2.52 | 0.57 |
| 3:E:1:MET:HG3 | 3:E:2:TYR:N | 2.16 | 0.57 |
| 2:C:5:ARG:HA | 3:E:3:GLU:CA | 2.34 | 0.57 |
| 3:F:53:GLN:OE1 | 3:F:102:LYS:HE3 | 2.03 | 0.57 |
| 1:B:182:ARG:HG2 | 1:B:183:TYR:N | 2.20 | 0.57 |
| 1:B:51:ARG:HD2 | 1:B:57:ASN:OD1 | 2.04 | 0.57 |
| 2:D:34:ASP:HB3 | 2:D:35:GLU:CA | 2.35 | 0.57 |
| 3:E:37:HIS:HB2 | 3:F:89:ASP:OD1 | 2.04 | 0.57 |
| 4:G:32:THR:HG21 | 4:G:43:TYR:CB | 2.31 | 0.57 |
| 4:G:37:LYS:HD3 | 4:G:37:LYS:H | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:LYS:O | 1:A:116:GLU:HG3 | 2.05 | 0.57 |
| 1:A:290:ASN:HB2 | 1:A:291:TYR:HB2 | 1.87 | 0.57 |
| 1:A:415:THR:HB | 1:A:417:THR:OG1 | 2.04 | 0.57 |
| 1:A:88:TRP:HZ3 | 1:A:91:LEU:HD22 | 1.68 | 0.57 |
| 1:A:96:LYS:HE3 | 1:A:377:ALA:CB | 2.34 | 0.57 |
| 1:B:216:GLN:HG2 | 1:B:217:MET:H | 1.70 | 0.57 |
| 2:C:71:THR:N | 2:C:72:GLY:HA3 | 2.18 | 0.57 |
| 5:H:52:ARG:CD | 5:H:54:LEU:HA | 2.21 | 0.57 |
| 5:H:59:VAL:HG12 | 5:H:60:ALA:N | 2.18 | 0.57 |
| 1:A:201:THR:HG22 | 1:A:202:ASP:N | 2.18 | 0.57 |
| 1:A:216:GLN:HG2 | 1:A:217:MET:H | 1.70 | 0.57 |
| 1:A:460:ILE:HG22 | 1:B:467:TYR:HB3 | 1.85 | 0.57 |
| 2:C:34:ASP:HB3 | 2:C:35:GLU:CA | 2.35 | 0.57 |
| 2:C:36:CYS:N | 2:C:37:HIS:HA | 2.20 | 0.57 |
| 2:C:100:MET:HE1 | 2:D:100:MET:HB3 | 1.86 | 0.57 |
| 3:E:97:THR:HG22 | 3:E:98:ARG:N | 2.18 | 0.57 |
| 3:F:106:ALA:O | 3:F:107:TYR:HB2 | 2.05 | 0.57 |
| 4:G:6:ALA:O | 4:G:9:ALA:HB3 | 2.05 | 0.57 |
| 5:H:108:PHE:HD2 | 5:H:150:ILE:HG23 | 1.68 | 0.57 |
| 1:A:159:ILE:O | 1:A:160:PHE:HD1 | 1.87 | 0.57 |
| 1:A:202:ASP:HB2 | 1:A:242:VAL:CG2 | 2.35 | 0.57 |
| 1:A:207:TYR:O | 1:A:208:TYR:HD1 | 1.88 | 0.57 |
| 1:B:207:TYR:O | 1:B:208:TYR:HD1 | 1.88 | 0.57 |
| 1:B:46:LEU:O | 1:B:50:VAL:HG23 | 2.04 | 0.57 |
| 4:G:76:ARG:HD2 | 4:G:125:ILE:HG13 | 1.87 | 0.57 |
| 4:G:73:GLY:HA2 | 4:G:76:ARG:NH2 | 2.20 | 0.57 |
| 4:G:98:GLU:N | 5:H:49:LYS:HD3 | 2.20 | 0.57 |
| 4:G:9:ALA:O | 4:G:12:LYS:HB3 | 2.04 | 0.57 |
| 1:A:46:LEU:HG | 1:A:143:GLU:HB2 | 1.85 | 0.57 |
| 1:A:162:ALA:HB1 | 1:A:164:GLU:CA | 2.35 | 0.57 |
| 1:A:202:ASP:CA | 1:A:242:VAL:HG23 | 2.32 | 0.57 |
| 1:B:159:ILE:O | 1:B:160:PHE:HD1 | 1.87 | 0.57 |
| 1:B:183:TYR:HB2 | 1:B:197:ALA:HA | 1.85 | 0.57 |
| 2:D:70:LEU:CB | 3:E:2:TYR:CE1 | 2.87 | 0.57 |
| 3:E:62:THR:H | 3:E:65:ASP:HB2 | 1.68 | 0.57 |
| 1:A:317:VAL:HG23 | 1:A:317:VAL:O | 2.05 | 0.57 |
| 1:A:51:ARG:HD2 | 1:A:57:ASN:OD1 | 2.04 | 0.57 |
| 2:D:71:THR:N | 2:D:72:GLY:HA3 | 2.18 | 0.57 |
| 5:H:46:GLU:H | 5:H:151:VAL:HG11 | 1.70 | 0.57 |
| 1:A:136:ASN:HB2 | 1:A:145:TRP:CZ3 | 2.40 | 0.57 |
| 1:A:204:HIS:NE2 | 1:A:226:PRO:HG2 | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:187:LYS:CE | 1:B:193:GLU:HB3 | 2.35 | 0.57 |
| 3:E:16:GLU:HB3 | 3:E:24:LYS:HD3 | 1.87 | 0.57 |
| 3:E:58:TYR:CD2 | 3:F:100:LYS:HG2 | 2.39 | 0.57 |
| 3:F:12:GLN:NE2 | 3:F:75:ILE:HG12 | 2.20 | 0.57 |
| 3:F:88:VAL:O | 3:F:97:THR:HA | 2.02 | 0.57 |
| 5:H:112:TYR:HD2 | 5:H:114:GLU:HG2 | 1.68 | 0.57 |
| 1:A:169:TYR:CD1 | 1:A:174:ARG:HA | 2.40 | 0.56 |
| 1:A:387:LEU:HD11 | 1:A:391:PHE:CZ | 2.40 | 0.56 |
| 1:A:422:ASP:C | 1:A:425:ILE:HG22 | 2.25 | 0.56 |
| 1:A:440:LYS:C | 1:A:440:LYS:HD3 | 2.26 | 0.56 |
| 1:A:92:PHE:CZ | 1:A:369:LEU:HD22 | 2.40 | 0.56 |
| 1:B:204:HIS:NE2 | 1:B:226:PRO:HG2 | 2.19 | 0.56 |
| 1:B:52:TYR:HE1 | 1:B:56:GLU:CB | 2.18 | 0.56 |
| 2:C:40:PHE:O | 2:C:48:SER:HB3 | 2.04 | 0.56 |
| 2:C:84:THR:CG2 | 2:D:86:ILE:HD11 | 2.35 | 0.56 |
| 3:E:105:GLY:O | 4:G:41:TYR:CE1 | 2.48 | 0.56 |
| 3:F:83:PHE:O | 3:F:83:PHE:HD1 | 1.88 | 0.56 |
| 1:A:100:LEU:HD11 | 1:A:381:ILE:HG13 | 1.87 | 0.56 |
| 1:A:38:ILE:HG23 | 1:A:163:GLU:CG | 2.21 | 0.56 |
| 1:A:417:THR:CB | 1:A:418:ARG:HA | 2.28 | 0.56 |
| 1:A:83:ARG:N | 1:A:83:ARG:HD3 | 2.19 | 0.56 |
| 1:B:134:VAL:HA | 1:B:137:MET:HE2 | 1.87 | 0.56 |
| 1:B:99:TYR:HB3 | 1:B:373:LYS:HZ1 | 1.70 | 0.56 |
| 2:C:100:MET:CE | 2:D:100:MET:HB3 | 2.33 | 0.56 |
| 2:D:63:PHE:CB | 2:D:85:GLU:HG2 | 2.35 | 0.56 |
| 3:F:57:GLY:O | 3:F:58:TYR:HD1 | 1.88 | 0.56 |
| 3:F:90:LEU:HB3 | 3:F:98:ARG:CZ | 2.35 | 0.56 |
| 5:H:89:ILE:CG2 | 5:H:91:PHE:HE1 | 2.18 | 0.56 |
| 1:A:104:PRO:HG2 | 1:A:127:ASP:OD2 | 2.05 | 0.56 |
| 1:A:140:LYS:HD3 | 1:A:261:LYS:CE | 2.30 | 0.56 |
| 1:B:112:LYS:O | 1:B:116:GLU:HG3 | 2.05 | 0.56 |
| 1:A:439:SER:O | 1:B:459:ARG:NH1 | 2.38 | 0.56 |
| 2:C:63:PHE:CB | 2:C:85:GLU:HG2 | 2.35 | 0.56 |
| 3:E:12:GLN:O | 3:E:13:SER:HB3 | 2.04 | 0.56 |
| 3:E:13:SER:CB | 3:E:75:ILE:HD13 | 2.35 | 0.56 |
| 3:E:58:TYR:HD2 | 3:F:86:ASP:CG | 2.09 | 0.56 |
| 1:A:364:GLU:C | 1:A:368:ALA:HB3 | 2.25 | 0.56 |
| 1:A:59:ILE:HG23 | 1:A:62:LYS:HZ3 | 1.69 | 0.56 |
| 1:B:390:TRP:O | 1:B:394:GLU:HG2 | 2.05 | 0.56 |
| 2:C:29:VAL:CG1 | 2:C:50:PRO:HG3 | 2.35 | 0.56 |
| 2:C:98:ARG:NH1 | 2:D:102:ARG:CA | 2.67 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:36:CYS:N | 2:D:37:HIS:HA | 2.19 | 0.56 |
| 2:D:5:ARG:CD | 2:D:7:LYS:HB2 | 2.29 | 0.56 |
| 4:G:57:LYS:HG2 | 4:G:57:LYS:O | 2.05 | 0.56 |
| 4:G:46:ILE:HG22 | 4:G:66:MET:HE1 | 1.86 | 0.56 |
| 5:H:99:ASN:CB | 5:H:104:TYR:HB2 | 2.35 | 0.56 |
| 1:A:52:TYR:HE1 | 1:A:56:GLU:CB | 2.18 | 0.56 |
| 1:A:270:ILE:CD1 | 1:B:275:MET:SD | 2.93 | 0.56 |
| 1:B:46:LEU:HG | 1:B:143:GLU:HB2 | 1.86 | 0.56 |
| 1:B:96:LYS:HE3 | 1:B:377:ALA:CB | 2.34 | 0.56 |
| 1:A:319:THR:O | 1:A:319:THR:HG22 | 2.06 | 0.56 |
| 1:B:109:SER:H | 1:B:115:LEU:HD13 | 1.69 | 0.56 |
| 1:B:148:PHE:CB | 1:B:205:VAL:HG21 | 2.35 | 0.56 |
| 1:B:202:ASP:HB2 | 1:B:242:VAL:CG2 | 2.35 | 0.56 |
| 1:B:294:GLU:CG | 2:C:42:ASP:CG | 2.74 | 0.56 |
| 1:B:317:VAL:O | 1:B:317:VAL:HG23 | 2.05 | 0.56 |
| 3:F:26:TYR:HD1 | 3:F:26:TYR:O | 1.89 | 0.56 |
| 3:F:44:GLU:O | 3:F:45:GLU:HB3 | 2.05 | 0.56 |
| 4:G:113:ILE:CB | 4:G:121:LYS:HB3 | 2.35 | 0.56 |
| 5:H:52:ARG:NE | 5:H:54:LEU:N | 2.51 | 0.56 |
| 1:A:163:GLU:HA | 1:A:182:ARG:HG3 | 1.85 | 0.56 |
| 1:A:148:PHE:CB | 1:A:205:VAL:HG21 | 2.35 | 0.56 |
| 1:A:367:TYR:N | 1:A:368:ALA:HB2 | 2.21 | 0.56 |
| 1:A:63:ARG:HD2 | 1:A:76:ASP:O | 2.05 | 0.56 |
| 1:B:177:ILE:HG23 | 1:B:177:ILE:O | 2.05 | 0.56 |
| 1:B:255:SER:HB2 | 1:B:256:ASP:CA | 2.34 | 0.56 |
| 1:B:319:THR:O | 1:B:319:THR:HG22 | 2.06 | 0.56 |
| 1:B:367:TYR:H | 1:B:368:ALA:HB2 | 1.70 | 0.56 |
| 1:B:100:LEU:HD11 | 1:B:381:ILE:HG13 | 1.87 | 0.56 |
| 1:B:46:LEU:HD13 | 1:B:164:GLU:HB2 | 1.88 | 0.56 |
| 2:D:54:LEU:CA | 2:D:57:VAL:HG22 | 2.35 | 0.56 |
| 3:E:79:LYS:HE3 | 3:F:86:ASP:CA | 2.35 | 0.56 |
| 1:A:111:ASN:ND2 | 1:A:114:LEU:H | 2.04 | 0.56 |
| 1:B:111:ASN:ND2 | 1:B:114:LEU:H | 2.04 | 0.56 |
| 1:B:136:ASN:HB2 | 1:B:145:TRP:CZ3 | 2.41 | 0.56 |
| 1:B:367:TYR:N | 1:B:368:ALA:HB2 | 2.21 | 0.56 |
| 1:B:83:ARG:HD3 | 1:B:83:ARG:N | 2.19 | 0.56 |
| 1:B:298:GLU:CB | 2:C:42:ASP:HB3 | 2.36 | 0.56 |
| 2:D:75:MET:N | 2:D:78:VAL:HG11 | 2.21 | 0.56 |
| 3:E:88:VAL:O | 3:E:97:THR:HG23 | 2.06 | 0.56 |
| 5:H:116:ARG:NH2 | 5:H:128:ILE:HD13 | 2.20 | 0.56 |
| 4:G:133:ASN:ND2 | 5:H:42:GLU:HG3 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:ASP:HB2 | 1:A:124:ASP:HA | 1.87 | 0.56 |
| 1:A:365:LYS:O | 1:A:365:LYS:HD3 | 2.05 | 0.56 |
| 1:A:390:TRP:O | 1:A:394:GLU:HG2 | 2.05 | 0.56 |
| 1:B:123:ASP:HB2 | 1:B:124:ASP:HA | 1.87 | 0.56 |
| 1:B:243:PRO:CB | 1:B:244:ILE:HG22 | 2.36 | 0.56 |
| 1:B:254:VAL:HB | 1:B:259:PHE:CD1 | 2.40 | 0.56 |
| 1:B:290:ASN:HB2 | 1:B:291:TYR:HB2 | 1.87 | 0.56 |
| 1:B:46:LEU:HD22 | 1:B:162:ALA:HA | 1.88 | 0.56 |
| 3:E:15:VAL:HG11 | 3:E:73:ARG:HB2 | 1.88 | 0.56 |
| 3:E:83:PHE:HB2 | 3:E:99:ILE:HD13 | 1.88 | 0.56 |
| 3:F:69:ASP:OD1 | 3:F:97:THR:HG21 | 2.06 | 0.56 |
| 5:H:54:LEU:HD12 | 5:H:54:LEU:N | 2.18 | 0.56 |
| 1:A:134:VAL:HA | 1:A:137:MET:HE2 | 1.87 | 0.56 |
| 1:A:177:ILE:HG23 | 1:A:177:ILE:O | 2.05 | 0.56 |
| 1:A:254:VAL:HB | 1:A:259:PHE:CD1 | 2.40 | 0.56 |
| 1:B:165:MET:HG3 | 1:B:182:ARG:HB2 | 1.87 | 0.56 |
| 1:A:46:LEU:HD13 | 1:A:164:GLU:HB2 | 1.88 | 0.56 |
| 1:A:292:ASP:CG | 2:C:31:PHE:O | 2.43 | 0.56 |
| 1:A:367:TYR:H | 1:A:368:ALA:HB2 | 1.71 | 0.56 |
| 1:A:439:SER:HB2 | 1:A:442:THR:HB | 1.88 | 0.56 |
| 1:B:292:ASP:CG | 2:D:31:PHE:O | 2.43 | 0.56 |
| 1:B:293:GLY:O | 2:D:31:PHE:HD2 | 1.89 | 0.56 |
| 1:B:365:LYS:O | 1:B:365:LYS:HD3 | 2.05 | 0.56 |
| 1:B:422:ASP:C | 1:B:425:ILE:HG22 | 2.25 | 0.56 |
| 1:B:63:ARG:HD2 | 1:B:76:ASP:O | 2.05 | 0.56 |
| 2:C:54:LEU:CA | 2:C:57:VAL:HG22 | 2.35 | 0.56 |
| 2:C:95:ASN:HB2 | 2:D:97:TYR:HD2 | 1.70 | 0.56 |
| 3:E:55:PRO:HG2 | 3:F:100:LYS:HZ3 | 1.71 | 0.56 |
| 2:C:73:ARG:HG2 | 3:E:91:SER:CB | 2.36 | 0.56 |
| 3:E:98:ARG:HG2 | 3:E:98:ARG:NH1 | 2.20 | 0.56 |
| 5:H:110:PHE:O | 5:H:132:LEU:HD12 | 2.07 | 0.56 |
| 5:H:138:LEU:HB2 | 5:H:140:ASN:O | 2.05 | 0.56 |
| 5:H:143:ILE:HB | 5:H:144:ASP:O | 2.06 | 0.56 |
| 5:H:15:PHE:CE1 | 5:H:91:PHE:CG | 2.94 | 0.56 |
| 1:A:254:VAL:HG12 | 1:B:85:SER:OG | 2.06 | 0.55 |
| 1:A:348:ASP:OD2 | 1:A:350:SER:HB2 | 2.06 | 0.55 |
| 1:B:104:PRO:HG2 | 1:B:127:ASP:OD2 | 2.05 | 0.55 |
| 1:B:34:ILE:HG22 | 1:B:181:LEU:CG | 2.35 | 0.55 |
| 1:B:284:ILE:HG23 | 1:B:284:ILE:O | 2.06 | 0.55 |
| 1:A:456:GLU:CG | 1:B:466:GLN:OE1 | 2.54 | 0.55 |
| 5:H:110:PHE:HE1 | 5:H:150:ILE:CD1 | 2.18 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:HIS:HB2 | 1:A:166:ILE:HG13 | 1.87 | 0.55 |
| 1:A:34:ILE:HG22 | 1:A:181:LEU:CG | 2.35 | 0.55 |
| 1:A:438:MET:SD | 1:B:434:THR:N | 2.78 | 0.55 |
| 1:A:63:ARG:CZ | 1:A:75:VAL:HG11 | 2.36 | 0.55 |
| 1:B:41:HIS:HB2 | 1:B:166:ILE:HG13 | 1.87 | 0.55 |
| 1:B:440:LYS:C | 1:B:440:LYS:HD3 | 2.26 | 0.55 |
| 1:B:63:ARG:CZ | 1:B:75:VAL:HG11 | 2.36 | 0.55 |
| 1:B:92:PHE:CZ | 1:B:369:LEU:HD22 | 2.40 | 0.55 |
| 2:C:99:LYS:HZ3 | 2:D:102:ARG:HG2 | 1.71 | 0.55 |
| 3:E:38:VAL:HG22 | 3:E:60:ILE:HG22 | 1.87 | 0.55 |
| 3:E:36:ALA:HB1 | 3:E:68:ILE:HD13 | 1.87 | 0.55 |
| 3:E:89:ASP:CB | 3:E:95:GLU:HB3 | 2.36 | 0.55 |
| 1:A:165:MET:HG3 | 1:A:182:ARG:HB2 | 1.87 | 0.55 |
| 1:A:410:LEU:HB3 | 1:A:412:MET:HG3 | 1.86 | 0.55 |
| 1:A:453:PRO:CB | 1:B:462:GLU:OE2 | 2.54 | 0.55 |
| 1:A:48:LYS:HA | 1:A:51:ARG:NH1 | 2.21 | 0.55 |
| 1:B:182:ARG:NH2 | 1:B:184:TYR:HB3 | 2.22 | 0.55 |
| 1:B:298:GLU:CD | 2:C:43:LYS:NZ | 2.60 | 0.55 |
| 1:B:410:LEU:HB3 | 1:B:412:MET:HG3 | 1.86 | 0.55 |
| 1:A:299:PHE:CD2 | 2:C:35:GLU:O | 2.56 | 0.55 |
| 2:C:69:GLY:CA | 2:C:73:ARG:HB3 | 2.25 | 0.55 |
| 3:E:109:GLY:HA2 | 4:G:114:THR:OG1 | 2.05 | 0.55 |
| 3:E:89:ASP:HA | 3:E:96:ILE:O | 2.05 | 0.55 |
| 3:F:45:GLU:O | 3:F:45:GLU:HG2 | 2.06 | 0.55 |
| 3:F:8:VAL:HG23 | 3:F:8:VAL:O | 2.06 | 0.55 |
| 4:G:113:ILE:HG21 | 4:G:121:LYS:CG | 2.36 | 0.55 |
| 5:H:42:GLU:HB2 | 5:H:43:LEU:CA | 2.37 | 0.55 |
| 1:A:335:ARG:C | 1:A:335:ARG:HD2 | 2.27 | 0.55 |
| 1:B:169:TYR:CD1 | 1:B:174:ARG:HA | 2.40 | 0.55 |
| 1:B:163:GLU:HB2 | 1:B:182:ARG:HB2 | 1.89 | 0.55 |
| 1:B:146:HIS:HA | 1:B:244:ILE:HG21 | 1.89 | 0.55 |
| 1:A:68:ASP:CG | 1:B:300:THR:CB | 2.73 | 0.55 |
| 1:B:335:ARG:HH11 | 1:B:336:ILE:HA | 1.71 | 0.55 |
| 1:B:367:TYR:CD2 | 1:B:369:LEU:HD23 | 2.31 | 0.55 |
| 1:B:48:LYS:HA | 1:B:51:ARG:NH1 | 2.21 | 0.55 |
| 1:B:59:ILE:HG23 | 1:B:62:LYS:HZ3 | 1.72 | 0.55 |
| 1:B:74:LEU:HD22 | 1:B:75:VAL:O | 2.07 | 0.55 |
| 2:D:87:PRO:HG3 | 2:D:90:ILE:CD1 | 2.22 | 0.55 |
| 3:E:45:GLU:HA | 3:E:47:TYR:CZ | 2.41 | 0.55 |
| 3:E:47:TYR:O | 3:E:50:GLN:HB2 | 2.07 | 0.55 |
| 3:F:9:ILE:HB | 3:F:76:TYR:HA | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:11:VAL:HG23 | 5:H:11:VAL:O | 2.05 | 0.55 |
| 5:H:58:SER:HB3 | 5:H:143:ILE:HD12 | 1.86 | 0.55 |
| 1:A:460:ILE:HG21 | 1:B:467:TYR:CA | 2.35 | 0.55 |
| 1:A:335:ARG:CZ | 1:B:278:PHE:HE1 | 2.19 | 0.55 |
| 1:B:86:HIS:ND1 | 1:B:88:TRP:HB2 | 2.20 | 0.55 |
| 2:C:50:PRO:O | 2:C:54:LEU:HB2 | 2.07 | 0.55 |
| 2:D:33:LYS:CE | 2:D:50:PRO:HB3 | 2.36 | 0.55 |
| 3:F:32:PHE:CG | 3:F:67:ARG:HD2 | 2.41 | 0.55 |
| 4:G:44:VAL:HG21 | 4:G:74:THR:HB | 1.88 | 0.55 |
| 5:H:167:THR:HG23 | 5:H:167:THR:O | 2.07 | 0.55 |
| 5:H:42:GLU:H | 5:H:43:LEU:HA | 1.69 | 0.55 |
| 1:A:46:LEU:HD22 | 1:A:162:ALA:HA | 1.88 | 0.55 |
| 1:B:335:ARG:C | 1:B:335:ARG:HD2 | 2.27 | 0.55 |
| 1:B:379:ARG:HA | 1:B:382:ARG:O | 2.07 | 0.55 |
| 1:B:439:SER:HB2 | 1:B:442:THR:HB | 1.88 | 0.55 |
| 1:B:63:ARG:HD2 | 1:B:75:VAL:HG12 | 1.88 | 0.55 |
| 1:B:99:TYR:HD2 | 1:B:370:LEU:HB3 | 1.68 | 0.55 |
| 1:A:296:PRO:HG2 | 2:C:37:HIS:CD2 | 2.41 | 0.55 |
| 3:F:12:GLN:HG2 | 3:F:75:ILE:HD13 | 1.86 | 0.55 |
| 3:F:93:LEU:H | 3:F:93:LEU:HD22 | 1.71 | 0.55 |
| 4:G:133:ASN:HB2 | 5:H:56:PRO:CD | 2.37 | 0.55 |
| 4:G:25:MET:O | 4:G:28:VAL:HA | 2.05 | 0.55 |
| 1:A:100:LEU:HD13 | 1:A:100:LEU:C | 2.27 | 0.55 |
| 1:A:335:ARG:HH11 | 1:A:336:ILE:HA | 1.71 | 0.55 |
| 1:A:86:HIS:ND1 | 1:A:88:TRP:HB2 | 2.20 | 0.55 |
| 1:B:147:PRO:HB3 | 1:B:155:PHE:CZ | 2.42 | 0.55 |
| 2:C:98:ARG:HH12 | 2:D:102:ARG:CB | 2.04 | 0.55 |
| 3:E:55:PRO:HG2 | 3:F:100:LYS:NZ | 2.21 | 0.55 |
| 3:F:9:ILE:HG13 | 3:F:11:PHE:HE1 | 1.68 | 0.55 |
| 5:H:18:ILE:H | 5:H:23:GLY:CA | 2.19 | 0.55 |
| 1:A:163:GLU:HB2 | 1:A:182:ARG:HB2 | 1.89 | 0.55 |
| 1:A:187:LYS:HE2 | 1:A:193:GLU:CB | 2.37 | 0.55 |
| 1:A:146:HIS:HA | 1:A:244:ILE:HG21 | 1.88 | 0.55 |
| 1:A:251:GLU:CG | 1:B:54:MET:N | 2.59 | 0.55 |
| 1:B:224:ASN:HD22 | 1:B:227:ARG:HA | 1.70 | 0.55 |
| 1:B:417:THR:CB | 1:B:418:ARG:HA | 2.28 | 0.55 |
| 1:A:441:GLU:HG2 | 1:B:462:GLU:OE2 | 1.98 | 0.55 |
| 1:A:291:TYR:HE1 | 2:C:33:LYS:HA | 1.70 | 0.55 |
| 2:C:94:LEU:C | 2:C:96:PRO:HA | 2.27 | 0.55 |
| 2:D:73:ARG:CG | 3:F:91:SER:CB | 2.70 | 0.55 |
| 3:F:88:VAL:HG22 | 3:F:98:ARG:CB | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:96:ILE:CG1 | 3:F:98:ARG:HE | 2.20 | 0.55 |
| 3:F:59:ASN:HD22 | 3:F:99:ILE:HG21 | 1.72 | 0.55 |
| 3:F:104:ASP:OD1 | 4:G:34:SER:O | 2.24 | 0.55 |
| 5:H:104:TYR:CE1 | 5:H:160:PHE:CG | 2.95 | 0.55 |
| 1:A:284:ILE:O | 1:A:284:ILE:HG23 | 2.06 | 0.55 |
| 1:A:63:ARG:HD2 | 1:A:75:VAL:HG12 | 1.88 | 0.55 |
| 1:A:74:LEU:HD22 | 1:A:75:VAL:O | 2.07 | 0.55 |
| 1:B:166:ILE:HG22 | 1:B:167:VAL:O | 2.07 | 0.55 |
| 1:B:179:PHE:CE2 | 1:B:200:TYR:CD2 | 2.95 | 0.55 |
| 1:B:178:LEU:CA | 1:B:242:VAL:HG13 | 2.37 | 0.55 |
| 2:C:84:THR:CB | 2:D:83:ALA:HA | 2.37 | 0.55 |
| 3:F:90:LEU:CB | 3:F:98:ARG:HD3 | 2.33 | 0.55 |
| 5:H:39:GLY:CA | 5:H:43:LEU:HB3 | 2.36 | 0.55 |
| 5:H:57:GLY:C | 5:H:58:SER:N | 2.60 | 0.55 |
| 1:A:147:PRO:HB3 | 1:A:155:PHE:CZ | 2.42 | 0.55 |
| 1:A:293:GLY:O | 2:C:31:PHE:HD2 | 1.89 | 0.55 |
| 1:A:379:ARG:HA | 1:A:382:ARG:O | 2.07 | 0.55 |
| 2:C:33:LYS:CE | 2:C:50:PRO:HB3 | 2.36 | 0.55 |
| 2:D:93:LYS:O | 2:D:94:LEU:HB2 | 2.07 | 0.55 |
| 3:E:32:PHE:HD1 | 3:E:34:ALA:O | 1.90 | 0.55 |
| 3:E:57:GLY:O | 3:E:58:TYR:HD1 | 1.88 | 0.55 |
| 2:D:7:LYS:HD3 | 3:F:4:GLU:CD | 2.26 | 0.55 |
| 3:E:37:HIS:HD2 | 3:F:89:ASP:N | 2.05 | 0.55 |
| 3:F:93:LEU:HD22 | 3:F:93:LEU:N | 2.22 | 0.55 |
| 5:H:91:PHE:HE2 | 5:H:132:LEU:CD2 | 2.20 | 0.55 |
| 5:H:14:LEU:CD1 | 5:H:26:PRO:HB3 | 2.36 | 0.55 |
| 5:H:96:THR:HA | 5:H:99:ASN:OD1 | 2.07 | 0.55 |
| 1:A:178:LEU:CA | 1:A:242:VAL:HG13 | 2.37 | 0.54 |
| 1:B:284:ILE:HD11 | 1:B:321:ARG:NH1 | 2.22 | 0.54 |
| 1:A:289:LYS:HG2 | 1:B:315:GLY:C | 2.27 | 0.54 |
| 1:B:294:GLU:CG | 2:C:42:ASP:OD1 | 2.55 | 0.54 |
| 2:C:93:LYS:O | 2:C:94:LEU:HB2 | 2.07 | 0.54 |
| 2:D:70:LEU:HD21 | 3:F:90:LEU:C | 1.90 | 0.54 |
| 2:D:94:LEU:C | 2:D:96:PRO:HA | 2.27 | 0.54 |
| 3:E:38:VAL:HG22 | 3:E:60:ILE:HG21 | 1.87 | 0.54 |
| 3:E:76:TYR:HB2 | 3:F:87:PRO:HD2 | 1.89 | 0.54 |
| 3:E:81:VAL:HG21 | 3:F:86:ASP:CB | 2.31 | 0.54 |
| 3:E:84:ILE:HD13 | 3:E:84:ILE:N | 2.18 | 0.54 |
| 4:G:30:GLN:HG2 | 4:G:34:SER:OG | 2.07 | 0.54 |
| 5:H:94:VAL:HG13 | 5:H:104:TYR:CD2 | 2.41 | 0.54 |
| 5:H:94:VAL:HG22 | 5:H:104:TYR:HE2 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:MET:HB3 | 1:A:180:ALA:HB1 | 1.89 | 0.54 |
| 1:A:216:GLN:HG2 | 1:A:217:MET:N | 2.22 | 0.54 |
| 1:A:243:PRO:CB | 1:A:244:ILE:HG22 | 2.36 | 0.54 |
| 1:A:99:TYR:HD2 | 1:A:370:LEU:HB3 | 1.68 | 0.54 |
| 1:B:216:GLN:HG2 | 1:B:217:MET:N | 2.22 | 0.54 |
| 3:E:66:ASP:HA | 3:E:97:THR:HG21 | 1.89 | 0.54 |
| 3:F:14:TYR:CZ | 3:F:28:TRP:CE2 | 2.95 | 0.54 |
| 2:D:7:LYS:HD3 | 3:F:4:GLU:OE2 | 2.08 | 0.54 |
| 3:F:69:ASP:CG | 3:F:97:THR:HG21 | 2.27 | 0.54 |
| 5:H:37:VAL:HG12 | 5:H:63:GLY:HA2 | 1.89 | 0.54 |
| 1:A:165:MET:HB2 | 1:A:180:ALA:CB | 2.37 | 0.54 |
| 1:A:179:PHE:CE2 | 1:A:200:TYR:CD2 | 2.95 | 0.54 |
| 1:A:336:ILE:HD13 | 1:B:278:PHE:CA | 2.25 | 0.54 |
| 1:B:348:ASP:OD2 | 1:B:350:SER:HB2 | 2.06 | 0.54 |
| 1:B:364:GLU:C | 1:B:368:ALA:HB3 | 2.25 | 0.54 |
| 2:C:75:MET:N | 2:C:78:VAL:HG11 | 2.21 | 0.54 |
| 2:C:94:LEU:HG | 2:D:97:TYR:HA | 1.89 | 0.54 |
| 1:B:296:PRO:HG2 | 2:D:37:HIS:CD2 | 2.41 | 0.54 |
| 2:D:50:PRO:O | 2:D:54:LEU:HB2 | 2.07 | 0.54 |
| 3:E:40:PRO:HB3 | 3:F:100:LYS:HA | 1.89 | 0.54 |
| 3:E:96:ILE:CD1 | 3:E:98:ARG:HH21 | 2.19 | 0.54 |
| 5:H:42:GLU:HB2 | 5:H:43:LEU:C | 2.28 | 0.54 |
| 5:H:15:PHE:CZ | 5:H:91:PHE:CE2 | 2.96 | 0.54 |
| 1:A:368:ALA:C | 1:A:370:LEU:HD22 | 2.28 | 0.54 |
| 1:A:422:ASP:O | 1:A:425:ILE:HG22 | 2.07 | 0.54 |
| 1:A:59:ILE:HA | 1:A:81:ASN:CG | 2.28 | 0.54 |
| 1:A:175:ARG:NH2 | 1:B:148:PHE:CZ | 2.76 | 0.54 |
| 1:B:111:ASN:N | 1:B:396:LEU:HD22 | 2.23 | 0.54 |
| 1:B:425:ILE:HG23 | 1:B:426:VAL:N | 2.22 | 0.54 |
| 1:B:59:ILE:HA | 1:B:81:ASN:CG | 2.28 | 0.54 |
| 3:F:89:ASP:HA | 3:F:96:ILE:O | 2.06 | 0.54 |
| 4:G:103:VAL:HG12 | 4:G:104:ALA:N | 2.21 | 0.54 |
| 4:G:18:LEU:HB3 | 4:G:24:LEU:HD21 | 1.90 | 0.54 |
| 4:G:4:LYS:CB | 4:G:5:LEU:HD13 | 2.38 | 0.54 |
| 5:H:104:TYR:CE1 | 5:H:160:PHE:HB2 | 2.43 | 0.54 |
| 1:A:166:ILE:HG22 | 1:A:167:VAL:O | 2.07 | 0.54 |
| 1:A:224:ASN:HD22 | 1:A:227:ARG:HA | 1.70 | 0.54 |
| 1:A:425:ILE:HG23 | 1:A:426:VAL:N | 2.22 | 0.54 |
| 1:B:165:MET:HB2 | 1:B:180:ALA:CB | 2.37 | 0.54 |
| 1:B:165:MET:HB3 | 1:B:180:ALA:HB1 | 1.89 | 0.54 |
| 1:B:421:ASN:O | 1:B:425:ILE:HG22 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:442:THR:HA | 1:B:445:ALA:HB2 | 1.90 | 0.54 |
| 2:C:98:ARG:CB | 2:D:97:TYR:CD2 | 2.78 | 0.54 |
| 3:E:44:GLU:HG2 | 3:E:47:TYR:N | 2.18 | 0.54 |
| 2:C:70:LEU:HA | 3:E:91:SER:HB2 | 1.90 | 0.54 |
| 3:F:51:GLN:HG3 | 3:F:52:LEU:HD23 | 1.89 | 0.54 |
| 4:G:127:VAL:HG22 | 4:G:129:PHE:CE1 | 2.43 | 0.54 |
| 4:G:62:GLU:HG2 | 4:G:63:ASN:H | 1.72 | 0.54 |
| 3:E:19:ASN:ND2 | 4:G:81:ASP:OD2 | 2.41 | 0.54 |
| 5:H:88:GLN:O | 5:H:89:ILE:HD13 | 2.07 | 0.54 |
| 5:H:22:THR:H | 5:H:90:LYS:HB2 | 1.71 | 0.54 |
| 1:A:142:ILE:HG21 | 1:A:145:TRP:HB2 | 1.89 | 0.54 |
| 1:A:140:LYS:CB | 1:A:257:LEU:HD23 | 2.35 | 0.54 |
| 1:A:311:VAL:HG13 | 1:A:311:VAL:O | 2.08 | 0.54 |
| 1:A:445:ALA:CA | 1:A:448:PRO:HB3 | 2.34 | 0.54 |
| 1:A:48:LYS:HG3 | 1:A:49:GLY:N | 2.22 | 0.54 |
| 2:C:94:LEU:CG | 2:D:97:TYR:HA | 2.38 | 0.54 |
| 1:B:299:PHE:CD2 | 2:D:35:GLU:O | 2.56 | 0.54 |
| 2:C:4:GLN:HA | 3:E:1:MET:H3 | 1.69 | 0.54 |
| 2:C:73:ARG:HE | 3:E:91:SER:HB3 | 1.72 | 0.54 |
| 3:F:74:VAL:HG13 | 3:F:81:VAL:CG1 | 2.37 | 0.54 |
| 4:G:32:THR:HB | 4:G:44:VAL:O | 2.07 | 0.54 |
| 5:H:22:THR:HG23 | 5:H:24:SER:H | 1.73 | 0.54 |
| 1:B:187:LYS:HE2 | 1:B:193:GLU:CB | 2.37 | 0.54 |
| 1:B:368:ALA:N | 1:B:370:LEU:H | 2.06 | 0.54 |
| 2:C:19:GLU:OE2 | 2:C:23:GLU:HG2 | 2.08 | 0.54 |
| 2:C:70:LEU:HD21 | 3:E:90:LEU:O | 1.97 | 0.54 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:HG3 | 2.01 | 0.54 |
| 3:F:11:PHE:H | 3:F:33:THR:HA | 1.73 | 0.54 |
| 3:F:58:TYR:O | 3:F:83:PHE:HB2 | 2.07 | 0.54 |
| 5:H:39:GLY:HA2 | 5:H:43:LEU:HB3 | 1.89 | 0.54 |
| 1:A:182:ARG:NH2 | 1:A:184:TYR:HB3 | 2.22 | 0.54 |
| 1:B:100:LEU:HD13 | 1:B:100:LEU:C | 2.27 | 0.54 |
| 1:B:368:ALA:C | 1:B:370:LEU:HD22 | 2.28 | 0.54 |
| 3:E:77:ARG:HH12 | 3:F:64:TYR:CA | 2.18 | 0.54 |
| 3:F:76:TYR:HE1 | 3:F:81:VAL:HG12 | 1.73 | 0.54 |
| 3:F:22:GLY:O | 4:G:19:GLU:CD | 2.47 | 0.54 |
| 1:A:162:ALA:HB1 | 1:A:164:GLU:HA | 1.90 | 0.54 |
| 1:A:167:VAL:HG22 | 1:A:246:PRO:HG3 | 1.90 | 0.54 |
| 1:A:421:ASN:O | 1:A:425:ILE:HG22 | 2.08 | 0.54 |
| 1:B:142:ILE:HG21 | 1:B:145:TRP:HB2 | 1.89 | 0.54 |
| 1:B:291:TYR:HE1 | 2:D:33:LYS:HA | 1.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:338:ASP:OD2 | 1:B:337:GLN:NE2 | 2.41 | 0.54 |
| 1:B:48:LYS:HG3 | 1:B:49:GLY:N | 2.22 | 0.54 |
| 2:D:19:GLU:OE2 | 2:D:23:GLU:HG2 | 2.08 | 0.54 |
| 2:D:5:ARG:CB | 3:F:3:GLU:CA | 2.84 | 0.54 |
| 4:G:21:TYR:CE1 | 4:G:23:PRO:HG2 | 2.42 | 0.54 |
| 5:H:142:GLU:HG2 | 5:H:144:ASP:N | 2.22 | 0.54 |
| 1:A:138:SER:HB3 | 1:A:256:ASP:CB | 2.38 | 0.54 |
| 1:A:199:LEU:C | 1:A:200:TYR:HD1 | 2.11 | 0.54 |
| 1:A:368:ALA:N | 1:A:370:LEU:H | 2.06 | 0.54 |
| 1:B:422:ASP:O | 1:B:425:ILE:HG22 | 2.07 | 0.54 |
| 2:C:73:ARG:HD3 | 3:E:91:SER:CB | 2.38 | 0.54 |
| 2:D:41:ILE:HG22 | 2:D:42:ASP:N | 2.23 | 0.54 |
| 3:E:36:ALA:HB3 | 3:E:76:TYR:CE2 | 2.42 | 0.54 |
| 3:F:87:PRO:CB | 3:F:97:THR:HG23 | 2.36 | 0.54 |
| 4:G:21:TYR:CD2 | 4:G:24:LEU:HD12 | 2.40 | 0.54 |
| 4:G:49:GLN:HB3 | 4:G:69:HIS:CE1 | 2.40 | 0.54 |
| 1:A:231:THR:HA | 1:A:237:ILE:HG22 | 1.90 | 0.53 |
| 1:A:138:SER:HB3 | 1:A:256:ASP:HB2 | 1.90 | 0.53 |
| 1:A:88:TRP:CH2 | 1:A:369:LEU:HD21 | 2.43 | 0.53 |
| 1:A:96:LYS:HG2 | 1:A:373:LYS:HB2 | 1.89 | 0.53 |
| 1:A:59:ILE:HG13 | 1:A:81:ASN:CB | 2.39 | 0.53 |
| 1:A:332:GLU:OE2 | 1:B:330:ALA:HB2 | 2.08 | 0.53 |
| 1:B:88:TRP:CH2 | 1:B:369:LEU:HD21 | 2.43 | 0.53 |
| 3:F:24:LYS:HG2 | 3:F:25:THR:N | 2.21 | 0.53 |
| 4:G:86:VAL:HG13 | 4:G:87:LEU:CD1 | 2.37 | 0.53 |
| 5:H:31:TYR:HE1 | 5:H:70:LYS:HG3 | 1.72 | 0.53 |
| 1:A:89:HIS:ND1 | 1:A:260:TYR:HD2 | 2.07 | 0.53 |
| 1:B:138:SER:HB3 | 1:B:256:ASP:HB2 | 1.90 | 0.53 |
| 1:B:148:PHE:HZ | 1:B:156:ASP:OD2 | 1.91 | 0.53 |
| 1:B:167:VAL:HG22 | 1:B:246:PRO:HG3 | 1.90 | 0.53 |
| 1:B:311:VAL:O | 1:B:311:VAL:HG13 | 2.08 | 0.53 |
| 1:B:76:ASP:CG | 1:B:79:LYS:HG2 | 2.29 | 0.53 |
| 2:C:99:LYS:HA | 2:D:100:MET:C | 2.27 | 0.53 |
| 2:C:99:LYS:HA | 2:D:100:MET:O | 2.07 | 0.53 |
| 2:D:29:VAL:CG1 | 2:D:50:PRO:HG3 | 2.35 | 0.53 |
| 3:E:59:ASN:H | 3:F:100:LYS:CE | 2.19 | 0.53 |
| 3:F:10:THR:O | 3:F:75:ILE:HG22 | 2.09 | 0.53 |
| 3:F:87:PRO:HA | 3:F:98:ARG:O | 2.09 | 0.53 |
| 1:A:148:PHE:HZ | 1:A:156:ASP:OD2 | 1.91 | 0.53 |
| 1:A:250:ASN:ND2 | 1:B:90:LYS:HD2 | 2.24 | 0.53 |
| 1:A:442:THR:HA | 1:A:445:ALA:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:84:THR:HG22 | 1:A:85:SER:N | 2.22 | 0.53 |
| 1:A:89:HIS:HD1 | 1:A:260:TYR:HD2 | 1.56 | 0.53 |
| 1:B:162:ALA:HB1 | 1:B:164:GLU:HA | 1.90 | 0.53 |
| 1:B:178:LEU:CB | 1:B:242:VAL:HG11 | 2.38 | 0.53 |
| 1:B:292:ASP:OD2 | 2:D:31:PHE:O | 2.25 | 0.53 |
| 1:A:371:ASP:O | 1:B:363:LEU:CD2 | 2.54 | 0.53 |
| 4:G:41:TYR:CZ | 4:G:43:TYR:CE1 | 2.96 | 0.53 |
| 4:G:46:ILE:HG22 | 4:G:66:MET:CE | 2.38 | 0.53 |
| 4:G:61:GLY:HA2 | 5:H:139:LYS:CD | 2.38 | 0.53 |
| 4:G:86:VAL:HG13 | 4:G:87:LEU:HD12 | 1.88 | 0.53 |
| 5:H:94:VAL:HG12 | 5:H:95:ASP:O | 2.09 | 0.53 |
| 5:H:97:VAL:HG13 | 5:H:97:VAL:O | 2.08 | 0.53 |
| 1:A:311:VAL:HG22 | 1:A:312:SER:O | 2.09 | 0.53 |
| 1:B:199:LEU:C | 1:B:200:TYR:HD1 | 2.11 | 0.53 |
| 1:B:138:SER:HB3 | 1:B:256:ASP:CB | 2.38 | 0.53 |
| 2:C:70:LEU:H | 3:E:93:LEU:N | 2.05 | 0.53 |
| 2:C:4:GLN:HB3 | 2:C:8:ARG:HB3 | 1.89 | 0.53 |
| 2:D:5:ARG:CA | 3:F:3:GLU:HA | 2.27 | 0.53 |
| 2:D:70:LEU:N | 3:F:93:LEU:CA | 2.70 | 0.53 |
| 1:A:289:LYS:CG | 1:B:315:GLY:HA3 | 2.38 | 0.53 |
| 1:A:456:GLU:CD | 1:B:466:GLN:OE1 | 2.46 | 0.53 |
| 1:B:294:GLU:HG3 | 2:C:42:ASP:OD1 | 2.08 | 0.53 |
| 1:B:311:VAL:HG22 | 1:B:312:SER:O | 2.09 | 0.53 |
| 1:A:418:ARG:NH1 | 1:B:426:VAL:HG21 | 2.22 | 0.53 |
| 1:B:89:HIS:HD1 | 1:B:260:TYR:HD2 | 1.55 | 0.53 |
| 1:A:378:GLU:HG2 | 1:B:98:GLN:OE1 | 2.09 | 0.53 |
| 2:C:21:LEU:HD13 | 2:C:21:LEU:C | 2.28 | 0.53 |
| 2:D:21:LEU:C | 2:D:21:LEU:HD13 | 2.28 | 0.53 |
| 3:E:74:VAL:CG1 | 3:E:76:TYR:HE1 | 2.20 | 0.53 |
| 3:E:74:VAL:C | 3:E:75:ILE:HD12 | 2.29 | 0.53 |
| 3:E:48:LYS:NZ | 3:F:48:LYS:HE3 | 2.23 | 0.53 |
| 3:F:11:PHE:HE2 | 3:F:68:ILE:CG2 | 2.22 | 0.53 |
| 4:G:109:LEU:C | 4:G:109:LEU:HD13 | 2.29 | 0.53 |
| 4:G:113:ILE:HD12 | 4:G:114:THR:N | 2.23 | 0.53 |
| 4:G:117:ASP:CB | 4:G:119:VAL:HG23 | 2.18 | 0.53 |
| 3:E:105:GLY:C | 4:G:41:TYR:CE2 | 2.70 | 0.53 |
| 4:G:52:THR:CG2 | 4:G:53:PRO:HD2 | 2.39 | 0.53 |
| 1:A:142:ILE:N | 1:A:143:GLU:HA | 2.23 | 0.53 |
| 1:A:284:ILE:HD11 | 1:A:321:ARG:NH1 | 2.22 | 0.53 |
| 1:A:292:ASP:OD2 | 2:C:31:PHE:O | 2.25 | 0.53 |
| 1:B:235:GLN:HA | 1:B:235:GLN:OE1 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:453:PRO:CA | 1:B:462:GLU:OE2 | 2.57 | 0.53 |
| 2:C:100:MET:CE | 2:D:100:MET:CG | 2.86 | 0.53 |
| 2:C:12:ILE:HA | 3:E:93:LEU:CG | 2.39 | 0.53 |
| 2:C:5:ARG:CD | 2:C:7:LYS:HB2 | 2.29 | 0.53 |
| 3:E:79:LYS:HB3 | 3:F:87:PRO:HD3 | 1.90 | 0.53 |
| 3:F:1:MET:HG2 | 3:F:2:TYR:N | 2.23 | 0.53 |
| 3:F:70:LYS:CE | 3:F:71:LYS:HB2 | 2.39 | 0.53 |
| 3:F:69:ASP:CG | 3:F:87:PRO:HG3 | 2.27 | 0.53 |
| 3:F:9:ILE:CG1 | 3:F:11:PHE:HE1 | 2.21 | 0.53 |
| 4:G:32:THR:HB | 4:G:44:VAL:H | 1.73 | 0.53 |
| 1:A:178:LEU:CB | 1:A:242:VAL:HG11 | 2.38 | 0.53 |
| 1:B:195:GLN:NE2 | 1:B:195:GLN:HA | 2.24 | 0.53 |
| 1:A:379:ARG:CD | 1:B:94:ASP:CB | 2.79 | 0.53 |
| 2:C:34:ASP:H | 2:C:35:GLU:HA | 1.72 | 0.53 |
| 2:C:90:ILE:CG1 | 2:D:91:LEU:CG | 2.58 | 0.53 |
| 3:E:9:ILE:CD1 | 3:E:11:PHE:HZ | 2.21 | 0.53 |
| 4:G:43:TYR:CE1 | 4:G:71:TRP:CG | 2.97 | 0.53 |
| 5:H:39:GLY:O | 5:H:43:LEU:HB3 | 2.07 | 0.53 |
| 5:H:90:LYS:CE | 5:H:150:ILE:HD11 | 2.38 | 0.53 |
| 1:A:121:LEU:CD1 | 1:A:124:ASP:H | 2.18 | 0.53 |
| 1:A:209:GLU:OE1 | 1:A:209:GLU:HA | 2.08 | 0.53 |
| 1:A:225:ASN:HB2 | 1:A:226:PRO:CA | 2.34 | 0.53 |
| 1:A:320:LEU:HD21 | 1:B:318:ASP:HA | 1.91 | 0.53 |
| 3:F:73:ARG:HG2 | 3:F:75:ILE:HD12 | 1.89 | 0.53 |
| 3:F:75:ILE:HG21 | 3:F:78:GLY:HA2 | 1.91 | 0.53 |
| 3:E:79:LYS:HG2 | 3:F:86:ASP:HA | 1.90 | 0.53 |
| 5:H:120:ASP:O | 5:H:126:VAL:HG23 | 2.09 | 0.53 |
| 1:A:171:ASP:HB3 | 1:A:178:LEU:HD11 | 1.90 | 0.53 |
| 1:A:146:HIS:HB2 | 1:A:244:ILE:HG21 | 1.89 | 0.53 |
| 2:C:41:ILE:HG22 | 2:C:42:ASP:N | 2.23 | 0.53 |
| 3:E:81:VAL:HG12 | 3:E:82:THR:N | 2.24 | 0.53 |
| 3:E:2:TYR:CZ | 3:F:95:GLU:HA | 2.44 | 0.53 |
| 3:F:9:ILE:CD1 | 3:F:11:PHE:HE1 | 2.21 | 0.53 |
| 5:H:14:LEU:CD1 | 5:H:16:GLN:HE21 | 2.21 | 0.53 |
| 1:A:76:ASP:CG | 1:A:79:LYS:HG2 | 2.29 | 0.53 |
| 1:A:80:THR:HG22 | 1:A:81:ASN:H | 1.73 | 0.53 |
| 1:B:142:ILE:N | 1:B:143:GLU:HA | 2.23 | 0.53 |
| 1:A:314:ASP:OD2 | 2:D:97:TYR:OH | 2.27 | 0.53 |
| 3:E:21:GLU:HG3 | 3:E:22:GLY:N | 2.19 | 0.53 |
| 3:E:38:VAL:CG2 | 3:E:60:ILE:HG22 | 2.39 | 0.53 |
| 4:G:42:PRO:HB3 | 4:G:72:GLY:CA | 2.28 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:H:100:GLU:HB3 | 5:H:103:LYS:CB | 2.38 | 0.53 |
| 1:B:146:HIS:HB2 | 1:B:244:ILE:HG21 | 1.89 | 0.52 |
| 5:H:18:ILE:HG12 | 5:H:23:GLY:HA2 | 1.91 | 0.52 |
| 1:A:195:GLN:NE2 | 1:A:195:GLN:HA | 2.24 | 0.52 |
| 1:A:199:LEU:HB2 | 1:A:208:TYR:CE2 | 2.44 | 0.52 |
| 1:B:199:LEU:HB2 | 1:B:208:TYR:CE2 | 2.44 | 0.52 |
| 1:B:59:ILE:HG13 | 1:B:81:ASN:CB | 2.38 | 0.52 |
| 3:E:15:VAL:HG13 | 3:E:29:VAL:HG23 | 1.91 | 0.52 |
| 3:F:41:ILE:HG23 | 3:F:53:GLN:HG2 | 1.91 | 0.52 |
| 1:A:132:GLU:HA | 1:A:132:GLU:OE1 | 2.10 | 0.52 |
| 1:A:433:VAL:HB | 1:A:440:LYS:CG | 2.38 | 0.52 |
| 1:B:209:GLU:OE1 | 1:B:209:GLU:HA | 2.08 | 0.52 |
| 1:B:140:LYS:CB | 1:B:257:LEU:HD23 | 2.35 | 0.52 |
| 1:B:84:THR:HG22 | 1:B:85:SER:N | 2.22 | 0.52 |
| 1:B:89:HIS:ND1 | 1:B:260:TYR:HD2 | 2.06 | 0.52 |
| 2:C:11:SER:CB | 3:E:93:LEU:HB2 | 2.39 | 0.52 |
| 2:C:84:THR:OG1 | 2:D:86:ILE:HD11 | 2.10 | 0.52 |
| 2:C:98:ARG:NH2 | 2:D:102:ARG:HG2 | 2.23 | 0.52 |
| 3:E:47:TYR:HB3 | 3:E:50:GLN:CD | 2.30 | 0.52 |
| 3:F:7:ASP:CB | 3:F:9:ILE:HG12 | 2.40 | 0.52 |
| 3:F:96:ILE:CD1 | 3:F:98:ARG:HE | 2.22 | 0.52 |
| 5:H:119:SER:CB | 5:H:128:ILE:HG12 | 2.39 | 0.52 |
| 1:B:111:ASN:CG | 1:B:399:THR:HG21 | 2.30 | 0.52 |
| 1:B:174:ARG:NH1 | 1:B:174:ARG:HG2 | 2.25 | 0.52 |
| 1:B:99:TYR:HB2 | 1:B:370:LEU:CD1 | 2.38 | 0.52 |
| 2:C:25:VAL:HG12 | 2:C:29:VAL:HG23 | 1.90 | 0.52 |
| 2:D:4:GLN:HB3 | 2:D:8:ARG:HB3 | 1.90 | 0.52 |
| 3:F:65:ASP:HB3 | 3:F:68:ILE:CG2 | 2.30 | 0.52 |
| 4:G:131:ILE:O | 4:G:131:ILE:HG13 | 2.09 | 0.52 |
| 5:H:18:ILE:H | 5:H:23:GLY:HA3 | 1.74 | 0.52 |
| 5:H:64:GLU:OE1 | 5:H:64:GLU:HA | 2.08 | 0.52 |
| 1:A:111:ASN:CG | 1:A:399:THR:HG21 | 2.30 | 0.52 |
| 1:A:289:LYS:HB3 | 1:B:315:GLY:HA3 | 1.91 | 0.52 |
| 1:A:324:ILE:CB | 1:A:325:PRO:HD3 | 2.36 | 0.52 |
| 1:B:121:LEU:CD1 | 1:B:124:ASP:H | 2.18 | 0.52 |
| 1:B:33:MET:O | 1:B:37:LEU:HG | 2.09 | 0.52 |
| 2:C:21:LEU:HD13 | 2:C:21:LEU:O | 2.10 | 0.52 |
| 2:C:94:LEU:HD12 | 2:C:94:LEU:N | 2.25 | 0.52 |
| 2:C:9:LEU:HD13 | 2:D:20:TYR:HE2 | 1.74 | 0.52 |
| 2:D:94:LEU:HD12 | 2:D:94:LEU:N | 2.25 | 0.52 |
| 3:E:58:TYR:HB3 | 3:F:100:LYS:CG | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:93:LEU:H | 3:E:93:LEU:CD2 | 2.21 | 0.52 |
| 3:E:104:ASP:CA | 4:G:119:VAL:HG21 | 2.39 | 0.52 |
| 5:H:110:PHE:CE1 | 5:H:150:ILE:HD12 | 2.45 | 0.52 |
| 5:H:22:THR:O | 5:H:22:THR:HG23 | 2.09 | 0.52 |
| 1:A:211:ILE:HG13 | 1:A:212:ASP:OD1 | 2.10 | 0.52 |
| 1:A:308:VAL:HG22 | 1:A:309:ILE:N | 2.25 | 0.52 |
| 1:A:367:TYR:CZ | 1:A:372:LEU:HB2 | 2.45 | 0.52 |
| 1:A:99:TYR:HB2 | 1:A:370:LEU:CD1 | 2.38 | 0.52 |
| 1:B:190:MET:HE1 | 1:B:194:THR:HG21 | 1.91 | 0.52 |
| 1:B:433:VAL:HB | 1:B:440:LYS:CG | 2.38 | 0.52 |
| 3:E:58:TYR:HA | 3:F:100:LYS:NZ | 2.24 | 0.52 |
| 3:F:17:GLN:HB3 | 3:F:19:ASN:ND2 | 2.21 | 0.52 |
| 2:D:7:LYS:HG3 | 3:F:4:GLU:HA | 1.91 | 0.52 |
| 3:F:14:TYR:HB3 | 3:F:73:ARG:NE | 2.24 | 0.52 |
| 4:G:22:GLN:CG | 4:G:23:PRO:HD3 | 2.38 | 0.52 |
| 4:G:33:GLU:HG2 | 4:G:34:SER:N | 2.25 | 0.52 |
| 4:G:44:VAL:CG2 | 4:G:74:THR:H | 2.14 | 0.52 |
| 1:A:151:GLU:HA | 1:A:151:GLU:OE1 | 2.10 | 0.52 |
| 1:A:341:TYR:CA | 1:A:344:ALA:HB2 | 2.40 | 0.52 |
| 1:B:132:GLU:HA | 1:B:132:GLU:OE1 | 2.10 | 0.52 |
| 1:B:179:PHE:HD2 | 1:B:200:TYR:HB2 | 1.69 | 0.52 |
| 2:D:33:LYS:CD | 2:D:50:PRO:HB3 | 2.40 | 0.52 |
| 2:D:5:ARG:HD3 | 2:D:7:LYS:HE3 | 1.92 | 0.52 |
| 3:E:9:ILE:HD11 | 3:E:11:PHE:HZ | 1.75 | 0.52 |
| 3:E:40:PRO:CB | 3:F:100:LYS:HB2 | 2.40 | 0.52 |
| 2:D:5:ARG:HB3 | 3:F:3:GLU:O | 2.08 | 0.52 |
| 4:G:127:VAL:HG21 | 4:G:129:PHE:CZ | 2.45 | 0.52 |
| 4:G:18:LEU:O | 4:G:24:LEU:HD22 | 2.10 | 0.52 |
| 5:H:91:PHE:CD2 | 5:H:111:ALA:HB1 | 2.44 | 0.52 |
| 1:A:292:ASP:OD1 | 2:C:33:LYS:O | 2.26 | 0.52 |
| 1:A:329:ALA:O | 1:A:333:LEU:HG | 2.09 | 0.52 |
| 1:B:130:LEU:O | 1:B:134:VAL:HG22 | 2.10 | 0.52 |
| 1:B:211:ILE:HG13 | 1:B:212:ASP:OD1 | 2.10 | 0.52 |
| 1:B:232:LYS:N | 1:B:237:ILE:HB | 2.24 | 0.52 |
| 1:B:231:THR:HA | 1:B:237:ILE:HG22 | 1.90 | 0.52 |
| 1:B:367:TYR:CZ | 1:B:372:LEU:HB2 | 2.45 | 0.52 |
| 2:C:4:GLN:HG2 | 2:D:68:ALA:HB1 | 1.91 | 0.52 |
| 1:A:101:VAL:HG23 | 1:A:102:GLY:H | 1.73 | 0.52 |
| 1:A:146:HIS:CB | 1:A:244:ILE:HG21 | 2.40 | 0.52 |
| 1:A:441:GLU:HG2 | 1:A:456:GLU:CB | 2.38 | 0.52 |
| 1:B:101:VAL:HG23 | 1:B:102:GLY:H | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:151:GLU:OE1 | 1:B:151:GLU:HA | 2.10 | 0.52 |
| 1:B:80:THR:HG22 | 1:B:81:ASN:H | 1.73 | 0.52 |
| 2:C:30:GLU:HA | 2:C:40:PHE:CZ | 2.45 | 0.52 |
| 2:C:4:GLN:HB2 | 2:C:8:ARG:NH2 | 2.25 | 0.52 |
| 2:D:21:LEU:HD13 | 2:D:21:LEU:O | 2.09 | 0.52 |
| 2:D:4:GLN:HB2 | 2:D:8:ARG:NH2 | 2.25 | 0.52 |
| 3:E:58:TYR:HB3 | 3:F:100:LYS:HG2 | 1.92 | 0.52 |
| 5:H:43:LEU:HD22 | 5:H:43:LEU:C | 2.31 | 0.52 |
| 1:A:159:ILE:HD13 | 1:A:159:ILE:C | 2.30 | 0.52 |
| 1:B:146:HIS:CB | 1:B:244:ILE:HG21 | 2.40 | 0.52 |
| 1:B:308:VAL:HG22 | 1:B:309:ILE:N | 2.25 | 0.52 |
| 1:B:387:LEU:HG | 1:B:391:PHE:CZ | 2.45 | 0.52 |
| 1:B:439:SER:CB | 1:B:442:THR:HB | 2.40 | 0.52 |
| 1:B:88:TRP:CD1 | 1:B:92:PHE:CZ | 2.98 | 0.52 |
| 2:D:35:GLU:OE1 | 2:D:37:HIS:HA | 2.10 | 0.52 |
| 2:C:94:LEU:HB3 | 2:D:97:TYR:CE1 | 2.45 | 0.52 |
| 3:E:108:VAL:HG22 | 3:E:109:GLY:N | 2.24 | 0.52 |
| 3:F:13:SER:HA | 3:F:73:ARG:HB3 | 1.91 | 0.52 |
| 4:G:75:THR:O | 4:G:75:THR:HG23 | 2.10 | 0.52 |
| 5:H:22:THR:HB | 5:H:108:PHE:CZ | 2.44 | 0.52 |
| 5:H:58:SER:HA | 5:H:143:ILE:HD11 | 1.91 | 0.52 |
| 1:A:165:MET:CB | 1:A:180:ALA:HB1 | 2.40 | 0.51 |
| 1:A:222:GLY:HA2 | 1:A:223:GLU:C | 2.30 | 0.51 |
| 1:A:249:ASN:HD22 | 1:A:249:ASN:H | 1.56 | 0.51 |
| 1:A:368:ALA:O | 1:A:370:LEU:HD22 | 2.10 | 0.51 |
| 1:A:387:LEU:HG | 1:A:391:PHE:CZ | 2.45 | 0.51 |
| 1:B:249:ASN:H | 1:B:249:ASN:HD22 | 1.56 | 0.51 |
| 1:B:32:THR:HG22 | 1:B:36:LYS:HE2 | 1.91 | 0.51 |
| 3:E:31:GLU:HG2 | 3:E:67:ARG:O | 2.11 | 0.51 |
| 3:F:75:ILE:HA | 3:F:79:LYS:O | 2.09 | 0.51 |
| 3:F:9:ILE:HG13 | 3:F:34:ALA:O | 2.10 | 0.51 |
| 1:A:130:LEU:O | 1:A:134:VAL:HG22 | 2.10 | 0.51 |
| 1:A:232:LYS:N | 1:A:237:ILE:HB | 2.24 | 0.51 |
| 1:B:159:ILE:C | 1:B:159:ILE:HD13 | 2.30 | 0.51 |
| 1:B:165:MET:CB | 1:B:180:ALA:HB1 | 2.40 | 0.51 |
| 1:B:147:PRO:HD2 | 1:B:243:PRO:CB | 2.40 | 0.51 |
| 3:E:84:ILE:CG1 | 3:E:103:GLU:HG2 | 2.40 | 0.51 |
| 3:F:17:GLN:OE1 | 3:F:24:LYS:HB3 | 2.10 | 0.51 |
| 4:G:124:ILE:C | 4:G:124:ILE:HD13 | 2.31 | 0.51 |
| 4:G:63:ASN:N | 5:H:139:LYS:HB2 | 2.25 | 0.51 |
| 5:H:104:TYR:HE1 | 5:H:160:PHE:HB2 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:235:GLN:HA | 1:A:235:GLN:OE1 | 2.08 | 0.51 |
| 1:A:441:GLU:O | 1:A:444:VAL:HB | 2.10 | 0.51 |
| 1:B:222:GLY:HA2 | 1:B:223:GLU:C | 2.30 | 0.51 |
| 1:B:368:ALA:O | 1:B:370:LEU:HD22 | 2.10 | 0.51 |
| 1:B:376:MET:O | 1:B:379:ARG:HB2 | 2.10 | 0.51 |
| 1:B:441:GLU:HG2 | 1:B:456:GLU:CB | 2.38 | 0.51 |
| 1:B:466:GLN:CG | 1:B:467:TYR:HB2 | 2.39 | 0.51 |
| 1:A:460:ILE:HD12 | 1:B:466:GLN:NE2 | 2.23 | 0.51 |
| 2:C:4:GLN:CD | 2:C:5:ARG:H | 2.14 | 0.51 |
| 2:D:14:ASN:HD21 | 2:D:21:LEU:CG | 2.23 | 0.51 |
| 3:E:44:GLU:H | 3:E:44:GLU:CD | 2.14 | 0.51 |
| 3:E:60:ILE:O | 3:E:98:ARG:HA | 2.09 | 0.51 |
| 3:F:12:GLN:NE2 | 3:F:28:TRP:HZ3 | 2.09 | 0.51 |
| 5:H:110:PHE:HE1 | 5:H:150:ILE:HD12 | 1.75 | 0.51 |
| 5:H:145:THR:HG23 | 5:H:146:LEU:HD23 | 1.91 | 0.51 |
| 5:H:52:ARG:HD2 | 5:H:52:ARG:C | 2.30 | 0.51 |
| 5:H:37:VAL:HG11 | 5:H:63:GLY:CA | 2.40 | 0.51 |
| 1:A:110:ASP:HA | 1:A:409:GLU:CD | 2.30 | 0.51 |
| 1:A:150:ASP:HB2 | 1:A:156:ASP:HB2 | 1.91 | 0.51 |
| 1:A:33:MET:O | 1:A:37:LEU:HG | 2.09 | 0.51 |
| 1:A:100:LEU:HD23 | 1:A:377:ALA:HB3 | 1.93 | 0.51 |
| 1:A:439:SER:CB | 1:A:442:THR:H | 2.24 | 0.51 |
| 1:B:324:ILE:CB | 1:B:325:PRO:HD3 | 2.36 | 0.51 |
| 2:C:7:LYS:NZ | 3:E:4:GLU:CD | 2.61 | 0.51 |
| 3:F:38:VAL:HG22 | 3:F:60:ILE:HB | 1.93 | 0.51 |
| 3:F:60:ILE:HG13 | 3:F:83:PHE:HE2 | 1.76 | 0.51 |
| 3:F:6:ARG:HH11 | 3:F:33:THR:HG23 | 1.74 | 0.51 |
| 2:D:70:LEU:N | 3:F:93:LEU:HA | 2.25 | 0.51 |
| 5:H:91:PHE:CE1 | 5:H:111:ALA:HB1 | 2.46 | 0.51 |
| 5:H:14:LEU:HG | 5:H:160:PHE:CE1 | 2.45 | 0.51 |
| 4:G:3:TRP:HZ2 | 5:H:52:ARG:HH21 | 1.51 | 0.51 |
| 1:A:174:ARG:NH1 | 1:A:174:ARG:HG2 | 2.25 | 0.51 |
| 1:B:283:GLN:CD | 1:B:284:ILE:HG22 | 2.31 | 0.51 |
| 1:B:329:ALA:O | 1:B:333:LEU:HG | 2.09 | 0.51 |
| 1:B:341:TYR:CA | 1:B:344:ALA:HB2 | 2.40 | 0.51 |
| 1:B:38:ILE:HG12 | 1:B:181:LEU:O | 2.11 | 0.51 |
| 1:B:110:ASP:CB | 1:B:396:LEU:HD13 | 2.22 | 0.51 |
| 1:B:439:SER:CB | 1:B:442:THR:H | 2.24 | 0.51 |
| 1:B:88:TRP:CD2 | 1:B:92:PHE:CE1 | 2.99 | 0.51 |
| 2:C:5:ARG:HD3 | 2:C:7:LYS:HE3 | 1.92 | 0.51 |
| 4:G:73:GLY:CA | 4:G:76:ARG:HH21 | 2.22 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:GLU:HB3 | 1:A:165:MET:N | 2.24 | 0.51 |
| 1:A:394:GLU:O | 1:A:397:ARG:HB3 | 2.11 | 0.51 |
| 1:A:62:LYS:HD3 | 1:A:63:ARG:H | 1.75 | 0.51 |
| 1:B:95:GLN:HG2 | 1:B:370:LEU:HD13 | 1.92 | 0.51 |
| 3:E:80:ILE:O | 3:E:80:ILE:HG13 | 2.10 | 0.51 |
| 3:E:65:ASP:HB3 | 3:E:97:THR:C | 2.31 | 0.51 |
| 3:E:40:PRO:HG3 | 3:F:100:LYS:CB | 2.41 | 0.51 |
| 3:F:14:TYR:H | 3:F:73:ARG:HB3 | 1.75 | 0.51 |
| 4:G:128:ARG:N | 4:G:128:ARG:HD2 | 2.20 | 0.51 |
| 4:G:41:TYR:CE1 | 4:G:43:TYR:CE1 | 2.98 | 0.51 |
| 1:A:147:PRO:HD2 | 1:A:243:PRO:CB | 2.40 | 0.51 |
| 1:A:460:ILE:CG1 | 1:B:467:TYR:CG | 2.84 | 0.51 |
| 1:A:46:LEU:CG | 1:A:143:GLU:H | 2.23 | 0.51 |
| 1:A:88:TRP:CD2 | 1:A:92:PHE:CE1 | 2.99 | 0.51 |
| 1:A:96:LYS:HB2 | 1:A:373:LYS:CB | 2.38 | 0.51 |
| 1:B:110:ASP:HA | 1:B:409:GLU:CD | 2.30 | 0.51 |
| 1:B:150:ASP:HB2 | 1:B:156:ASP:HB2 | 1.91 | 0.51 |
| 1:B:163:GLU:HB3 | 1:B:165:MET:N | 2.24 | 0.51 |
| 1:B:34:ILE:HG21 | 1:B:199:LEU:HD13 | 1.92 | 0.51 |
| 1:B:382:ARG:HA | 1:B:383:ALA:C | 2.31 | 0.51 |
| 1:B:441:GLU:O | 1:B:444:VAL:HB | 2.10 | 0.51 |
| 1:A:439:SER:OG | 1:B:459:ARG:CD | 2.58 | 0.51 |
| 2:D:30:GLU:HA | 2:D:40:PHE:CZ | 2.45 | 0.51 |
| 2:D:4:GLN:CD | 2:D:5:ARG:H | 2.14 | 0.51 |
| 3:E:43:GLN:HE22 | 3:F:53:GLN:CD | 2.14 | 0.51 |
| 3:E:5:PHE:CZ | 3:F:64:TYR:CE1 | 2.98 | 0.51 |
| 3:F:22:GLY:C | 4:G:19:GLU:HB2 | 2.30 | 0.51 |
| 5:H:108:PHE:CB | 5:H:150:ILE:HG23 | 2.40 | 0.51 |
| 1:A:175:ARG:HH22 | 1:B:148:PHE:HZ | 1.58 | 0.51 |
| 1:A:382:ARG:HA | 1:A:383:ALA:C | 2.31 | 0.51 |
| 1:A:111:ASN:N | 1:A:396:LEU:HD22 | 2.23 | 0.51 |
| 1:B:225:ASN:HB2 | 1:B:226:PRO:CA | 2.34 | 0.51 |
| 2:C:8:ARG:NH1 | 2:D:64:TYR:OH | 2.43 | 0.51 |
| 3:E:48:LYS:HZ3 | 3:F:48:LYS:HE3 | 1.75 | 0.51 |
| 3:E:79:LYS:CD | 3:F:69:ASP:HB3 | 2.40 | 0.51 |
| 3:F:75:ILE:HG13 | 3:F:80:ILE:HG22 | 1.91 | 0.51 |
| 3:F:88:VAL:H | 3:F:98:ARG:H | 1.58 | 0.51 |
| 3:E:104:ASP:CB | 4:G:119:VAL:HG21 | 2.41 | 0.51 |
| 4:G:124:ILE:O | 4:G:124:ILE:HG23 | 2.10 | 0.51 |
| 4:G:98:GLU:H | 5:H:49:LYS:HD3 | 1.76 | 0.51 |
| 1:A:243:PRO:HB2 | 1:A:244:ILE:HG22 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:PRO:HG3 | 1:A:170:LYS:CD | 2.41 | 0.51 |
| 1:A:34:ILE:HG21 | 1:A:199:LEU:HD13 | 1.92 | 0.51 |
| 1:A:95:GLN:HG2 | 1:A:370:LEU:HD13 | 1.92 | 0.51 |
| 1:A:439:SER:CB | 1:A:442:THR:HB | 2.40 | 0.51 |
| 1:A:63:ARG:HG2 | 1:A:79:LYS:CB | 2.22 | 0.51 |
| 1:A:69:ALA:HB2 | 1:B:300:THR:HG23 | 1.92 | 0.51 |
| 1:A:88:TRP:CD1 | 1:A:92:PHE:CZ | 2.98 | 0.51 |
| 1:B:186:TYR:O | 1:B:196:LYS:HE3 | 2.11 | 0.51 |
| 1:A:64:ARG:HH21 | 1:B:284:ILE:CG1 | 2.24 | 0.51 |
| 1:B:292:ASP:OD1 | 2:D:33:LYS:O | 2.26 | 0.51 |
| 2:C:33:LYS:CD | 2:C:50:PRO:HB3 | 2.40 | 0.51 |
| 2:C:35:GLU:OE1 | 2:C:37:HIS:HA | 2.10 | 0.51 |
| 1:B:298:GLU:CD | 2:C:43:LYS:HG2 | 2.28 | 0.51 |
| 2:D:34:ASP:H | 2:D:35:GLU:HA | 1.72 | 0.51 |
| 2:C:93:LYS:CE | 2:D:96:PRO:O | 2.58 | 0.51 |
| 3:E:14:TYR:OH | 3:E:26:TYR:HB2 | 2.10 | 0.51 |
| 4:G:33:GLU:HB2 | 4:G:46:ILE:H | 1.76 | 0.51 |
| 4:G:61:GLY:HA2 | 5:H:139:LYS:H | 1.76 | 0.51 |
| 5:H:26:PRO:HB2 | 5:H:162:GLN:OE1 | 2.11 | 0.51 |
| 5:H:29:PRO:HA | 5:H:30:ALA:O | 2.10 | 0.51 |
| 1:A:186:TYR:O | 1:A:196:LYS:HE3 | 2.11 | 0.51 |
| 1:A:204:HIS:CD2 | 1:A:206:TYR:CE1 | 2.99 | 0.51 |
| 1:A:210:LYS:C | 1:A:210:LYS:HD3 | 2.31 | 0.51 |
| 1:B:204:HIS:CD2 | 1:B:206:TYR:CE1 | 2.99 | 0.51 |
| 1:B:195:GLN:O | 1:B:210:LYS:HB2 | 2.11 | 0.51 |
| 1:B:239:TRP:HB2 | 1:B:241:ARG:O | 2.11 | 0.51 |
| 1:B:345:GLN:CD | 1:B:345:GLN:H | 2.13 | 0.51 |
| 1:B:63:ARG:HG2 | 1:B:79:LYS:CB | 2.22 | 0.51 |
| 1:B:294:GLU:CB | 2:C:42:ASP:CG | 2.77 | 0.51 |
| 2:C:54:LEU:HD23 | 2:C:54:LEU:C | 2.32 | 0.51 |
| 2:C:63:PHE:HB2 | 2:C:85:GLU:HG2 | 1.93 | 0.51 |
| 2:D:25:VAL:HG12 | 2:D:29:VAL:HG23 | 1.90 | 0.51 |
| 4:G:44:VAL:CG2 | 4:G:74:THR:HB | 2.41 | 0.51 |
| 5:H:47:GLN:HE22 | 5:H:55:GLY:N | 2.09 | 0.51 |
| 1:A:283:GLN:CD | 1:A:284:ILE:HG22 | 2.31 | 0.50 |
| 1:A:96:LYS:HA | 1:A:373:LYS:CG | 2.41 | 0.50 |
| 1:A:460:ILE:HG13 | 1:B:467:TYR:CG | 2.46 | 0.50 |
| 1:A:466:GLN:CG | 1:A:467:TYR:HB2 | 2.39 | 0.50 |
| 1:A:46:LEU:HD23 | 1:A:143:GLU:H | 1.76 | 0.50 |
| 1:A:332:GLU:CG | 1:B:326:VAL:HG13 | 2.40 | 0.50 |
| 1:B:62:LYS:HG3 | 1:B:81:ASN:HA | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:42:SER:C | 3:E:43:GLN:HG3 | 2.30 | 0.50 |
| 3:E:46:TYR:CG | 3:E:48:LYS:HE2 | 2.46 | 0.50 |
| 3:E:96:ILE:HG13 | 3:E:96:ILE:O | 2.09 | 0.50 |
| 4:G:100:PHE:CD2 | 5:H:47:GLN:CG | 2.94 | 0.50 |
| 5:H:15:PHE:CZ | 5:H:91:PHE:CD2 | 2.99 | 0.50 |
| 5:H:91:PHE:CG | 5:H:111:ALA:CB | 2.94 | 0.50 |
| 1:A:148:PHE:CE1 | 1:A:156:ASP:HB3 | 2.47 | 0.50 |
| 1:A:345:GLN:CD | 1:A:345:GLN:H | 2.13 | 0.50 |
| 1:A:376:MET:O | 1:A:379:ARG:HB2 | 2.10 | 0.50 |
| 1:A:38:ILE:HG12 | 1:A:181:LEU:O | 2.11 | 0.50 |
| 1:A:457:LEU:C | 1:A:457:LEU:HD23 | 2.31 | 0.50 |
| 1:A:62:LYS:HG3 | 1:A:81:ASN:HA | 1.93 | 0.50 |
| 1:A:89:HIS:HE1 | 1:A:257:LEU:HG | 1.75 | 0.50 |
| 1:B:221:TYR:HB2 | 1:B:222:GLY:HA2 | 1.93 | 0.50 |
| 2:D:87:PRO:CG | 2:D:90:ILE:HB | 2.41 | 0.50 |
| 3:E:61:TYR:CD1 | 3:E:96:ILE:HB | 2.46 | 0.50 |
| 3:F:24:LYS:CG | 3:F:25:THR:H | 2.19 | 0.50 |
| 3:F:46:TYR:CD2 | 3:F:48:LYS:HE2 | 2.46 | 0.50 |
| 3:E:43:GLN:HE22 | 3:F:53:GLN:NE2 | 2.09 | 0.50 |
| 3:F:76:TYR:CE1 | 3:F:81:VAL:HG12 | 2.47 | 0.50 |
| 5:H:108:PHE:CE2 | 5:H:153:VAL:HG11 | 2.47 | 0.50 |
| 5:H:66:THR:O | 5:H:67:TYR:HD1 | 1.93 | 0.50 |
| 1:A:239:TRP:HB2 | 1:A:241:ARG:O | 2.11 | 0.50 |
| 1:A:290:ASN:O | 1:A:317:VAL:HG11 | 2.12 | 0.50 |
| 1:A:379:ARG:HB2 | 1:A:380:LYS:HZ3 | 1.76 | 0.50 |
| 1:A:439:SER:CA | 1:B:459:ARG:HD2 | 2.40 | 0.50 |
| 1:B:142:ILE:HB | 1:B:144:TYR:N | 2.26 | 0.50 |
| 1:B:46:LEU:CG | 1:B:143:GLU:H | 2.23 | 0.50 |
| 1:B:46:LEU:HD23 | 1:B:143:GLU:H | 1.76 | 0.50 |
| 1:B:373:LYS:HE3 | 1:B:374:ALA:CA | 2.41 | 0.50 |
| 1:B:394:GLU:O | 1:B:397:ARG:HB3 | 2.11 | 0.50 |
| 1:B:63:ARG:HD2 | 1:B:75:VAL:CG1 | 2.42 | 0.50 |
| 2:D:54:LEU:HD23 | 2:D:54:LEU:C | 2.32 | 0.50 |
| 3:E:6:ARG:NE | 3:E:6:ARG:HA | 2.27 | 0.50 |
| 3:F:43:GLN:H | 3:F:53:GLN:CB | 2.18 | 0.50 |
| 4:G:24:LEU:O | 4:G:28:VAL:HG23 | 2.12 | 0.50 |
| 5:H:53:ILE:HG13 | 5:H:53:ILE:O | 2.10 | 0.50 |
| 5:H:52:ARG:NH2 | 5:H:54:LEU:HD21 | 2.03 | 0.50 |
| 1:A:121:LEU:HD12 | 1:A:124:ASP:N | 2.23 | 0.50 |
| 1:A:146:HIS:CD2 | 1:A:200:TYR:CD2 | 2.99 | 0.50 |
| 1:A:255:SER:HB2 | 1:A:256:ASP:CA | 2.34 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:THR:HB | 1:A:419:ILE:N | 2.27 | 0.50 |
| 1:B:158:VAL:HG12 | 1:B:159:ILE:N | 2.27 | 0.50 |
| 1:B:96:LYS:HA | 1:B:373:LYS:CG | 2.41 | 0.50 |
| 1:B:100:LEU:HD23 | 1:B:377:ALA:HB3 | 1.93 | 0.50 |
| 1:B:62:LYS:HE3 | 1:B:80:THR:C | 2.32 | 0.50 |
| 2:C:87:PRO:CG | 2:C:90:ILE:HB | 2.41 | 0.50 |
| 2:C:94:LEU:CB | 2:D:97:TYR:CG | 2.78 | 0.50 |
| 4:G:32:THR:HG22 | 4:G:37:LYS:HA | 1.91 | 0.50 |
| 1:A:29:PRO:HG3 | 1:A:170:LYS:CE | 2.42 | 0.50 |
| 1:A:175:ARG:CZ | 1:B:148:PHE:HE2 | 2.24 | 0.50 |
| 1:A:235:GLN:HG3 | 1:A:236:ALA:N | 2.27 | 0.50 |
| 1:A:438:MET:HA | 1:A:439:SER:C | 2.31 | 0.50 |
| 1:B:146:HIS:CD2 | 1:B:200:TYR:CD2 | 2.99 | 0.50 |
| 1:B:288:LEU:HD23 | 1:B:288:LEU:N | 2.27 | 0.50 |
| 1:B:433:VAL:CG2 | 1:B:440:LYS:HG3 | 2.42 | 0.50 |
| 1:B:445:ALA:CA | 1:B:448:PRO:HB3 | 2.34 | 0.50 |
| 3:E:46:TYR:CD2 | 3:E:48:LYS:HE2 | 2.46 | 0.50 |
| 3:F:104:ASP:OD1 | 4:G:34:SER:C | 2.49 | 0.50 |
| 4:G:134:ASN:CA | 5:H:138:LEU:O | 2.60 | 0.50 |
| 5:H:65:VAL:HG12 | 5:H:66:THR:N | 2.27 | 0.50 |
| 1:A:158:VAL:HG12 | 1:A:159:ILE:N | 2.27 | 0.50 |
| 1:A:221:TYR:HB2 | 1:A:222:GLY:HA2 | 1.93 | 0.50 |
| 1:A:373:LYS:HE3 | 1:A:374:ALA:CA | 2.41 | 0.50 |
| 1:A:96:LYS:CE | 1:A:377:ALA:HA | 2.36 | 0.50 |
| 1:A:376:MET:SD | 1:A:380:LYS:HE2 | 2.52 | 0.50 |
| 1:A:62:LYS:HE3 | 1:A:80:THR:C | 2.32 | 0.50 |
| 1:B:235:GLN:HG3 | 1:B:236:ALA:N | 2.27 | 0.50 |
| 1:B:391:PHE:O | 1:B:394:GLU:HB2 | 2.12 | 0.50 |
| 1:B:417:THR:HB | 1:B:419:ILE:N | 2.27 | 0.50 |
| 1:B:51:ARG:HB3 | 1:B:51:ARG:NH1 | 2.26 | 0.50 |
| 2:C:11:SER:HB3 | 3:E:93:LEU:HB2 | 1.94 | 0.50 |
| 2:D:49:ILE:CD1 | 2:D:54:LEU:HD12 | 2.40 | 0.50 |
| 2:D:5:ARG:NH2 | 3:F:2:TYR:HD2 | 2.07 | 0.50 |
| 4:G:10:LEU:HD12 | 4:G:10:LEU:C | 2.31 | 0.50 |
| 4:G:91:THR:O | 4:G:92:TYR:HD1 | 1.95 | 0.50 |
| 1:B:121:LEU:N | 1:B:122:ALA:HA | 2.27 | 0.50 |
| 1:B:148:PHE:CE1 | 1:B:156:ASP:HB3 | 2.47 | 0.50 |
| 1:B:457:LEU:C | 1:B:457:LEU:HD23 | 2.31 | 0.50 |
| 2:C:25:VAL:CB | 2:C:26:PRO:HD3 | 2.36 | 0.50 |
| 2:D:63:PHE:CE1 | 2:D:85:GLU:CB | 2.95 | 0.50 |
| 3:E:2:TYR:HD1 | 3:F:93:LEU:O | 1.95 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:61:TYR:HE1 | 3:E:96:ILE:CG2 | 2.25 | 0.50 |
| 3:F:60:ILE:CG1 | 3:F:83:PHE:CE2 | 2.95 | 0.50 |
| 4:G:33:GLU:CB | 4:G:46:ILE:H | 2.24 | 0.50 |
| 4:G:74:THR:HG23 | 4:G:75:THR:H | 1.77 | 0.50 |
| 4:G:79:ALA:O | 4:G:82:ILE:HG12 | 2.10 | 0.50 |
| 5:H:108:PHE:CE2 | 5:H:153:VAL:CG1 | 2.95 | 0.50 |
| 5:H:91:PHE:CD1 | 5:H:111:ALA:CB | 2.95 | 0.50 |
| 5:H:14:LEU:CD2 | 5:H:160:PHE:CZ | 2.95 | 0.50 |
| 5:H:42:GLU:HG2 | 5:H:56:PRO:HG2 | 1.76 | 0.50 |
| 1:A:391:PHE:O | 1:A:394:GLU:HB2 | 2.12 | 0.50 |
| 1:B:190:MET:HE1 | 1:B:194:THR:CG2 | 2.42 | 0.50 |
| 1:B:254:VAL:CG2 | 1:B:259:PHE:CE1 | 2.95 | 0.50 |
| 1:B:295:ASN:OD1 | 2:C:42:ASP:OD2 | 2.30 | 0.50 |
| 2:C:98:ARG:HG3 | 2:D:97:TYR:CD2 | 2.47 | 0.50 |
| 3:F:14:TYR:CZ | 3:F:28:TRP:NE1 | 2.80 | 0.50 |
| 3:F:47:TYR:CB | 3:F:50:GLN:HB3 | 2.34 | 0.50 |
| 4:G:127:VAL:CG2 | 4:G:129:PHE:CE1 | 2.95 | 0.50 |
| 1:A:195:GLN:O | 1:A:210:LYS:HB2 | 2.11 | 0.50 |
| 1:A:433:VAL:HG23 | 1:A:440:LYS:HG3 | 1.93 | 0.50 |
| 1:A:51:ARG:HB3 | 1:A:51:ARG:NH1 | 2.26 | 0.50 |
| 1:A:64:ARG:NE | 1:B:283:GLN:O | 2.45 | 0.50 |
| 1:B:210:LYS:C | 1:B:210:LYS:HD3 | 2.31 | 0.50 |
| 1:B:433:VAL:HG23 | 1:B:440:LYS:HG3 | 1.93 | 0.50 |
| 2:C:59:LYS:HB2 | 2:C:90:ILE:HD13 | 1.94 | 0.50 |
| 2:C:99:LYS:NZ | 2:D:102:ARG:CB | 2.75 | 0.50 |
| 2:D:8:ARG:CZ | 2:D:12:ILE:HD11 | 2.41 | 0.50 |
| 3:F:9:ILE:CD1 | 3:F:11:PHE:CE1 | 2.95 | 0.50 |
| 3:F:2:TYR:O | 3:F:3:GLU:HB3 | 2.12 | 0.50 |
| 3:F:46:TYR:HB3 | 3:F:48:LYS:CE | 2.32 | 0.50 |
| 3:F:14:TYR:HD2 | 3:F:73:ARG:NH1 | 2.09 | 0.50 |
| 4:G:10:LEU:O | 4:G:13:ALA:HB3 | 2.10 | 0.50 |
| 4:G:22:GLN:CB | 4:G:23:PRO:HD3 | 2.42 | 0.50 |
| 1:A:121:LEU:N | 1:A:122:ALA:HA | 2.27 | 0.49 |
| 1:A:52:TYR:CZ | 1:A:265:ASP:CB | 2.95 | 0.49 |
| 1:A:288:LEU:N | 1:A:288:LEU:HD23 | 2.27 | 0.49 |
| 1:B:144:TYR:C | 1:B:244:ILE:HD12 | 2.32 | 0.49 |
| 1:B:298:GLU:HB3 | 2:C:42:ASP:HB3 | 1.92 | 0.49 |
| 1:A:365:LYS:O | 1:B:359:THR:HG21 | 2.08 | 0.49 |
| 1:B:376:MET:SD | 1:B:380:LYS:HE2 | 2.52 | 0.49 |
| 2:C:8:ARG:CZ | 2:C:12:ILE:HD11 | 2.41 | 0.49 |
| 2:D:59:LYS:HB2 | 2:D:90:ILE:HD13 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:103:GLU:HG3 | 4:G:41:TYR:C | 2.32 | 0.49 |
| 3:F:68:ILE:HD13 | 3:F:69:ASP:H | 1.76 | 0.49 |
| 3:F:74:VAL:CB | 3:F:83:PHE:CE2 | 2.95 | 0.49 |
| 3:F:74:VAL:HG13 | 3:F:81:VAL:HG13 | 1.94 | 0.49 |
| 3:E:109:GLY:C | 4:G:114:THR:OG1 | 2.51 | 0.49 |
| 5:H:92:TRP:CE3 | 5:H:106:ALA:CB | 2.95 | 0.49 |
| 1:A:142:ILE:HB | 1:A:144:TYR:N | 2.26 | 0.49 |
| 1:A:387:LEU:CD1 | 1:A:391:PHE:CE1 | 2.95 | 0.49 |
| 1:B:29:PRO:HG3 | 1:B:170:LYS:CE | 2.42 | 0.49 |
| 2:C:14:ASN:HD21 | 2:C:21:LEU:CG | 2.23 | 0.49 |
| 2:C:37:HIS:O | 2:C:39:PRO:HD3 | 2.12 | 0.49 |
| 2:D:75:MET:H | 2:D:78:VAL:CB | 2.25 | 0.49 |
| 3:E:53:GLN:CG | 3:E:55:PRO:HD3 | 2.40 | 0.49 |
| 3:E:60:ILE:HG12 | 3:E:99:ILE:CD1 | 2.42 | 0.49 |
| 3:F:12:GLN:HE21 | 3:F:80:ILE:CG2 | 2.24 | 0.49 |
| 3:F:59:ASN:HD22 | 3:F:99:ILE:CG2 | 2.25 | 0.49 |
| 3:F:76:TYR:CE2 | 3:F:79:LYS:CG | 2.95 | 0.49 |
| 5:H:46:GLU:H | 5:H:151:VAL:HG21 | 1.75 | 0.49 |
| 5:H:160:PHE:C | 5:H:163:PRO:HD2 | 2.32 | 0.49 |
| 1:A:254:VAL:CG2 | 1:A:259:PHE:CE1 | 2.95 | 0.49 |
| 1:A:373:LYS:C | 1:A:373:LYS:HD2 | 2.33 | 0.49 |
| 1:A:99:TYR:CD2 | 1:A:373:LYS:CE | 2.95 | 0.49 |
| 1:A:387:LEU:CG | 1:A:391:PHE:CZ | 2.95 | 0.49 |
| 1:A:65:THR:HB | 1:A:73:GLN:HG3 | 1.94 | 0.49 |
| 1:A:63:ARG:HD2 | 1:A:75:VAL:CG1 | 2.42 | 0.49 |
| 1:B:136:ASN:CB | 1:B:145:TRP:CH2 | 2.95 | 0.49 |
| 1:B:243:PRO:HB2 | 1:B:244:ILE:HG22 | 1.93 | 0.49 |
| 1:B:298:GLU:HA | 2:C:43:LYS:HZ1 | 1.77 | 0.49 |
| 2:C:49:ILE:CD1 | 2:C:54:LEU:HD12 | 2.40 | 0.49 |
| 2:D:16:LYS:CD | 3:E:3:GLU:OE1 | 2.59 | 0.49 |
| 1:A:255:SER:CB | 1:A:259:PHE:CE2 | 2.95 | 0.49 |
| 1:B:52:TYR:CZ | 1:B:265:ASP:CB | 2.95 | 0.49 |
| 1:B:290:ASN:O | 1:B:317:VAL:HG11 | 2.12 | 0.49 |
| 1:B:373:LYS:HD2 | 1:B:373:LYS:C | 2.33 | 0.49 |
| 1:B:130:LEU:HD13 | 1:B:388:PHE:CZ | 2.47 | 0.49 |
| 2:C:7:LYS:CD | 3:E:4:GLU:CD | 2.61 | 0.49 |
| 2:C:85:GLU:CA | 2:D:86:ILE:CD1 | 2.87 | 0.49 |
| 2:C:84:THR:HB | 2:D:83:ALA:CB | 2.43 | 0.49 |
| 3:E:38:VAL:CB | 3:E:60:ILE:HG22 | 2.41 | 0.49 |
| 3:F:14:TYR:H | 3:F:73:ARG:CB | 2.26 | 0.49 |
| 3:F:21:GLU:HA | 4:G:20:SER:CA | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:43:GLN:CB | 3:F:47:TYR:CE1 | 2.95 | 0.49 |
| 3:F:60:ILE:HD13 | 3:F:99:ILE:CD1 | 2.42 | 0.49 |
| 3:F:96:ILE:HD11 | 3:F:98:ARG:HE | 1.77 | 0.49 |
| 5:H:119:SER:OG | 5:H:128:ILE:HG12 | 2.12 | 0.49 |
| 1:A:198:GLU:HB2 | 1:A:200:TYR:HE1 | 1.77 | 0.49 |
| 1:A:306:HIS:HB3 | 1:A:308:VAL:CG1 | 2.23 | 0.49 |
| 1:A:99:TYR:CE2 | 1:A:370:LEU:HB3 | 2.48 | 0.49 |
| 1:B:142:ILE:CG2 | 1:B:145:TRP:HB2 | 2.42 | 0.49 |
| 1:B:159:ILE:HG23 | 1:B:159:ILE:O | 2.12 | 0.49 |
| 1:A:336:ILE:CD1 | 1:B:278:PHE:HA | 2.34 | 0.49 |
| 1:B:48:LYS:HE3 | 1:B:258:LYS:NZ | 2.27 | 0.49 |
| 1:B:65:THR:HB | 1:B:73:GLN:HG3 | 1.94 | 0.49 |
| 1:B:81:ASN:ND2 | 1:B:83:ARG:HD2 | 2.27 | 0.49 |
| 2:C:95:ASN:HB3 | 2:C:98:ARG:N | 2.28 | 0.49 |
| 5:H:143:ILE:HG21 | 5:H:146:LEU:HB2 | 1.93 | 0.49 |
| 1:A:140:LYS:HG2 | 1:A:141:GLY:H | 1.77 | 0.49 |
| 1:A:142:ILE:CG2 | 1:A:145:TRP:HB2 | 2.42 | 0.49 |
| 1:B:136:ASN:O | 1:B:139:ASN:HB2 | 2.12 | 0.49 |
| 1:B:64:ARG:H | 1:B:79:LYS:HG3 | 1.78 | 0.49 |
| 1:B:96:LYS:HB2 | 1:B:373:LYS:CB | 2.38 | 0.49 |
| 2:C:7:LYS:HE2 | 3:E:4:GLU:HA | 0.74 | 0.49 |
| 2:D:63:PHE:HB2 | 2:D:85:GLU:HG2 | 1.93 | 0.49 |
| 2:D:77:THR:HG21 | 3:E:46:TYR:CZ | 2.47 | 0.49 |
| 3:F:7:ASP:HB2 | 3:F:9:ILE:HG12 | 1.95 | 0.49 |
| 5:H:68:TYR:HA | 5:H:127:GLU:HG3 | 1.94 | 0.49 |
| 5:H:16:GLN:CG | 5:H:92:TRP:CD1 | 2.95 | 0.49 |
| 5:H:32:GLN:CA | 5:H:67:TYR:CE1 | 2.95 | 0.49 |
| 5:H:42:GLU:HB2 | 5:H:43:LEU:HA | 1.94 | 0.49 |
| 1:A:144:TYR:C | 1:A:244:ILE:HD12 | 2.32 | 0.49 |
| 1:A:167:VAL:HG22 | 1:A:246:PRO:CG | 2.43 | 0.49 |
| 1:A:179:PHE:CE2 | 1:A:200:TYR:CB | 2.95 | 0.49 |
| 1:A:387:LEU:HD21 | 1:A:391:PHE:CZ | 2.48 | 0.49 |
| 1:A:418:ARG:HH22 | 1:B:426:VAL:HG13 | 1.77 | 0.49 |
| 1:A:433:VAL:CG2 | 1:A:440:LYS:HG3 | 2.42 | 0.49 |
| 1:A:64:ARG:H | 1:A:79:LYS:HG3 | 1.78 | 0.49 |
| 1:A:175:ARG:NH1 | 1:B:150:ASP:OD1 | 2.45 | 0.49 |
| 1:B:167:VAL:HG13 | 1:B:177:ILE:CB | 2.42 | 0.49 |
| 1:B:29:PRO:HG3 | 1:B:170:LYS:CD | 2.41 | 0.49 |
| 1:B:146:HIS:HA | 1:B:244:ILE:HG22 | 1.94 | 0.49 |
| 1:B:438:MET:HA | 1:B:439:SER:C | 2.31 | 0.49 |
| 2:D:55:ILE:CD1 | 2:D:93:LYS:HZ2 | 2.22 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:2:TYR:CE1 | 3:F:95:GLU:CA | 2.95 | 0.49 |
| 3:F:22:GLY:O | 4:G:19:GLU:OE2 | 2.31 | 0.49 |
| 4:G:41:TYR:CE1 | 4:G:43:TYR:CD1 | 3.00 | 0.49 |
| 5:H:92:TRP:HE3 | 5:H:106:ALA:CB | 2.25 | 0.49 |
| 5:H:91:PHE:CD2 | 5:H:111:ALA:CB | 2.95 | 0.49 |
| 5:H:157:GLY:O | 5:H:158:TYR:HD1 | 1.95 | 0.49 |
| 1:A:136:ASN:O | 1:A:139:ASN:HB2 | 2.12 | 0.49 |
| 1:A:159:ILE:O | 1:A:159:ILE:HG23 | 2.12 | 0.49 |
| 1:A:430:VAL:O | 1:A:433:VAL:HG12 | 2.13 | 0.49 |
| 1:B:167:VAL:HG22 | 1:B:246:PRO:CG | 2.43 | 0.49 |
| 1:B:179:PHE:CE2 | 1:B:200:TYR:CB | 2.95 | 0.49 |
| 1:B:198:GLU:HB2 | 1:B:200:TYR:HE1 | 1.77 | 0.49 |
| 1:A:379:ARG:CD | 1:B:94:ASP:OD2 | 2.54 | 0.49 |
| 1:B:99:TYR:CD2 | 1:B:373:LYS:CE | 2.95 | 0.49 |
| 2:C:5:ARG:HG3 | 2:C:8:ARG:HB2 | 1.95 | 0.49 |
| 2:D:35:GLU:HA | 2:D:35:GLU:OE1 | 2.13 | 0.49 |
| 3:E:15:VAL:CG1 | 3:E:29:VAL:HG23 | 2.42 | 0.49 |
| 3:E:24:LYS:HB2 | 3:E:24:LYS:NZ | 2.27 | 0.49 |
| 3:E:74:VAL:CG1 | 3:E:83:PHE:CE2 | 2.95 | 0.49 |
| 3:E:50:GLN:HB3 | 3:F:49:ALA:HB3 | 1.95 | 0.49 |
| 1:A:111:ASN:H | 1:A:396:LEU:CD2 | 2.26 | 0.49 |
| 1:A:175:ARG:CZ | 1:B:148:PHE:CE2 | 2.96 | 0.49 |
| 1:A:195:GLN:HE21 | 1:A:195:GLN:HA | 1.78 | 0.49 |
| 1:A:365:LYS:C | 1:B:359:THR:HG21 | 2.30 | 0.49 |
| 1:A:88:TRP:NE1 | 1:A:92:PHE:CZ | 2.79 | 0.49 |
| 1:B:195:GLN:HE21 | 1:B:195:GLN:HA | 1.78 | 0.49 |
| 1:B:231:THR:C | 1:B:237:ILE:HG22 | 2.34 | 0.49 |
| 1:B:387:LEU:CG | 1:B:391:PHE:CZ | 2.95 | 0.49 |
| 1:B:387:LEU:HD21 | 1:B:391:PHE:CZ | 2.48 | 0.49 |
| 1:B:62:LYS:HD3 | 1:B:63:ARG:H | 1.75 | 0.49 |
| 1:B:89:HIS:HE1 | 1:B:257:LEU:HG | 1.75 | 0.49 |
| 2:C:33:LYS:HB2 | 2:C:35:GLU:CD | 2.33 | 0.49 |
| 2:C:75:MET:H | 2:C:78:VAL:CB | 2.26 | 0.49 |
| 3:E:9:ILE:CD1 | 3:E:11:PHE:CZ | 2.95 | 0.49 |
| 3:E:38:VAL:CG2 | 3:E:76:TYR:CZ | 2.95 | 0.49 |
| 3:E:48:LYS:CD | 3:F:48:LYS:HG3 | 2.39 | 0.49 |
| 4:G:81:ASP:O | 4:G:85:ARG:HG2 | 2.13 | 0.49 |
| 5:H:32:GLN:HE22 | 5:H:93:ARG:HG2 | 1.78 | 0.49 |
| 5:H:97:VAL:O | 5:H:98:LYS:HG3 | 2.13 | 0.49 |
| 1:A:136:ASN:CB | 1:A:145:TRP:CH2 | 2.95 | 0.49 |
| 1:A:149:VAL:HG22 | 1:A:150:ASP:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:VAL:HG11 | 1:A:160:PHE:HE1 | 1.78 | 0.49 |
| 1:A:341:TYR:O | 1:A:344:ALA:HB3 | 2.12 | 0.49 |
| 1:A:68:ASP:OD2 | 1:B:300:THR:HG21 | 2.13 | 0.49 |
| 1:B:149:VAL:HG22 | 1:B:150:ASP:O | 2.13 | 0.49 |
| 1:B:145:TRP:O | 1:B:244:ILE:HB | 2.12 | 0.49 |
| 1:B:51:ARG:HD2 | 1:B:57:ASN:HD21 | 1.78 | 0.49 |
| 1:B:52:TYR:CE1 | 1:B:56:GLU:HB3 | 2.48 | 0.49 |
| 1:B:88:TRP:NE1 | 1:B:92:PHE:CZ | 2.79 | 0.49 |
| 1:B:291:TYR:CD2 | 2:C:51:SER:OG | 2.65 | 0.49 |
| 2:D:33:LYS:HB2 | 2:D:35:GLU:CD | 2.33 | 0.49 |
| 3:E:13:SER:O | 3:E:28:TRP:HB3 | 2.12 | 0.49 |
| 3:E:74:VAL:CG2 | 3:E:76:TYR:CE1 | 2.96 | 0.49 |
| 4:G:44:VAL:HA | 4:G:71:TRP:H | 1.78 | 0.49 |
| 5:H:121:GLY:CA | 5:H:126:VAL:HA | 2.39 | 0.49 |
| 5:H:53:ILE:CA | 5:H:54:LEU:N | 2.69 | 0.49 |
| 5:H:55:GLY:HA2 | 5:H:57:GLY:N | 2.24 | 0.49 |
| 1:A:146:HIS:HA | 1:A:244:ILE:HG22 | 1.94 | 0.48 |
| 1:A:62:LYS:CD | 1:A:63:ARG:HG3 | 2.43 | 0.48 |
| 1:A:91:LEU:N | 1:A:91:LEU:HD12 | 2.28 | 0.48 |
| 1:B:140:LYS:HG2 | 1:B:141:GLY:H | 1.77 | 0.48 |
| 1:B:158:VAL:HG11 | 1:B:160:PHE:HE1 | 1.78 | 0.48 |
| 1:B:387:LEU:CD1 | 1:B:391:PHE:CE1 | 2.95 | 0.48 |
| 1:B:38:ILE:CD1 | 1:B:183:TYR:HD2 | 2.26 | 0.48 |
| 1:B:467:TYR:HA | 1:B:467:TYR:HD1 | 1.42 | 0.48 |
| 2:D:37:HIS:O | 2:D:39:PRO:HD3 | 2.12 | 0.48 |
| 3:E:44:GLU:O | 3:E:45:GLU:HB3 | 2.12 | 0.48 |
| 3:F:70:LYS:HG2 | 3:F:71:LYS:H | 1.78 | 0.48 |
| 5:H:91:PHE:CE2 | 5:H:132:LEU:CD2 | 2.95 | 0.48 |
| 5:H:17:SER:HB2 | 5:H:90:LYS:O | 2.13 | 0.48 |
| 1:A:48:LYS:HE3 | 1:A:258:LYS:NZ | 2.27 | 0.48 |
| 1:A:52:TYR:CE1 | 1:A:56:GLU:HB3 | 2.48 | 0.48 |
| 1:B:187:LYS:HD3 | 1:B:193:GLU:CB | 2.41 | 0.48 |
| 1:B:334:GLU:HA | 1:B:337:GLN:HG2 | 1.95 | 0.48 |
| 3:E:40:PRO:HB3 | 3:F:100:LYS:CB | 2.43 | 0.48 |
| 3:E:52:LEU:HD12 | 3:E:53:GLN:NE2 | 2.28 | 0.48 |
| 5:H:148:GLU:HA | 5:H:148:GLU:OE1 | 2.13 | 0.48 |
| 1:A:158:VAL:CG1 | 1:A:160:PHE:CE1 | 2.96 | 0.48 |
| 1:A:231:THR:C | 1:A:237:ILE:HG22 | 2.34 | 0.48 |
| 1:A:51:ARG:HD2 | 1:A:57:ASN:HD21 | 1.78 | 0.48 |
| 1:A:64:ARG:NH2 | 1:B:284:ILE:CG1 | 2.76 | 0.48 |
| 1:A:81:ASN:ND2 | 1:A:83:ARG:HD2 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:170:LYS:HE2 | 1:B:170:LYS:O | 2.13 | 0.48 |
| 1:A:66:TYR:OH | 1:B:304:ARG:CD | 2.61 | 0.48 |
| 1:B:326:VAL:O | 1:B:329:ALA:HB3 | 2.14 | 0.48 |
| 1:B:341:TYR:O | 1:B:344:ALA:HB3 | 2.12 | 0.48 |
| 1:B:347:VAL:HB | 1:B:349:ASN:OD1 | 2.13 | 0.48 |
| 2:D:4:GLN:OE1 | 3:F:1:MET:SD | 2.70 | 0.48 |
| 3:E:70:LYS:HD3 | 3:E:84:ILE:CA | 2.43 | 0.48 |
| 3:F:74:VAL:CG1 | 3:F:83:PHE:CE2 | 2.96 | 0.48 |
| 5:H:58:SER:HB2 | 5:H:143:ILE:HG13 | 1.95 | 0.48 |
| 1:A:130:LEU:HD13 | 1:A:388:PHE:CZ | 2.47 | 0.48 |
| 1:A:170:LYS:HE2 | 1:A:170:LYS:O | 2.14 | 0.48 |
| 1:A:200:TYR:CE1 | 1:A:205:VAL:CG1 | 2.95 | 0.48 |
| 1:A:267:TYR:CD2 | 1:A:345:GLN:CG | 2.96 | 0.48 |
| 1:A:38:ILE:CD1 | 1:A:183:TYR:HD2 | 2.26 | 0.48 |
| 1:B:430:VAL:O | 1:B:433:VAL:HG12 | 2.13 | 0.48 |
| 2:C:48:SER:HG | 2:D:31:PHE:HE2 | 1.60 | 0.48 |
| 2:D:4:GLN:OE1 | 3:F:2:TYR:HB2 | 2.13 | 0.48 |
| 2:D:5:ARG:CZ | 3:F:2:TYR:HD2 | 2.25 | 0.48 |
| 3:F:70:LYS:HG2 | 3:F:71:LYS:N | 2.28 | 0.48 |
| 3:F:7:ASP:HB3 | 3:F:8:VAL:C | 2.33 | 0.48 |
| 4:G:27:MET:HB2 | 4:G:28:VAL:O | 2.13 | 0.48 |
| 4:G:3:TRP:O | 4:G:6:ALA:HB3 | 2.13 | 0.48 |
| 5:H:94:VAL:CG2 | 5:H:104:TYR:CE2 | 2.96 | 0.48 |
| 1:A:111:ASN:ND2 | 1:A:399:THR:HG21 | 2.28 | 0.48 |
| 1:A:296:PRO:HA | 1:A:299:PHE:CB | 2.44 | 0.48 |
| 1:A:318:ASP:OD1 | 2:D:102:ARG:HD3 | 2.12 | 0.48 |
| 1:A:326:VAL:O | 1:A:329:ALA:HB3 | 2.14 | 0.48 |
| 1:A:334:GLU:HA | 1:A:337:GLN:HG2 | 1.95 | 0.48 |
| 1:A:110:ASP:CB | 1:A:396:LEU:HD13 | 2.22 | 0.48 |
| 1:B:158:VAL:CG1 | 1:B:160:PHE:CE1 | 2.96 | 0.48 |
| 1:B:179:PHE:CG | 1:B:180:ALA:N | 2.82 | 0.48 |
| 1:B:370:LEU:H | 1:B:370:LEU:HD22 | 1.79 | 0.48 |
| 1:B:91:LEU:N | 1:B:91:LEU:HD12 | 2.28 | 0.48 |
| 2:C:63:PHE:CD2 | 2:C:86:ILE:HG23 | 2.48 | 0.48 |
| 2:C:5:ARG:HG3 | 2:C:8:ARG:CB | 2.43 | 0.48 |
| 2:C:94:LEU:HD12 | 2:D:96:PRO:C | 2.33 | 0.48 |
| 3:F:11:PHE:CE2 | 3:F:68:ILE:CG2 | 2.96 | 0.48 |
| 3:F:22:GLY:H | 4:G:19:GLU:CG | 2.18 | 0.48 |
| 3:F:43:GLN:CB | 3:F:47:TYR:HE1 | 2.20 | 0.48 |
| 3:F:103:GLU:CA | 4:G:31:VAL:HG21 | 2.43 | 0.48 |
| 5:H:91:PHE:CE1 | 5:H:111:ALA:CB | 2.97 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:VAL:HG13 | 1:A:177:ILE:CB | 2.42 | 0.48 |
| 1:A:335:ARG:CG | 1:B:333:LEU:CB | 2.89 | 0.48 |
| 1:A:43:PRO:CB | 1:A:47:LEU:HD11 | 2.43 | 0.48 |
| 1:B:198:GLU:CB | 1:B:200:TYR:HE1 | 2.27 | 0.48 |
| 1:B:111:ASN:ND2 | 1:B:399:THR:HG21 | 2.28 | 0.48 |
| 1:B:99:TYR:CE2 | 1:B:370:LEU:HB3 | 2.48 | 0.48 |
| 2:C:78:VAL:HG22 | 2:C:79:SER:H | 1.79 | 0.48 |
| 2:D:63:PHE:CD1 | 2:D:85:GLU:CB | 2.97 | 0.48 |
| 5:H:52:ARG:NH2 | 5:H:54:LEU:HG | 1.28 | 0.48 |
| 1:A:179:PHE:CG | 1:A:180:ALA:N | 2.82 | 0.48 |
| 1:A:96:LYS:HE3 | 1:A:377:ALA:HB2 | 1.96 | 0.48 |
| 1:B:83:ARG:HD3 | 1:B:83:ARG:H | 1.78 | 0.48 |
| 2:C:82:PHE:HD1 | 2:C:82:PHE:HA | 1.49 | 0.48 |
| 2:C:89:THR:CB | 2:D:88:SER:CB | 2.86 | 0.48 |
| 2:D:13:THR:HB | 3:E:1:MET:N | 2.27 | 0.48 |
| 1:A:426:VAL:HA | 1:A:429:LEU:CG | 2.43 | 0.48 |
| 1:A:83:ARG:H | 1:A:83:ARG:HD3 | 1.78 | 0.48 |
| 1:B:267:TYR:CD2 | 1:B:345:GLN:CG | 2.96 | 0.48 |
| 2:D:5:ARG:HG3 | 2:D:8:ARG:HB2 | 1.95 | 0.48 |
| 2:D:78:VAL:HG22 | 2:D:79:SER:H | 1.79 | 0.48 |
| 3:E:36:ALA:HA | 3:E:62:THR:HG23 | 1.94 | 0.48 |
| 3:E:40:PRO:HA | 3:F:100:LYS:HE2 | 1.95 | 0.48 |
| 3:E:43:GLN:CG | 3:E:53:GLN:H | 2.10 | 0.48 |
| 3:F:104:ASP:HB2 | 4:G:31:VAL:CB | 2.40 | 0.48 |
| 3:F:43:GLN:N | 3:F:53:GLN:HB2 | 2.19 | 0.48 |
| 4:G:102:PHE:CD1 | 5:H:56:PRO:CD | 2.91 | 0.48 |
| 4:G:63:ASN:HB3 | 4:G:130:THR:OG1 | 2.14 | 0.48 |
| 3:E:108:VAL:CG1 | 4:G:43:TYR:HH | 2.11 | 0.48 |
| 4:G:97:PHE:HB3 | 4:G:100:PHE:HB2 | 1.96 | 0.48 |
| 1:A:198:GLU:CB | 1:A:200:TYR:HE1 | 2.27 | 0.48 |
| 1:A:66:TYR:CE2 | 1:B:304:ARG:HG2 | 2.49 | 0.48 |
| 1:B:158:VAL:CG1 | 1:B:160:PHE:HE1 | 2.27 | 0.48 |
| 1:B:200:TYR:CE1 | 1:B:205:VAL:CG1 | 2.95 | 0.48 |
| 2:C:63:PHE:CD1 | 2:C:85:GLU:CB | 2.97 | 0.48 |
| 2:C:70:LEU:C | 3:E:91:SER:HB2 | 2.34 | 0.48 |
| 2:D:95:ASN:HB3 | 2:D:98:ARG:N | 2.28 | 0.48 |
| 3:F:32:PHE:CE1 | 3:F:67:ARG:CB | 2.95 | 0.48 |
| 3:F:60:ILE:CD1 | 3:F:83:PHE:CE2 | 2.97 | 0.48 |
| 4:G:10:LEU:HG | 4:G:11:GLN:N | 2.29 | 0.48 |
| 4:G:34:SER:HB3 | 4:G:35:PRO:CD | 2.43 | 0.48 |
| 4:G:70:VAL:HG11 | 4:G:76:ARG:HH12 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 5:H:100:GLU:HB3 | 5:H:103:LYS:H | 1.79 | 0.48 |
| 1:A:158:VAL:CG1 | 1:A:160:PHE:HE1 | 2.27 | 0.48 |
| 1:A:370:LEU:HD22 | 1:A:370:LEU:H | 1.79 | 0.48 |
| 1:B:379:ARG:HB2 | 1:B:380:LYS:NZ | 2.29 | 0.48 |
| 2:C:35:GLU:HA | 2:C:35:GLU:OE1 | 2.13 | 0.48 |
| 2:C:98:ARG:HD3 | 2:D:97:TYR:CE1 | 2.47 | 0.48 |
| 3:E:65:ASP:OD1 | 3:E:68:ILE:HB | 2.14 | 0.48 |
| 3:F:105:GLY:N | 4:G:39:ASP:CG | 2.33 | 0.48 |
| 5:H:16:GLN:NE2 | 5:H:26:PRO:HA | 2.28 | 0.48 |
| 4:G:100:PHE:HD1 | 5:H:45:ASP:H | 1.59 | 0.48 |
| 1:A:379:ARG:HB2 | 1:A:380:LYS:NZ | 2.29 | 0.47 |
| 1:B:144:TYR:CD1 | 1:B:144:TYR:N | 2.82 | 0.47 |
| 1:B:426:VAL:HA | 1:B:429:LEU:CG | 2.43 | 0.47 |
| 1:B:466:GLN:HA | 1:B:467:TYR:HD1 | 1.74 | 0.47 |
| 1:B:52:TYR:CE1 | 1:B:56:GLU:CB | 2.97 | 0.47 |
| 2:C:63:PHE:CE1 | 2:C:85:GLU:CB | 2.95 | 0.47 |
| 3:E:108:VAL:HB | 4:G:43:TYR:CZ | 2.48 | 0.47 |
| 4:G:100:PHE:CZ | 5:H:46:GLU:CA | 2.49 | 0.47 |
| 1:A:145:TRP:O | 1:A:244:ILE:HB | 2.12 | 0.47 |
| 1:A:155:PHE:CD1 | 1:A:156:ASP:N | 2.82 | 0.47 |
| 1:A:187:LYS:HD3 | 1:A:193:GLU:CB | 2.41 | 0.47 |
| 1:B:291:TYR:HD2 | 2:C:51:SER:OG | 1.97 | 0.47 |
| 1:B:59:ILE:HG13 | 1:B:81:ASN:CG | 2.35 | 0.47 |
| 3:E:38:VAL:HA | 3:E:60:ILE:CB | 2.43 | 0.47 |
| 3:E:62:THR:HG22 | 3:E:63:PRO:CD | 2.43 | 0.47 |
| 3:F:69:ASP:OD2 | 3:F:87:PRO:HB3 | 2.13 | 0.47 |
| 5:H:14:LEU:HG | 5:H:160:PHE:CZ | 2.49 | 0.47 |
| 1:A:144:TYR:CD1 | 1:A:144:TYR:N | 2.82 | 0.47 |
| 1:A:290:ASN:HB2 | 1:A:291:TYR:HA | 1.96 | 0.47 |
| 1:A:59:ILE:HG13 | 1:A:81:ASN:CG | 2.35 | 0.47 |
| 1:B:227:ARG:HE | 1:B:227:ARG:N | 2.12 | 0.47 |
| 1:B:442:THR:HA | 1:B:445:ALA:HB3 | 1.96 | 0.47 |
| 1:B:96:LYS:HE3 | 1:B:377:ALA:HB2 | 1.96 | 0.47 |
| 2:D:56:PHE:HA | 2:D:59:LYS:HZ2 | 1.78 | 0.47 |
| 3:E:85:GLY:CA | 3:E:99:ILE:HG23 | 2.41 | 0.47 |
| 4:G:131:ILE:HG22 | 5:H:53:ILE:HD12 | 1.95 | 0.47 |
| 4:G:18:LEU:C | 4:G:24:LEU:HD22 | 2.35 | 0.47 |
| 5:H:58:SER:HB3 | 5:H:143:ILE:N | 2.29 | 0.47 |
| 5:H:30:ALA:CB | 5:H:67:TYR:CD2 | 2.97 | 0.47 |
| 1:B:43:PRO:CA | 1:B:164:GLU:H | 2.17 | 0.47 |
| 1:B:298:GLU:CD | 2:C:43:LYS:HZ1 | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:D:5:ARG:HG3 | 2:D:8:ARG:CB | 2.43 | 0.47 |
| 3:E:60:ILE:HG23 | 3:E:99:ILE:HD12 | 1.97 | 0.47 |
| 2:D:4:GLN:OE1 | 3:F:1:MET:HG2 | 2.13 | 0.47 |
| 3:E:77:ARG:HD2 | 3:F:87:PRO:CB | 2.44 | 0.47 |
| 1:A:179:PHE:CD1 | 1:A:244:ILE:N | 2.83 | 0.47 |
| 1:A:186:TYR:CD1 | 1:A:187:LYS:N | 2.83 | 0.47 |
| 1:A:347:VAL:HB | 1:A:349:ASN:OD1 | 2.13 | 0.47 |
| 1:A:88:TRP:CE2 | 1:A:92:PHE:CE1 | 3.03 | 0.47 |
| 1:B:171:ASP:HB3 | 1:B:178:LEU:HD11 | 1.90 | 0.47 |
| 1:B:186:TYR:CD1 | 1:B:187:LYS:N | 2.83 | 0.47 |
| 1:B:53:TYR:HA | 1:B:261:LYS:HZ2 | 1.79 | 0.47 |
| 1:A:64:ARG:NE | 1:B:283:GLN:NE2 | 2.60 | 0.47 |
| 1:B:96:LYS:HG2 | 1:B:373:LYS:HB2 | 1.89 | 0.47 |
| 1:B:291:TYR:HD2 | 2:C:51:SER:HG | 1.61 | 0.47 |
| 2:C:98:ARG:HH11 | 2:D:102:ARG:N | 2.06 | 0.47 |
| 2:D:38:ASN:O | 2:D:40:PHE:HD2 | 1.97 | 0.47 |
| 3:E:21:GLU:CG | 3:E:22:GLY:H | 2.21 | 0.47 |
| 3:F:74:VAL:HG11 | 3:F:83:PHE:CE2 | 2.50 | 0.47 |
| 3:E:107:TYR:N | 4:G:117:ASP:N | 2.62 | 0.47 |
| 5:H:112:TYR:H | 5:H:132:LEU:CB | 2.14 | 0.47 |
| 5:H:150:ILE:O | 5:H:154:SER:HB3 | 2.14 | 0.47 |
| 5:H:94:VAL:CG2 | 5:H:160:PHE:CZ | 2.95 | 0.47 |
| 1:A:107:PHE:CD1 | 1:A:108:THR:N | 2.83 | 0.47 |
| 1:A:438:MET:SD | 1:B:434:THR:OG1 | 2.68 | 0.47 |
| 1:A:52:TYR:CE1 | 1:A:56:GLU:CB | 2.97 | 0.47 |
| 1:A:99:TYR:CD2 | 1:A:370:LEU:CD1 | 2.95 | 0.47 |
| 1:A:99:TYR:HD2 | 1:A:373:LYS:CE | 2.28 | 0.47 |
| 1:B:46:LEU:CG | 1:B:143:GLU:HB2 | 2.45 | 0.47 |
| 1:B:255:SER:CB | 1:B:259:PHE:CE2 | 2.95 | 0.47 |
| 1:B:296:PRO:HA | 1:B:299:PHE:CB | 2.44 | 0.47 |
| 1:B:361:PRO:O | 1:B:364:GLU:HG2 | 2.15 | 0.47 |
| 1:B:368:ALA:HA | 1:B:369:LEU:HA | 1.63 | 0.47 |
| 1:B:375:ASN:O | 1:B:379:ARG:HG3 | 2.15 | 0.47 |
| 2:D:93:LYS:C | 2:D:95:ASN:H | 2.16 | 0.47 |
| 3:E:2:TYR:CE1 | 3:F:95:GLU:N | 2.83 | 0.47 |
| 3:F:41:ILE:HG21 | 3:F:53:GLN:HG2 | 1.97 | 0.47 |
| 3:F:70:LYS:HD3 | 3:F:70:LYS:C | 2.35 | 0.47 |
| 4:G:105:LYS:NZ | 4:G:105:LYS:HB2 | 2.30 | 0.47 |
| 3:E:108:VAL:CG2 | 4:G:43:TYR:OH | 2.63 | 0.47 |
| 4:G:44:VAL:HG13 | 4:G:70:VAL:CB | 2.44 | 0.47 |
| 5:H:111:ALA:HA | 5:H:132:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:H:16:GLN:CB | 5:H:26:PRO:HA | 2.44 | 0.47 |
| 5:H:22:THR:HB | 5:H:108:PHE:CG | 2.47 | 0.47 |
| 5:H:39:GLY:HA2 | 5:H:43:LEU:HG | 1.96 | 0.47 |
| 1:A:148:PHE:CD1 | 1:A:148:PHE:N | 2.83 | 0.47 |
| 1:A:199:LEU:CB | 1:A:208:TYR:CE2 | 2.98 | 0.47 |
| 1:A:32:THR:HG22 | 1:A:36:LYS:HE2 | 1.91 | 0.47 |
| 1:A:46:LEU:CG | 1:A:143:GLU:HB2 | 2.45 | 0.47 |
| 1:B:148:PHE:CD1 | 1:B:148:PHE:N | 2.83 | 0.47 |
| 1:B:198:GLU:HB2 | 1:B:200:TYR:CE1 | 2.49 | 0.47 |
| 1:B:52:TYR:CE1 | 1:B:265:ASP:HB3 | 2.50 | 0.47 |
| 1:B:290:ASN:HB2 | 1:B:291:TYR:HA | 1.96 | 0.47 |
| 1:A:460:ILE:CB | 1:B:466:GLN:HG3 | 2.42 | 0.47 |
| 1:B:53:TYR:HB2 | 1:B:140:LYS:CE | 2.45 | 0.47 |
| 1:B:62:LYS:CD | 1:B:63:ARG:HG3 | 2.43 | 0.47 |
| 1:B:66:TYR:N | 1:B:66:TYR:CD1 | 2.83 | 0.47 |
| 2:C:31:PHE:CD2 | 2:C:32:ALA:N | 2.83 | 0.47 |
| 2:C:98:ARG:CA | 2:D:97:TYR:CD2 | 2.97 | 0.47 |
| 4:G:32:THR:OG1 | 4:G:43:TYR:HB2 | 2.14 | 0.47 |
| 5:H:68:TYR:CD1 | 5:H:69:GLY:N | 2.83 | 0.47 |
| 5:H:17:SER:OG | 5:H:89:ILE:HG22 | 2.14 | 0.47 |
| 1:A:139:ASN:HA | 1:A:257:LEU:HB2 | 1.96 | 0.47 |
| 1:A:251:GLU:HG2 | 1:B:54:MET:H | 1.78 | 0.47 |
| 1:A:382:ARG:HE | 1:A:386:ARG:NH1 | 2.13 | 0.47 |
| 1:A:64:ARG:HD3 | 1:A:79:LYS:HZ3 | 1.78 | 0.47 |
| 1:B:155:PHE:CD1 | 1:B:156:ASP:N | 2.83 | 0.47 |
| 1:B:382:ARG:HE | 1:B:386:ARG:NH1 | 2.13 | 0.47 |
| 2:C:56:PHE:CD1 | 2:C:59:LYS:CE | 2.95 | 0.47 |
| 2:D:102:ARG:CZ | 2:D:102:ARG:HB2 | 2.45 | 0.47 |
| 2:D:56:PHE:CD1 | 2:D:59:LYS:CE | 2.95 | 0.47 |
| 4:G:43:TYR:CD1 | 4:G:71:TRP:HB2 | 2.49 | 0.47 |
| 5:H:143:ILE:N | 5:H:143:ILE:HD12 | 2.23 | 0.47 |
| 1:A:52:TYR:CE1 | 1:A:265:ASP:HB3 | 2.50 | 0.47 |
| 1:B:107:PHE:CD1 | 1:B:108:THR:N | 2.83 | 0.47 |
| 1:B:441:GLU:CD | 1:B:456:GLU:HB2 | 2.35 | 0.47 |
| 1:B:88:TRP:CE2 | 1:B:92:PHE:CE1 | 3.03 | 0.47 |
| 2:C:55:ILE:HD12 | 2:C:93:LYS:HZ2 | 1.79 | 0.47 |
| 2:C:8:ARG:HD2 | 2:C:8:ARG:C | 2.35 | 0.47 |
| 3:E:109:GLY:CA | 4:G:114:THR:OG1 | 2.62 | 0.47 |
| 3:E:74:VAL:HG21 | 3:E:76:TYR:CE1 | 2.49 | 0.47 |
| 3:F:32:PHE:N | 3:F:32:PHE:HD1 | 2.13 | 0.47 |
| 3:F:57:GLY:HA3 | 3:F:84:ILE:HG12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:97:PHE:CD1 | 4:G:98:GLU:N | 2.83 | 0.47 |
| 5:H:21:ALA:HB1 | 5:H:108:PHE:HD2 | 1.79 | 0.47 |
| 5:H:21:ALA:HB1 | 5:H:150:ILE:HA | 1.97 | 0.47 |
| 5:H:31:TYR:N | 5:H:31:TYR:CD1 | 2.83 | 0.47 |
| 1:A:206:TYR:HB3 | 1:A:208:TYR:CE1 | 2.50 | 0.47 |
| 1:A:375:ASN:O | 1:A:379:ARG:HG3 | 2.15 | 0.47 |
| 1:B:111:ASN:H | 1:B:396:LEU:CD2 | 2.26 | 0.47 |
| 1:B:121:LEU:HD12 | 1:B:124:ASP:N | 2.23 | 0.47 |
| 1:B:155:PHE:CD1 | 1:B:229:HIS:CE1 | 3.03 | 0.47 |
| 1:B:164:GLU:OE1 | 1:B:164:GLU:HA | 2.15 | 0.47 |
| 1:B:199:LEU:CB | 1:B:208:TYR:CE2 | 2.98 | 0.47 |
| 2:C:38:ASN:O | 2:C:40:PHE:HD2 | 1.97 | 0.47 |
| 2:D:73:ARG:HG3 | 2:D:74:SER:O | 2.15 | 0.47 |
| 3:E:2:TYR:O | 3:E:3:GLU:HB3 | 2.15 | 0.47 |
| 3:E:79:LYS:CB | 3:F:87:PRO:HD3 | 2.44 | 0.47 |
| 3:E:79:LYS:HE2 | 3:F:87:PRO:CD | 2.45 | 0.47 |
| 3:F:96:ILE:O | 3:F:96:ILE:HG13 | 2.15 | 0.47 |
| 4:G:133:ASN:CB | 5:H:56:PRO:CD | 2.92 | 0.47 |
| 4:G:4:LYS:HG2 | 4:G:5:LEU:N | 2.29 | 0.47 |
| 1:A:121:LEU:CB | 1:A:124:ASP:H | 2.28 | 0.47 |
| 1:A:287:VAL:HG12 | 1:A:319:THR:HG21 | 1.97 | 0.47 |
| 1:B:121:LEU:CB | 1:B:124:ASP:H | 2.28 | 0.47 |
| 1:B:184:TYR:CD1 | 1:B:184:TYR:N | 2.82 | 0.47 |
| 1:B:206:TYR:CD1 | 1:B:206:TYR:N | 2.83 | 0.47 |
| 1:B:291:TYR:CD1 | 1:B:292:ASP:N | 2.83 | 0.47 |
| 1:B:395:TYR:O | 1:B:398:ASN:HB2 | 2.15 | 0.47 |
| 2:C:34:ASP:CB | 2:C:35:GLU:CA | 2.93 | 0.47 |
| 1:B:298:GLU:CG | 2:C:42:ASP:OD2 | 2.61 | 0.47 |
| 2:D:31:PHE:CD2 | 2:D:32:ALA:N | 2.83 | 0.47 |
| 2:C:84:THR:HG21 | 2:D:83:ALA:HA | 1.96 | 0.47 |
| 3:E:2:TYR:HE1 | 3:F:94:GLN:C | 2.18 | 0.47 |
| 3:E:30:ASP:OD2 | 3:E:32:PHE:HE2 | 1.98 | 0.47 |
| 3:E:45:GLU:CA | 3:E:47:TYR:CE1 | 2.94 | 0.47 |
| 3:E:62:THR:HG22 | 3:E:63:PRO:O | 2.15 | 0.47 |
| 3:E:15:VAL:CG1 | 3:E:73:ARG:HE | 2.08 | 0.47 |
| 3:E:66:ASP:OD1 | 3:E:97:THR:HG21 | 2.14 | 0.47 |
| 3:F:26:TYR:N | 3:F:26:TYR:CD1 | 2.83 | 0.47 |
| 3:E:79:LYS:HE2 | 3:F:87:PRO:HD3 | 1.96 | 0.47 |
| 3:F:96:ILE:HD11 | 3:F:98:ARG:NH2 | 2.29 | 0.47 |
| 4:G:54:PHE:CD1 | 4:G:54:PHE:N | 2.83 | 0.47 |
| 5:H:90:LYS:CE | 5:H:146:LEU:HB3 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:HIS:CD2 | 1:A:164:GLU:HB3 | 2.47 | 0.46 |
| 1:A:395:TYR:O | 1:A:398:ASN:HB2 | 2.15 | 0.46 |
| 1:A:440:LYS:CD | 1:A:444:VAL:HG23 | 2.46 | 0.46 |
| 1:A:441:GLU:CD | 1:A:456:GLU:HB2 | 2.35 | 0.46 |
| 1:A:88:TRP:CE2 | 1:A:92:PHE:CZ | 3.04 | 0.46 |
| 1:B:206:TYR:HB3 | 1:B:208:TYR:CE1 | 2.50 | 0.46 |
| 1:B:96:LYS:HG2 | 1:B:373:LYS:HD3 | 1.95 | 0.46 |
| 1:B:99:TYR:CD2 | 1:B:370:LEU:CB | 2.97 | 0.46 |
| 2:C:93:LYS:C | 2:C:95:ASN:H | 2.16 | 0.46 |
| 2:D:82:PHE:HD1 | 2:D:82:PHE:HA | 1.49 | 0.46 |
| 3:E:70:LYS:HD3 | 3:E:84:ILE:CB | 2.45 | 0.46 |
| 4:G:76:ARG:HG3 | 4:G:76:ARG:HH11 | 1.80 | 0.46 |
| 5:H:135:ILE:O | 5:H:135:ILE:HG23 | 2.14 | 0.46 |
| 1:A:184:TYR:N | 1:A:184:TYR:CD1 | 2.83 | 0.46 |
| 1:A:291:TYR:CD1 | 1:A:292:ASP:N | 2.83 | 0.46 |
| 1:A:308:VAL:HG21 | 1:A:310:LYS:HE2 | 1.97 | 0.46 |
| 1:B:232:LYS:CA | 1:B:237:ILE:HB | 2.46 | 0.46 |
| 1:B:287:VAL:HG12 | 1:B:319:THR:HG21 | 1.97 | 0.46 |
| 1:B:401:LYS:HG2 | 1:B:402:GLY:N | 2.31 | 0.46 |
| 1:A:418:ARG:NH2 | 1:B:426:VAL:HG11 | 2.30 | 0.46 |
| 1:B:58:ASP:HB3 | 1:B:81:ASN:OD1 | 2.15 | 0.46 |
| 2:D:99:LYS:O | 2:D:99:LYS:HG2 | 2.16 | 0.46 |
| 3:E:64:TYR:O | 3:E:68:ILE:HG13 | 2.16 | 0.46 |
| 3:E:40:PRO:HB3 | 3:F:100:LYS:CA | 2.45 | 0.46 |
| 4:G:37:LYS:CD | 4:G:37:LYS:H | 2.28 | 0.46 |
| 1:A:292:ASP:HB3 | 1:A:293:GLY:O | 2.16 | 0.46 |
| 1:B:305:TYR:CD1 | 1:B:305:TYR:N | 2.83 | 0.46 |
| 1:B:369:LEU:HD12 | 1:B:369:LEU:H | 1.80 | 0.46 |
| 1:B:99:TYR:CD2 | 1:B:370:LEU:CD1 | 2.95 | 0.46 |
| 3:E:74:VAL:HG13 | 3:E:74:VAL:O | 2.15 | 0.46 |
| 3:F:21:GLU:OE1 | 4:G:16:GLU:HG2 | 2.15 | 0.46 |
| 3:F:5:PHE:HD1 | 3:F:5:PHE:HA | 1.53 | 0.46 |
| 3:F:67:ARG:O | 3:F:72:MET:HB2 | 2.15 | 0.46 |
| 3:F:60:ILE:CD1 | 3:F:83:PHE:CD2 | 2.95 | 0.46 |
| 4:G:65:THR:HA | 4:G:128:ARG:HA | 1.97 | 0.46 |
| 4:G:27:MET:HB3 | 4:G:29:ASN:O | 2.16 | 0.46 |
| 4:G:68:PHE:N | 4:G:68:PHE:CD1 | 2.83 | 0.46 |
| 5:H:13:TYR:CE1 | 5:H:31:TYR:CB | 2.95 | 0.46 |
| 5:H:15:PHE:HE1 | 5:H:91:PHE:CD1 | 2.33 | 0.46 |
| 1:A:164:GLU:HA | 1:A:164:GLU:OE1 | 2.15 | 0.46 |
| 1:A:361:PRO:O | 1:A:364:GLU:HG2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:51:ARG:HD2 | 1:A:57:ASN:ND2 | 2.30 | 0.46 |
| 1:A:99:TYR:HB3 | 1:A:373:LYS:HZ1 | 1.81 | 0.46 |
| 1:B:206:TYR:C | 1:B:207:TYR:HD1 | 2.19 | 0.46 |
| 1:B:179:PHE:CD1 | 1:B:244:ILE:N | 2.83 | 0.46 |
| 1:B:292:ASP:HB3 | 1:B:293:GLY:O | 2.16 | 0.46 |
| 1:B:308:VAL:HG21 | 1:B:310:LYS:HE2 | 1.97 | 0.46 |
| 1:B:130:LEU:CD2 | 1:B:388:PHE:CE2 | 2.95 | 0.46 |
| 1:B:92:PHE:N | 1:B:92:PHE:CD1 | 2.82 | 0.46 |
| 2:C:102:ARG:HB2 | 2:C:102:ARG:CZ | 2.45 | 0.46 |
| 2:C:11:SER:OG | 3:E:94:GLN:HB3 | 2.15 | 0.46 |
| 3:E:5:PHE:CD1 | 3:E:6:ARG:N | 2.83 | 0.46 |
| 5:H:13:TYR:CD1 | 5:H:13:TYR:N | 2.82 | 0.46 |
| 5:H:14:LEU:CD2 | 5:H:160:PHE:CE2 | 2.99 | 0.46 |
| 1:A:155:PHE:CE1 | 1:A:229:HIS:CE1 | 3.03 | 0.46 |
| 1:A:232:LYS:CA | 1:A:237:ILE:HB | 2.46 | 0.46 |
| 1:A:66:TYR:N | 1:A:66:TYR:CD1 | 2.83 | 0.46 |
| 1:A:55:CYS:HG | 1:A:83:ARG:HB2 | 1.81 | 0.46 |
| 1:B:205:VAL:HG12 | 1:B:206:TYR:N | 2.30 | 0.46 |
| 1:B:56:GLU:HB3 | 1:B:265:ASP:HB3 | 1.97 | 0.46 |
| 1:B:43:PRO:CB | 1:B:47:LEU:HD11 | 2.43 | 0.46 |
| 1:B:99:TYR:HD2 | 1:B:373:LYS:CE | 2.28 | 0.46 |
| 2:C:73:ARG:HG3 | 2:C:74:SER:O | 2.15 | 0.46 |
| 3:E:39:GLN:HG3 | 3:F:90:LEU:HD13 | 1.97 | 0.46 |
| 2:C:5:ARG:CA | 3:E:3:GLU:H | 2.26 | 0.46 |
| 3:E:58:TYR:O | 3:E:83:PHE:HB3 | 2.15 | 0.46 |
| 3:F:68:ILE:HD13 | 3:F:69:ASP:N | 2.31 | 0.46 |
| 4:G:31:VAL:HA | 4:G:32:THR:C | 2.35 | 0.46 |
| 5:H:143:ILE:HG12 | 5:H:147:PRO:HD2 | 1.95 | 0.46 |
| 1:A:158:VAL:HG12 | 1:A:160:PHE:CE1 | 2.51 | 0.46 |
| 1:A:43:PRO:CA | 1:A:164:GLU:H | 2.17 | 0.46 |
| 1:A:227:ARG:N | 1:A:227:ARG:HE | 2.12 | 0.46 |
| 1:A:401:LYS:HG2 | 1:A:402:GLY:N | 2.31 | 0.46 |
| 1:A:442:THR:HA | 1:A:445:ALA:HB3 | 1.96 | 0.46 |
| 1:A:466:GLN:HA | 1:A:467:TYR:HD1 | 1.74 | 0.46 |
| 1:B:98:GLN:O | 1:B:101:VAL:HG22 | 2.16 | 0.46 |
| 2:D:63:PHE:CG | 2:D:85:GLU:CG | 2.96 | 0.46 |
| 3:E:19:ASN:HB3 | 3:E:24:LYS:HG3 | 1.95 | 0.46 |
| 3:F:16:GLU:O | 3:F:17:GLN:HG3 | 2.16 | 0.46 |
| 3:F:60:ILE:O | 3:F:60:ILE:HD13 | 2.16 | 0.46 |
| 4:G:62:GLU:HG2 | 5:H:139:LYS:HB3 | 1.66 | 0.46 |
| 4:G:3:TRP:HH2 | 5:H:52:ARG:NH2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:H:37:VAL:HG23 | 5:H:64:GLU:HG2 | 1.97 | 0.46 |
| 5:H:91:PHE:H | 5:H:111:ALA:HB2 | 1.80 | 0.46 |
| 1:A:41:HIS:CD2 | 1:A:164:GLU:CG | 2.99 | 0.46 |
| 1:A:206:TYR:N | 1:A:206:TYR:CD1 | 2.83 | 0.46 |
| 1:A:290:ASN:HD22 | 1:A:291:TYR:HB2 | 1.81 | 0.46 |
| 1:A:428:SER:CB | 1:B:430:VAL:HG11 | 2.46 | 0.46 |
| 1:A:58:ASP:HB3 | 1:A:81:ASN:OD1 | 2.15 | 0.46 |
| 1:B:41:HIS:CD2 | 1:B:164:GLU:CG | 2.99 | 0.46 |
| 1:B:241:ARG:NE | 1:B:245:ILE:HD11 | 2.28 | 0.46 |
| 1:B:306:HIS:NE2 | 2:C:39:PRO:CG | 2.57 | 0.46 |
| 1:B:51:ARG:CZ | 1:B:51:ARG:HB3 | 2.46 | 0.46 |
| 4:G:7:SER:O | 4:G:10:LEU:HG | 2.16 | 0.46 |
| 5:H:14:LEU:CG | 5:H:160:PHE:CE1 | 2.99 | 0.46 |
| 4:G:97:PHE:C | 5:H:49:LYS:HD3 | 2.34 | 0.46 |
| 1:A:46:LEU:HD23 | 1:A:143:GLU:N | 2.30 | 0.46 |
| 1:A:148:PHE:CZ | 1:A:156:ASP:HB3 | 2.50 | 0.46 |
| 1:A:190:MET:HE1 | 1:A:194:THR:HG21 | 1.97 | 0.46 |
| 1:A:198:GLU:HB2 | 1:A:200:TYR:CE1 | 2.49 | 0.46 |
| 1:A:305:TYR:CD1 | 1:A:305:TYR:N | 2.83 | 0.46 |
| 1:A:439:SER:HB3 | 1:A:443:ALA:H | 1.81 | 0.46 |
| 1:A:92:PHE:N | 1:A:92:PHE:HD1 | 2.13 | 0.46 |
| 1:B:225:ASN:HA | 1:B:226:PRO:C | 2.37 | 0.46 |
| 1:B:155:PHE:CE1 | 1:B:229:HIS:CE1 | 3.03 | 0.46 |
| 1:B:439:SER:HB3 | 1:B:443:ALA:H | 1.81 | 0.46 |
| 1:B:86:HIS:CD2 | 1:B:264:ILE:CG2 | 2.99 | 0.46 |
| 2:C:99:LYS:O | 2:C:99:LYS:HG2 | 2.16 | 0.46 |
| 2:C:94:LEU:HD12 | 2:D:97:TYR:HA | 1.97 | 0.46 |
| 3:E:38:VAL:O | 3:F:88:VAL:HG11 | 2.16 | 0.46 |
| 3:F:11:PHE:CD2 | 3:F:68:ILE:HG22 | 2.51 | 0.46 |
| 4:G:41:TYR:HA | 4:G:42:PRO:C | 2.23 | 0.46 |
| 1:A:155:PHE:CD1 | 1:A:229:HIS:CE1 | 3.03 | 0.46 |
| 1:A:99:TYR:CD2 | 1:A:370:LEU:CG | 2.99 | 0.46 |
| 1:B:139:ASN:HA | 1:B:257:LEU:HB2 | 1.96 | 0.46 |
| 1:B:148:PHE:CZ | 1:B:156:ASP:HB3 | 2.50 | 0.46 |
| 1:B:158:VAL:HG12 | 1:B:160:PHE:CE1 | 2.51 | 0.46 |
| 1:B:179:PHE:CD1 | 1:B:180:ALA:N | 2.83 | 0.46 |
| 1:B:51:ARG:HD2 | 1:B:57:ASN:ND2 | 2.30 | 0.46 |
| 2:D:4:GLN:HG3 | 2:D:8:ARG:HG3 | 1.97 | 0.46 |
| 3:E:14:TYR:CD1 | 3:E:15:VAL:N | 2.84 | 0.46 |
| 3:F:32:PHE:CD1 | 3:F:32:PHE:N | 2.83 | 0.46 |
| 3:F:71:LYS:HG2 | 3:F:71:LYS:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:41:TYR:N | 4:G:41:TYR:CD1 | 2.82 | 0.46 |
| 1:A:109:SER:CB | 1:A:114:LEU:HD23 | 2.45 | 0.46 |
| 1:A:163:GLU:HA | 1:A:182:ARG:HE | 1.81 | 0.46 |
| 1:A:205:VAL:HG12 | 1:A:206:TYR:N | 2.30 | 0.46 |
| 1:A:225:ASN:HA | 1:A:226:PRO:C | 2.37 | 0.46 |
| 1:A:56:GLU:HB3 | 1:A:265:ASP:HB3 | 1.97 | 0.46 |
| 1:A:96:LYS:HG2 | 1:A:373:LYS:HD3 | 1.95 | 0.46 |
| 1:B:290:ASN:HD22 | 1:B:291:TYR:HB2 | 1.81 | 0.46 |
| 1:B:440:LYS:CD | 1:B:444:VAL:HG23 | 2.46 | 0.46 |
| 1:B:81:ASN:HD22 | 1:B:83:ARG:HD2 | 1.81 | 0.46 |
| 1:B:99:TYR:CD2 | 1:B:370:LEU:CG | 2.99 | 0.46 |
| 2:C:36:CYS:N | 2:C:37:HIS:CA | 2.80 | 0.46 |
| 2:D:63:PHE:CE2 | 2:D:86:ILE:N | 2.84 | 0.46 |
| 3:E:59:ASN:HA | 3:E:99:ILE:HB | 1.97 | 0.46 |
| 2:C:73:ARG:HD3 | 3:E:91:SER:HB2 | 1.98 | 0.46 |
| 3:F:6:ARG:NH1 | 3:F:33:THR:HG23 | 2.32 | 0.46 |
| 3:F:60:ILE:N | 3:F:60:ILE:HD13 | 2.28 | 0.46 |
| 4:G:71:TRP:N | 4:G:71:TRP:CE3 | 2.84 | 0.46 |
| 1:A:206:TYR:C | 1:A:207:TYR:HD1 | 2.19 | 0.45 |
| 1:A:232:LYS:HG2 | 1:A:233:GLY:N | 2.31 | 0.45 |
| 1:A:425:ILE:HG12 | 1:A:429:LEU:CD2 | 2.46 | 0.45 |
| 1:A:58:ASP:HB3 | 1:A:81:ASN:CG | 2.37 | 0.45 |
| 1:B:163:GLU:HA | 1:B:182:ARG:HE | 1.81 | 0.45 |
| 1:B:88:TRP:CE2 | 1:B:92:PHE:CZ | 3.04 | 0.45 |
| 2:C:63:PHE:CE2 | 2:C:86:ILE:N | 2.84 | 0.45 |
| 2:C:4:GLN:HG3 | 2:C:8:ARG:HG3 | 1.97 | 0.45 |
| 2:D:75:MET:H | 2:D:78:VAL:HG11 | 1.80 | 0.45 |
| 3:F:36:ALA:HB2 | 3:F:62:THR:HG23 | 1.98 | 0.45 |
| 3:E:81:VAL:CB | 3:F:86:ASP:HB3 | 2.45 | 0.45 |
| 5:H:143:ILE:HG21 | 5:H:147:PRO:HD2 | 1.97 | 0.45 |
| 5:H:14:LEU:N | 5:H:14:LEU:HD23 | 2.31 | 0.45 |
| 1:A:165:MET:CB | 1:A:180:ALA:CB | 2.94 | 0.45 |
| 1:A:184:TYR:N | 1:A:184:TYR:HD1 | 2.14 | 0.45 |
| 1:A:46:LEU:HG | 1:A:143:GLU:CB | 2.46 | 0.45 |
| 1:B:389:PHE:N | 1:B:389:PHE:CD1 | 2.83 | 0.45 |
| 1:B:403:ASP:C | 1:B:404:PHE:HD1 | 2.20 | 0.45 |
| 2:C:71:THR:HB | 2:C:72:GLY:HA3 | 1.98 | 0.45 |
| 2:D:63:PHE:CD2 | 2:D:86:ILE:HG23 | 2.48 | 0.45 |
| 3:E:60:ILE:HG13 | 3:E:65:ASP:CG | 2.37 | 0.45 |
| 4:G:129:PHE:CD1 | 4:G:129:PHE:N | 2.83 | 0.45 |
| 5:H:17:SER:HB3 | 5:H:89:ILE:CG2 | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:TYR:HB2 | 1:A:140:LYS:CE | 2.45 | 0.45 |
| 1:A:167:VAL:CG2 | 1:A:246:PRO:HG2 | 2.46 | 0.45 |
| 1:A:378:GLU:CD | 1:B:98:GLN:CD | 2.75 | 0.45 |
| 1:A:419:ILE:O | 1:A:422:ASP:HB2 | 2.17 | 0.45 |
| 1:A:92:PHE:CD1 | 1:A:92:PHE:N | 2.82 | 0.45 |
| 1:A:98:GLN:O | 1:A:101:VAL:HG22 | 2.16 | 0.45 |
| 1:B:109:SER:CB | 1:B:114:LEU:HD23 | 2.45 | 0.45 |
| 1:B:46:LEU:HG | 1:B:143:GLU:CB | 2.46 | 0.45 |
| 1:B:46:LEU:H | 1:B:46:LEU:CD1 | 2.30 | 0.45 |
| 1:B:63:ARG:CD | 1:B:75:VAL:CG1 | 2.95 | 0.45 |
| 2:D:86:ILE:HG13 | 2:D:86:ILE:O | 2.16 | 0.45 |
| 2:D:8:ARG:HD2 | 2:D:8:ARG:C | 2.35 | 0.45 |
| 3:E:48:LYS:HA | 3:F:48:LYS:HB2 | 1.98 | 0.45 |
| 3:E:38:VAL:HG13 | 3:E:59:ASN:O | 2.17 | 0.45 |
| 5:H:14:LEU:CD2 | 5:H:160:PHE:CE1 | 2.99 | 0.45 |
| 5:H:43:LEU:HD22 | 5:H:44:PHE:N | 2.31 | 0.45 |
| 5:H:91:PHE:N | 5:H:91:PHE:CD1 | 2.82 | 0.45 |
| 1:A:169:TYR:HB2 | 1:A:173:THR:O | 2.17 | 0.45 |
| 1:A:171:ASP:N | 1:A:178:LEU:HD22 | 2.31 | 0.45 |
| 1:A:403:ASP:C | 1:A:404:PHE:HD1 | 2.20 | 0.45 |
| 1:B:171:ASP:N | 1:B:178:LEU:HD22 | 2.31 | 0.45 |
| 1:B:215:TYR:O | 1:B:216:GLN:HB3 | 2.16 | 0.45 |
| 1:B:99:TYR:CB | 1:B:373:LYS:HE2 | 2.46 | 0.45 |
| 1:B:46:LEU:HD23 | 1:B:143:GLU:N | 2.30 | 0.45 |
| 1:A:252:GLU:HG3 | 1:B:85:SER:HB2 | 1.98 | 0.45 |
| 3:F:17:GLN:HE21 | 3:F:19:ASN:ND2 | 2.14 | 0.45 |
| 3:F:70:LYS:HB2 | 3:F:84:ILE:HA | 1.98 | 0.45 |
| 1:A:178:LEU:CA | 1:A:242:VAL:CG1 | 2.95 | 0.45 |
| 1:A:363:LEU:C | 1:A:363:LEU:HD23 | 2.36 | 0.45 |
| 1:A:369:LEU:H | 1:A:369:LEU:HD12 | 1.80 | 0.45 |
| 1:A:130:LEU:CD2 | 1:A:388:PHE:CE2 | 2.95 | 0.45 |
| 1:A:63:ARG:CD | 1:A:75:VAL:CG1 | 2.95 | 0.45 |
| 1:B:169:TYR:CD1 | 1:B:169:TYR:N | 2.84 | 0.45 |
| 1:B:169:TYR:HB2 | 1:B:173:THR:O | 2.17 | 0.45 |
| 1:B:317:VAL:HB | 1:B:319:THR:OG1 | 2.16 | 0.45 |
| 1:A:460:ILE:HG21 | 1:B:467:TYR:N | 2.32 | 0.45 |
| 2:C:63:PHE:CG | 2:C:85:GLU:CG | 2.96 | 0.45 |
| 2:D:67:ASN:HA | 2:D:81:ASN:OD1 | 2.17 | 0.45 |
| 3:E:37:HIS:CE1 | 3:E:39:GLN:HB2 | 2.51 | 0.45 |
| 3:E:58:TYR:HA | 3:F:100:LYS:HZ2 | 1.81 | 0.45 |
| 3:F:62:THR:HB | 3:F:65:ASP:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:11:GLN:O | 4:G:14:THR:HB | 2.16 | 0.45 |
| 5:H:42:GLU:CB | 5:H:43:LEU:CA | 2.95 | 0.45 |
| 5:H:43:LEU:HD13 | 5:H:43:LEU:C | 2.36 | 0.45 |
| 5:H:44:PHE:CD1 | 5:H:44:PHE:N | 2.83 | 0.45 |
| 1:A:179:PHE:CD1 | 1:A:180:ALA:N | 2.83 | 0.45 |
| 1:B:165:MET:CB | 1:B:180:ALA:CB | 2.94 | 0.45 |
| 1:A:64:ARG:NH2 | 1:B:284:ILE:HG12 | 2.31 | 0.45 |
| 1:B:92:PHE:N | 1:B:92:PHE:HD1 | 2.13 | 0.45 |
| 2:C:12:ILE:HG12 | 3:E:93:LEU:HG | 1.99 | 0.45 |
| 2:D:75:MET:O | 2:D:78:VAL:HG12 | 2.16 | 0.45 |
| 2:C:5:ARG:CA | 3:E:3:GLU:N | 2.80 | 0.45 |
| 3:E:50:GLN:CG | 3:F:52:LEU:HB2 | 2.46 | 0.45 |
| 3:E:65:ASP:CA | 3:E:97:THR:HB | 2.46 | 0.45 |
| 3:F:44:GLU:HG2 | 3:F:46:TYR:HB2 | 1.95 | 0.45 |
| 3:E:50:GLN:CB | 3:F:49:ALA:HB3 | 2.46 | 0.45 |
| 4:G:105:LYS:HA | 4:G:106:LYS:HA | 1.65 | 0.45 |
| 1:A:190:MET:HE1 | 1:A:194:THR:CG2 | 2.47 | 0.45 |
| 1:A:206:TYR:HD1 | 1:A:206:TYR:N | 2.15 | 0.45 |
| 1:A:289:LYS:HD2 | 1:A:319:THR:HG23 | 1.94 | 0.45 |
| 1:A:418:ARG:HH21 | 1:A:446:ARG:NH2 | 2.15 | 0.45 |
| 1:A:86:HIS:CB | 1:A:264:ILE:HG21 | 2.47 | 0.45 |
| 2:C:75:MET:O | 2:C:78:VAL:HG12 | 2.16 | 0.45 |
| 2:C:84:THR:CG2 | 2:D:83:ALA:HA | 2.47 | 0.45 |
| 2:C:98:ARG:HH12 | 2:D:102:ARG:H | 1.63 | 0.45 |
| 3:E:35:ALA:O | 3:E:36:ALA:HB3 | 2.16 | 0.45 |
| 3:E:38:VAL:H | 3:F:88:VAL:HB | 1.82 | 0.45 |
| 3:F:28:TRP:HZ3 | 3:F:80:ILE:CG2 | 2.26 | 0.45 |
| 3:F:21:GLU:HG3 | 4:G:19:GLU:OE2 | 2.08 | 0.45 |
| 1:A:142:ILE:CD1 | 1:A:145:TRP:HB2 | 2.46 | 0.45 |
| 1:A:187:LYS:CE | 1:A:193:GLU:CB | 2.95 | 0.45 |
| 1:A:390:TRP:CZ3 | 1:B:125:ASP:OD2 | 2.69 | 0.45 |
| 1:A:466:GLN:HA | 1:A:467:TYR:HA | 1.58 | 0.45 |
| 1:A:88:TRP:CD2 | 1:A:92:PHE:HE1 | 2.34 | 0.45 |
| 1:A:99:TYR:CD2 | 1:A:370:LEU:CB | 2.97 | 0.45 |
| 2:C:67:ASN:HA | 2:C:81:ASN:OD1 | 2.17 | 0.45 |
| 2:D:59:LYS:HB2 | 2:D:90:ILE:CD1 | 2.47 | 0.45 |
| 2:D:75:MET:H | 2:D:78:VAL:HB | 1.81 | 0.45 |
| 3:E:47:TYR:OH | 3:F:41:ILE:HD11 | 2.17 | 0.45 |
| 3:E:53:GLN:O | 3:F:102:LYS:HE2 | 2.17 | 0.45 |
| 3:F:103:GLU:OE1 | 4:G:31:VAL:HG11 | 2.17 | 0.45 |
| 5:H:65:VAL:HG11 | 5:H:67:TYR:CE1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:291:TYR:CB | 1:A:312:SER:HB2 | 2.43 | 0.45 |
| 1:A:51:ARG:CZ | 1:A:51:ARG:HB3 | 2.46 | 0.45 |
| 1:A:62:LYS:HB3 | 1:A:81:ASN:OD1 | 2.17 | 0.45 |
| 1:A:63:ARG:CD | 1:A:75:VAL:HG11 | 2.46 | 0.45 |
| 1:B:183:TYR:CB | 1:B:197:ALA:CB | 2.95 | 0.45 |
| 1:B:232:LYS:HG2 | 1:B:233:GLY:N | 2.31 | 0.45 |
| 1:B:320:LEU:N | 1:B:321:ARG:CA | 2.80 | 0.45 |
| 1:B:99:TYR:CB | 1:B:373:LYS:HZ1 | 2.29 | 0.45 |
| 1:B:379:ARG:HB2 | 1:B:380:LYS:HZ3 | 1.81 | 0.45 |
| 1:B:419:ILE:O | 1:B:422:ASP:HB2 | 2.17 | 0.45 |
| 2:C:53:VAL:O | 2:C:57:VAL:HG13 | 2.17 | 0.45 |
| 2:D:36:CYS:N | 2:D:37:HIS:CA | 2.80 | 0.45 |
| 2:C:95:ASN:N | 2:D:97:TYR:HB2 | 2.30 | 0.45 |
| 2:D:95:ASN:CB | 2:D:98:ARG:N | 2.80 | 0.45 |
| 3:E:60:ILE:HD11 | 3:E:69:ASP:OD1 | 2.16 | 0.45 |
| 3:E:74:VAL:CG1 | 3:E:76:TYR:CE1 | 2.99 | 0.45 |
| 3:F:63:PRO:CA | 3:F:96:ILE:HA | 2.24 | 0.45 |
| 4:G:33:GLU:O | 4:G:34:SER:HB2 | 2.17 | 0.45 |
| 1:A:317:VAL:HB | 1:A:319:THR:OG1 | 2.16 | 0.45 |
| 1:A:320:LEU:N | 1:A:321:ARG:CA | 2.80 | 0.45 |
| 1:A:382:ARG:CZ | 1:A:385:LEU:HD23 | 2.47 | 0.45 |
| 1:A:81:ASN:HD22 | 1:A:83:ARG:HD2 | 1.81 | 0.45 |
| 1:B:300:THR:O | 1:B:304:ARG:HG3 | 2.17 | 0.45 |
| 1:B:382:ARG:CZ | 1:B:385:LEU:HD23 | 2.47 | 0.45 |
| 1:B:418:ARG:HH21 | 1:B:446:ARG:NH2 | 2.15 | 0.45 |
| 1:B:63:ARG:CD | 1:B:75:VAL:HG11 | 2.46 | 0.45 |
| 2:D:53:VAL:O | 2:D:57:VAL:HG13 | 2.17 | 0.45 |
| 2:D:71:THR:HB | 2:D:72:GLY:HA3 | 1.98 | 0.45 |
| 3:E:50:GLN:HB3 | 3:F:49:ALA:CB | 2.47 | 0.45 |
| 3:F:60:ILE:CG2 | 3:F:83:PHE:HD2 | 2.29 | 0.45 |
| 5:H:108:PHE:CZ | 5:H:153:VAL:CG2 | 3.00 | 0.45 |
| 5:H:15:PHE:HZ | 5:H:91:PHE:CZ | 2.33 | 0.45 |
| 5:H:22:THR:CG2 | 5:H:92:TRP:NE1 | 2.79 | 0.45 |
| 1:A:146:HIS:CE1 | 1:A:243:PRO:HB2 | 2.52 | 0.44 |
| 1:A:99:TYR:CB | 1:A:373:LYS:HE2 | 2.46 | 0.44 |
| 1:B:254:VAL:CB | 1:B:259:PHE:CE1 | 2.95 | 0.44 |
| 2:C:49:ILE:CD1 | 2:C:54:LEU:CG | 2.95 | 0.44 |
| 3:E:14:TYR:HD1 | 3:E:15:VAL:H | 1.66 | 0.44 |
| 3:E:12:GLN:C | 3:E:30:ASP:HB2 | 2.36 | 0.44 |
| 3:E:45:GLU:O | 3:F:44:GLU:HB3 | 2.17 | 0.44 |
| 1:A:215:TYR:O | 1:A:216:GLN:HB3 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:206:TYR:HD1 | 1:B:206:TYR:N | 2.15 | 0.44 |
| 1:B:178:LEU:CA | 1:B:242:VAL:CG1 | 2.95 | 0.44 |
| 1:B:258:LYS:HA | 1:B:261:LYS:HB3 | 1.98 | 0.44 |
| 2:C:75:MET:H | 2:C:78:VAL:HG11 | 1.81 | 0.44 |
| 2:C:86:ILE:HG13 | 2:C:86:ILE:O | 2.16 | 0.44 |
| 2:D:23:GLU:O | 2:D:26:PRO:HD2 | 2.18 | 0.44 |
| 3:E:83:PHE:CD1 | 3:E:83:PHE:N | 2.83 | 0.44 |
| 3:E:85:GLY:HA3 | 3:E:99:ILE:HG22 | 1.98 | 0.44 |
| 3:F:60:ILE:HD13 | 3:F:99:ILE:HD11 | 1.98 | 0.44 |
| 4:G:33:GLU:HB2 | 4:G:45:VAL:HA | 1.98 | 0.44 |
| 4:G:41:TYR:N | 4:G:41:TYR:HD1 | 2.14 | 0.44 |
| 5:H:128:ILE:HG22 | 5:H:129:SER:N | 2.33 | 0.44 |
| 5:H:108:PHE:CB | 5:H:150:ILE:CG2 | 2.95 | 0.44 |
| 1:A:211:ILE:HG13 | 1:A:212:ASP:H | 1.81 | 0.44 |
| 1:A:389:PHE:CD1 | 1:A:389:PHE:N | 2.83 | 0.44 |
| 1:B:167:VAL:CG2 | 1:B:246:PRO:HG2 | 2.46 | 0.44 |
| 1:B:58:ASP:HB3 | 1:B:81:ASN:CG | 2.37 | 0.44 |
| 1:B:88:TRP:CD2 | 1:B:92:PHE:HE1 | 2.34 | 0.44 |
| 2:C:23:GLU:O | 2:C:26:PRO:HD2 | 2.18 | 0.44 |
| 3:E:108:VAL:CB | 4:G:43:TYR:HH | 2.23 | 0.44 |
| 2:C:4:GLN:O | 3:E:1:MET:N | 2.50 | 0.44 |
| 3:E:5:PHE:CE2 | 3:E:7:ASP:HB2 | 2.49 | 0.44 |
| 3:F:15:VAL:HG12 | 3:F:17:GLN:N | 2.32 | 0.44 |
| 3:F:76:TYR:HE1 | 3:F:81:VAL:HG11 | 1.80 | 0.44 |
| 4:G:44:VAL:HG21 | 4:G:74:THR:CA | 2.45 | 0.44 |
| 4:G:44:VAL:HG12 | 4:G:45:VAL:N | 2.32 | 0.44 |
| 4:G:4:LYS:CD | 4:G:5:LEU:CD1 | 2.96 | 0.44 |
| 4:G:42:PRO:CB | 4:G:72:GLY:HA3 | 2.32 | 0.44 |
| 5:H:43:LEU:CD1 | 5:H:43:LEU:H | 2.30 | 0.44 |
| 5:H:47:GLN:HE22 | 5:H:55:GLY:H | 1.64 | 0.44 |
| 5:H:89:ILE:N | 5:H:89:ILE:HD13 | 2.32 | 0.44 |
| 1:A:187:LYS:CD | 1:A:193:GLU:CB | 2.95 | 0.44 |
| 1:A:138:SER:HB3 | 1:A:256:ASP:CG | 2.37 | 0.44 |
| 1:A:63:ARG:CB | 1:A:75:VAL:CG1 | 2.95 | 0.44 |
| 1:B:179:PHE:CE1 | 1:B:244:ILE:CG2 | 2.98 | 0.44 |
| 1:B:292:ASP:HA | 1:B:293:GLY:HA3 | 1.73 | 0.44 |
| 1:B:392:PHE:HD1 | 1:B:392:PHE:HA | 1.56 | 0.44 |
| 1:B:86:HIS:CB | 1:B:264:ILE:HG21 | 2.47 | 0.44 |
| 1:A:292:ASP:OD2 | 2:C:31:PHE:C | 2.56 | 0.44 |
| 2:C:95:ASN:CB | 2:C:98:ARG:N | 2.80 | 0.44 |
| 2:D:49:ILE:CD1 | 2:D:54:LEU:CG | 2.95 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:93:LYS:NZ | 2:D:94:LEU:HD11 | 2.30 | 0.44 |
| 3:F:6:ARG:HD2 | 3:F:33:THR:HG21 | 1.99 | 0.44 |
| 4:G:18:LEU:HA | 4:G:24:LEU:HD13 | 1.98 | 0.44 |
| 4:G:35:PRO:HA | 4:G:37:LYS:HZ3 | 1.82 | 0.44 |
| 1:A:178:LEU:CG | 1:A:242:VAL:HG11 | 2.45 | 0.44 |
| 1:A:300:THR:O | 1:A:304:ARG:HG3 | 2.17 | 0.44 |
| 1:A:335:ARG:NH2 | 1:A:336:ILE:HG12 | 2.32 | 0.44 |
| 1:A:96:LYS:CE | 1:A:377:ALA:HB2 | 2.47 | 0.44 |
| 1:A:387:LEU:HG | 1:A:391:PHE:CE2 | 2.53 | 0.44 |
| 1:A:86:HIS:CD2 | 1:A:264:ILE:CG2 | 2.99 | 0.44 |
| 1:B:38:ILE:CD1 | 1:B:181:LEU:CD1 | 2.95 | 0.44 |
| 1:B:146:HIS:CE1 | 1:B:243:PRO:HB2 | 2.52 | 0.44 |
| 1:B:44:GLU:HB3 | 1:B:45:PRO:CD | 2.37 | 0.44 |
| 2:C:75:MET:H | 2:C:78:VAL:HB | 1.81 | 0.44 |
| 4:G:113:ILE:HG12 | 4:G:122:HIS:N | 2.32 | 0.44 |
| 4:G:48:ASP:HB2 | 4:G:51:SER:HB3 | 1.99 | 0.44 |
| 5:H:68:TYR:HH | 5:H:125:ALA:HB3 | 1.82 | 0.44 |
| 5:H:160:PHE:CB | 5:H:163:PRO:HG2 | 2.45 | 0.44 |
| 1:A:199:LEU:HB3 | 1:A:208:TYR:CZ | 2.53 | 0.44 |
| 1:A:243:PRO:HA | 1:A:244:ILE:HA | 1.53 | 0.44 |
| 1:B:108:THR:CG2 | 1:B:412:MET:CE | 2.95 | 0.44 |
| 1:B:138:SER:HB3 | 1:B:256:ASP:CG | 2.37 | 0.44 |
| 1:B:157:TYR:CD1 | 1:B:157:TYR:N | 2.85 | 0.44 |
| 1:B:310:LYS:HG3 | 2:C:38:ASN:CB | 2.44 | 0.44 |
| 1:B:425:ILE:HG12 | 1:B:429:LEU:CD2 | 2.46 | 0.44 |
| 1:B:62:LYS:HB3 | 1:B:81:ASN:OD1 | 2.17 | 0.44 |
| 2:D:41:ILE:HG22 | 2:D:45:GLY:HA2 | 1.97 | 0.44 |
| 3:E:37:HIS:NE2 | 3:F:90:LEU:HA | 2.32 | 0.44 |
| 3:E:79:LYS:HD3 | 3:F:69:ASP:HB3 | 1.98 | 0.44 |
| 3:F:75:ILE:CG2 | 3:F:78:GLY:H | 2.30 | 0.44 |
| 4:G:113:ILE:CG1 | 4:G:122:HIS:H | 2.31 | 0.44 |
| 4:G:59:SER:HB2 | 5:H:138:LEU:HB3 | 2.00 | 0.44 |
| 5:H:53:ILE:C | 5:H:54:LEU:CA | 2.75 | 0.44 |
| 5:H:89:ILE:CG2 | 5:H:91:PHE:CE1 | 3.01 | 0.44 |
| 1:A:148:PHE:CB | 1:A:205:VAL:CG2 | 2.96 | 0.44 |
| 1:A:183:TYR:CB | 1:A:197:ALA:CB | 2.95 | 0.44 |
| 1:A:258:LYS:HA | 1:A:261:LYS:HB3 | 1.98 | 0.44 |
| 1:A:288:LEU:CD2 | 1:B:310:LYS:NZ | 2.81 | 0.44 |
| 1:A:426:VAL:HA | 1:A:429:LEU:HG | 2.00 | 0.44 |
| 1:B:452:ASP:OD1 | 1:B:453:PRO:HD2 | 2.18 | 0.44 |
| 2:C:73:ARG:HD3 | 3:E:91:SER:HB3 | 1.95 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:64:TYR:CE1 | 3:F:95:GLU:CB | 2.95 | 0.44 |
| 4:G:113:ILE:HG13 | 4:G:115:ASP:OD1 | 2.17 | 0.44 |
| 5:H:32:GLN:NE2 | 5:H:93:ARG:HG2 | 2.32 | 0.44 |
| 1:A:247:PHE:CD1 | 1:A:247:PHE:N | 2.83 | 0.44 |
| 1:B:187:LYS:CE | 1:B:193:GLU:CB | 2.95 | 0.44 |
| 1:B:187:LYS:CD | 1:B:193:GLU:CB | 2.95 | 0.44 |
| 1:B:149:VAL:CG2 | 1:B:227:ARG:CD | 2.95 | 0.44 |
| 1:B:370:LEU:N | 1:B:370:LEU:HD22 | 2.33 | 0.44 |
| 1:B:426:VAL:HA | 1:B:429:LEU:HG | 2.00 | 0.44 |
| 1:B:42:ASN:OD1 | 1:B:44:GLU:HB2 | 2.18 | 0.44 |
| 2:C:59:LYS:HB2 | 2:C:90:ILE:CD1 | 2.47 | 0.44 |
| 3:E:52:LEU:CB | 3:E:53:GLN:HA | 2.46 | 0.44 |
| 3:E:74:VAL:HB | 3:E:83:PHE:HZ | 1.79 | 0.44 |
| 3:F:15:VAL:HG12 | 3:F:17:GLN:H | 1.82 | 0.44 |
| 3:F:37:HIS:ND1 | 3:F:61:TYR:HE2 | 2.15 | 0.44 |
| 4:G:32:THR:OG1 | 4:G:43:TYR:HA | 2.17 | 0.44 |
| 4:G:4:LYS:HG2 | 4:G:5:LEU:H | 1.83 | 0.44 |
| 5:H:120:ASP:C | 5:H:126:VAL:HG23 | 2.38 | 0.44 |
| 5:H:42:GLU:CG | 5:H:56:PRO:CD | 2.90 | 0.44 |
| 1:A:167:VAL:HG21 | 1:A:246:PRO:HG2 | 1.99 | 0.44 |
| 1:A:439:SER:N | 1:A:440:LYS:CA | 2.81 | 0.44 |
| 1:B:117:TYR:O | 1:B:121:LEU:HD23 | 2.18 | 0.44 |
| 1:B:211:ILE:HG13 | 1:B:212:ASP:H | 1.81 | 0.44 |
| 1:B:96:LYS:CE | 1:B:377:ALA:HB2 | 2.47 | 0.44 |
| 2:C:95:ASN:CB | 2:C:98:ARG:H | 2.31 | 0.44 |
| 2:C:98:ARG:NH2 | 2:D:102:ARG:HD2 | 2.33 | 0.44 |
| 2:C:98:ARG:CZ | 2:D:102:ARG:CG | 2.90 | 0.44 |
| 1:B:292:ASP:OD2 | 2:D:31:PHE:C | 2.56 | 0.44 |
| 2:D:34:ASP:CB | 2:D:35:GLU:CA | 2.93 | 0.44 |
| 2:D:95:ASN:CB | 2:D:98:ARG:H | 2.31 | 0.44 |
| 3:E:15:VAL:CG1 | 3:E:73:ARG:HB2 | 2.47 | 0.44 |
| 3:F:46:TYR:CG | 3:F:48:LYS:HE2 | 2.52 | 0.44 |
| 3:E:38:VAL:O | 3:F:88:VAL:HB | 2.17 | 0.44 |
| 4:G:45:VAL:HG22 | 4:G:71:TRP:CZ3 | 2.41 | 0.44 |
| 5:H:143:ILE:CG1 | 5:H:147:PRO:HG2 | 2.37 | 0.44 |
| 1:A:120:GLU:HG3 | 1:A:121:LEU:N | 2.33 | 0.43 |
| 1:A:252:GLU:CG | 1:B:85:SER:CB | 2.95 | 0.43 |
| 1:A:370:LEU:HD22 | 1:A:370:LEU:N | 2.33 | 0.43 |
| 1:A:130:LEU:CD1 | 1:A:388:PHE:CE2 | 2.98 | 0.43 |
| 1:A:389:PHE:HD2 | 1:A:407:ASP:OD2 | 2.01 | 0.43 |
| 1:A:126:PHE:CE2 | 1:A:392:PHE:CZ | 3.03 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:48:LYS:O | 1:A:52:TYR:HB2 | 2.18 | 0.43 |
| 1:B:120:GLU:HG3 | 1:B:121:LEU:N | 2.33 | 0.43 |
| 1:B:204:HIS:NE2 | 1:B:206:TYR:CE1 | 2.86 | 0.43 |
| 1:B:148:PHE:CB | 1:B:205:VAL:CG2 | 2.96 | 0.43 |
| 1:B:439:SER:N | 1:B:440:LYS:CA | 2.81 | 0.43 |
| 1:B:63:ARG:CB | 1:B:75:VAL:CG1 | 2.95 | 0.43 |
| 2:C:4:GLN:OE1 | 3:E:2:TYR:N | 2.46 | 0.43 |
| 2:D:4:GLN:HG2 | 3:F:1:MET:HE3 | 1.93 | 0.43 |
| 3:F:93:LEU:CD2 | 3:F:93:LEU:H | 2.30 | 0.43 |
| 1:A:219:TYR:N | 1:A:219:TYR:CD1 | 2.83 | 0.43 |
| 1:A:42:ASN:OD1 | 1:A:44:GLU:HB2 | 2.18 | 0.43 |
| 1:A:452:ASP:OD1 | 1:A:453:PRO:HD2 | 2.18 | 0.43 |
| 1:A:466:GLN:CG | 1:A:467:TYR:CB | 2.95 | 0.43 |
| 1:A:53:TYR:O | 1:A:53:TYR:HD1 | 2.01 | 0.43 |
| 1:B:142:ILE:CD1 | 1:B:145:TRP:HB2 | 2.46 | 0.43 |
| 1:B:199:LEU:HB3 | 1:B:208:TYR:CZ | 2.53 | 0.43 |
| 3:E:38:VAL:CB | 3:F:88:VAL:HG12 | 2.36 | 0.43 |
| 4:G:32:THR:CB | 4:G:43:TYR:HB2 | 2.47 | 0.43 |
| 1:A:43:PRO:HB2 | 1:A:47:LEU:HD12 | 2.00 | 0.43 |
| 1:B:146:HIS:CG | 1:B:200:TYR:HD2 | 2.37 | 0.43 |
| 1:B:163:GLU:N | 1:B:182:ARG:HD2 | 2.33 | 0.43 |
| 1:B:178:LEU:CG | 1:B:242:VAL:HG11 | 2.45 | 0.43 |
| 2:C:94:LEU:HD12 | 2:D:97:TYR:CA | 2.46 | 0.43 |
| 2:D:4:GLN:HB2 | 2:D:8:ARG:NE | 2.33 | 0.43 |
| 3:E:53:GLN:NE2 | 3:E:102:LYS:HD2 | 2.34 | 0.43 |
| 2:C:71:THR:HA | 3:E:92:GLY:CA | 2.49 | 0.43 |
| 4:G:28:VAL:HG22 | 4:G:29:ASN:N | 2.33 | 0.43 |
| 4:G:44:VAL:HG13 | 4:G:70:VAL:CG1 | 2.44 | 0.43 |
| 4:G:4:LYS:HG2 | 4:G:5:LEU:CD1 | 2.46 | 0.43 |
| 4:G:48:ASP:HB2 | 4:G:51:SER:CB | 2.49 | 0.43 |
| 4:G:63:ASN:CB | 4:G:130:THR:HA | 2.48 | 0.43 |
| 5:H:112:TYR:HA | 5:H:112:TYR:HD1 | 1.56 | 0.43 |
| 4:G:63:ASN:OD1 | 5:H:139:LYS:HG2 | 2.18 | 0.43 |
| 5:H:15:PHE:HE1 | 5:H:91:PHE:CG | 2.36 | 0.43 |
| 1:A:144:TYR:HD2 | 1:A:165:MET:HE2 | 1.82 | 0.43 |
| 1:A:38:ILE:CD1 | 1:A:181:LEU:CD1 | 2.95 | 0.43 |
| 1:B:389:PHE:HD2 | 1:B:407:ASP:OD2 | 2.01 | 0.43 |
| 1:B:53:TYR:HD1 | 1:B:53:TYR:O | 2.01 | 0.43 |
| 3:E:12:GLN:CB | 3:E:28:TRP:CE3 | 2.95 | 0.43 |
| 3:F:41:ILE:CG2 | 3:F:42:SER:H | 2.24 | 0.43 |
| 1:A:169:TYR:CD1 | 1:A:169:TYR:N | 2.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:146:HIS:CG | 1:A:200:TYR:HD2 | 2.37 | 0.43 |
| 1:A:290:ASN:CB | 1:A:291:TYR:CA | 2.95 | 0.43 |
| 1:B:167:VAL:HG21 | 1:B:246:PRO:HG2 | 1.99 | 0.43 |
| 1:B:335:ARG:NH2 | 1:B:336:ILE:HG12 | 2.32 | 0.43 |
| 2:C:4:GLN:HB2 | 2:C:8:ARG:NE | 2.33 | 0.43 |
| 3:E:50:GLN:OE1 | 3:F:49:ALA:HB3 | 2.18 | 0.43 |
| 3:E:55:PRO:HB3 | 3:E:102:LYS:HB2 | 1.99 | 0.43 |
| 3:F:80:ILE:HG13 | 3:F:80:ILE:O | 2.17 | 0.43 |
| 3:F:90:LEU:CB | 3:F:98:ARG:CD | 2.97 | 0.43 |
| 4:G:70:VAL:HG11 | 4:G:76:ARG:HH22 | 1.80 | 0.43 |
| 1:A:148:PHE:HD1 | 1:A:148:PHE:N | 2.14 | 0.43 |
| 1:A:204:HIS:NE2 | 1:A:206:TYR:CE1 | 2.86 | 0.43 |
| 1:A:221:TYR:CD1 | 1:A:221:TYR:N | 2.83 | 0.43 |
| 1:A:230:MET:SD | 1:A:239:TRP:NE1 | 2.91 | 0.43 |
| 1:A:410:LEU:CB | 1:A:412:MET:CG | 2.95 | 0.43 |
| 1:B:147:PRO:HB2 | 1:B:229:HIS:NE2 | 2.33 | 0.43 |
| 1:B:376:MET:HG3 | 1:B:377:ALA:N | 2.30 | 0.43 |
| 2:C:41:ILE:HG22 | 2:C:45:GLY:HA2 | 1.97 | 0.43 |
| 2:D:41:ILE:HG21 | 2:D:45:GLY:HA2 | 1.95 | 0.43 |
| 3:E:52:LEU:CB | 3:E:53:GLN:CA | 2.95 | 0.43 |
| 3:E:62:THR:CB | 3:E:68:ILE:CD1 | 2.95 | 0.43 |
| 4:G:74:THR:CG2 | 4:G:75:THR:N | 2.81 | 0.43 |
| 4:G:96:MET:HG2 | 4:G:97:PHE:N | 2.33 | 0.43 |
| 5:H:108:PHE:CZ | 5:H:153:VAL:HG22 | 2.54 | 0.43 |
| 5:H:32:GLN:CB | 5:H:67:TYR:CE1 | 3.01 | 0.43 |
| 1:A:163:GLU:N | 1:A:182:ARG:HD2 | 2.33 | 0.43 |
| 1:A:179:PHE:CE1 | 1:A:244:ILE:CG2 | 2.98 | 0.43 |
| 1:A:254:VAL:CB | 1:A:259:PHE:CE1 | 2.95 | 0.43 |
| 1:A:417:THR:N | 1:A:418:ARG:CA | 2.82 | 0.43 |
| 1:A:46:LEU:H | 1:A:46:LEU:CD1 | 2.30 | 0.43 |
| 1:B:142:ILE:N | 1:B:143:GLU:CA | 2.81 | 0.43 |
| 1:B:144:TYR:HD2 | 1:B:165:MET:HE2 | 1.83 | 0.43 |
| 1:B:219:TYR:CD1 | 1:B:219:TYR:N | 2.83 | 0.43 |
| 1:B:291:TYR:CB | 1:B:312:SER:HB2 | 2.43 | 0.43 |
| 1:B:364:GLU:HG3 | 1:B:365:LYS:N | 2.34 | 0.43 |
| 1:B:387:LEU:HG | 1:B:391:PHE:CE2 | 2.53 | 0.43 |
| 2:C:95:ASN:OD1 | 2:C:97:TYR:HB3 | 2.18 | 0.43 |
| 2:D:95:ASN:OD1 | 2:D:97:TYR:HB3 | 2.18 | 0.43 |
| 3:E:84:ILE:HG13 | 3:E:103:GLU:HG2 | 2.01 | 0.43 |
| 2:C:11:SER:HB3 | 3:E:93:LEU:CB | 2.49 | 0.43 |
| 3:F:76:TYR:N | 3:F:76:TYR:CD1 | 2.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:76:TYR:CE2 | 3:F:79:LYS:CB | 3.01 | 0.43 |
| 5:H:58:SER:CB | 5:H:143:ILE:CD1 | 2.95 | 0.43 |
| 1:A:117:TYR:O | 1:A:121:LEU:HD23 | 2.18 | 0.43 |
| 1:A:157:TYR:CD1 | 1:A:157:TYR:N | 2.85 | 0.43 |
| 1:A:347:VAL:HG12 | 1:A:348:ASP:N | 2.34 | 0.43 |
| 1:B:221:TYR:N | 1:B:221:TYR:CD1 | 2.82 | 0.43 |
| 1:B:290:ASN:CB | 1:B:291:TYR:CA | 2.95 | 0.43 |
| 1:B:404:PHE:CD1 | 1:B:404:PHE:N | 2.84 | 0.43 |
| 1:B:48:LYS:O | 1:B:52:TYR:HB2 | 2.18 | 0.43 |
| 3:E:105:GLY:N | 4:G:119:VAL:HG22 | 2.11 | 0.43 |
| 3:E:81:VAL:CG1 | 3:E:82:THR:N | 2.82 | 0.43 |
| 3:F:17:GLN:HB2 | 3:F:19:ASN:OD1 | 2.18 | 0.43 |
| 3:F:43:GLN:HG2 | 3:F:52:LEU:C | 2.39 | 0.43 |
| 3:F:42:SER:O | 3:F:43:GLN:HG3 | 2.19 | 0.43 |
| 3:F:45:GLU:CA | 3:F:47:TYR:CE1 | 2.95 | 0.43 |
| 3:F:57:GLY:C | 3:F:58:TYR:HD1 | 2.21 | 0.43 |
| 3:E:77:ARG:HD3 | 3:F:65:ASP:O | 2.18 | 0.43 |
| 3:F:70:LYS:CG | 3:F:71:LYS:N | 2.82 | 0.43 |
| 3:F:9:ILE:HD12 | 3:F:11:PHE:HE1 | 1.83 | 0.43 |
| 3:E:109:GLY:N | 4:G:113:ILE:HD12 | 2.30 | 0.43 |
| 4:G:33:GLU:CB | 4:G:45:VAL:HA | 2.49 | 0.43 |
| 4:G:48:ASP:CA | 4:G:67:ASP:HB2 | 2.47 | 0.43 |
| 4:G:134:ASN:C | 5:H:57:GLY:C | 2.77 | 0.43 |
| 1:A:163:GLU:OE1 | 1:A:163:GLU:HA | 2.19 | 0.43 |
| 1:A:288:LEU:HG | 1:A:288:LEU:O | 2.19 | 0.43 |
| 1:B:149:VAL:CG2 | 1:B:227:ARG:HD3 | 2.49 | 0.43 |
| 1:A:339:GLU:CD | 1:B:274:THR:HG21 | 2.38 | 0.43 |
| 1:A:438:MET:HG2 | 1:B:433:VAL:O | 2.19 | 0.43 |
| 2:C:5:ARG:CB | 3:E:3:GLU:C | 2.85 | 0.43 |
| 2:C:99:LYS:HZ3 | 2:D:102:ARG:N | 1.89 | 0.43 |
| 2:D:76:ASP:OD1 | 3:F:90:LEU:HD11 | 2.18 | 0.43 |
| 2:D:80:TYR:HA | 2:D:80:TYR:HD1 | 1.38 | 0.43 |
| 3:E:13:SER:CB | 3:E:75:ILE:CD1 | 2.96 | 0.43 |
| 3:E:58:TYR:CE2 | 3:E:81:VAL:HG11 | 2.50 | 0.43 |
| 3:E:58:TYR:CG | 3:E:81:VAL:HG11 | 2.51 | 0.43 |
| 3:F:103:GLU:CB | 4:G:31:VAL:HG21 | 2.49 | 0.43 |
| 5:H:37:VAL:HB | 5:H:64:GLU:N | 2.34 | 0.43 |
| 1:A:44:GLU:HB3 | 1:A:45:PRO:CD | 2.37 | 0.43 |
| 1:B:140:LYS:N | 1:B:257:LEU:CB | 2.82 | 0.43 |
| 1:B:221:TYR:CB | 1:B:222:GLY:CA | 2.94 | 0.43 |
| 3:E:62:THR:CG2 | 3:E:68:ILE:CD1 | 2.95 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:8:VAL:HG22 | 3:E:34:ALA:CA | 2.38 | 0.43 |
| 3:F:55:PRO:HG3 | 3:F:102:LYS:CB | 2.48 | 0.43 |
| 3:E:54:THR:HG23 | 3:F:102:LYS:HG3 | 2.01 | 0.43 |
| 3:F:76:TYR:CE2 | 3:F:79:LYS:HG2 | 2.53 | 0.43 |
| 4:G:4:LYS:CG | 4:G:5:LEU:CD1 | 2.95 | 0.43 |
| 4:G:100:PHE:CZ | 5:H:47:GLN:N | 2.46 | 0.43 |
| 5:H:67:TYR:O | 5:H:127:GLU:HG3 | 2.19 | 0.43 |
| 1:A:221:TYR:CB | 1:A:222:GLY:CA | 2.94 | 0.42 |
| 1:A:37:LEU:O | 1:A:166:ILE:HD12 | 2.19 | 0.42 |
| 1:A:112:LYS:N | 1:A:401:LYS:HZ2 | 2.17 | 0.42 |
| 1:A:52:TYR:CZ | 1:A:265:ASP:HB2 | 2.54 | 0.42 |
| 1:B:148:PHE:HD1 | 1:B:148:PHE:N | 2.14 | 0.42 |
| 1:B:140:LYS:N | 1:B:257:LEU:HB3 | 2.34 | 0.42 |
| 1:B:260:TYR:N | 1:B:260:TYR:CD1 | 2.82 | 0.42 |
| 1:B:347:VAL:HG12 | 1:B:348:ASP:N | 2.34 | 0.42 |
| 1:B:417:THR:N | 1:B:418:ARG:CA | 2.82 | 0.42 |
| 1:B:439:SER:CB | 1:B:442:THR:N | 2.82 | 0.42 |
| 1:B:466:GLN:CG | 1:B:467:TYR:CG | 2.95 | 0.42 |
| 1:B:52:TYR:CZ | 1:B:265:ASP:HB2 | 2.54 | 0.42 |
| 2:C:94:LEU:O | 2:C:96:PRO:HA | 2.19 | 0.42 |
| 2:D:49:ILE:HD11 | 2:D:54:LEU:HG | 2.01 | 0.42 |
| 3:F:12:GLN:HB2 | 3:F:29:VAL:O | 2.19 | 0.42 |
| 4:G:7:SER:O | 4:G:10:LEU:HD23 | 2.19 | 0.42 |
| 4:G:46:ILE:CG2 | 4:G:66:MET:CE | 2.96 | 0.42 |
| 5:H:143:ILE:H | 5:H:143:ILE:CD1 | 2.23 | 0.42 |
| 5:H:41:ARG:NE | 5:H:61:ASP:HB2 | 2.30 | 0.42 |
| 1:A:142:ILE:N | 1:A:143:GLU:CA | 2.81 | 0.42 |
| 1:A:364:GLU:HG3 | 1:A:365:LYS:N | 2.34 | 0.42 |
| 1:A:373:LYS:CE | 1:A:374:ALA:HA | 2.49 | 0.42 |
| 1:A:376:MET:HA | 1:A:379:ARG:CZ | 2.50 | 0.42 |
| 2:D:94:LEU:O | 2:D:96:PRO:HA | 2.19 | 0.42 |
| 3:F:75:ILE:CG1 | 3:F:80:ILE:HG22 | 2.49 | 0.42 |
| 4:G:63:ASN:C | 5:H:140:ASN:ND2 | 2.68 | 0.42 |
| 5:H:46:GLU:HB3 | 5:H:151:VAL:HB | 1.99 | 0.42 |
| 5:H:26:PRO:O | 5:H:27:LEU:HD23 | 2.20 | 0.42 |
| 1:A:288:LEU:CD2 | 1:A:288:LEU:H | 2.30 | 0.42 |
| 1:A:361:PRO:O | 1:A:365:LYS:HB2 | 2.19 | 0.42 |
| 1:A:452:ASP:OD2 | 1:A:454:GLU:HB2 | 2.19 | 0.42 |
| 1:B:41:HIS:CD2 | 1:B:164:GLU:HB3 | 2.47 | 0.42 |
| 1:B:185:SER:HB3 | 1:B:195:GLN:NE2 | 2.35 | 0.42 |
| 1:B:247:PHE:CD1 | 1:B:247:PHE:N | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:425:ILE:CG2 | 1:B:426:VAL:N | 2.83 | 0.42 |
| 1:B:440:LYS:HE2 | 1:B:444:VAL:HG23 | 1.99 | 0.42 |
| 1:B:46:LEU:CD2 | 1:B:143:GLU:N | 2.82 | 0.42 |
| 2:C:84:THR:CB | 2:D:83:ALA:CB | 2.97 | 0.42 |
| 2:D:84:THR:HG23 | 2:D:85:GLU:H | 1.82 | 0.42 |
| 3:F:105:GLY:O | 4:G:38:ASP:N | 2.44 | 0.42 |
| 3:F:9:ILE:CG1 | 3:F:11:PHE:CE1 | 2.95 | 0.42 |
| 3:F:14:TYR:N | 3:F:73:ARG:HB3 | 2.34 | 0.42 |
| 3:F:68:ILE:CG1 | 3:F:69:ASP:N | 2.82 | 0.42 |
| 4:G:22:GLN:HG3 | 4:G:23:PRO:CD | 2.43 | 0.42 |
| 4:G:27:MET:N | 4:G:28:VAL:CA | 2.82 | 0.42 |
| 4:G:43:TYR:CE1 | 4:G:71:TRP:HB2 | 2.54 | 0.42 |
| 4:G:134:ASN:ND2 | 5:H:58:SER:O | 2.53 | 0.42 |
| 5:H:96:THR:CG2 | 5:H:97:VAL:H | 2.30 | 0.42 |
| 1:A:140:LYS:N | 1:A:257:LEU:CB | 2.82 | 0.42 |
| 1:A:177:ILE:HG23 | 1:A:241:ARG:HH22 | 1.85 | 0.42 |
| 1:A:425:ILE:CG2 | 1:A:426:VAL:N | 2.83 | 0.42 |
| 1:A:439:SER:HB3 | 1:A:442:THR:N | 2.34 | 0.42 |
| 1:A:447:ASN:ND2 | 1:A:449:PHE:CE1 | 2.87 | 0.42 |
| 1:B:138:SER:HB3 | 1:B:256:ASP:OD2 | 2.20 | 0.42 |
| 1:B:177:ILE:HG23 | 1:B:241:ARG:HH22 | 1.85 | 0.42 |
| 1:B:112:LYS:N | 1:B:401:LYS:HZ2 | 2.17 | 0.42 |
| 1:B:80:THR:CG2 | 1:B:81:ASN:N | 2.83 | 0.42 |
| 1:B:96:LYS:HD3 | 1:B:377:ALA:CB | 2.50 | 0.42 |
| 2:C:80:TYR:HA | 2:C:80:TYR:HD1 | 1.38 | 0.42 |
| 2:D:78:VAL:CG2 | 2:D:79:SER:N | 2.82 | 0.42 |
| 3:E:85:GLY:O | 3:E:87:PRO:HD3 | 2.19 | 0.42 |
| 3:F:12:GLN:HE21 | 3:F:75:ILE:HG12 | 1.82 | 0.42 |
| 3:F:76:TYR:HE2 | 3:F:79:LYS:HG2 | 1.84 | 0.42 |
| 5:H:111:ALA:HA | 5:H:132:LEU:CB | 2.49 | 0.42 |
| 5:H:150:ILE:O | 5:H:153:VAL:HG13 | 2.20 | 0.42 |
| 1:A:146:HIS:CG | 1:A:200:TYR:CD2 | 3.07 | 0.42 |
| 1:A:171:ASP:N | 1:A:178:LEU:CD2 | 2.83 | 0.42 |
| 1:A:147:PRO:HB2 | 1:A:229:HIS:NE2 | 2.33 | 0.42 |
| 1:A:138:SER:HB3 | 1:A:256:ASP:OD2 | 2.20 | 0.42 |
| 1:A:286:TYR:O | 1:A:321:ARG:HG2 | 2.20 | 0.42 |
| 1:A:441:GLU:HB2 | 1:B:462:GLU:CD | 2.39 | 0.42 |
| 1:A:48:LYS:CG | 1:A:49:GLY:N | 2.83 | 0.42 |
| 1:B:136:ASN:HB2 | 1:B:145:TRP:CH2 | 2.54 | 0.42 |
| 1:B:216:GLN:CG | 1:B:217:MET:N | 2.83 | 0.42 |
| 1:B:298:GLU:OE1 | 2:C:44:ASP:N | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:334:GLU:HG3 | 1:B:335:ARG:N | 2.35 | 0.42 |
| 1:B:345:GLN:CG | 1:B:346:ALA:H | 2.33 | 0.42 |
| 1:B:410:LEU:CB | 1:B:412:MET:CG | 2.95 | 0.42 |
| 1:B:439:SER:HB3 | 1:B:442:THR:N | 2.35 | 0.42 |
| 2:C:55:ILE:CG1 | 2:C:56:PHE:N | 2.82 | 0.42 |
| 2:C:97:TYR:O | 2:C:98:ARG:HB3 | 2.19 | 0.42 |
| 2:D:71:THR:N | 2:D:72:GLY:CA | 2.83 | 0.42 |
| 3:E:31:GLU:CA | 3:E:72:MET:SD | 3.07 | 0.42 |
| 3:F:45:GLU:CA | 3:F:47:TYR:CD1 | 2.96 | 0.42 |
| 3:F:65:ASP:CB | 3:F:68:ILE:CG2 | 2.95 | 0.42 |
| 5:H:29:PRO:HG2 | 5:H:31:TYR:CE2 | 2.55 | 0.42 |
| 5:H:53:ILE:C | 5:H:54:LEU:C | 2.78 | 0.42 |
| 1:A:159:ILE:HD13 | 1:A:160:PHE:C | 2.40 | 0.42 |
| 1:A:140:LYS:N | 1:A:257:LEU:HB3 | 2.34 | 0.42 |
| 1:A:320:LEU:HB2 | 1:A:321:ARG:C | 2.38 | 0.42 |
| 1:A:80:THR:CG2 | 1:A:81:ASN:N | 2.83 | 0.42 |
| 1:A:83:ARG:N | 1:A:83:ARG:CD | 2.83 | 0.42 |
| 1:B:106:THR:CG2 | 1:B:107:PHE:N | 2.83 | 0.42 |
| 1:B:171:ASP:N | 1:B:178:LEU:CD2 | 2.83 | 0.42 |
| 1:B:255:SER:HB3 | 1:B:259:PHE:CZ | 2.54 | 0.42 |
| 1:B:361:PRO:O | 1:B:365:LYS:HB2 | 2.19 | 0.42 |
| 1:B:373:LYS:CE | 1:B:374:ALA:HA | 2.49 | 0.42 |
| 1:B:96:LYS:CE | 1:B:377:ALA:HA | 2.36 | 0.42 |
| 1:B:452:ASP:OD2 | 1:B:454:GLU:HB2 | 2.19 | 0.42 |
| 2:C:84:THR:CG2 | 2:C:85:GLU:N | 2.82 | 0.42 |
| 2:C:98:ARG:HH22 | 2:D:102:ARG:HG2 | 1.81 | 0.42 |
| 2:D:59:LYS:CB | 2:D:90:ILE:HD13 | 2.50 | 0.42 |
| 3:E:8:VAL:HG11 | 3:E:33:THR:HG22 | 2.01 | 0.42 |
| 3:E:84:ILE:CD1 | 3:E:84:ILE:N | 2.83 | 0.42 |
| 2:D:5:ARG:CB | 3:F:2:TYR:HB2 | 2.46 | 0.42 |
| 5:H:22:THR:CG2 | 5:H:24:SER:H | 2.32 | 0.42 |
| 5:H:44:PHE:CZ | 5:H:60:ALA:CB | 3.02 | 0.42 |
| 1:A:106:THR:CG2 | 1:A:107:PHE:N | 2.83 | 0.42 |
| 1:A:150:ASP:OD2 | 1:A:152:GLU:HG3 | 2.20 | 0.42 |
| 1:A:270:ILE:HD13 | 1:B:275:MET:SD | 2.60 | 0.42 |
| 1:A:46:LEU:CD2 | 1:A:143:GLU:N | 2.82 | 0.42 |
| 1:A:69:ALA:N | 1:B:300:THR:HG22 | 2.28 | 0.42 |
| 1:B:150:ASP:OD2 | 1:B:152:GLU:HG3 | 2.20 | 0.42 |
| 1:B:230:MET:SD | 1:B:239:TRP:NE1 | 2.91 | 0.42 |
| 1:B:243:PRO:HA | 1:B:244:ILE:HA | 1.53 | 0.42 |
| 1:B:350:SER:OG | 1:B:351:PRO:HD2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:417:THR:CB | 1:B:418:ARG:CA | 2.95 | 0.42 |
| 2:C:59:LYS:CB | 2:C:90:ILE:HD13 | 2.50 | 0.42 |
| 3:E:24:LYS:HG2 | 3:E:25:THR:N | 2.35 | 0.42 |
| 3:F:42:SER:C | 3:F:43:GLN:HG3 | 2.40 | 0.42 |
| 3:F:6:ARG:HD2 | 3:F:33:THR:CG2 | 2.49 | 0.42 |
| 3:F:70:LYS:HE2 | 3:F:71:LYS:HB2 | 2.02 | 0.42 |
| 4:G:134:ASN:HB2 | 5:H:138:LEU:O | 2.15 | 0.42 |
| 1:A:149:VAL:CG2 | 1:A:227:ARG:HD3 | 2.49 | 0.42 |
| 1:A:211:ILE:CG1 | 1:A:212:ASP:N | 2.83 | 0.42 |
| 1:A:440:LYS:HE2 | 1:A:444:VAL:HG23 | 2.00 | 0.42 |
| 1:A:89:HIS:CE1 | 1:A:257:LEU:CD1 | 3.03 | 0.42 |
| 1:B:134:VAL:CG2 | 1:B:135:LYS:N | 2.83 | 0.42 |
| 1:B:37:LEU:O | 1:B:166:ILE:HD12 | 2.19 | 0.42 |
| 1:B:286:TYR:O | 1:B:321:ARG:HG2 | 2.20 | 0.42 |
| 1:A:438:MET:CE | 1:B:433:VAL:C | 2.88 | 0.42 |
| 1:B:43:PRO:HB2 | 1:B:47:LEU:HD12 | 2.00 | 0.42 |
| 1:B:447:ASN:ND2 | 1:B:449:PHE:CE1 | 2.87 | 0.42 |
| 1:B:67:TYR:N | 1:B:67:TYR:CD1 | 2.83 | 0.42 |
| 2:C:49:ILE:HD11 | 2:C:54:LEU:HG | 2.01 | 0.42 |
| 2:C:90:ILE:HG23 | 2:D:96:PRO:CG | 2.48 | 0.42 |
| 3:E:41:ILE:CG2 | 3:E:42:SER:H | 2.29 | 0.42 |
| 3:E:83:PHE:CD2 | 3:E:99:ILE:CD1 | 3.02 | 0.42 |
| 3:F:17:GLN:CB | 3:F:19:ASN:HD21 | 2.25 | 0.42 |
| 3:E:37:HIS:HB2 | 3:F:89:ASP:CG | 2.40 | 0.42 |
| 4:G:68:PHE:N | 4:G:68:PHE:HD1 | 2.18 | 0.42 |
| 5:H:22:THR:C | 5:H:24:SER:H | 2.22 | 0.42 |
| 1:A:108:THR:CG2 | 1:A:412:MET:CE | 2.95 | 0.42 |
| 1:A:201:THR:CG2 | 1:A:202:ASP:N | 2.82 | 0.42 |
| 1:A:350:SER:OG | 1:A:351:PRO:HD2 | 2.20 | 0.42 |
| 1:A:65:THR:HB | 1:A:73:GLN:CG | 2.49 | 0.42 |
| 1:B:227:ARG:HD2 | 1:B:227:ARG:O | 2.19 | 0.42 |
| 1:B:288:LEU:O | 1:B:288:LEU:HG | 2.19 | 0.42 |
| 1:B:130:LEU:CD1 | 1:B:388:PHE:CE2 | 2.98 | 0.42 |
| 1:B:66:TYR:N | 1:B:66:TYR:HD1 | 2.12 | 0.42 |
| 1:B:310:LYS:O | 2:C:38:ASN:ND2 | 2.52 | 0.42 |
| 2:C:87:PRO:HB3 | 2:C:90:ILE:CA | 2.49 | 0.42 |
| 2:D:29:VAL:HG22 | 2:D:50:PRO:CG | 2.48 | 0.42 |
| 2:D:75:MET:N | 2:D:78:VAL:CG1 | 2.83 | 0.42 |
| 2:D:97:TYR:O | 2:D:98:ARG:HB3 | 2.19 | 0.42 |
| 3:F:87:PRO:HB3 | 3:F:97:THR:HG21 | 2.01 | 0.42 |
| 2:D:70:LEU:HD23 | 3:F:91:SER:HB2 | 1.28 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:F:97:THR:CG2 | 3:F:98:ARG:N | 2.83 | 0.42 |
| 4:G:100:PHE:CZ | 5:H:45:ASP:CB | 2.59 | 0.42 |
| 4:G:49:GLN:HA | 4:G:69:HIS:HE2 | 1.85 | 0.42 |
| 5:H:122:VAL:CG1 | 5:H:125:ALA:H | 2.30 | 0.42 |
| 5:H:21:ALA:C | 5:H:23:GLY:H | 2.23 | 0.42 |
| 1:A:146:HIS:CB | 1:A:244:ILE:CG2 | 2.98 | 0.42 |
| 1:A:38:ILE:HD12 | 1:A:183:TYR:HD2 | 1.84 | 0.42 |
| 1:B:201:THR:CG2 | 1:B:202:ASP:N | 2.82 | 0.42 |
| 1:B:367:TYR:N | 1:B:368:ALA:CA | 2.82 | 0.42 |
| 2:C:84:THR:HG23 | 2:C:85:GLU:H | 1.82 | 0.42 |
| 2:D:73:ARG:NE | 3:F:91:SER:CB | 2.80 | 0.42 |
| 3:E:12:GLN:HB3 | 3:E:28:TRP:CB | 2.50 | 0.42 |
| 3:E:47:TYR:CB | 3:E:50:GLN:HB2 | 2.41 | 0.42 |
| 3:E:70:LYS:HE2 | 3:E:85:GLY:C | 2.40 | 0.42 |
| 3:F:11:PHE:HE2 | 3:F:68:ILE:HG21 | 1.85 | 0.42 |
| 3:F:47:TYR:CB | 3:F:50:GLN:CB | 2.95 | 0.42 |
| 3:F:60:ILE:CG2 | 3:F:83:PHE:CD2 | 3.03 | 0.42 |
| 3:F:75:ILE:HG21 | 3:F:78:GLY:CA | 2.50 | 0.42 |
| 5:H:126:VAL:HG13 | 5:H:126:VAL:O | 2.20 | 0.42 |
| 4:G:61:GLY:O | 5:H:140:ASN:OD1 | 2.38 | 0.42 |
| 5:H:21:ALA:CB | 5:H:150:ILE:HA | 2.50 | 0.42 |
| 5:H:37:VAL:CG1 | 5:H:63:GLY:CA | 2.95 | 0.42 |
| 5:H:61:ASP:O | 5:H:62:SER:HB3 | 2.20 | 0.42 |
| 1:A:149:VAL:CG1 | 1:A:227:ARG:CZ | 2.98 | 0.41 |
| 1:A:215:TYR:HD1 | 1:A:215:TYR:HA | 1.36 | 0.41 |
| 1:A:216:GLN:CG | 1:A:217:MET:N | 2.83 | 0.41 |
| 1:A:227:ARG:HD2 | 1:A:227:ARG:O | 2.19 | 0.41 |
| 1:A:278:PHE:HD1 | 1:A:278:PHE:HA | 1.66 | 0.41 |
| 1:A:345:GLN:CG | 1:A:346:ALA:H | 2.33 | 0.41 |
| 1:A:367:TYR:N | 1:A:368:ALA:CA | 2.82 | 0.41 |
| 1:A:439:SER:CB | 1:A:442:THR:N | 2.82 | 0.41 |
| 1:A:67:TYR:CD1 | 1:A:67:TYR:N | 2.83 | 0.41 |
| 1:B:146:HIS:CG | 1:B:200:TYR:CD2 | 3.07 | 0.41 |
| 1:B:211:ILE:CG1 | 1:B:212:ASP:N | 2.83 | 0.41 |
| 1:B:292:ASP:HB3 | 1:B:293:GLY:C | 2.40 | 0.41 |
| 1:B:320:LEU:HB2 | 1:B:321:ARG:C | 2.39 | 0.41 |
| 2:C:33:LYS:HE3 | 2:C:50:PRO:HG3 | 2.02 | 0.41 |
| 1:B:313:GLY:CA | 2:C:51:SER:H | 2.24 | 0.41 |
| 2:C:5:ARG:CD | 2:C:7:LYS:HE3 | 2.50 | 0.41 |
| 2:D:5:ARG:CD | 2:D:7:LYS:HE3 | 2.50 | 0.41 |
| 3:E:29:VAL:CG1 | 3:E:72:MET:CB | 2.97 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:107:LEU:HD23 | 4:G:107:LEU:HA | 1.80 | 0.41 |
| 4:G:128:ARG:N | 4:G:128:ARG:CD | 2.83 | 0.41 |
| 4:G:28:VAL:HG12 | 4:G:28:VAL:H | 1.52 | 0.41 |
| 5:H:118:TYR:HA | 5:H:118:TYR:HD1 | 1.43 | 0.41 |
| 5:H:10:ASP:CG | 5:H:167:THR:HG21 | 2.39 | 0.41 |
| 5:H:39:GLY:HA2 | 5:H:43:LEU:CG | 2.49 | 0.41 |
| 1:A:171:ASP:HB2 | 1:A:178:LEU:CD1 | 2.39 | 0.41 |
| 1:A:190:MET:HE2 | 1:A:190:MET:HB2 | 1.91 | 0.41 |
| 1:A:292:ASP:HA | 1:A:293:GLY:HA3 | 1.73 | 0.41 |
| 1:A:29:PRO:HG3 | 1:A:170:LYS:HZ2 | 1.83 | 0.41 |
| 1:A:335:ARG:HB2 | 1:B:330:ALA:HB1 | 2.02 | 0.41 |
| 1:A:334:GLU:HG3 | 1:A:335:ARG:N | 2.35 | 0.41 |
| 1:A:433:VAL:CG1 | 1:A:434:THR:N | 2.83 | 0.41 |
| 1:A:66:TYR:N | 1:A:66:TYR:HD1 | 2.12 | 0.41 |
| 1:B:149:VAL:CG1 | 1:B:227:ARG:CZ | 2.98 | 0.41 |
| 1:B:433:VAL:CG1 | 1:B:434:THR:N | 2.83 | 0.41 |
| 2:D:95:ASN:HB2 | 2:D:98:ARG:HA | 2.01 | 0.41 |
| 3:E:29:VAL:CG1 | 3:E:72:MET:CA | 2.95 | 0.41 |
| 3:E:72:MET:HE2 | 3:E:72:MET:HB3 | 1.78 | 0.41 |
| 3:E:87:PRO:HB3 | 3:E:97:THR:CG2 | 2.50 | 0.41 |
| 3:E:58:TYR:CA | 3:F:100:LYS:HD3 | 2.49 | 0.41 |
| 3:F:64:TYR:HD1 | 3:F:64:TYR:HA | 1.53 | 0.41 |
| 3:E:104:ASP:OD2 | 4:G:43:TYR:CE1 | 2.73 | 0.41 |
| 4:G:63:ASN:C | 4:G:64:ILE:HD12 | 2.40 | 0.41 |
| 4:G:82:ILE:CG1 | 4:G:83:SER:N | 2.83 | 0.41 |
| 5:H:17:SER:CA | 5:H:23:GLY:HA3 | 2.40 | 0.41 |
| 5:H:29:PRO:CG | 5:H:31:TYR:CE2 | 3.04 | 0.41 |
| 1:A:158:VAL:HG11 | 1:A:160:PHE:CE1 | 2.55 | 0.41 |
| 1:A:185:SER:HB3 | 1:A:195:GLN:NE2 | 2.35 | 0.41 |
| 1:A:251:GLU:C | 1:B:54:MET:SD | 2.96 | 0.41 |
| 1:A:387:LEU:CD1 | 1:A:391:PHE:CZ | 3.03 | 0.41 |
| 1:A:456:GLU:O | 1:A:460:ILE:HG12 | 2.21 | 0.41 |
| 1:B:100:LEU:O | 1:B:100:LEU:HD13 | 2.20 | 0.41 |
| 1:B:146:HIS:CB | 1:B:244:ILE:CG2 | 2.98 | 0.41 |
| 1:B:159:ILE:HD13 | 1:B:160:PHE:C | 2.40 | 0.41 |
| 1:B:163:GLU:HA | 1:B:163:GLU:OE1 | 2.19 | 0.41 |
| 1:B:289:LYS:HD2 | 1:B:319:THR:HG23 | 1.94 | 0.41 |
| 1:B:376:MET:HA | 1:B:379:ARG:CZ | 2.50 | 0.41 |
| 1:B:65:THR:HB | 1:B:73:GLN:CG | 2.49 | 0.41 |
| 1:B:89:HIS:CE1 | 1:B:257:LEU:CD1 | 3.03 | 0.41 |
| 2:C:39:PRO:O | 2:C:40:PHE:CG | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:57:VAL:CG2 | 2:C:58:ALA:N | 2.83 | 0.41 |
| 2:C:75:MET:H | 2:C:78:VAL:CG1 | 2.33 | 0.41 |
| 2:D:33:LYS:HE3 | 2:D:50:PRO:HG3 | 2.02 | 0.41 |
| 2:D:57:VAL:CG2 | 2:D:58:ALA:N | 2.83 | 0.41 |
| 2:D:59:LYS:CD | 2:D:90:ILE:CD1 | 2.95 | 0.41 |
| 3:E:38:VAL:HG11 | 3:F:86:ASP:OD2 | 2.20 | 0.41 |
| 3:E:41:ILE:CG2 | 3:E:42:SER:N | 2.82 | 0.41 |
| 3:E:74:VAL:HG11 | 3:E:76:TYR:CE1 | 2.52 | 0.41 |
| 3:E:47:TYR:CE2 | 3:F:53:GLN:NE2 | 2.88 | 0.41 |
| 4:G:103:VAL:CG1 | 4:G:104:ALA:N | 2.83 | 0.41 |
| 4:G:33:GLU:N | 4:G:45:VAL:HA | 2.35 | 0.41 |
| 4:G:76:ARG:CZ | 4:G:76:ARG:N | 2.83 | 0.41 |
| 4:G:86:VAL:CG1 | 4:G:87:LEU:N | 2.83 | 0.41 |
| 5:H:145:THR:CG2 | 5:H:146:LEU:N | 2.83 | 0.41 |
| 5:H:17:SER:HB3 | 5:H:91:PHE:HD1 | 1.85 | 0.41 |
| 5:H:18:ILE:HG12 | 5:H:23:GLY:CA | 2.50 | 0.41 |
| 1:A:121:LEU:HB3 | 1:A:122:ALA:C | 2.40 | 0.41 |
| 1:A:441:GLU:CG | 1:A:456:GLU:CB | 2.95 | 0.41 |
| 1:A:442:THR:OG1 | 1:B:459:ARG:CB | 2.66 | 0.41 |
| 1:B:34:ILE:HG23 | 1:B:181:LEU:HD22 | 2.00 | 0.41 |
| 1:B:373:LYS:CD | 1:B:374:ALA:N | 2.83 | 0.41 |
| 1:B:373:LYS:CE | 1:B:374:ALA:CA | 2.99 | 0.41 |
| 1:B:456:GLU:O | 1:B:460:ILE:HG12 | 2.21 | 0.41 |
| 1:B:48:LYS:CG | 1:B:49:GLY:N | 2.83 | 0.41 |
| 2:C:71:THR:N | 2:C:72:GLY:CA | 2.83 | 0.41 |
| 3:E:84:ILE:HD11 | 3:E:103:GLU:HG2 | 1.96 | 0.41 |
| 3:E:62:THR:HG21 | 3:E:68:ILE:HD11 | 2.02 | 0.41 |
| 3:F:14:TYR:CE2 | 3:F:28:TRP:CZ2 | 3.09 | 0.41 |
| 3:F:81:VAL:CG2 | 3:F:82:THR:N | 2.83 | 0.41 |
| 4:G:64:ILE:CD1 | 4:G:64:ILE:N | 2.83 | 0.41 |
| 5:H:134:VAL:HG22 | 5:H:135:ILE:N | 2.34 | 0.41 |
| 4:G:64:ILE:HD11 | 5:H:140:ASN:OD1 | 2.16 | 0.41 |
| 5:H:147:PRO:O | 5:H:151:VAL:HG23 | 2.20 | 0.41 |
| 5:H:162:GLN:HB2 | 5:H:163:PRO:CD | 2.39 | 0.41 |
| 5:H:21:ALA:HB1 | 5:H:108:PHE:CD2 | 2.54 | 0.41 |
| 1:A:183:TYR:CB | 1:A:197:ALA:CA | 2.97 | 0.41 |
| 1:A:149:VAL:CG2 | 1:A:227:ARG:CD | 2.95 | 0.41 |
| 1:A:334:GLU:CG | 1:A:335:ARG:N | 2.84 | 0.41 |
| 1:A:61:LYS:NZ | 1:A:61:LYS:HB3 | 2.35 | 0.41 |
| 1:B:334:GLU:CG | 1:B:335:ARG:N | 2.84 | 0.41 |
| 1:B:89:HIS:HB2 | 1:B:264:ILE:CD1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:49:ILE:CD1 | 2:C:54:LEU:CD1 | 2.95 | 0.41 |
| 2:C:95:ASN:HB2 | 2:C:98:ARG:HA | 2.01 | 0.41 |
| 2:C:100:MET:CE | 2:D:100:MET:HG3 | 2.50 | 0.41 |
| 2:D:69:GLY:HA3 | 2:D:73:ARG:CB | 2.27 | 0.41 |
| 2:D:70:LEU:HD23 | 2:D:73:ARG:HG2 | 1.96 | 0.41 |
| 2:D:75:MET:H | 2:D:78:VAL:CG1 | 2.33 | 0.41 |
| 2:D:84:THR:CG2 | 2:D:85:GLU:N | 2.82 | 0.41 |
| 3:E:47:TYR:HB3 | 3:E:50:GLN:HG3 | 1.99 | 0.41 |
| 3:E:62:THR:N | 3:E:65:ASP:HB2 | 2.35 | 0.41 |
| 3:E:40:PRO:CB | 3:F:100:LYS:HA | 2.51 | 0.41 |
| 2:D:5:ARG:HB3 | 3:F:2:TYR:C | 2.41 | 0.41 |
| 3:F:62:THR:HG22 | 3:F:65:ASP:OD1 | 2.20 | 0.41 |
| 3:F:75:ILE:CG2 | 3:F:76:TYR:N | 2.83 | 0.41 |
| 3:F:60:ILE:HG23 | 3:F:83:PHE:HD2 | 1.85 | 0.41 |
| 3:E:37:HIS:HD2 | 3:F:88:VAL:HB | 1.73 | 0.41 |
| 5:H:113:ILE:CG2 | 5:H:114:GLU:N | 2.83 | 0.41 |
| 4:G:64:ILE:N | 5:H:140:ASN:HD21 | 2.19 | 0.41 |
| 5:H:15:PHE:CD1 | 5:H:15:PHE:C | 2.94 | 0.41 |
| 5:H:54:LEU:CD1 | 5:H:54:LEU:N | 2.84 | 0.41 |
| 5:H:59:VAL:CG1 | 5:H:60:ALA:N | 2.83 | 0.41 |
| 5:H:31:TYR:CE1 | 5:H:70:LYS:HG3 | 2.53 | 0.41 |
| 1:A:100:LEU:HD13 | 1:A:100:LEU:O | 2.20 | 0.41 |
| 1:A:373:LYS:CD | 1:A:374:ALA:N | 2.83 | 0.41 |
| 1:A:91:LEU:N | 1:A:91:LEU:CD1 | 2.83 | 0.41 |
| 1:B:101:VAL:CG2 | 1:B:102:GLY:N | 2.82 | 0.41 |
| 1:B:181:LEU:HG | 1:B:181:LEU:O | 2.21 | 0.41 |
| 1:B:387:LEU:CD1 | 1:B:391:PHE:CZ | 3.03 | 0.41 |
| 2:C:59:LYS:HD3 | 2:C:90:ILE:CB | 2.50 | 0.41 |
| 2:D:41:ILE:CG2 | 2:D:42:ASP:N | 2.83 | 0.41 |
| 3:E:64:TYR:HA | 3:E:64:TYR:HD1 | 1.35 | 0.41 |
| 3:F:106:ALA:N | 4:G:38:ASP:C | 2.53 | 0.41 |
| 3:F:68:ILE:HG12 | 3:F:69:ASP:N | 2.33 | 0.41 |
| 3:E:109:GLY:N | 4:G:113:ILE:CD1 | 2.84 | 0.41 |
| 4:G:32:THR:HG23 | 4:G:36:GLY:O | 2.20 | 0.41 |
| 4:G:96:MET:HG2 | 4:G:97:PHE:O | 2.19 | 0.41 |
| 5:H:33:THR:O | 5:H:34:ASP:HB3 | 2.20 | 0.41 |
| 1:A:100:LEU:HG | 1:A:377:ALA:CB | 2.42 | 0.41 |
| 1:A:136:ASN:HB2 | 1:A:145:TRP:CH2 | 2.54 | 0.41 |
| 1:A:235:GLN:CG | 1:A:236:ALA:N | 2.84 | 0.41 |
| 1:A:439:SER:OG | 1:B:459:ARG:HD2 | 2.20 | 0.41 |
| 1:A:62:LYS:CG | 1:A:63:ARG:N | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:HIS:HB2 | 1:A:264:ILE:CD1 | 2.51 | 0.41 |
| 1:B:167:VAL:CA | 1:B:177:ILE:HD12 | 2.50 | 0.41 |
| 1:B:227:ARG:HD2 | 1:B:227:ARG:C | 2.41 | 0.41 |
| 1:A:69:ALA:HB1 | 1:B:296:PRO:HB2 | 2.03 | 0.41 |
| 1:B:419:ILE:CG2 | 1:B:420:GLN:N | 2.83 | 0.41 |
| 1:B:46:LEU:HD21 | 1:B:144:TYR:H | 1.86 | 0.41 |
| 1:B:61:LYS:NZ | 1:B:61:LYS:HB3 | 2.35 | 0.41 |
| 1:B:84:THR:CG2 | 1:B:85:SER:N | 2.84 | 0.41 |
| 1:B:91:LEU:N | 1:B:91:LEU:CD1 | 2.83 | 0.41 |
| 2:C:29:VAL:HG22 | 2:C:50:PRO:CG | 2.48 | 0.41 |
| 2:C:35:GLU:HB3 | 2:C:37:HIS:ND1 | 2.36 | 0.41 |
| 2:C:59:LYS:CD | 2:C:90:ILE:CD1 | 2.95 | 0.41 |
| 3:E:109:GLY:N | 4:G:71:TRP:HE1 | 2.14 | 0.41 |
| 3:F:13:SER:HB2 | 3:F:29:VAL:HG23 | 2.03 | 0.41 |
| 3:F:38:VAL:CG2 | 3:F:60:ILE:HB | 2.51 | 0.41 |
| 3:F:60:ILE:HD12 | 3:F:83:PHE:CE2 | 2.53 | 0.41 |
| 4:G:119:VAL:CG1 | 4:G:120:THR:N | 2.83 | 0.41 |
| 5:H:13:TYR:O | 5:H:31:TYR:HA | 2.21 | 0.41 |
| 1:A:167:VAL:CA | 1:A:177:ILE:HD12 | 2.50 | 0.41 |
| 1:A:289:LYS:HG3 | 1:B:316:GLY:H | 1.66 | 0.41 |
| 1:A:292:ASP:HB3 | 1:A:293:GLY:C | 2.40 | 0.41 |
| 1:A:46:LEU:HD21 | 1:A:144:TYR:H | 1.86 | 0.41 |
| 1:A:53:TYR:HA | 1:A:261:LYS:HZ1 | 1.86 | 0.41 |
| 1:B:183:TYR:CB | 1:B:197:ALA:CA | 2.97 | 0.41 |
| 1:B:215:TYR:HA | 1:B:215:TYR:HD1 | 1.36 | 0.41 |
| 1:B:235:GLN:CG | 1:B:236:ALA:N | 2.84 | 0.41 |
| 1:B:306:HIS:CE1 | 2:C:39:PRO:CG | 3.03 | 0.41 |
| 1:B:38:ILE:HD12 | 1:B:183:TYR:HD2 | 1.84 | 0.41 |
| 1:B:417:THR:H | 1:B:418:ARG:HA | 1.85 | 0.41 |
| 2:C:56:PHE:HA | 2:C:59:LYS:HZ2 | 1.79 | 0.41 |
| 2:D:4:GLN:OE1 | 3:F:2:TYR:CB | 2.68 | 0.41 |
| 3:E:37:HIS:ND1 | 3:E:61:TYR:CD2 | 2.86 | 0.41 |
| 3:E:70:LYS:CD | 3:E:85:GLY:N | 2.83 | 0.41 |
| 3:F:14:TYR:CB | 3:F:73:ARG:CD | 2.95 | 0.41 |
| 3:F:73:ARG:CG | 3:F:74:VAL:N | 2.84 | 0.41 |
| 5:H:92:TRP:HZ3 | 5:H:106:ALA:HB3 | 1.84 | 0.41 |
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CE2 | 2.55 | 0.41 |
| 1:A:130:LEU:HD22 | 1:A:388:PHE:CD2 | 2.55 | 0.41 |
| 1:A:149:VAL:HG21 | 1:A:227:ARG:HD3 | 2.02 | 0.41 |
| 1:A:177:ILE:HG21 | 1:A:246:PRO:CD | 2.51 | 0.41 |
| 1:A:288:LEU:CD2 | 1:B:310:LYS:HZ2 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:376:MET:HG3 | 1:A:377:ALA:N | 2.30 | 0.41 |
| 1:A:376:MET:CB | 1:A:379:ARG:CZ | 2.96 | 0.41 |
| 1:A:419:ILE:CG2 | 1:A:420:GLN:N | 2.83 | 0.41 |
| 1:A:74:LEU:HD11 | 1:B:304:ARG:NH2 | 2.35 | 0.41 |
| 1:A:84:THR:CG2 | 1:A:85:SER:N | 2.84 | 0.41 |
| 1:B:291:TYR:HB3 | 1:B:312:SER:C | 2.40 | 0.41 |
| 1:B:96:LYS:HG3 | 1:B:373:LYS:HB2 | 1.97 | 0.41 |
| 2:C:54:LEU:C | 2:C:57:VAL:HG22 | 2.41 | 0.41 |
| 2:D:35:GLU:HB3 | 2:D:37:HIS:ND1 | 2.36 | 0.41 |
| 3:E:37:HIS:CG | 3:E:38:VAL:N | 2.87 | 0.41 |
| 3:F:75:ILE:CG2 | 3:F:78:GLY:CA | 2.99 | 0.41 |
| 2:D:12:ILE:HG12 | 3:F:93:LEU:HG | 2.03 | 0.41 |
| 5:H:143:ILE:H | 5:H:144:ASP:HA | 1.84 | 0.41 |
| 5:H:14:LEU:HD21 | 5:H:160:PHE:CZ | 2.55 | 0.41 |
| 5:H:43:LEU:CD1 | 5:H:43:LEU:N | 2.83 | 0.41 |
| 1:A:285:VAL:CG1 | 1:A:287:VAL:CG2 | 2.95 | 0.41 |
| 1:A:290:ASN:CB | 1:A:291:TYR:HA | 2.49 | 0.41 |
| 1:A:42:ASN:HA | 1:A:43:PRO:HD3 | 1.81 | 0.41 |
| 1:B:121:LEU:HB3 | 1:B:122:ALA:C | 2.40 | 0.41 |
| 1:B:171:ASP:HB2 | 1:B:178:LEU:CD1 | 2.39 | 0.41 |
| 1:B:376:MET:CB | 1:B:379:ARG:CZ | 2.96 | 0.41 |
| 2:C:41:ILE:CG2 | 2:C:42:ASP:N | 2.83 | 0.41 |
| 2:C:75:MET:N | 2:C:78:VAL:CG1 | 2.83 | 0.41 |
| 2:D:54:LEU:C | 2:D:57:VAL:HG22 | 2.41 | 0.41 |
| 2:D:87:PRO:HB3 | 2:D:90:ILE:CA | 2.49 | 0.41 |
| 3:E:6:ARG:HE | 3:E:6:ARG:HA | 1.86 | 0.41 |
| 2:C:73:ARG:CG | 3:E:91:SER:CB | 2.99 | 0.41 |
| 3:E:89:ASP:HB2 | 3:E:95:GLU:HB3 | 2.01 | 0.41 |
| 3:F:51:GLN:HG3 | 3:F:52:LEU:N | 2.36 | 0.41 |
| 3:E:37:HIS:CD2 | 3:F:89:ASP:N | 2.87 | 0.41 |
| 3:E:1:MET:HB3 | 3:F:93:LEU:HD13 | 2.03 | 0.41 |
| 4:G:43:TYR:CG | 4:G:43:TYR:O | 2.74 | 0.41 |
| 4:G:91:THR:C | 4:G:93:LYS:H | 2.24 | 0.41 |
| 5:H:98:LYS:HG3 | 5:H:98:LYS:O | 2.20 | 0.41 |
| 1:A:260:TYR:N | 1:A:260:TYR:CD1 | 2.82 | 0.41 |
| 1:A:373:LYS:HD2 | 1:A:374:ALA:N | 2.36 | 0.41 |
| 1:A:410:LEU:N | 1:A:411:THR:CA | 2.82 | 0.41 |
| 1:B:227:ARG:NE | 1:B:227:ARG:H | 2.19 | 0.41 |
| 1:B:29:PRO:HG3 | 1:B:170:LYS:HZ2 | 1.84 | 0.41 |
| 1:B:410:LEU:N | 1:B:411:THR:CA | 2.83 | 0.41 |
| 1:B:441:GLU:CG | 1:B:456:GLU:CB | 2.95 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:456:GLU:O | 1:B:467:TYR:CD2 | 2.63 | 0.41 |
| 1:B:52:TYR:HE1 | 1:B:56:GLU:HB2 | 1.84 | 0.41 |
| 2:D:28:LEU:O | 2:D:31:PHE:CE1 | 2.74 | 0.41 |
| 2:D:27:LEU:O | 2:D:31:PHE:CE1 | 2.74 | 0.41 |
| 2:D:29:VAL:HG21 | 2:D:50:PRO:CD | 2.51 | 0.41 |
| 2:D:49:ILE:HA | 2:D:50:PRO:HD3 | 1.84 | 0.41 |
| 3:E:98:ARG:HD2 | 3:E:98:ARG:N | 2.35 | 0.41 |
| 3:E:40:PRO:HG3 | 3:F:100:LYS:CA | 2.51 | 0.41 |
| 3:E:47:TYR:CZ | 3:F:53:GLN:NE2 | 2.89 | 0.41 |
| 3:F:61:TYR:CG | 3:F:61:TYR:O | 2.74 | 0.41 |
| 3:F:83:PHE:N | 3:F:83:PHE:CD1 | 2.83 | 0.41 |
| 4:G:21:TYR:CZ | 4:G:23:PRO:HG2 | 2.56 | 0.41 |
| 4:G:92:TYR:CG | 4:G:92:TYR:O | 2.74 | 0.41 |
| 5:H:117:GLU:OE1 | 5:H:117:GLU:HA | 2.21 | 0.41 |
| 5:H:21:ALA:CB | 5:H:150:ILE:CG1 | 2.95 | 0.41 |
| 5:H:97:VAL:HG22 | 5:H:97:VAL:O | 2.20 | 0.41 |
| 1:A:291:TYR:HB3 | 1:A:312:SER:C | 2.40 | 0.40 |
| 1:A:373:LYS:CE | 1:A:374:ALA:CA | 2.99 | 0.40 |
| 1:A:69:ALA:HB2 | 1:B:300:THR:CG2 | 2.51 | 0.40 |
| 1:B:136:ASN:CB | 1:B:145:TRP:CZ3 | 3.05 | 0.40 |
| 1:B:184:TYR:CE1 | 1:B:198:GLU:OE2 | 2.75 | 0.40 |
| 1:B:96:LYS:CE | 1:B:377:ALA:CB | 2.99 | 0.40 |
| 1:B:418:ARG:CB | 1:B:421:ASN:CB | 2.95 | 0.40 |
| 2:C:29:VAL:HG21 | 2:C:50:PRO:CD | 2.51 | 0.40 |
| 2:D:13:THR:CG2 | 2:D:14:ASN:N | 2.83 | 0.40 |
| 2:D:39:PRO:O | 2:D:40:PHE:CG | 2.74 | 0.40 |
| 2:C:5:ARG:HH21 | 3:E:2:TYR:HB3 | 1.86 | 0.40 |
| 3:E:29:VAL:CG1 | 3:E:72:MET:HE3 | 2.51 | 0.40 |
| 3:F:75:ILE:HG13 | 3:F:79:LYS:O | 2.20 | 0.40 |
| 5:H:108:PHE:HB2 | 5:H:150:ILE:CG2 | 2.50 | 0.40 |
| 5:H:143:ILE:CG1 | 5:H:147:PRO:HD2 | 2.51 | 0.40 |
| 5:H:18:ILE:N | 5:H:23:GLY:HA3 | 2.36 | 0.40 |
| 5:H:89:ILE:HG21 | 5:H:91:PHE:HE1 | 1.84 | 0.40 |
| 1:A:181:LEU:O | 1:A:181:LEU:HG | 2.21 | 0.40 |
| 1:A:163:GLU:OE2 | 1:A:183:TYR:CD2 | 2.75 | 0.40 |
| 1:A:184:TYR:O | 1:A:184:TYR:CD1 | 2.75 | 0.40 |
| 1:A:369:LEU:HD12 | 1:A:369:LEU:N | 2.35 | 0.40 |
| 1:A:52:TYR:CD2 | 1:A:265:ASP:OD2 | 2.75 | 0.40 |
| 1:A:89:HIS:CE1 | 1:A:257:LEU:CG | 3.03 | 0.40 |
| 1:B:183:TYR:HB3 | 1:B:197:ALA:HB2 | 2.01 | 0.40 |
| 1:B:393:ALA:O | 1:B:396:LEU:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:6:VAL:HG23 | 3:E:3:GLU:HG3 | 2.03 | 0.40 |
| 2:D:65:MET:HG3 | 2:D:66:THR:N | 2.36 | 0.40 |
| 3:F:37:HIS:O | 3:F:61:TYR:CD2 | 2.74 | 0.40 |
| 5:H:112:TYR:CG | 5:H:133:GLN:O | 2.75 | 0.40 |
| 4:G:61:GLY:CA | 5:H:139:LYS:H | 2.34 | 0.40 |
| 5:H:13:TYR:CD1 | 5:H:32:GLN:O | 2.75 | 0.40 |
| 5:H:37:VAL:CG1 | 5:H:38:SER:N | 2.82 | 0.40 |
| 5:H:22:THR:O | 5:H:92:TRP:CD1 | 2.74 | 0.40 |
| 1:A:227:ARG:H | 1:A:227:ARG:NE | 2.19 | 0.40 |
| 1:A:64:ARG:HH21 | 1:B:284:ILE:HG12 | 1.86 | 0.40 |
| 1:A:66:TYR:OH | 1:B:304:ARG:HD2 | 2.21 | 0.40 |
| 1:A:74:LEU:CD1 | 1:B:304:ARG:CZ | 2.99 | 0.40 |
| 1:B:183:TYR:HB2 | 1:B:197:ALA:CA | 2.52 | 0.40 |
| 1:B:52:TYR:CD2 | 1:B:265:ASP:OD2 | 2.75 | 0.40 |
| 1:B:345:GLN:HE21 | 1:B:345:GLN:HB3 | 1.60 | 0.40 |
| 1:B:369:LEU:HD12 | 1:B:369:LEU:N | 2.35 | 0.40 |
| 1:B:126:PHE:CE2 | 1:B:392:PHE:CZ | 3.03 | 0.40 |
| 2:C:27:LEU:HD12 | 2:C:27:LEU:N | 2.36 | 0.40 |
| 2:C:38:ASN:O | 2:C:40:PHE:CD2 | 2.75 | 0.40 |
| 2:C:69:GLY:HA3 | 2:C:73:ARG:CB | 2.27 | 0.40 |
| 5:H:101:ASN:O | 5:H:104:TYR:HD1 | 2.04 | 0.40 |
| 5:H:117:GLU:O | 5:H:118:TYR:CD1 | 2.75 | 0.40 |
| 5:H:16:GLN:HB3 | 5:H:26:PRO:HA | 2.03 | 0.40 |
| 5:H:20:ALA:C | 5:H:90:LYS:HD2 | 2.41 | 0.40 |
| 1:A:146:HIS:NE2 | 1:A:200:TYR:HB3 | 2.37 | 0.40 |
| 1:A:206:TYR:C | 1:A:207:TYR:CD1 | 2.95 | 0.40 |
| 1:A:221:TYR:HB2 | 1:A:222:GLY:HA3 | 2.03 | 0.40 |
| 1:A:241:ARG:NE | 1:A:245:ILE:HD11 | 2.28 | 0.40 |
| 1:A:366:LEU:N | 1:A:368:ALA:HB2 | 2.36 | 0.40 |
| 1:A:417:THR:H | 1:A:418:ARG:HA | 1.85 | 0.40 |
| 1:A:426:VAL:O | 1:A:430:VAL:HG23 | 2.21 | 0.40 |
| 1:B:183:TYR:CD1 | 1:B:183:TYR:O | 2.74 | 0.40 |
| 1:B:62:LYS:CG | 1:B:63:ARG:N | 2.83 | 0.40 |
| 2:C:40:PHE:CD1 | 2:C:40:PHE:O | 2.74 | 0.40 |
| 2:C:63:PHE:O | 2:C:63:PHE:CD1 | 2.74 | 0.40 |
| 1:B:292:ASP:CG | 2:D:35:GLU:N | 2.73 | 0.40 |
| 2:D:63:PHE:O | 2:D:63:PHE:CD1 | 2.74 | 0.40 |
| 2:D:75:MET:HE1 | 3:F:90:LEU:HD23 | 2.01 | 0.40 |
| 3:E:97:THR:CG2 | 3:E:98:ARG:N | 2.82 | 0.40 |
| 3:E:40:PRO:CG | 3:F:100:LYS:HA | 2.51 | 0.40 |
| 3:E:58:TYR:CE2 | 3:F:100:LYS:O | 2.75 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:F:21:GLU:HG3 | 3:F:22:GLY:N | 2.37 | 0.40 |
| 3:F:57:GLY:C | 3:F:58:TYR:CD1 | 2.95 | 0.40 |
| 3:F:37:HIS:HD1 | 3:F:61:TYR:HE2 | 1.69 | 0.40 |
| 4:G:97:PHE:CD2 | 5:H:52:ARG:NH1 | 2.82 | 0.40 |
| 5:H:104:TYR:CE1 | 5:H:160:PHE:CB | 3.04 | 0.40 |
| 1:A:101:VAL:CG2 | 1:A:102:GLY:N | 2.82 | 0.40 |
| 1:A:134:VAL:CG2 | 1:A:135:LYS:N | 2.83 | 0.40 |
| 1:A:183:TYR:HB3 | 1:A:197:ALA:HB2 | 2.01 | 0.40 |
| 1:A:255:SER:HB3 | 1:A:259:PHE:CZ | 2.54 | 0.40 |
| 1:A:267:TYR:O | 1:A:267:TYR:CD1 | 2.75 | 0.40 |
| 1:A:332:GLU:HG3 | 1:B:326:VAL:HG13 | 2.02 | 0.40 |
| 1:A:403:ASP:C | 1:A:404:PHE:CD1 | 2.95 | 0.40 |
| 1:B:159:ILE:C | 1:B:160:PHE:CD1 | 2.95 | 0.40 |
| 1:B:159:ILE:C | 1:B:160:PHE:HD1 | 2.24 | 0.40 |
| 1:B:146:HIS:NE2 | 1:B:200:TYR:HB3 | 2.37 | 0.40 |
| 1:B:206:TYR:C | 1:B:207:TYR:CD1 | 2.95 | 0.40 |
| 1:B:373:LYS:HD2 | 1:B:374:ALA:N | 2.36 | 0.40 |
| 2:C:41:ILE:HG21 | 2:C:45:GLY:HA2 | 1.95 | 0.40 |
| 2:C:65:MET:HG3 | 2:C:66:THR:N | 2.36 | 0.40 |
| 2:D:63:PHE:CD1 | 2:D:85:GLU:OE1 | 2.74 | 0.40 |
| 3:F:44:GLU:CG | 3:F:46:TYR:CB | 2.95 | 0.40 |
| 4:G:112:VAL:O | 4:G:122:HIS:HE1 | 2.04 | 0.40 |
| 4:G:43:TYR:O | 4:G:43:TYR:CD1 | 2.75 | 0.40 |
| 4:G:61:GLY:CA | 5:H:139:LYS:CE | 2.82 | 0.40 |
| 5:H:162:GLN:CB | 5:H:163:PRO:HD3 | 2.37 | 0.40 |
| 4:G:100:PHE:HE2 | 5:H:47:GLN:CA | 2.06 | 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 | 438/503 (87%) | 426 (97%) | 7 (2%) | 5 (1%) | 17 | 60 |
| 1 | B | 438/503 (87%) | 426 (97%) | 7 (2%) | 5 (1%) | 17 | 60 |
| 2 | C | 97/102 (95%) | 90 (93%) | 4 (4%) | 3 (3%) | 5 | 36 |
| 2 | D | 97/102 (95%) | 90 (93%) | 4 (4%) | 3 (3%) | 5 | 36 |
| 3 | E | 107/109 (98%) | 98 (92%) | 7 (6%) | 2 (2%) | 9 | 47 |
| 3 | F | 107/109 (98%) | 98 (92%) | 7 (6%) | 2 (2%) | 9 | 47 |
| 4 | G | 131/134 (98%) | 122 (93%) | 6 (5%) | 3 (2%) | 7 | 43 |
| 5 | H | 155/177 (88%) | 140 (90%) | 7 (4%) | 8 (5%) | 2 | 26 |
| All | All | 1570/1739 (90%) | 1490 (95%) | 49 (3%) | 31 (2%) | 13 | 46 |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 284 | ILE |
| 1 | A | 287 | VAL |
| 1 | B | 284 | ILE |
| 1 | B | 287 | VAL |
| 2 | C | 95 | ASN |
| 2 | C | 101 | ALA |
| 2 | D | 95 | ASN |
| 2 | D | 101 | ALA |
| 5 | H | 54 | LEU |
| 5 | H | 142 | GLU |
| 1 | A | 103 | GLU |
| 1 | A | 320 | LEU |
| 1 | B | 103 | GLU |
| 1 | B | 320 | LEU |
| 2 | C | 98 | ARG |
| 2 | D | 98 | ARG |
| 5 | H | 19 | ASP |
| 5 | H | 38 | SER |
| 3 | E | 43 | GLN |
| 5 | H | 34 | ASP |
| 5 | H | 62 | SER |
| 5 | H | 166 | THR |
| 1 | A | 345 | GLN |
| 1 | B | 345 | GLN |
| 3 | E | 36 | ALA |
| 3 | F | 43 | GLN |
| 4 | G | 28 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | G | 34 | SER |
| 3 | F | 107 | TYR |
| 4 | G | 55 | GLU |
| 5 | H | 97 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 388/436 (89%) | 349 (90%) | 39 (10%) | 9 | 33 |
| 1 | B | 388/436 (89%) | 349 (90%) | 39 (10%) | 9 | 33 |
| 2 | C | 88/91 (97%) | 81 (92%) | 7 (8%) | 14 | 45 |
| 2 | D | 88/91 (97%) | 81 (92%) | 7 (8%) | 14 | 45 |
| 3 | E | 94/94 (100%) | 81 (86%) | 13 (14%) | 4 | 23 |
| 3 | F | 94/94 (100%) | 77 (82%) | 17 (18%) | 2 | 13 |
| 4 | G | 117/118 (99%) | 102 (87%) | 15 (13%) | 5 | 25 |
| 5 | H | 130/142 (92%) | 111 (85%) | 19 (15%) | 3 | 21 |
| All | All | 1387/1502 (92%) | 1231 (89%) | 156 (11%) | 11 | 29 |

All (156) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 52 | TYR |
| 1 | A | 53 | TYR |
| 1 | A | 62 | LYS |
| 1 | A | 66 | TYR |
| 1 | A | 83 | ARG |
| 1 | A | 88 | TRP |
| 1 | A | 96 | LYS |
| 1 | A | 107 | PHE |
| 1 | A | 121 | LEU |
| 1 | A | 140 | LYS |
| 1 | A | 143 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 148 | PHE |
| 1 | A | 159 | ILE |
| 1 | A | 165 | MET |
| 1 | A | 170 | LYS |
| 1 | A | 184 | TYR |
| 1 | A | 215 | TYR |
| 1 | A | 225 | ASN |
| 1 | A | 227 | ARG |
| 1 | A | 242 | VAL |
| 1 | A | 244 | ILE |
| 1 | A | 249 | ASN |
| 1 | A | 250 | ASN |
| 1 | A | 254 | VAL |
| 1 | A | 259 | PHE |
| 1 | A | 260 | TYR |
| 1 | A | 286 | TYR |
| 1 | A | 291 | TYR |
| 1 | A | 318 | ASP |
| 1 | A | 323 | GLU |
| 1 | A | 345 | GLN |
| 1 | A | 365 | LYS |
| 1 | A | 367 | TYR |
| 1 | A | 373 | LYS |
| 1 | A | 376 | MET |
| 1 | A | 392 | PHE |
| 1 | A | 440 | LYS |
| 1 | A | 465 | ASN |
| 1 | A | 467 | TYR |
| 1 | B | 52 | TYR |
| 1 | B | 53 | TYR |
| 1 | B | 62 | LYS |
| 1 | B | 66 | TYR |
| 1 | B | 83 | ARG |
| 1 | B | 88 | TRP |
| 1 | B | 96 | LYS |
| 1 | B | 107 | PHE |
| 1 | B | 121 | LEU |
| 1 | B | 140 | LYS |
| 1 | B | 143 | GLU |
| 1 | B | 148 | PHE |
| 1 | B | 159 | ILE |
| 1 | B | 165 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 170 | LYS |
| 1 | B | 184 | TYR |
| 1 | B | 215 | TYR |
| 1 | B | 225 | ASN |
| 1 | B | 227 | ARG |
| 1 | B | 242 | VAL |
| 1 | B | 244 | ILE |
| 1 | B | 249 | ASN |
| 1 | B | 250 | ASN |
| 1 | B | 254 | VAL |
| 1 | B | 259 | PHE |
| 1 | B | 260 | TYR |
| 1 | B | 286 | TYR |
| 1 | B | 291 | TYR |
| 1 | B | 318 | ASP |
| 1 | B | 323 | GLU |
| 1 | B | 345 | GLN |
| 1 | B | 365 | LYS |
| 1 | B | 367 | TYR |
| 1 | B | 373 | LYS |
| 1 | B | 376 | MET |
| 1 | B | 392 | PHE |
| 1 | B | 440 | LYS |
| 1 | B | 465 | ASN |
| 1 | B | 467 | TYR |
| 2 | C | 4 | GLN |
| 2 | C | 64 | TYR |
| 2 | C | 80 | TYR |
| 2 | C | 82 | PHE |
| 2 | C | 97 | TYR |
| 2 | C | 100 | MET |
| 2 | C | 102 | ARG |
| 2 | D | 4 | GLN |
| 2 | D | 64 | TYR |
| 2 | D | 80 | TYR |
| 2 | D | 82 | PHE |
| 2 | D | 97 | TYR |
| 2 | D | 100 | MET |
| 2 | D | 102 | ARG |
| 3 | E | 6 | ARG |
| 3 | E | 14 | TYR |
| 3 | E | 21 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | E | 26 | TYR |
| 3 | E | 29 | VAL |
| 3 | E | 43 | GLN |
| 3 | E | 44 | GLU |
| 3 | E | 61 | TYR |
| 3 | E | 64 | TYR |
| 3 | E | 83 | PHE |
| 3 | E | 84 | ILE |
| 3 | E | 98 | ARG |
| 3 | E | 102 | LYS |
| 3 | F | 5 | PHE |
| 3 | F | 14 | TYR |
| 3 | F | 16 | GLU |
| 3 | F | 19 | ASN |
| 3 | F | 26 | TYR |
| 3 | F | 32 | PHE |
| 3 | F | 44 | GLU |
| 3 | F | 60 | ILE |
| 3 | F | 61 | TYR |
| 3 | F | 64 | TYR |
| 3 | F | 65 | ASP |
| 3 | F | 68 | ILE |
| 3 | F | 76 | TYR |
| 3 | F | 83 | PHE |
| 3 | F | 98 | ARG |
| 3 | F | 100 | LYS |
| 3 | F | 102 | LYS |
| 4 | G | 5 | LEU |
| 4 | G | 12 | LYS |
| 4 | G | 21 | TYR |
| 4 | G | 22 | GLN |
| 4 | G | 24 | LEU |
| 4 | G | 27 | MET |
| 4 | G | 28 | VAL |
| 4 | G | 30 | GLN |
| 4 | G | 37 | LYS |
| 4 | G | 43 | TYR |
| 4 | G | 66 | MET |
| 4 | G | 76 | ARG |
| 4 | G | 92 | TYR |
| 4 | G | 124 | ILE |
| 4 | G | 128 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | H | 10 | ASP |
| 5 | H | 13 | TYR |
| 5 | H | 14 | LEU |
| 5 | H | 15 | PHE |
| 5 | H | 19 | ASP |
| 5 | H | 22 | THR |
| 5 | H | 28 | PHE |
| 5 | H | 43 | LEU |
| 5 | H | 44 | PHE |
| 5 | H | 52 | ARG |
| 5 | H | 67 | TYR |
| 5 | H | 87 | LYS |
| 5 | H | 98 | LYS |
| 5 | H | 110 | PHE |
| 5 | H | 112 | TYR |
| 5 | H | 118 | TYR |
| 5 | H | 139 | LYS |
| 5 | H | 142 | GLU |
| 5 | H | 150 | ILE |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 41 | HIS |
| 1 | A | 119 | ASN |
| 1 | A | 131 | ASN |
| 1 | A | 136 | ASN |
| 1 | A | 195 | GLN |
| 1 | A | 224 | ASN |
| 1 | A | 225 | ASN |
| 1 | A | 302 | ASN |
| 1 | A | 337 | GLN |
| 1 | A | 345 | GLN |
| 1 | A | 398 | ASN |
| 1 | A | 405 | ASN |
| 1 | A | 420 | GLN |
| 1 | A | 431 | GLN |
| 1 | A | 451 | GLN |
| 1 | A | 465 | ASN |
| 1 | B | 41 | HIS |
| 1 | B | 119 | ASN |
| 1 | B | 131 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 136 | ASN |
| 1 | B | 195 | GLN |
| 1 | B | 224 | ASN |
| 1 | B | 225 | ASN |
| 1 | B | 282 | GLN |
| 1 | B | 302 | ASN |
| 1 | B | 337 | GLN |
| 1 | B | 345 | GLN |
| 1 | B | 398 | ASN |
| 1 | B | 405 | ASN |
| 1 | B | 420 | GLN |
| 1 | B | 431 | GLN |
| 1 | B | 451 | GLN |
| 1 | B | 465 | ASN |
| 2 | C | 14 | ASN |
| 2 | C | 37 | HIS |
| 2 | C | 38 | ASN |
| 2 | D | 14 | ASN |
| 2 | D | 17 | HIS |
| 2 | D | 37 | HIS |
| 3 | E | 19 | ASN |
| 3 | E | 43 | GLN |
| 3 | E | 51 | GLN |
| 3 | E | 53 | GLN |
| 3 | E | 59 | ASN |
| 3 | F | 12 | GLN |
| 3 | F | 19 | ASN |
| 3 | F | 53 | GLN |
| 4 | G | 22 | GLN |
| 4 | G | 49 | GLN |
| 5 | H | 16 | GLN |
| 5 | H | 47 | GLN |
| 5 | H | 85 | ASN |
| 5 | H | 88 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5 | H | 4 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | H | 137:GLU | C | 138:LEU | N | 2.84 |
| 1 | H | 57:GLY | C | 58:SER | N | 2.60 |
| 1 | H | 141:GLY | C | 142:GLU | N | 1.77 |
| 1 | H | 53:ILE | C | 54:LEU | N | 1.72 |