



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3J8I
EMDB ID: : EMD-6179
Title : Near-Atomic Resolution for One State of F-Actin
Authors : Galkin, V.E.
Deposited on : 2014-11-06
Resolution : 4.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

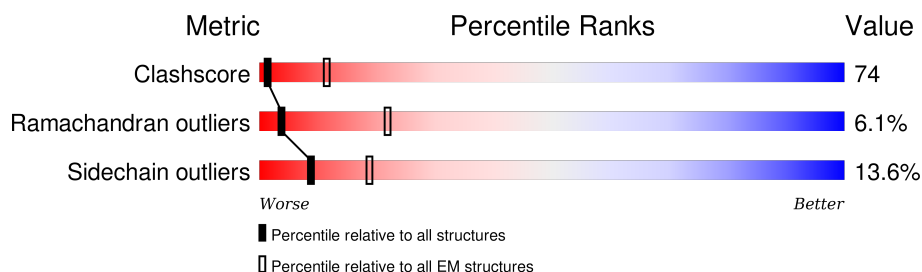
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 | D | 377 | |
| 1 | E | 377 | |
| 1 | F | 377 | |
| 1 | G | 377 | |
| 1 | H | 377 | |

2 Entry composition [i](#)

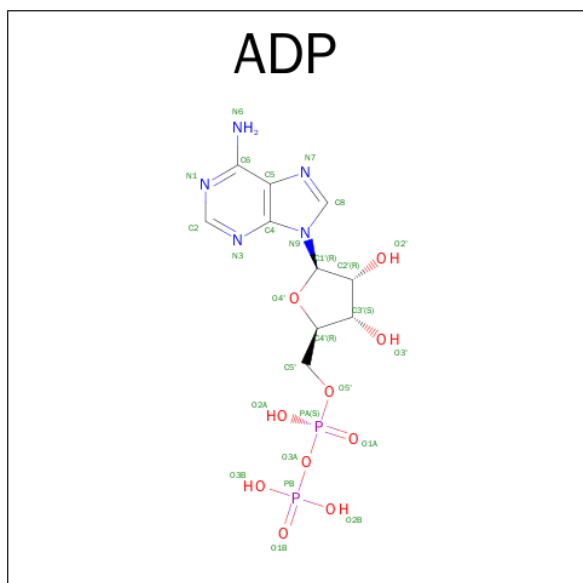
There are 3 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Actin, alpha skeletal muscle.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | D | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | E | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | F | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | G | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | H | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | G | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | H | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

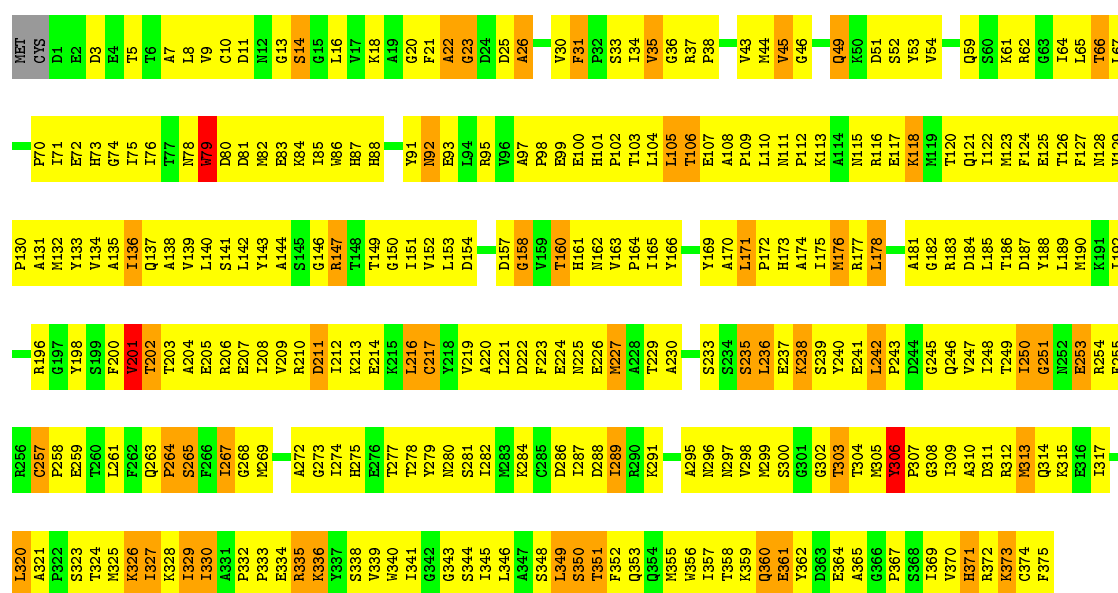
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 3 | H | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | G | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | F | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

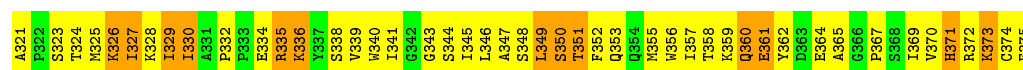
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Actin, alpha skeletal muscle

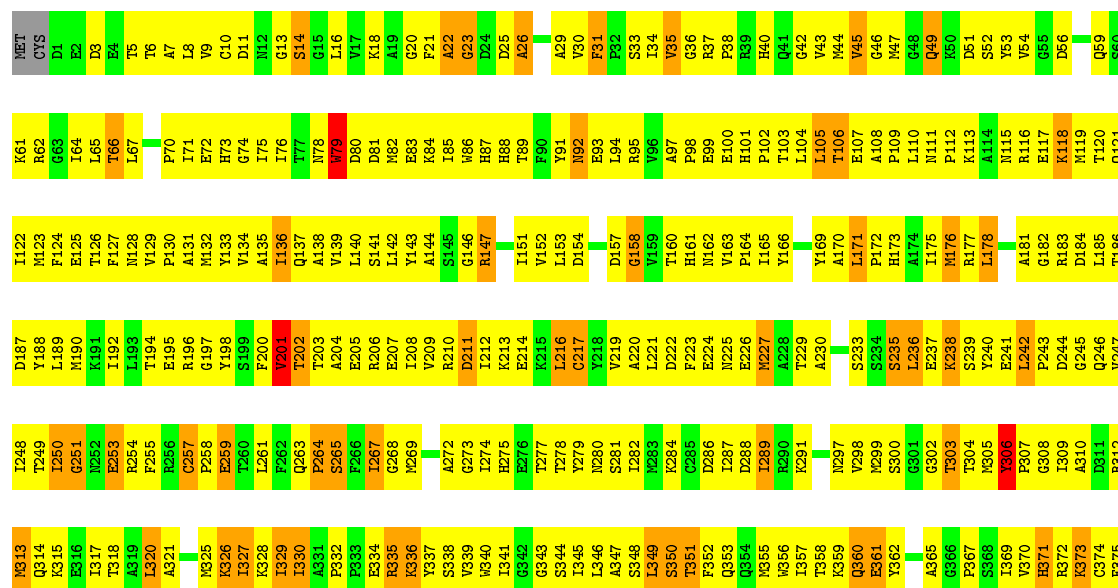
Chain D:  ..





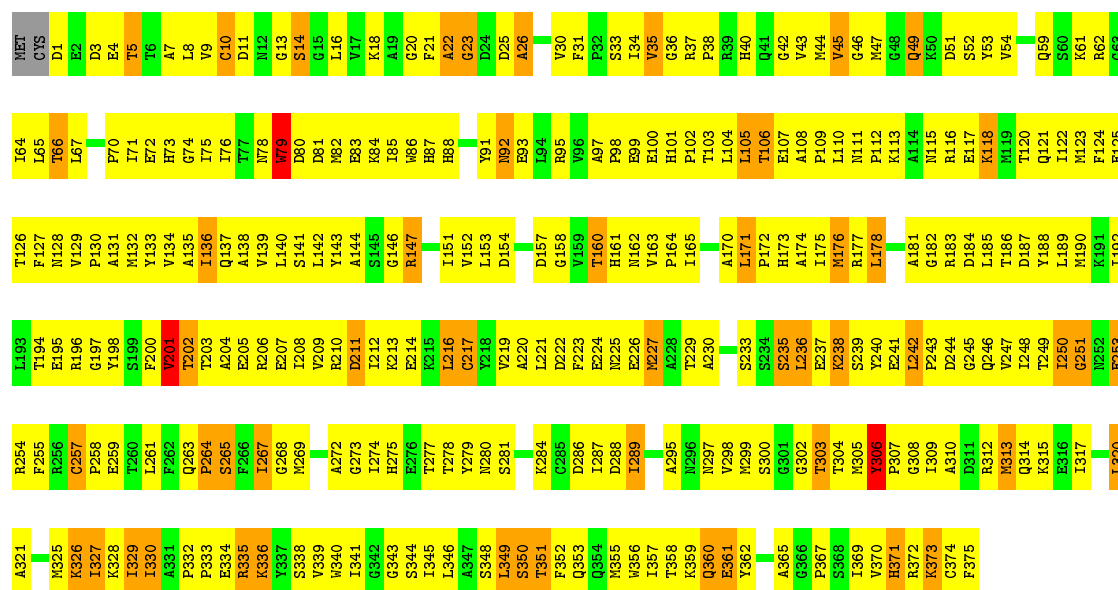
• Molecule 1: Actin, alpha skeletal muscle

Chain F: 21% 64% 14% ..



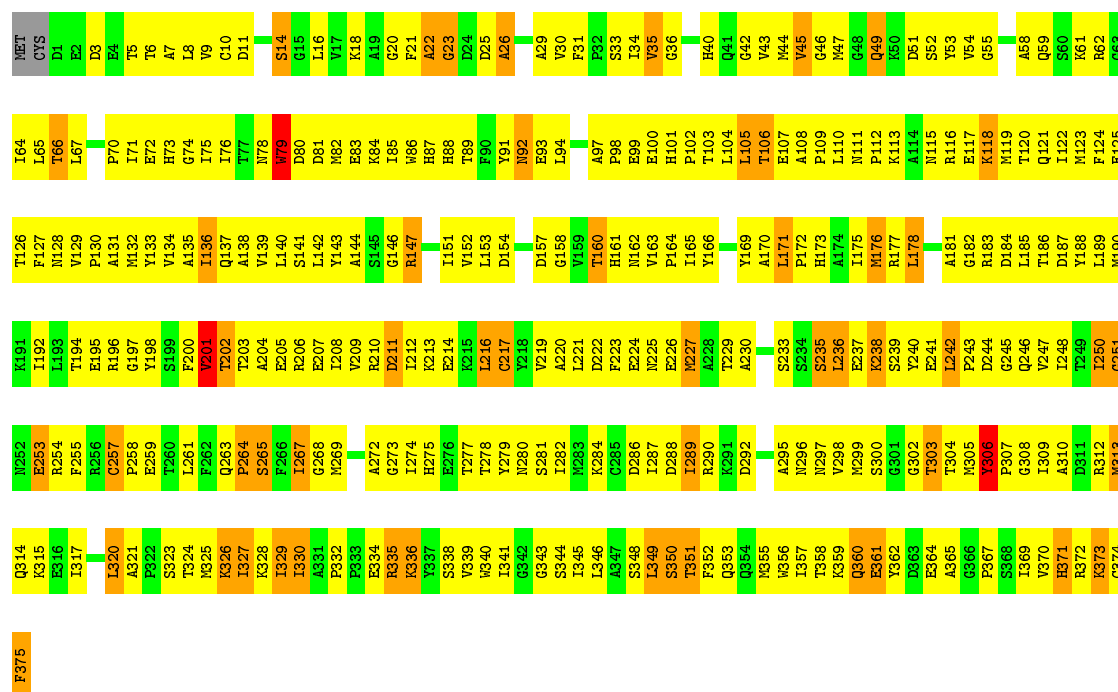
• Molecule 1: Actin, alpha skeletal muscle

Chain G: 23% 62% 14% ..



• Molecule 1: Actin, alpha skeletal muscle

Chain H: 21% 64% 14% ..



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------------------|-----------|
| Reconstruction method | HELICAL | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | FSC and comparison with atomic model | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI Falcon II (4k x 4k) | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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 | D | 0.81 | 0/2995 | 0.73 | 0/4058 |
| 1 | E | 0.81 | 0/2995 | 0.72 | 0/4058 |
| 1 | F | 0.80 | 0/2995 | 0.72 | 0/4058 |
| 1 | G | 0.82 | 1/2995 (0.0%) | 0.72 | 0/4058 |
| 1 | H | 0.82 | 1/2995 (0.0%) | 0.72 | 0/4058 |
| All | All | 0.81 | 2/14975 (0.0%) | 0.72 | 0/20290 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | G | 10 | CYS | CB-SG | 5.58 | 1.91 | 1.82 |
| 1 | H | 375 | PHE | CE1-CZ | 5.04 | 1.47 | 1.37 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | D | 2932 | 0 | 2894 | 445 | 0 |
| 1 | E | 2932 | 0 | 2894 | 438 | 0 |
| 1 | F | 2932 | 0 | 2894 | 475 | 0 |
| 1 | G | 2932 | 0 | 2894 | 439 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | H | 2932 | 0 | 2894 | 450 | 0 |
| 2 | D | 27 | 0 | 12 | 2 | 0 |
| 2 | E | 27 | 0 | 12 | 2 | 0 |
| 2 | F | 27 | 0 | 12 | 2 | 0 |
| 2 | G | 27 | 0 | 12 | 2 | 0 |
| 2 | H | 27 | 0 | 12 | 2 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| All | All | 14800 | 0 | 14530 | 2165 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (2165) 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:H:259:GLU:HB3 | 1:H:263:GLN:HE22 | 1.06 | 1.18 |
| 1:E:259:GLU:HB3 | 1:E:263:GLN:HE22 | 1.06 | 1.13 |
| 1:G:259:GLU:HB3 | 1:G:263:GLN:HE22 | 1.06 | 1.12 |
| 1:F:259:GLU:HB3 | 1:F:263:GLN:HE22 | 1.08 | 1.11 |
| 1:D:259:GLU:HB3 | 1:D:263:GLN:HE22 | 1.08 | 1.08 |
| 1:H:329:ILE:HD13 | 1:H:329:ILE:H | 1.21 | 1.02 |
| 1:D:329:ILE:H | 1:D:329:ILE:HD13 | 1.23 | 1.02 |
| 1:G:329:ILE:HD13 | 1:G:329:ILE:H | 1.23 | 1.01 |
| 1:E:109:PRO:HD2 | 1:E:161:HIS:NE2 | 1.77 | 1.00 |
| 1:D:109:PRO:HD2 | 1:D:161:HIS:NE2 | 1.77 | 1.00 |
| 1:E:329:ILE:HD13 | 1:E:329:ILE:H | 1.24 | 1.00 |
| 1:F:329:ILE:HD13 | 1:F:329:ILE:H | 1.27 | 1.00 |
| 1:G:66:THR:HG23 | 1:G:203:THR:HG21 | 1.44 | 0.99 |
| 1:E:66:THR:HG23 | 1:E:203:THR:HG21 | 1.45 | 0.99 |
| 1:H:109:PRO:HD2 | 1:H:161:HIS:NE2 | 1.77 | 0.99 |
| 1:F:147:ARG:HH12 | 1:F:330:ILE:HD13 | 1.28 | 0.98 |
| 1:F:109:PRO:HD2 | 1:F:161:HIS:NE2 | 1.78 | 0.98 |
| 1:D:66:THR:HG23 | 1:D:203:THR:HG21 | 1.42 | 0.98 |
| 1:H:147:ARG:HH12 | 1:H:330:ILE:HD13 | 1.29 | 0.98 |
| 1:G:109:PRO:HD2 | 1:G:161:HIS:NE2 | 1.77 | 0.98 |
| 1:H:66:THR:HG23 | 1:H:203:THR:HG21 | 1.44 | 0.98 |
| 1:E:147:ARG:HH12 | 1:E:330:ILE:HD13 | 1.29 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:147:ARG:HH12 | 1:D:330:ILE:HD13 | 1.28 | 0.97 |
| 1:E:190:MET:HE2 | 1:E:206:ARG:HG3 | 1.47 | 0.97 |
| 1:G:147:ARG:HH12 | 1:G:330:ILE:HD13 | 1.28 | 0.96 |
| 1:F:76:ILE:H | 1:F:115:ASN:HD21 | 1.11 | 0.95 |
| 1:F:66:THR:HG23 | 1:F:203:THR:HG21 | 1.44 | 0.94 |
| 1:G:190:MET:HE2 | 1:G:206:ARG:HG3 | 1.51 | 0.93 |
| 1:E:76:ILE:H | 1:E:115:ASN:HD21 | 1.15 | 0.92 |
| 1:G:76:ILE:H | 1:G:115:ASN:HD21 | 1.15 | 0.92 |
| 1:D:76:ILE:H | 1:D:115:ASN:HD21 | 1.14 | 0.91 |
| 1:E:367:PRO:O | 1:E:370:VAL:HG12 | 1.71 | 0.91 |
| 1:F:98:PRO:HB2 | 1:F:127:PHE:HB3 | 1.52 | 0.91 |
| 1:G:259:GLU:HB3 | 1:G:263:GLN:NE2 | 1.86 | 0.91 |
| 1:E:259:GLU:HB3 | 1:E:263:GLN:NE2 | 1.86 | 0.91 |
| 1:G:64:ILE:HD12 | 1:G:65:LEU:N | 1.86 | 0.91 |
| 1:E:64:ILE:HD12 | 1:E:65:LEU:N | 1.86 | 0.91 |
| 1:G:176:MET:HE1 | 1:G:277:THR:HB | 1.53 | 0.90 |
| 1:F:64:ILE:HD12 | 1:F:65:LEU:N | 1.86 | 0.90 |
| 1:D:367:PRO:O | 1:D:370:VAL:HG12 | 1.72 | 0.90 |
| 1:D:136:ILE:HD12 | 1:D:139:VAL:HG23 | 1.53 | 0.90 |
| 1:F:202:THR:HG22 | 1:F:205:GLU:H | 1.36 | 0.90 |
| 1:G:238:LYS:HG2 | 1:G:254:ARG:NH1 | 1.87 | 0.90 |
| 1:H:76:ILE:H | 1:H:115:ASN:HD21 | 1.14 | 0.90 |
| 1:G:98:PRO:HB2 | 1:G:127:PHE:HB3 | 1.53 | 0.89 |
| 1:E:98:PRO:HB2 | 1:E:127:PHE:HB3 | 1.52 | 0.89 |
| 1:D:64:ILE:HD12 | 1:D:65:LEU:N | 1.86 | 0.89 |
| 1:G:367:PRO:O | 1:G:370:VAL:HG12 | 1.73 | 0.89 |
| 1:E:202:THR:HG22 | 1:E:205:GLU:HB2 | 1.54 | 0.89 |
| 1:H:23:GLY:HA2 | 1:H:344:SER:HB3 | 1.52 | 0.89 |
| 1:H:259:GLU:HB3 | 1:H:263:GLN:NE2 | 1.87 | 0.89 |
| 1:D:98:PRO:HB2 | 1:D:127:PHE:HB3 | 1.53 | 0.89 |
| 1:G:202:THR:HG22 | 1:G:205:GLU:HB2 | 1.54 | 0.88 |
| 1:H:64:ILE:HD12 | 1:H:65:LEU:N | 1.88 | 0.88 |
| 1:H:202:THR:HG22 | 1:H:205:GLU:HB2 | 1.55 | 0.88 |
| 1:D:259:GLU:HB3 | 1:D:263:GLN:NE2 | 1.89 | 0.88 |
| 1:E:202:THR:HG22 | 1:E:205:GLU:H | 1.37 | 0.88 |
| 1:H:98:PRO:HB2 | 1:H:127:PHE:HB3 | 1.55 | 0.88 |
| 1:H:238:LYS:HG2 | 1:H:254:ARG:NH1 | 1.88 | 0.88 |
| 1:E:238:LYS:HG2 | 1:E:254:ARG:NH1 | 1.89 | 0.88 |
| 1:D:190:MET:HE2 | 1:D:206:ARG:HG3 | 1.53 | 0.88 |
| 1:G:23:GLY:HA2 | 1:G:344:SER:HB3 | 1.55 | 0.88 |
| 1:F:259:GLU:HB3 | 1:F:263:GLN:NE2 | 1.89 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:110:LEU:HB2 | 1:H:177:ARG:HG3 | 1.55 | 0.87 |
| 1:F:238:LYS:HG2 | 1:F:254:ARG:NH1 | 1.88 | 0.87 |
| 1:H:202:THR:HG22 | 1:H:205:GLU:H | 1.39 | 0.87 |
| 1:D:238:LYS:HG2 | 1:D:254:ARG:NH1 | 1.88 | 0.87 |
| 1:H:367:PRO:O | 1:H:370:VAL:HG12 | 1.73 | 0.87 |
| 1:F:71:ILE:HD12 | 1:F:76:ILE:HG13 | 1.57 | 0.87 |
| 1:D:202:THR:HG22 | 1:D:205:GLU:HB2 | 1.56 | 0.87 |
| 1:E:23:GLY:HA2 | 1:E:344:SER:HB3 | 1.55 | 0.87 |
| 1:D:23:GLY:HA2 | 1:D:344:SER:HB3 | 1.55 | 0.87 |
| 1:H:313:MET:O | 1:H:317:ILE:HG12 | 1.75 | 0.86 |
| 1:D:110:LEU:HB2 | 1:D:177:ARG:HG3 | 1.55 | 0.86 |
| 1:F:23:GLY:HA2 | 1:F:344:SER:HB3 | 1.55 | 0.86 |
| 1:G:202:THR:HG22 | 1:G:205:GLU:H | 1.38 | 0.86 |
| 1:E:273:GLY:H | 1:E:277:THR:HG23 | 1.40 | 0.86 |
| 1:D:202:THR:HG22 | 1:D:205:GLU:H | 1.39 | 0.86 |
| 1:F:72:GLU:HA | 1:F:183:ARG:HH22 | 1.41 | 0.86 |
| 1:E:110:LEU:HB2 | 1:E:177:ARG:HG3 | 1.56 | 0.86 |
| 1:F:110:LEU:HB2 | 1:F:177:ARG:HG3 | 1.56 | 0.86 |
| 1:H:162:ASN:HD21 | 1:H:278:THR:HG22 | 1.38 | 0.86 |
| 1:F:136:ILE:HD12 | 1:F:139:VAL:HG23 | 1.58 | 0.86 |
| 1:H:71:ILE:HD12 | 1:H:76:ILE:HG13 | 1.58 | 0.85 |
| 1:D:72:GLU:HA | 1:D:183:ARG:HH22 | 1.40 | 0.85 |
| 1:G:313:MET:O | 1:G:317:ILE:HG12 | 1.77 | 0.85 |
| 1:F:176:MET:HE1 | 1:F:277:THR:HB | 1.59 | 0.85 |
| 1:G:162:ASN:HD21 | 1:G:278:THR:HG22 | 1.40 | 0.85 |
| 1:F:367:PRO:O | 1:F:370:VAL:HG12 | 1.76 | 0.85 |
| 1:E:162:ASN:HD21 | 1:E:278:THR:HG22 | 1.41 | 0.85 |
| 1:E:313:MET:O | 1:E:317:ILE:HG12 | 1.75 | 0.85 |
| 1:E:136:ILE:HD12 | 1:E:139:VAL:HG23 | 1.59 | 0.85 |
| 1:E:129:VAL:HG21 | 1:E:132:MET:HG2 | 1.59 | 0.85 |
| 1:G:273:GLY:H | 1:G:277:THR:HG23 | 1.41 | 0.84 |
| 1:G:72:GLU:HA | 1:G:183:ARG:HH22 | 1.42 | 0.84 |
| 1:H:273:GLY:H | 1:H:277:THR:HG23 | 1.41 | 0.84 |
| 1:F:178:LEU:HD12 | 1:F:178:LEU:H | 1.40 | 0.84 |
| 1:F:202:THR:HG22 | 1:F:205:GLU:HB2 | 1.58 | 0.84 |
| 1:E:64:ILE:HD12 | 1:E:65:LEU:H | 1.40 | 0.84 |
| 1:F:162:ASN:HD21 | 1:F:278:THR:HG22 | 1.40 | 0.84 |
| 1:D:313:MET:O | 1:D:317:ILE:HG12 | 1.77 | 0.84 |
| 1:D:7:ALA:H | 1:D:22:ALA:HB2 | 1.43 | 0.84 |
| 1:G:110:LEU:HB2 | 1:G:177:ARG:HG3 | 1.57 | 0.84 |
| 1:G:136:ILE:HD12 | 1:G:139:VAL:HG23 | 1.60 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:273:GLY:H | 1:F:277:THR:HG23 | 1.42 | 0.84 |
| 1:G:8:LEU:O | 1:G:103:THR:HA | 1.78 | 0.84 |
| 1:F:313:MET:O | 1:F:317:ILE:HG12 | 1.76 | 0.84 |
| 1:H:72:GLU:HA | 1:H:183:ARG:HH22 | 1.41 | 0.84 |
| 1:H:178:LEU:H | 1:H:178:LEU:HD12 | 1.41 | 0.84 |
| 1:E:178:LEU:H | 1:E:178:LEU:HD12 | 1.41 | 0.84 |
| 1:G:178:LEU:H | 1:G:178:LEU:HD12 | 1.42 | 0.83 |
| 1:E:71:ILE:HD12 | 1:E:76:ILE:HG13 | 1.57 | 0.83 |
| 1:H:136:ILE:HD12 | 1:H:139:VAL:HG23 | 1.60 | 0.83 |
| 1:H:129:VAL:HG21 | 1:H:132:MET:HG2 | 1.58 | 0.83 |
| 1:D:273:GLY:H | 1:D:277:THR:HG23 | 1.43 | 0.83 |
| 1:G:71:ILE:HD12 | 1:G:76:ILE:HG13 | 1.59 | 0.83 |
| 1:D:71:ILE:HD12 | 1:D:76:ILE:HG13 | 1.61 | 0.83 |
| 1:F:7:ALA:H | 1:F:22:ALA:HB2 | 1.43 | 0.83 |
| 1:E:8:LEU:O | 1:E:103:THR:HA | 1.79 | 0.83 |
| 1:H:109:PRO:HG3 | 1:H:136:ILE:HG12 | 1.59 | 0.83 |
| 1:F:129:VAL:HG21 | 1:F:132:MET:HG2 | 1.58 | 0.83 |
| 1:D:176:MET:HE1 | 1:D:277:THR:HB | 1.59 | 0.83 |
| 1:D:178:LEU:H | 1:D:178:LEU:HD12 | 1.43 | 0.82 |
| 1:E:72:GLU:HA | 1:E:183:ARG:HH22 | 1.43 | 0.82 |
| 1:D:129:VAL:HG21 | 1:D:132:MET:HG2 | 1.59 | 0.82 |
| 1:H:7:ALA:H | 1:H:22:ALA:HB2 | 1.45 | 0.82 |
| 1:E:216:LEU:HD13 | 1:E:250:ILE:HG12 | 1.62 | 0.82 |
| 1:F:350:SER:O | 1:F:352:PHE:N | 2.13 | 0.82 |
| 1:D:169:TYR:HA | 1:F:42:GLY:HA3 | 1.61 | 0.82 |
| 1:E:104:LEU:HD11 | 1:E:135:ALA:HB2 | 1.60 | 0.82 |
| 1:F:242:LEU:HD23 | 1:F:248:ILE:HG23 | 1.62 | 0.82 |
| 1:D:8:LEU:O | 1:D:103:THR:HA | 1.79 | 0.81 |
| 1:H:62:ARG:HB3 | 1:H:204:ALA:HB1 | 1.61 | 0.81 |
| 1:E:196:ARG:HH21 | 1:E:251:GLY:HA3 | 1.45 | 0.81 |
| 1:F:71:ILE:HG13 | 1:F:75:ILE:O | 1.80 | 0.81 |
| 1:G:362:TYR:CE2 | 1:G:367:PRO:HA | 2.15 | 0.81 |
| 1:D:264:PRO:HB2 | 1:D:269:MET:O | 1.79 | 0.81 |
| 1:H:196:ARG:HH21 | 1:H:251:GLY:HA3 | 1.46 | 0.81 |
| 1:G:7:ALA:H | 1:G:22:ALA:HB2 | 1.45 | 0.81 |
| 1:E:7:ALA:H | 1:E:22:ALA:HB2 | 1.44 | 0.81 |
| 1:D:104:LEU:HD11 | 1:D:135:ALA:HB2 | 1.62 | 0.81 |
| 1:F:169:TYR:HA | 1:H:42:GLY:HA3 | 1.62 | 0.81 |
| 1:D:64:ILE:HD12 | 1:D:65:LEU:H | 1.44 | 0.81 |
| 1:G:129:VAL:HG21 | 1:G:132:MET:HG2 | 1.63 | 0.81 |
| 1:H:264:PRO:HB2 | 1:H:269:MET:O | 1.80 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:242:LEU:HD21 | 1:E:246:GLN:HB2 | 1.63 | 0.81 |
| 1:D:162:ASN:HD21 | 1:D:278:THR:HG22 | 1.43 | 0.81 |
| 1:H:104:LEU:HD11 | 1:H:135:ALA:HB2 | 1.62 | 0.81 |
| 1:F:62:ARG:HB3 | 1:F:204:ALA:HB1 | 1.62 | 0.81 |
| 1:F:196:ARG:HH21 | 1:F:251:GLY:HA3 | 1.47 | 0.80 |
| 1:G:216:LEU:HD13 | 1:G:250:ILE:HG12 | 1.64 | 0.80 |
| 1:E:220:ALA:HB1 | 1:E:226:GLU:HG3 | 1.63 | 0.80 |
| 1:F:104:LEU:HD11 | 1:F:135:ALA:HB2 | 1.63 | 0.80 |
| 1:E:264:PRO:HB2 | 1:E:269:MET:O | 1.80 | 0.80 |
| 1:G:264:PRO:HB2 | 1:G:269:MET:O | 1.81 | 0.80 |
| 1:H:216:LEU:HD13 | 1:H:250:ILE:HG12 | 1.62 | 0.80 |
| 1:D:147:ARG:NH1 | 1:D:330:ILE:HD13 | 1.97 | 0.80 |
| 1:H:220:ALA:HB1 | 1:H:226:GLU:HG3 | 1.63 | 0.80 |
| 1:E:169:TYR:HA | 1:G:42:GLY:HA3 | 1.64 | 0.80 |
| 1:H:8:LEU:O | 1:H:103:THR:HA | 1.79 | 0.80 |
| 1:G:104:LEU:HD11 | 1:G:135:ALA:HB2 | 1.62 | 0.80 |
| 1:F:109:PRO:HG3 | 1:F:136:ILE:HG12 | 1.62 | 0.80 |
| 1:E:109:PRO:HG3 | 1:E:136:ILE:HG12 | 1.62 | 0.80 |
| 1:F:147:ARG:NH1 | 1:F:330:ILE:HD13 | 1.97 | 0.80 |
| 1:E:362:TYR:CE2 | 1:E:367:PRO:HA | 2.17 | 0.80 |
| 1:H:83:GLU:HA | 1:H:86:TRP:HE3 | 1.47 | 0.80 |
| 1:E:176:MET:HE1 | 1:E:277:THR:HB | 1.61 | 0.80 |
| 1:H:71:ILE:HG13 | 1:H:75:ILE:O | 1.82 | 0.80 |
| 1:G:242:LEU:HD23 | 1:G:248:ILE:HG23 | 1.64 | 0.80 |
| 1:G:71:ILE:HG13 | 1:G:75:ILE:O | 1.80 | 0.79 |
| 1:G:147:ARG:NH1 | 1:G:330:ILE:HD13 | 1.96 | 0.79 |
| 1:E:62:ARG:HB3 | 1:E:204:ALA:HB1 | 1.63 | 0.79 |
| 1:D:286:ASP:HB3 | 1:D:289:ILE:HG22 | 1.64 | 0.79 |
| 1:H:242:LEU:HD23 | 1:H:248:ILE:HG23 | 1.64 | 0.79 |
| 1:H:147:ARG:NH1 | 1:H:330:ILE:HD13 | 1.97 | 0.79 |
| 1:D:171:LEU:HD12 | 1:F:40:HIS:HE1 | 1.48 | 0.79 |
| 1:F:264:PRO:HB2 | 1:F:269:MET:O | 1.81 | 0.79 |
| 1:D:216:LEU:HD13 | 1:D:250:ILE:HG12 | 1.63 | 0.79 |
| 1:G:189:LEU:HD11 | 1:G:213:LYS:HB3 | 1.65 | 0.79 |
| 1:D:62:ARG:HB3 | 1:D:204:ALA:HB1 | 1.65 | 0.79 |
| 1:E:83:GLU:HA | 1:E:86:TRP:HE3 | 1.48 | 0.79 |
| 1:F:83:GLU:HA | 1:F:86:TRP:HE3 | 1.47 | 0.79 |
| 1:F:189:LEU:HD11 | 1:F:213:LYS:HB3 | 1.64 | 0.79 |
| 1:F:216:LEU:HD13 | 1:F:250:ILE:HG12 | 1.64 | 0.79 |
| 1:G:196:ARG:HH21 | 1:G:251:GLY:HA3 | 1.47 | 0.79 |
| 1:H:242:LEU:HG | 1:H:246:GLN:O | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:62:ARG:HB3 | 1:G:204:ALA:HB1 | 1.65 | 0.79 |
| 1:F:8:LEU:O | 1:F:103:THR:HA | 1.82 | 0.78 |
| 1:H:362:TYR:CE2 | 1:H:367:PRO:HA | 2.17 | 0.78 |
| 1:G:109:PRO:HG3 | 1:G:136:ILE:HG12 | 1.65 | 0.78 |
| 1:D:350:SER:O | 1:D:352:PHE:N | 2.16 | 0.78 |
| 1:F:362:TYR:CE2 | 1:F:367:PRO:HA | 2.18 | 0.78 |
| 1:H:176:MET:HE1 | 1:H:277:THR:HB | 1.64 | 0.78 |
| 1:E:221:LEU:H | 1:E:221:LEU:HD12 | 1.49 | 0.78 |
| 1:G:106:THR:HG22 | 1:G:137:GLN:NE2 | 1.98 | 0.78 |
| 1:G:362:TYR:HE2 | 1:G:367:PRO:HA | 1.49 | 0.78 |
| 1:D:242:LEU:HD23 | 1:D:248:ILE:HG23 | 1.65 | 0.78 |
| 1:E:286:ASP:HB3 | 1:E:289:ILE:HG22 | 1.65 | 0.78 |
| 1:F:220:ALA:HB1 | 1:F:226:GLU:HG3 | 1.65 | 0.78 |
| 1:E:106:THR:HG22 | 1:E:137:GLN:NE2 | 1.98 | 0.78 |
| 1:H:264:PRO:O | 1:H:267:ILE:HG22 | 1.83 | 0.78 |
| 1:D:83:GLU:HA | 1:D:86:TRP:HE3 | 1.48 | 0.78 |
| 1:G:83:GLU:HA | 1:G:86:TRP:HE3 | 1.48 | 0.78 |
| 1:D:362:TYR:CE2 | 1:D:367:PRO:HA | 2.18 | 0.78 |
| 1:E:189:LEU:HD11 | 1:E:213:LYS:HB3 | 1.66 | 0.78 |
| 1:D:196:ARG:HH21 | 1:D:251:GLY:HA3 | 1.46 | 0.78 |
| 1:D:171:LEU:HD12 | 1:F:40:HIS:CE1 | 2.19 | 0.78 |
| 1:F:190:MET:HE2 | 1:F:206:ARG:HG3 | 1.65 | 0.78 |
| 1:H:165:ILE:HG13 | 1:H:170:ALA:CB | 2.14 | 0.77 |
| 1:D:189:LEU:HD11 | 1:D:213:LYS:HB3 | 1.66 | 0.77 |
| 1:G:242:LEU:HD21 | 1:G:246:GLN:HB2 | 1.67 | 0.77 |
| 1:H:165:ILE:HG13 | 1:H:170:ALA:HB2 | 1.65 | 0.77 |
| 1:E:71:ILE:HG13 | 1:E:75:ILE:O | 1.83 | 0.77 |
| 1:E:242:LEU:HD23 | 1:E:248:ILE:HG23 | 1.67 | 0.77 |
| 1:E:147:ARG:NH1 | 1:E:330:ILE:HD13 | 1.98 | 0.77 |
| 1:G:350:SER:O | 1:G:352:PHE:N | 2.18 | 0.77 |
| 1:H:189:LEU:HD11 | 1:H:213:LYS:HB3 | 1.65 | 0.77 |
| 1:H:190:MET:HE2 | 1:H:206:ARG:HG3 | 1.65 | 0.77 |
| 1:G:64:ILE:HD12 | 1:G:65:LEU:H | 1.47 | 0.77 |
| 1:H:64:ILE:HD12 | 1:H:65:LEU:H | 1.49 | 0.77 |
| 1:E:362:TYR:HE2 | 1:E:367:PRO:HA | 1.50 | 0.77 |
| 1:H:286:ASP:HB3 | 1:H:289:ILE:HG22 | 1.67 | 0.77 |
| 1:D:109:PRO:HG3 | 1:D:136:ILE:HG12 | 1.65 | 0.77 |
| 1:H:106:THR:HG22 | 1:H:137:GLN:NE2 | 1.99 | 0.76 |
| 1:G:154:ASP:OD1 | 1:G:161:HIS:HB2 | 1.85 | 0.76 |
| 1:H:242:LEU:HD21 | 1:H:246:GLN:HB2 | 1.66 | 0.76 |
| 1:D:154:ASP:OD1 | 1:D:161:HIS:HB2 | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:242:LEU:HD21 | 1:F:246:GLN:HB2 | 1.66 | 0.76 |
| 1:F:64:ILE:HD12 | 1:F:65:LEU:H | 1.49 | 0.76 |
| 1:E:154:ASP:OD1 | 1:E:161:HIS:HB2 | 1.85 | 0.76 |
| 1:G:220:ALA:HB1 | 1:G:226:GLU:HG3 | 1.66 | 0.76 |
| 1:H:362:TYR:HE2 | 1:H:367:PRO:HA | 1.50 | 0.75 |
| 1:H:99:GLU:HG3 | 1:H:128:ASN:HB2 | 1.69 | 0.75 |
| 1:D:242:LEU:HD21 | 1:D:246:GLN:HB2 | 1.67 | 0.75 |
| 1:G:286:ASP:HB3 | 1:G:289:ILE:HG22 | 1.67 | 0.75 |
| 1:F:106:THR:HG22 | 1:F:137:GLN:NE2 | 2.00 | 0.75 |
| 1:G:165:ILE:HG13 | 1:G:170:ALA:HB2 | 1.67 | 0.75 |
| 1:E:242:LEU:HG | 1:E:246:GLN:O | 1.87 | 0.75 |
| 1:F:237:GLU:O | 1:F:238:LYS:HG3 | 1.86 | 0.75 |
| 1:D:220:ALA:HB1 | 1:D:226:GLU:HG3 | 1.69 | 0.75 |
| 1:F:286:ASP:HB3 | 1:F:289:ILE:HG22 | 1.68 | 0.75 |
| 1:G:237:GLU:O | 1:G:238:LYS:HG3 | 1.87 | 0.75 |
| 1:G:242:LEU:HG | 1:G:246:GLN:O | 1.86 | 0.75 |
| 1:D:71:ILE:HG13 | 1:D:75:ILE:O | 1.85 | 0.75 |
| 1:G:264:PRO:O | 1:G:267:ILE:HG22 | 1.87 | 0.75 |
| 1:F:99:GLU:HG3 | 1:F:128:ASN:HB2 | 1.69 | 0.74 |
| 1:G:105:LEU:HD21 | 1:G:132:MET:HB2 | 1.69 | 0.74 |
| 1:H:221:LEU:HD12 | 1:H:221:LEU:H | 1.52 | 0.74 |
| 1:H:154:ASP:OD1 | 1:H:161:HIS:HB2 | 1.86 | 0.74 |
| 1:H:238:LYS:NZ | 1:H:254:ARG:HH22 | 1.86 | 0.74 |
| 1:F:83:GLU:HA | 1:F:86:TRP:CE3 | 2.23 | 0.74 |
| 1:H:83:GLU:HA | 1:H:86:TRP:CE3 | 2.22 | 0.74 |
| 1:E:171:LEU:HD12 | 1:G:40:HIS:HE1 | 1.52 | 0.74 |
| 1:F:362:TYR:HE2 | 1:F:367:PRO:HA | 1.52 | 0.74 |
| 1:H:141:SER:HA | 1:H:338:SER:HB2 | 1.70 | 0.74 |
| 1:E:350:SER:O | 1:E:352:PHE:N | 2.20 | 0.74 |
| 1:E:171:LEU:HD12 | 1:G:40:HIS:CE1 | 2.23 | 0.74 |
| 1:E:165:ILE:HG13 | 1:E:170:ALA:HB2 | 1.70 | 0.74 |
| 1:D:106:THR:HG22 | 1:D:137:GLN:NE2 | 2.01 | 0.74 |
| 1:E:105:LEU:HD21 | 1:E:132:MET:HB2 | 1.70 | 0.74 |
| 1:H:81:ASP:O | 1:H:84:LYS:HG2 | 1.87 | 0.74 |
| 1:F:154:ASP:OD1 | 1:F:161:HIS:HB2 | 1.88 | 0.73 |
| 1:G:112:PRO:HG3 | 1:H:197:GLY:HA2 | 1.68 | 0.73 |
| 1:D:303:THR:O | 1:D:306:TYR:HB2 | 1.88 | 0.73 |
| 1:F:171:LEU:HD12 | 1:H:40:HIS:HE1 | 1.53 | 0.73 |
| 1:D:362:TYR:HE2 | 1:D:367:PRO:HA | 1.53 | 0.73 |
| 1:H:105:LEU:HD21 | 1:H:132:MET:HB2 | 1.70 | 0.73 |
| 1:F:105:LEU:HD21 | 1:F:132:MET:HB2 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:81:ASP:O | 1:D:84:LYS:HG2 | 1.88 | 0.73 |
| 1:E:165:ILE:HG13 | 1:E:170:ALA:CB | 2.18 | 0.73 |
| 1:E:99:GLU:HG3 | 1:E:128:ASN:HB2 | 1.69 | 0.73 |
| 1:D:83:GLU:HA | 1:D:86:TRP:CE3 | 2.23 | 0.73 |
| 1:G:83:GLU:HA | 1:G:86:TRP:CE3 | 2.23 | 0.73 |
| 1:E:83:GLU:HA | 1:E:86:TRP:CE3 | 2.23 | 0.73 |
| 1:H:350:SER:O | 1:H:352:PHE:N | 2.21 | 0.73 |
| 1:D:105:LEU:HD21 | 1:D:132:MET:HB2 | 1.71 | 0.73 |
| 1:G:165:ILE:HG13 | 1:G:170:ALA:CB | 2.18 | 0.73 |
| 1:G:258:PRO:HG3 | 1:G:306:TYR:HE2 | 1.53 | 0.73 |
| 1:G:141:SER:HA | 1:G:338:SER:HB2 | 1.71 | 0.73 |
| 1:D:238:LYS:NZ | 1:D:254:ARG:HH22 | 1.87 | 0.72 |
| 1:F:112:PRO:HG3 | 1:G:197:GLY:HA2 | 1.69 | 0.72 |
| 1:H:258:PRO:HG3 | 1:H:306:TYR:HE2 | 1.54 | 0.72 |
| 1:F:171:LEU:HD12 | 1:H:40:HIS:CE1 | 2.24 | 0.72 |
| 1:D:258:PRO:HG3 | 1:D:306:TYR:HE2 | 1.55 | 0.72 |
| 1:D:264:PRO:O | 1:D:267:ILE:HG22 | 1.89 | 0.72 |
| 1:G:33:SER:HB2 | 1:G:85:ILE:HD13 | 1.71 | 0.72 |
| 1:D:221:LEU:H | 1:D:221:LEU:HD12 | 1.55 | 0.72 |
| 1:F:221:LEU:HD12 | 1:F:221:LEU:H | 1.55 | 0.72 |
| 1:E:81:ASP:O | 1:E:84:LYS:HG2 | 1.90 | 0.72 |
| 1:D:165:ILE:HG13 | 1:D:170:ALA:HB2 | 1.72 | 0.72 |
| 1:D:171:LEU:HA | 1:F:40:HIS:NE2 | 2.05 | 0.72 |
| 1:F:258:PRO:HG3 | 1:F:306:TYR:HE2 | 1.55 | 0.72 |
| 1:F:303:THR:O | 1:F:306:TYR:HB2 | 1.90 | 0.72 |
| 1:D:141:SER:HA | 1:D:338:SER:HB2 | 1.70 | 0.72 |
| 1:H:152:VAL:HG12 | 1:H:298:VAL:HG13 | 1.70 | 0.71 |
| 1:D:99:GLU:HG3 | 1:D:128:ASN:HB2 | 1.72 | 0.71 |
| 1:D:165:ILE:HG13 | 1:D:170:ALA:CB | 2.20 | 0.71 |
| 1:F:264:PRO:O | 1:F:267:ILE:HG22 | 1.90 | 0.71 |
| 1:E:33:SER:HB2 | 1:E:85:ILE:HD13 | 1.72 | 0.71 |
| 1:E:46:GLY:H | 1:E:49:GLN:HB2 | 1.54 | 0.71 |
| 1:D:102:PRO:HB3 | 1:D:131:ALA:HB3 | 1.71 | 0.71 |
| 1:F:165:ILE:HG13 | 1:F:170:ALA:CB | 2.20 | 0.71 |
| 1:E:152:VAL:HG12 | 1:E:298:VAL:HG13 | 1.71 | 0.71 |
| 1:E:237:GLU:O | 1:E:238:LYS:HG3 | 1.90 | 0.71 |
| 1:H:124:PHE:CZ | 1:H:362:TYR:HB3 | 2.26 | 0.71 |
| 1:G:221:LEU:HD12 | 1:G:221:LEU:H | 1.56 | 0.71 |
| 1:H:310:ALA:HB1 | 1:H:329:ILE:HG13 | 1.71 | 0.71 |
| 1:E:141:SER:HA | 1:E:338:SER:HB2 | 1.72 | 0.71 |
| 1:F:81:ASP:O | 1:F:84:LYS:HG2 | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:217:CYS:SG | 1:F:307:PRO:HD2 | 2.31 | 0.71 |
| 1:H:219:VAL:HG21 | 1:H:308:GLY:O | 1.90 | 0.71 |
| 1:D:237:GLU:O | 1:D:238:LYS:HG3 | 1.91 | 0.71 |
| 1:H:102:PRO:HB3 | 1:H:131:ALA:HB3 | 1.72 | 0.71 |
| 1:G:81:ASP:O | 1:G:84:LYS:HG2 | 1.90 | 0.71 |
| 1:H:33:SER:HB2 | 1:H:85:ILE:HD13 | 1.71 | 0.71 |
| 1:G:310:ALA:HB1 | 1:G:329:ILE:HG13 | 1.72 | 0.71 |
| 1:F:350:SER:C | 1:F:352:PHE:H | 1.94 | 0.71 |
| 1:F:76:ILE:H | 1:F:115:ASN:ND2 | 1.87 | 0.71 |
| 1:G:219:VAL:HG21 | 1:G:308:GLY:O | 1.91 | 0.71 |
| 1:H:217:CYS:SG | 1:H:307:PRO:HD2 | 2.31 | 0.70 |
| 1:H:54:VAL:HG21 | 1:H:88:HIS:CG | 2.27 | 0.70 |
| 1:D:242:LEU:HG | 1:D:246:GLN:O | 1.92 | 0.70 |
| 1:F:157:ASP:O | 1:F:183:ARG:HB3 | 1.92 | 0.70 |
| 1:G:59:GLN:O | 1:G:62:ARG:HG3 | 1.91 | 0.70 |
| 1:G:238:LYS:NZ | 1:G:254:ARG:HH22 | 1.88 | 0.70 |
| 1:E:54:VAL:HG21 | 1:E:88:HIS:CG | 2.26 | 0.70 |
| 1:F:264:PRO:HD2 | 1:F:272:ALA:O | 1.92 | 0.70 |
| 1:E:203:THR:O | 1:E:207:GLU:HG2 | 1.92 | 0.70 |
| 1:E:76:ILE:H | 1:E:115:ASN:ND2 | 1.89 | 0.70 |
| 1:G:102:PRO:HB3 | 1:G:131:ALA:HB3 | 1.73 | 0.70 |
| 1:E:217:CYS:SG | 1:E:307:PRO:HD2 | 2.32 | 0.70 |
| 1:D:46:GLY:H | 1:D:49:GLN:HB2 | 1.56 | 0.70 |
| 1:D:302:GLY:C | 1:D:304:THR:H | 1.95 | 0.70 |
| 1:G:203:THR:O | 1:G:207:GLU:HG2 | 1.92 | 0.70 |
| 1:F:33:SER:HB2 | 1:F:85:ILE:HD13 | 1.72 | 0.70 |
| 1:E:152:VAL:HG12 | 1:E:298:VAL:CG1 | 2.21 | 0.70 |
| 1:H:71:ILE:HD11 | 1:H:74:GLY:C | 2.12 | 0.70 |
| 1:H:230:ALA:HB1 | 1:H:236:LEU:HD21 | 1.73 | 0.70 |
| 1:E:171:LEU:HA | 1:G:40:HIS:NE2 | 2.05 | 0.70 |
| 1:E:59:GLN:O | 1:E:62:ARG:HG3 | 1.92 | 0.70 |
| 1:F:118:LYS:HE2 | 1:F:118:LYS:HA | 1.74 | 0.70 |
| 1:F:124:PHE:CZ | 1:F:362:TYR:HB3 | 2.27 | 0.70 |
| 1:D:297:ASN:HB3 | 1:D:328:LYS:O | 1.92 | 0.70 |
| 1:F:310:ALA:HB1 | 1:F:329:ILE:HG13 | 1.72 | 0.70 |
| 1:F:242:LEU:HG | 1:F:246:GLN:O | 1.92 | 0.70 |
| 1:D:152:VAL:HG12 | 1:D:298:VAL:HG13 | 1.72 | 0.70 |
| 1:D:109:PRO:O | 1:D:177:ARG:HD3 | 1.91 | 0.70 |
| 1:E:264:PRO:O | 1:E:267:ILE:HG22 | 1.92 | 0.70 |
| 1:F:152:VAL:HG12 | 1:F:298:VAL:HG13 | 1.72 | 0.70 |
| 1:F:165:ILE:HG13 | 1:F:170:ALA:HB2 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:310:ALA:HB1 | 1:D:329:ILE:HG13 | 1.73 | 0.69 |
| 1:G:152:VAL:HG12 | 1:G:298:VAL:HG13 | 1.73 | 0.69 |
| 1:G:71:ILE:HD11 | 1:G:74:GLY:C | 2.12 | 0.69 |
| 1:E:124:PHE:CZ | 1:E:362:TYR:HB3 | 2.26 | 0.69 |
| 1:D:124:PHE:CZ | 1:D:362:TYR:HB3 | 2.27 | 0.69 |
| 1:H:152:VAL:HG12 | 1:H:298:VAL:CG1 | 2.20 | 0.69 |
| 1:F:238:LYS:NZ | 1:F:254:ARG:HH22 | 1.89 | 0.69 |
| 1:E:118:LYS:HE2 | 1:E:118:LYS:HA | 1.72 | 0.69 |
| 1:H:237:GLU:O | 1:H:238:LYS:HG3 | 1.92 | 0.69 |
| 1:E:238:LYS:NZ | 1:E:254:ARG:HH22 | 1.88 | 0.69 |
| 1:F:141:SER:HA | 1:F:338:SER:HB2 | 1.74 | 0.69 |
| 1:H:136:ILE:CD1 | 1:H:139:VAL:H | 2.06 | 0.69 |
| 1:D:136:ILE:CD1 | 1:D:139:VAL:H | 2.05 | 0.69 |
| 1:G:302:GLY:C | 1:G:304:THR:H | 1.96 | 0.69 |
| 1:F:230:ALA:HB1 | 1:F:236:LEU:HD21 | 1.75 | 0.69 |
| 1:H:203:THR:O | 1:H:207:GLU:HG2 | 1.93 | 0.69 |
| 1:E:236:LEU:H | 1:E:236:LEU:HD13 | 1.57 | 0.69 |
| 1:D:238:LYS:HZ2 | 1:D:254:ARG:HH22 | 1.41 | 0.69 |
| 1:H:59:GLN:O | 1:H:62:ARG:HG3 | 1.92 | 0.69 |
| 1:G:46:GLY:H | 1:G:49:GLN:HB2 | 1.57 | 0.69 |
| 1:E:340:TRP:HE3 | 1:E:341:ILE:HD13 | 1.57 | 0.69 |
| 1:E:112:PRO:HG3 | 1:F:197:GLY:HA2 | 1.73 | 0.69 |
| 1:G:99:GLU:HG3 | 1:G:128:ASN:HB2 | 1.73 | 0.69 |
| 1:H:303:THR:O | 1:H:306:TYR:HB2 | 1.93 | 0.69 |
| 1:D:329:ILE:H | 1:D:329:ILE:CD1 | 2.02 | 0.69 |
| 1:E:303:THR:O | 1:E:306:TYR:HB2 | 1.92 | 0.69 |
| 1:F:219:VAL:HG21 | 1:F:308:GLY:O | 1.92 | 0.69 |
| 1:F:136:ILE:CD1 | 1:F:139:VAL:H | 2.06 | 0.69 |
| 1:G:303:THR:O | 1:G:306:TYR:HB2 | 1.92 | 0.69 |
| 1:D:59:GLN:O | 1:D:62:ARG:HG3 | 1.93 | 0.69 |
| 1:F:59:GLN:O | 1:F:62:ARG:HG3 | 1.92 | 0.69 |
| 1:D:112:PRO:HG3 | 1:E:197:GLY:HA2 | 1.73 | 0.69 |
| 1:D:76:ILE:H | 1:D:115:ASN:ND2 | 1.89 | 0.69 |
| 1:H:118:LYS:HA | 1:H:118:LYS:HE2 | 1.75 | 0.69 |
| 1:F:190:MET:CE | 1:F:206:ARG:HG3 | 2.23 | 0.69 |
| 1:E:124:PHE:HA | 1:E:129:VAL:HG22 | 1.75 | 0.69 |
| 1:F:203:THR:O | 1:F:207:GLU:HG2 | 1.93 | 0.69 |
| 1:H:221:LEU:HB3 | 1:H:315:LYS:HE2 | 1.73 | 0.69 |
| 1:D:33:SER:HB2 | 1:D:85:ILE:HD13 | 1.73 | 0.69 |
| 1:F:54:VAL:HG21 | 1:F:88:HIS:CG | 2.28 | 0.69 |
| 1:G:106:THR:HG22 | 1:G:137:GLN:HE22 | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:310:ALA:HB1 | 1:E:329:ILE:HG13 | 1.73 | 0.68 |
| 1:F:102:PRO:HB3 | 1:F:131:ALA:HB3 | 1.73 | 0.68 |
| 1:G:264:PRO:HD2 | 1:G:272:ALA:O | 1.92 | 0.68 |
| 1:D:226:GLU:HA | 1:D:229:THR:HG22 | 1.73 | 0.68 |
| 1:D:230:ALA:HB1 | 1:D:236:LEU:HD21 | 1.75 | 0.68 |
| 1:H:302:GLY:C | 1:H:304:THR:H | 1.95 | 0.68 |
| 1:D:152:VAL:HG12 | 1:D:298:VAL:CG1 | 2.22 | 0.68 |
| 1:F:302:GLY:C | 1:F:304:THR:H | 1.96 | 0.68 |
| 1:H:190:MET:CE | 1:H:206:ARG:HG3 | 2.23 | 0.68 |
| 1:E:157:ASP:O | 1:E:183:ARG:HB3 | 1.94 | 0.68 |
| 1:F:297:ASN:HB3 | 1:F:328:LYS:O | 1.94 | 0.68 |
| 1:G:54:VAL:HG21 | 1:G:88:HIS:CG | 2.28 | 0.68 |
| 1:E:258:PRO:HG3 | 1:E:306:TYR:HE2 | 1.56 | 0.68 |
| 1:F:171:LEU:HA | 1:H:40:HIS:NE2 | 2.08 | 0.68 |
| 1:G:79:TRP:HA | 1:G:79:TRP:CE3 | 2.29 | 0.68 |
| 1:E:136:ILE:CD1 | 1:E:139:VAL:H | 2.06 | 0.68 |
| 1:E:106:THR:HG22 | 1:E:137:GLN:HE22 | 1.58 | 0.68 |
| 1:H:340:TRP:HE3 | 1:H:341:ILE:HD13 | 1.57 | 0.68 |
| 1:G:340:TRP:HE3 | 1:G:341:ILE:HD13 | 1.58 | 0.68 |
| 1:G:302:GLY:O | 1:G:304:THR:N | 2.27 | 0.68 |
| 1:E:330:ILE:HG22 | 1:E:330:ILE:O | 1.94 | 0.68 |
| 1:H:79:TRP:CE3 | 1:H:79:TRP:HA | 2.29 | 0.68 |
| 1:G:136:ILE:CD1 | 1:G:139:VAL:H | 2.05 | 0.68 |
| 1:D:203:THR:O | 1:D:207:GLU:HG2 | 1.94 | 0.68 |
| 1:H:46:GLY:H | 1:H:49:GLN:HB2 | 1.58 | 0.68 |
| 1:F:152:VAL:HG12 | 1:F:298:VAL:CG1 | 2.23 | 0.68 |
| 1:D:330:ILE:HG22 | 1:D:330:ILE:O | 1.93 | 0.68 |
| 1:H:76:ILE:H | 1:H:115:ASN:ND2 | 1.90 | 0.68 |
| 1:D:327:ILE:H | 1:D:327:ILE:HD13 | 1.58 | 0.68 |
| 1:H:329:ILE:N | 1:H:329:ILE:HD13 | 2.03 | 0.68 |
| 1:G:152:VAL:HG12 | 1:G:298:VAL:CG1 | 2.24 | 0.68 |
| 1:D:124:PHE:HA | 1:D:129:VAL:HG22 | 1.75 | 0.68 |
| 1:E:302:GLY:C | 1:E:304:THR:H | 1.97 | 0.68 |
| 1:E:297:ASN:HB3 | 1:E:328:LYS:O | 1.93 | 0.68 |
| 1:F:340:TRP:HE3 | 1:F:341:ILE:HD13 | 1.57 | 0.68 |
| 1:G:124:PHE:CZ | 1:G:362:TYR:HB3 | 2.28 | 0.67 |
| 1:G:217:CYS:SG | 1:G:307:PRO:HD2 | 2.34 | 0.67 |
| 1:D:91:TYR:O | 1:D:92:ASN:CB | 2.42 | 0.67 |
| 1:E:230:ALA:HB1 | 1:E:236:LEU:HD21 | 1.76 | 0.67 |
| 1:G:230:ALA:HB1 | 1:G:236:LEU:HD21 | 1.76 | 0.67 |
| 1:D:71:ILE:HD11 | 1:D:74:GLY:C | 2.14 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:PRO:HB3 | 1:E:131:ALA:HB3 | 1.76 | 0.67 |
| 1:D:219:VAL:HG21 | 1:D:308:GLY:O | 1.93 | 0.67 |
| 1:E:221:LEU:HB3 | 1:E:315:LYS:HE2 | 1.77 | 0.67 |
| 1:D:340:TRP:HE3 | 1:D:341:ILE:HD13 | 1.58 | 0.67 |
| 1:F:236:LEU:H | 1:F:236:LEU:HD13 | 1.60 | 0.67 |
| 1:F:238:LYS:HG2 | 1:F:254:ARG:HH12 | 1.60 | 0.67 |
| 1:G:202:THR:CG2 | 1:G:205:GLU:H | 2.08 | 0.67 |
| 1:D:54:VAL:HG21 | 1:D:88:HIS:CG | 2.29 | 0.67 |
| 1:G:124:PHE:HA | 1:G:129:VAL:HG22 | 1.77 | 0.67 |
| 1:G:352:PHE:O | 1:G:355:MET:HG2 | 1.94 | 0.67 |
| 1:H:297:ASN:HB3 | 1:H:328:LYS:O | 1.95 | 0.67 |
| 1:F:273:GLY:O | 1:F:277:THR:HG23 | 1.94 | 0.67 |
| 1:G:350:SER:C | 1:G:352:PHE:H | 1.98 | 0.67 |
| 1:G:330:ILE:HG22 | 1:G:330:ILE:O | 1.95 | 0.67 |
| 1:F:219:VAL:HG13 | 1:F:307:PRO:O | 1.95 | 0.67 |
| 1:G:190:MET:CE | 1:G:206:ARG:HG3 | 2.22 | 0.67 |
| 1:H:362:TYR:O | 1:H:365:ALA:O | 2.13 | 0.67 |
| 1:G:327:ILE:HD13 | 1:G:327:ILE:H | 1.59 | 0.67 |
| 1:D:350:SER:C | 1:D:352:PHE:H | 1.98 | 0.67 |
| 1:F:71:ILE:HD11 | 1:F:74:GLY:C | 2.16 | 0.67 |
| 1:G:76:ILE:H | 1:G:115:ASN:ND2 | 1.90 | 0.67 |
| 1:D:264:PRO:HD2 | 1:D:272:ALA:O | 1.95 | 0.67 |
| 1:E:78:ASN:HB3 | 1:E:81:ASP:OD2 | 1.95 | 0.67 |
| 1:F:124:PHE:HA | 1:F:129:VAL:HG22 | 1.77 | 0.66 |
| 1:G:219:VAL:HG13 | 1:G:307:PRO:O | 1.95 | 0.66 |
| 1:D:78:ASN:HB3 | 1:D:81:ASP:OD2 | 1.95 | 0.66 |
| 1:F:291:LYS:HB2 | 1:H:244:ASP:OD2 | 1.95 | 0.66 |
| 1:D:217:CYS:SG | 1:D:307:PRO:HD2 | 2.35 | 0.66 |
| 1:H:106:THR:HG22 | 1:H:137:GLN:HE22 | 1.59 | 0.66 |
| 1:E:190:MET:CE | 1:E:206:ARG:HG3 | 2.22 | 0.66 |
| 1:G:118:LYS:HE2 | 1:G:118:LYS:HA | 1.75 | 0.66 |
| 1:E:219:VAL:HG21 | 1:E:308:GLY:O | 1.95 | 0.66 |
| 1:D:171:LEU:HA | 1:F:40:HIS:HE2 | 1.61 | 0.66 |
| 1:D:118:LYS:HE2 | 1:D:118:LYS:HA | 1.77 | 0.66 |
| 1:E:264:PRO:HD2 | 1:E:272:ALA:O | 1.95 | 0.66 |
| 1:E:143:TYR:CZ | 1:G:44:MET:SD | 2.88 | 0.66 |
| 1:F:170:ALA:O | 1:H:40:HIS:NE2 | 2.28 | 0.66 |
| 1:E:71:ILE:HD11 | 1:E:74:GLY:C | 2.15 | 0.66 |
| 1:D:329:ILE:HD13 | 1:D:329:ILE:N | 2.06 | 0.66 |
| 1:D:170:ALA:O | 1:F:40:HIS:NE2 | 2.29 | 0.66 |
| 1:F:143:TYR:CZ | 1:H:44:MET:SD | 2.89 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:202:THR:CG2 | 1:H:205:GLU:H | 2.09 | 0.66 |
| 1:D:157:ASP:O | 1:D:183:ARG:HB3 | 1.95 | 0.66 |
| 1:F:362:TYR:O | 1:F:365:ALA:O | 2.14 | 0.66 |
| 1:D:273:GLY:O | 1:D:277:THR:HG23 | 1.96 | 0.66 |
| 1:F:221:LEU:HB3 | 1:F:315:LYS:HE2 | 1.76 | 0.66 |
| 1:H:110:LEU:HD11 | 1:H:175:ILE:HB | 1.76 | 0.66 |
| 1:E:52:SER:HB2 | 1:E:65:LEU:HD13 | 1.77 | 0.66 |
| 1:G:113:LYS:HE2 | 1:H:195:GLU:HG3 | 1.77 | 0.66 |
| 1:D:219:VAL:HG13 | 1:D:307:PRO:O | 1.96 | 0.66 |
| 1:E:255:PHE:O | 1:E:258:PRO:HD2 | 1.96 | 0.66 |
| 1:H:154:ASP:HA | 1:H:300:SER:O | 1.95 | 0.66 |
| 1:H:302:GLY:O | 1:H:304:THR:N | 2.26 | 0.66 |
| 1:E:352:PHE:O | 1:E:355:MET:HG2 | 1.95 | 0.66 |
| 1:H:109:PRO:O | 1:H:177:ARG:HD3 | 1.96 | 0.65 |
| 1:D:79:TRP:HA | 1:D:79:TRP:CE3 | 2.30 | 0.65 |
| 1:D:190:MET:CE | 1:D:206:ARG:HG3 | 2.26 | 0.65 |
| 1:F:46:GLY:H | 1:F:49:GLN:HB2 | 1.59 | 0.65 |
| 1:H:330:ILE:HG22 | 1:H:330:ILE:O | 1.96 | 0.65 |
| 1:G:157:ASP:O | 1:G:183:ARG:HB3 | 1.96 | 0.65 |
| 1:H:350:SER:C | 1:H:352:PHE:H | 2.00 | 0.65 |
| 1:F:78:ASN:HB3 | 1:F:81:ASP:OD2 | 1.96 | 0.65 |
| 1:E:273:GLY:O | 1:E:277:THR:HG23 | 1.96 | 0.65 |
| 1:H:236:LEU:H | 1:H:236:LEU:HD13 | 1.60 | 0.65 |
| 1:G:78:ASN:HB3 | 1:G:81:ASP:OD2 | 1.96 | 0.65 |
| 1:G:109:PRO:O | 1:G:177:ARG:HD3 | 1.96 | 0.65 |
| 1:F:113:LYS:HE2 | 1:G:195:GLU:HG3 | 1.78 | 0.65 |
| 1:H:274:ILE:HA | 1:H:277:THR:OG1 | 1.96 | 0.65 |
| 1:F:176:MET:CE | 1:F:277:THR:HB | 2.27 | 0.65 |
| 1:F:7:ALA:O | 1:F:22:ALA:N | 2.30 | 0.65 |
| 1:H:257:CYS:SG | 1:H:258:PRO:HD3 | 2.36 | 0.65 |
| 1:D:107:GLU:OE2 | 1:D:116:ARG:HG2 | 1.97 | 0.65 |
| 1:H:273:GLY:O | 1:H:277:THR:HG23 | 1.96 | 0.65 |
| 1:E:110:LEU:HD11 | 1:E:175:ILE:HB | 1.79 | 0.65 |
| 1:E:79:TRP:CE3 | 1:E:79:TRP:HA | 2.30 | 0.65 |
| 1:G:71:ILE:HG13 | 1:G:75:ILE:C | 2.17 | 0.65 |
| 1:E:302:GLY:O | 1:E:304:THR:N | 2.30 | 0.65 |
| 1:E:202:THR:CG2 | 1:E:205:GLU:H | 2.07 | 0.65 |
| 1:F:98:PRO:CB | 1:F:127:PHE:HB3 | 2.27 | 0.65 |
| 1:D:221:LEU:HB3 | 1:D:315:LYS:HE2 | 1.77 | 0.65 |
| 1:H:124:PHE:HA | 1:H:129:VAL:HG22 | 1.78 | 0.65 |
| 1:E:107:GLU:OE2 | 1:E:116:ARG:HG2 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:297:ASN:HB3 | 1:G:328:LYS:O | 1.95 | 0.65 |
| 1:F:274:ILE:HA | 1:F:277:THR:OG1 | 1.97 | 0.65 |
| 1:G:362:TYR:O | 1:G:365:ALA:O | 2.15 | 0.65 |
| 1:D:72:GLU:HA | 1:D:183:ARG:NH2 | 2.11 | 0.65 |
| 1:G:157:ASP:C | 1:G:181:ALA:HB1 | 2.17 | 0.65 |
| 1:H:264:PRO:HD2 | 1:H:272:ALA:O | 1.97 | 0.65 |
| 1:E:327:ILE:H | 1:E:327:ILE:HD13 | 1.62 | 0.65 |
| 1:D:143:TYR:CZ | 1:F:44:MET:SD | 2.90 | 0.64 |
| 1:D:176:MET:CE | 1:D:277:THR:HB | 2.27 | 0.64 |
| 1:H:78:ASN:HB3 | 1:H:81:ASP:OD2 | 1.97 | 0.64 |
| 1:E:279:TYR:CD2 | 1:E:320:LEU:HD13 | 2.32 | 0.64 |
| 1:F:302:GLY:O | 1:F:304:THR:N | 2.29 | 0.64 |
| 1:H:261:LEU:O | 1:H:274:ILE:HG12 | 1.97 | 0.64 |
| 1:F:327:ILE:H | 1:F:327:ILE:HD13 | 1.61 | 0.64 |
| 1:F:329:ILE:HD13 | 1:F:329:ILE:N | 2.08 | 0.64 |
| 1:H:219:VAL:HG13 | 1:H:307:PRO:O | 1.96 | 0.64 |
| 1:E:273:GLY:O | 1:E:277:THR:N | 2.25 | 0.64 |
| 1:E:349:LEU:HB3 | 1:E:352:PHE:CE2 | 2.32 | 0.64 |
| 1:G:273:GLY:O | 1:G:277:THR:HG23 | 1.97 | 0.64 |
| 1:E:147:ARG:HH22 | 1:E:330:ILE:CD1 | 2.11 | 0.64 |
| 1:F:157:ASP:C | 1:F:181:ALA:HB1 | 2.17 | 0.64 |
| 1:E:170:ALA:O | 1:G:40:HIS:NE2 | 2.31 | 0.64 |
| 1:F:147:ARG:HH22 | 1:F:330:ILE:CD1 | 2.11 | 0.64 |
| 1:F:154:ASP:HA | 1:F:300:SER:O | 1.98 | 0.64 |
| 1:H:273:GLY:O | 1:H:277:THR:N | 2.27 | 0.64 |
| 1:F:107:GLU:OE2 | 1:F:116:ARG:HG2 | 1.97 | 0.64 |
| 1:D:210:ARG:O | 1:D:211:ASP:HB3 | 1.98 | 0.64 |
| 1:G:91:TYR:O | 1:G:92:ASN:CB | 2.46 | 0.64 |
| 1:H:327:ILE:H | 1:H:327:ILE:HD13 | 1.61 | 0.64 |
| 1:D:136:ILE:HG23 | 1:D:139:VAL:HB | 1.80 | 0.64 |
| 1:D:52:SER:HB2 | 1:D:65:LEU:HD13 | 1.78 | 0.64 |
| 1:H:157:ASP:O | 1:H:183:ARG:HB3 | 1.98 | 0.64 |
| 1:E:157:ASP:C | 1:E:181:ALA:HB1 | 2.17 | 0.64 |
| 1:D:240:TYR:CE1 | 1:D:241:GLU:O | 2.51 | 0.64 |
| 1:H:329:ILE:CD1 | 1:H:329:ILE:H | 2.01 | 0.64 |
| 1:E:350:SER:C | 1:E:352:PHE:H | 2.01 | 0.64 |
| 1:F:79:TRP:CE3 | 1:F:79:TRP:HA | 2.32 | 0.64 |
| 1:G:147:ARG:HH22 | 1:G:330:ILE:CD1 | 2.10 | 0.64 |
| 1:E:171:LEU:HA | 1:G:40:HIS:HE2 | 1.63 | 0.64 |
| 1:F:330:ILE:O | 1:F:330:ILE:HG22 | 1.96 | 0.64 |
| 1:F:352:PHE:O | 1:F:355:MET:HG2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:210:ARG:O | 1:G:211:ASP:HB3 | 1.98 | 0.64 |
| 1:G:7:ALA:O | 1:G:22:ALA:N | 2.31 | 0.64 |
| 1:H:212:ILE:HG22 | 1:H:216:LEU:HD12 | 1.80 | 0.64 |
| 1:H:255:PHE:O | 1:H:258:PRO:HD2 | 1.97 | 0.64 |
| 1:F:106:THR:HG22 | 1:F:137:GLN:HE22 | 1.62 | 0.64 |
| 1:E:182:GLY:O | 1:E:185:LEU:HB3 | 1.98 | 0.64 |
| 1:D:147:ARG:HH22 | 1:D:330:ILE:CD1 | 2.11 | 0.63 |
| 1:G:110:LEU:HD11 | 1:G:175:ILE:HB | 1.80 | 0.63 |
| 1:E:109:PRO:O | 1:E:177:ARG:HD3 | 1.97 | 0.63 |
| 1:E:154:ASP:HA | 1:E:300:SER:O | 1.98 | 0.63 |
| 1:H:157:ASP:C | 1:H:181:ALA:HB1 | 2.17 | 0.63 |
| 1:H:238:LYS:HG2 | 1:H:254:ARG:HH12 | 1.61 | 0.63 |
| 1:E:7:ALA:O | 1:E:22:ALA:N | 2.30 | 0.63 |
| 1:H:176:MET:CE | 1:H:277:THR:HB | 2.28 | 0.63 |
| 1:D:302:GLY:O | 1:D:304:THR:N | 2.28 | 0.63 |
| 1:G:176:MET:CE | 1:G:277:THR:HB | 2.27 | 0.63 |
| 1:H:113:LYS:HG2 | 1:H:117:GLU:OE1 | 1.98 | 0.63 |
| 1:D:222:ASP:O | 1:D:224:GLU:N | 2.31 | 0.63 |
| 1:E:261:LEU:O | 1:E:274:ILE:HG12 | 1.99 | 0.63 |
| 1:E:113:LYS:HE2 | 1:F:195:GLU:HG3 | 1.79 | 0.63 |
| 1:G:236:LEU:HD13 | 1:G:236:LEU:H | 1.64 | 0.63 |
| 1:G:221:LEU:HB3 | 1:G:315:LYS:HE2 | 1.80 | 0.63 |
| 1:D:291:LYS:HB2 | 1:F:244:ASP:OD2 | 1.99 | 0.63 |
| 1:F:110:LEU:HD11 | 1:F:175:ILE:HB | 1.79 | 0.63 |
| 1:F:172:PRO:HA | 1:F:175:ILE:HD11 | 1.79 | 0.63 |
| 1:G:261:LEU:O | 1:G:274:ILE:HG12 | 1.98 | 0.63 |
| 1:G:274:ILE:HA | 1:G:277:THR:OG1 | 1.98 | 0.63 |
| 1:F:171:LEU:HA | 1:H:40:HIS:HE2 | 1.64 | 0.63 |
| 1:G:52:SER:HB2 | 1:G:65:LEU:HD13 | 1.79 | 0.63 |
| 1:D:202:THR:CG2 | 1:D:205:GLU:H | 2.09 | 0.63 |
| 1:H:202:THR:HG22 | 1:H:205:GLU:CB | 2.28 | 0.63 |
| 1:H:62:ARG:HB3 | 1:H:204:ALA:CB | 2.28 | 0.63 |
| 1:H:72:GLU:HA | 1:H:183:ARG:NH2 | 2.12 | 0.63 |
| 1:D:279:TYR:CD2 | 1:D:320:LEU:HD13 | 2.34 | 0.63 |
| 1:F:72:GLU:HA | 1:F:183:ARG:NH2 | 2.12 | 0.63 |
| 1:D:212:ILE:HG22 | 1:D:216:LEU:HD12 | 1.81 | 0.63 |
| 1:G:107:GLU:OE2 | 1:G:116:ARG:HG2 | 1.98 | 0.63 |
| 1:E:176:MET:CE | 1:E:277:THR:HB | 2.28 | 0.63 |
| 1:E:202:THR:HG22 | 1:E:205:GLU:CB | 2.27 | 0.63 |
| 1:G:212:ILE:HG22 | 1:G:216:LEU:HD12 | 1.80 | 0.63 |
| 1:D:157:ASP:C | 1:D:181:ALA:HB1 | 2.19 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:91:TYR:O | 1:F:92:ASN:CB | 2.46 | 0.63 |
| 1:H:109:PRO:CG | 1:H:136:ILE:HG12 | 2.29 | 0.63 |
| 1:E:210:ARG:O | 1:E:211:ASP:HB3 | 1.99 | 0.63 |
| 1:H:107:GLU:OE2 | 1:H:116:ARG:HG2 | 1.97 | 0.62 |
| 1:D:238:LYS:HG2 | 1:D:254:ARG:HH12 | 1.62 | 0.62 |
| 1:G:329:ILE:CD1 | 1:G:329:ILE:H | 2.03 | 0.62 |
| 1:F:212:ILE:HG22 | 1:F:216:LEU:HD12 | 1.81 | 0.62 |
| 1:F:240:TYR:CE1 | 1:F:241:GLU:O | 2.53 | 0.62 |
| 1:E:113:LYS:HG2 | 1:E:117:GLU:OE1 | 1.99 | 0.62 |
| 1:G:72:GLU:HA | 1:G:183:ARG:NH2 | 2.13 | 0.62 |
| 1:H:91:TYR:O | 1:H:92:ASN:CB | 2.47 | 0.62 |
| 1:F:349:LEU:HB3 | 1:F:352:PHE:CE2 | 2.33 | 0.62 |
| 1:E:71:ILE:HG13 | 1:E:75:ILE:C | 2.20 | 0.62 |
| 1:E:291:LYS:HB2 | 1:G:244:ASP:OD2 | 1.98 | 0.62 |
| 1:G:172:PRO:HA | 1:G:175:ILE:HD11 | 1.81 | 0.62 |
| 1:F:122:ILE:O | 1:F:126:THR:HB | 1.99 | 0.62 |
| 1:D:7:ALA:O | 1:D:22:ALA:N | 2.32 | 0.62 |
| 1:H:349:LEU:HB3 | 1:H:352:PHE:CE2 | 2.33 | 0.62 |
| 1:H:352:PHE:O | 1:H:355:MET:HG2 | 1.98 | 0.62 |
| 1:F:227:MET:HA | 1:F:255:PHE:HZ | 1.64 | 0.62 |
| 1:E:212:ILE:HG22 | 1:E:216:LEU:HD12 | 1.81 | 0.62 |
| 1:F:202:THR:CG2 | 1:F:205:GLU:H | 2.08 | 0.62 |
| 1:D:71:ILE:HG13 | 1:D:75:ILE:C | 2.20 | 0.62 |
| 1:D:106:THR:HG22 | 1:D:137:GLN:HE22 | 1.62 | 0.62 |
| 1:D:182:GLY:O | 1:D:185:LEU:HB3 | 1.99 | 0.62 |
| 1:H:147:ARG:HH22 | 1:H:330:ILE:CD1 | 2.12 | 0.62 |
| 1:F:209:VAL:O | 1:F:212:ILE:HG12 | 1.98 | 0.62 |
| 1:G:202:THR:HG22 | 1:G:205:GLU:CB | 2.28 | 0.62 |
| 1:E:219:VAL:HG13 | 1:E:307:PRO:O | 1.99 | 0.62 |
| 1:F:113:LYS:HG2 | 1:F:117:GLU:OE1 | 1.99 | 0.62 |
| 1:G:329:ILE:HD13 | 1:G:329:ILE:N | 2.04 | 0.62 |
| 1:F:109:PRO:O | 1:F:177:ARG:HD3 | 1.99 | 0.62 |
| 1:H:122:ILE:O | 1:H:126:THR:HB | 2.00 | 0.62 |
| 1:E:122:ILE:O | 1:E:126:THR:HB | 1.99 | 0.62 |
| 1:E:72:GLU:HA | 1:E:183:ARG:NH2 | 2.14 | 0.62 |
| 1:H:162:ASN:ND2 | 1:H:278:THR:HG22 | 2.12 | 0.62 |
| 1:H:315:LYS:NZ | 1:H:315:LYS:HB2 | 2.13 | 0.62 |
| 1:G:279:TYR:CD2 | 1:G:320:LEU:HD13 | 2.34 | 0.62 |
| 1:D:105:LEU:HD22 | 1:D:105:LEU:H | 1.65 | 0.62 |
| 1:H:136:ILE:HG23 | 1:H:139:VAL:HB | 1.82 | 0.62 |
| 1:D:202:THR:HG22 | 1:D:205:GLU:CB | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:113:LYS:HG2 | 1:D:117:GLU:OE1 | 2.00 | 0.62 |
| 1:H:71:ILE:HG13 | 1:H:75:ILE:C | 2.18 | 0.62 |
| 1:F:257:CYS:SG | 1:F:258:PRO:HD3 | 2.40 | 0.61 |
| 1:G:238:LYS:HG2 | 1:G:254:ARG:HH12 | 1.60 | 0.61 |
| 1:D:362:TYR:O | 1:D:365:ALA:O | 2.18 | 0.61 |
| 1:D:110:LEU:HD11 | 1:D:175:ILE:HB | 1.81 | 0.61 |
| 1:G:122:ILE:O | 1:G:126:THR:HB | 1.99 | 0.61 |
| 1:E:362:TYR:O | 1:E:365:ALA:O | 2.18 | 0.61 |
| 1:H:7:ALA:O | 1:H:22:ALA:N | 2.32 | 0.61 |
| 1:E:227:MET:HA | 1:E:255:PHE:HZ | 1.65 | 0.61 |
| 1:G:349:LEU:HB3 | 1:G:352:PHE:CE2 | 2.35 | 0.61 |
| 1:D:122:ILE:O | 1:D:126:THR:HB | 2.01 | 0.61 |
| 1:E:238:LYS:HG2 | 1:E:254:ARG:HH12 | 1.61 | 0.61 |
| 1:H:172:PRO:HA | 1:H:175:ILE:HD11 | 1.81 | 0.61 |
| 1:E:274:ILE:HA | 1:E:277:THR:OG1 | 2.00 | 0.61 |
| 1:F:255:PHE:O | 1:F:258:PRO:HD2 | 1.99 | 0.61 |
| 1:G:257:CYS:SG | 1:G:258:PRO:HD3 | 2.41 | 0.61 |
| 1:G:209:VAL:O | 1:G:212:ILE:HG12 | 2.00 | 0.61 |
| 1:D:257:CYS:SG | 1:D:258:PRO:HD3 | 2.40 | 0.61 |
| 1:H:289:ILE:HG23 | 1:H:289:ILE:O | 2.00 | 0.61 |
| 1:F:71:ILE:HG13 | 1:F:75:ILE:C | 2.20 | 0.61 |
| 1:G:226:GLU:HA | 1:G:229:THR:HG22 | 1.82 | 0.61 |
| 1:E:91:TYR:O | 1:E:92:ASN:CB | 2.48 | 0.61 |
| 1:F:226:GLU:HA | 1:F:229:THR:HG22 | 1.82 | 0.61 |
| 1:D:315:LYS:NZ | 1:D:315:LYS:HB2 | 2.16 | 0.61 |
| 1:F:279:TYR:CD2 | 1:F:320:LEU:HD13 | 2.36 | 0.61 |
| 1:F:136:ILE:HG23 | 1:F:139:VAL:HB | 1.83 | 0.61 |
| 1:H:279:TYR:CD2 | 1:H:320:LEU:HD13 | 2.35 | 0.61 |
| 1:E:221:LEU:N | 1:E:221:LEU:HD12 | 2.16 | 0.60 |
| 1:F:52:SER:HB2 | 1:F:65:LEU:HD13 | 1.81 | 0.60 |
| 1:D:372:ARG:O | 1:D:373:LYS:HB3 | 1.99 | 0.60 |
| 1:F:261:LEU:O | 1:F:274:ILE:HG12 | 2.00 | 0.60 |
| 1:F:162:ASN:ND2 | 1:F:278:THR:HG22 | 2.14 | 0.60 |
| 1:G:359:LYS:O | 1:G:360:GLN:HB3 | 2.02 | 0.60 |
| 1:E:51:ASP:HB3 | 1:E:53:TYR:CZ | 2.36 | 0.60 |
| 1:G:273:GLY:O | 1:G:277:THR:N | 2.32 | 0.60 |
| 1:E:240:TYR:CE1 | 1:E:241:GLU:O | 2.55 | 0.60 |
| 1:G:113:LYS:HG2 | 1:G:117:GLU:OE1 | 2.01 | 0.60 |
| 1:D:274:ILE:HA | 1:D:277:THR:OG1 | 2.01 | 0.60 |
| 1:G:97:ALA:HB3 | 1:G:100:GLU:OE2 | 2.02 | 0.60 |
| 1:F:187:ASP:HA | 1:F:190:MET:HE3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:62:ARG:HB3 | 1:F:204:ALA:CB | 2.30 | 0.60 |
| 1:D:261:LEU:O | 1:D:274:ILE:HG12 | 2.02 | 0.60 |
| 1:G:315:LYS:NZ | 1:G:315:LYS:HB2 | 2.14 | 0.60 |
| 1:F:238:LYS:HZ2 | 1:F:254:ARG:HH22 | 1.48 | 0.60 |
| 1:H:52:SER:HB2 | 1:H:65:LEU:HD13 | 1.81 | 0.60 |
| 1:D:113:LYS:HE2 | 1:E:195:GLU:HG3 | 1.84 | 0.60 |
| 1:D:209:VAL:O | 1:D:212:ILE:HG12 | 2.01 | 0.60 |
| 1:F:289:ILE:HG23 | 1:F:289:ILE:O | 2.02 | 0.60 |
| 1:F:315:LYS:NZ | 1:F:315:LYS:HB2 | 2.16 | 0.60 |
| 1:E:329:ILE:N | 1:E:329:ILE:HD13 | 2.06 | 0.60 |
| 1:F:51:ASP:HB3 | 1:F:53:TYR:CZ | 2.37 | 0.60 |
| 1:D:352:PHE:O | 1:D:355:MET:HG2 | 2.02 | 0.60 |
| 1:G:109:PRO:CG | 1:G:136:ILE:HG12 | 2.32 | 0.60 |
| 1:G:136:ILE:HG23 | 1:G:139:VAL:HB | 1.83 | 0.60 |
| 1:E:372:ARG:O | 1:E:373:LYS:HB3 | 2.02 | 0.60 |
| 1:H:7:ALA:O | 1:H:22:ALA:HA | 2.02 | 0.60 |
| 1:H:220:ALA:CB | 1:H:226:GLU:HG3 | 2.32 | 0.60 |
| 1:E:226:GLU:HA | 1:E:229:THR:HG22 | 1.83 | 0.60 |
| 1:F:352:PHE:HZ | 1:H:47:MET:HE1 | 1.66 | 0.59 |
| 1:E:238:LYS:HD3 | 1:E:239:SER:H | 1.66 | 0.59 |
| 1:E:62:ARG:HB3 | 1:E:204:ALA:CB | 2.31 | 0.59 |
| 1:F:7:ALA:O | 1:F:22:ALA:HA | 2.02 | 0.59 |
| 1:E:315:LYS:HB2 | 1:E:315:LYS:NZ | 2.17 | 0.59 |
| 1:D:349:LEU:HB3 | 1:D:352:PHE:CE2 | 2.36 | 0.59 |
| 1:G:210:ARG:O | 1:G:211:ASP:CB | 2.50 | 0.59 |
| 1:E:7:ALA:O | 1:E:22:ALA:HA | 2.02 | 0.59 |
| 1:F:105:LEU:H | 1:F:105:LEU:HD22 | 1.67 | 0.59 |
| 1:G:289:ILE:HG23 | 1:G:289:ILE:O | 2.01 | 0.59 |
| 1:E:257:CYS:SG | 1:E:258:PRO:HD3 | 2.43 | 0.59 |
| 1:G:76:ILE:HG21 | 1:G:79:TRP:CE3 | 2.37 | 0.59 |
| 1:F:359:LYS:O | 1:F:360:GLN:HB3 | 2.02 | 0.59 |
| 1:D:267:ILE:O | 1:D:267:ILE:HD13 | 2.02 | 0.59 |
| 1:D:238:LYS:HD3 | 1:D:239:SER:H | 1.67 | 0.59 |
| 1:D:173:HIS:CE1 | 1:E:268:GLY:HA3 | 2.37 | 0.59 |
| 1:E:170:ALA:C | 1:G:40:HIS:HE2 | 2.05 | 0.59 |
| 1:D:51:ASP:HB3 | 1:D:53:TYR:CZ | 2.36 | 0.59 |
| 1:D:210:ARG:O | 1:D:211:ASP:CB | 2.49 | 0.59 |
| 1:D:236:LEU:HD13 | 1:D:236:LEU:H | 1.68 | 0.59 |
| 1:E:272:ALA:HB1 | 1:E:277:THR:CG2 | 2.32 | 0.59 |
| 1:E:136:ILE:HG23 | 1:E:139:VAL:HB | 1.84 | 0.59 |
| 1:H:258:PRO:HG3 | 1:H:306:TYR:CE2 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:209:VAL:O | 1:E:212:ILE:HG12 | 2.03 | 0.59 |
| 1:G:98:PRO:CB | 1:G:127:PHE:HB3 | 2.28 | 0.59 |
| 1:H:76:ILE:HG21 | 1:H:79:TRP:CE3 | 2.37 | 0.59 |
| 1:E:98:PRO:CB | 1:E:127:PHE:HB3 | 2.28 | 0.59 |
| 1:H:187:ASP:HA | 1:H:190:MET:HE3 | 1.85 | 0.59 |
| 1:H:238:LYS:HD3 | 1:H:239:SER:H | 1.67 | 0.59 |
| 1:H:102:PRO:HB2 | 1:H:356:TRP:CZ3 | 2.38 | 0.59 |
| 1:F:273:GLY:O | 1:F:277:THR:N | 2.27 | 0.59 |
| 1:H:36:GLY:O | 1:H:65:LEU:HD11 | 2.03 | 0.59 |
| 1:F:76:ILE:HG21 | 1:F:79:TRP:CE3 | 2.38 | 0.59 |
| 1:D:76:ILE:HG21 | 1:D:79:TRP:CE3 | 2.38 | 0.59 |
| 1:H:226:GLU:HA | 1:H:229:THR:HG22 | 1.84 | 0.59 |
| 1:D:352:PHE:HZ | 1:F:47:MET:HE1 | 1.68 | 0.59 |
| 1:G:182:GLY:O | 1:G:185:LEU:HB3 | 2.03 | 0.59 |
| 1:H:51:ASP:HB3 | 1:H:53:TYR:CZ | 2.39 | 0.58 |
| 1:F:202:THR:HG22 | 1:F:205:GLU:CB | 2.31 | 0.58 |
| 1:D:34:ILE:HG12 | 1:D:67:LEU:HD23 | 1.85 | 0.58 |
| 1:F:164:PRO:C | 1:F:165:ILE:HD12 | 2.24 | 0.58 |
| 1:F:345:ILE:HG22 | 1:F:349:LEU:HD12 | 1.85 | 0.58 |
| 1:G:227:MET:HA | 1:G:255:PHE:HZ | 1.68 | 0.58 |
| 1:E:97:ALA:HB3 | 1:E:100:GLU:OE2 | 2.03 | 0.58 |
| 1:F:272:ALA:HB1 | 1:F:277:THR:CG2 | 2.34 | 0.58 |
| 1:D:227:MET:HA | 1:D:255:PHE:HZ | 1.67 | 0.58 |
| 1:G:62:ARG:HB3 | 1:G:204:ALA:CB | 2.32 | 0.58 |
| 1:F:182:GLY:O | 1:F:185:LEU:HB3 | 2.03 | 0.58 |
| 1:F:109:PRO:CG | 1:F:136:ILE:HG12 | 2.31 | 0.58 |
| 1:E:210:ARG:O | 1:E:211:ASP:CB | 2.51 | 0.58 |
| 1:F:123:MET:HA | 1:F:127:PHE:HD2 | 1.69 | 0.58 |
| 1:E:183:ARG:O | 1:E:186:THR:HB | 2.04 | 0.58 |
| 1:H:355:MET:HE2 | 1:H:356:TRP:HE1 | 1.69 | 0.58 |
| 1:G:51:ASP:HB3 | 1:G:53:TYR:CZ | 2.37 | 0.58 |
| 1:H:240:TYR:CE1 | 1:H:241:GLU:O | 2.57 | 0.58 |
| 1:G:238:LYS:HD3 | 1:G:239:SER:H | 1.68 | 0.58 |
| 1:H:209:VAL:O | 1:H:212:ILE:HG12 | 2.02 | 0.58 |
| 1:H:221:LEU:HD23 | 1:H:315:LYS:HD3 | 1.85 | 0.58 |
| 1:H:221:LEU:HD12 | 1:H:221:LEU:N | 2.19 | 0.58 |
| 1:H:372:ARG:O | 1:H:373:LYS:HB3 | 2.03 | 0.58 |
| 1:D:164:PRO:C | 1:D:165:ILE:HD12 | 2.24 | 0.58 |
| 1:D:170:ALA:C | 1:F:40:HIS:HE2 | 2.07 | 0.58 |
| 1:H:123:MET:HA | 1:H:127:PHE:HD2 | 1.69 | 0.58 |
| 1:H:183:ARG:O | 1:H:186:THR:HB | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:227:MET:HA | 1:H:255:PHE:HZ | 1.69 | 0.58 |
| 1:D:7:ALA:O | 1:D:22:ALA:HA | 2.04 | 0.58 |
| 1:H:258:PRO:O | 1:H:261:LEU:HD12 | 2.03 | 0.58 |
| 1:H:345:ILE:HG22 | 1:H:349:LEU:HD12 | 1.85 | 0.58 |
| 1:D:154:ASP:HA | 1:D:300:SER:O | 2.02 | 0.58 |
| 1:D:153:LEU:HA | 1:D:161:HIS:O | 2.03 | 0.58 |
| 1:F:220:ALA:CB | 1:F:226:GLU:HG3 | 2.34 | 0.58 |
| 1:G:36:GLY:O | 1:G:65:LEU:HD11 | 2.04 | 0.58 |
| 1:D:355:MET:HE2 | 1:D:356:TRP:HE1 | 1.68 | 0.57 |
| 1:G:355:MET:HE2 | 1:G:356:TRP:HE1 | 1.68 | 0.57 |
| 1:D:255:PHE:O | 1:D:258:PRO:HD2 | 2.03 | 0.57 |
| 1:D:305:MET:O | 1:D:306:TYR:C | 2.42 | 0.57 |
| 1:F:170:ALA:C | 1:H:40:HIS:HE2 | 2.08 | 0.57 |
| 1:E:79:TRP:CZ2 | 1:E:118:LYS:HB3 | 2.39 | 0.57 |
| 1:G:345:ILE:HG22 | 1:G:349:LEU:HD12 | 1.85 | 0.57 |
| 1:D:284:LYS:HE2 | 1:D:284:LYS:HA | 1.86 | 0.57 |
| 1:D:163:VAL:HG13 | 1:D:165:ILE:CD1 | 2.34 | 0.57 |
| 1:E:172:PRO:HA | 1:E:175:ILE:HD11 | 1.85 | 0.57 |
| 1:E:105:LEU:HD22 | 1:E:105:LEU:H | 1.67 | 0.57 |
| 1:G:221:LEU:N | 1:G:221:LEU:HD12 | 2.19 | 0.57 |
| 1:F:210:ARG:O | 1:F:211:ASP:HB3 | 2.05 | 0.57 |
| 1:F:258:PRO:HG3 | 1:F:306:TYR:CE2 | 2.39 | 0.57 |
| 1:F:136:ILE:HD12 | 1:F:139:VAL:H | 1.70 | 0.57 |
| 1:F:355:MET:HE2 | 1:F:356:TRP:HE1 | 1.70 | 0.57 |
| 1:F:372:ARG:O | 1:F:373:LYS:HB3 | 2.03 | 0.57 |
| 1:H:250:ILE:O | 1:H:251:GLY:O | 2.22 | 0.57 |
| 1:F:185:LEU:O | 1:F:185:LEU:HD13 | 2.05 | 0.57 |
| 1:E:258:PRO:O | 1:E:261:LEU:HD12 | 2.05 | 0.57 |
| 1:E:5:THR:OG1 | 1:E:102:PRO:HD2 | 2.04 | 0.57 |
| 1:G:372:ARG:O | 1:G:373:LYS:HB3 | 2.04 | 0.57 |
| 1:H:105:LEU:HD22 | 1:H:105:LEU:H | 1.68 | 0.57 |
| 1:H:242:LEU:HD12 | 1:H:242:LEU:C | 2.25 | 0.57 |
| 1:E:20:GLY:HA3 | 1:E:340:TRP:HZ2 | 1.68 | 0.57 |
| 1:H:284:LYS:HE2 | 1:H:284:LYS:HA | 1.87 | 0.57 |
| 1:F:36:GLY:O | 1:F:65:LEU:HD11 | 2.04 | 0.57 |
| 1:E:329:ILE:CD1 | 1:E:329:ILE:H | 2.04 | 0.57 |
| 1:H:225:ASN:O | 1:H:229:THR:HG22 | 2.05 | 0.57 |
| 1:G:7:ALA:O | 1:G:22:ALA:HA | 2.04 | 0.57 |
| 1:D:258:PRO:O | 1:D:261:LEU:HD12 | 2.05 | 0.57 |
| 1:F:34:ILE:HG12 | 1:F:67:LEU:HD23 | 1.87 | 0.57 |
| 1:D:172:PRO:HA | 1:D:175:ILE:HD11 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:258:PRO:HG3 | 1:G:306:TYR:CE2 | 2.36 | 0.57 |
| 1:F:221:LEU:HD12 | 1:F:221:LEU:N | 2.19 | 0.57 |
| 1:F:325:MET:SD | 1:H:244:ASP:CG | 2.82 | 0.57 |
| 1:G:136:ILE:HD12 | 1:G:139:VAL:H | 1.69 | 0.57 |
| 1:D:79:TRP:CZ2 | 1:D:118:LYS:HB3 | 2.39 | 0.57 |
| 1:D:98:PRO:CB | 1:D:127:PHE:HB3 | 2.29 | 0.57 |
| 1:F:20:GLY:HA3 | 1:F:340:TRP:HZ2 | 1.70 | 0.57 |
| 1:D:20:GLY:HA3 | 1:D:340:TRP:HZ2 | 1.70 | 0.57 |
| 1:D:97:ALA:HB3 | 1:D:100:GLU:OE2 | 2.04 | 0.57 |
| 1:F:345:ILE:O | 1:F:349:LEU:HB2 | 2.05 | 0.57 |
| 1:G:258:PRO:O | 1:G:261:LEU:HD12 | 2.05 | 0.57 |
| 1:D:9:VAL:HG21 | 1:D:344:SER:HA | 1.87 | 0.57 |
| 1:F:9:VAL:HG21 | 1:F:344:SER:HA | 1.87 | 0.57 |
| 1:G:162:ASN:ND2 | 1:G:278:THR:HG22 | 2.14 | 0.57 |
| 1:F:43:VAL:HG13 | 1:F:44:MET:N | 2.20 | 0.56 |
| 1:E:136:ILE:HD12 | 1:E:139:VAL:H | 1.70 | 0.56 |
| 1:E:163:VAL:HG13 | 1:E:165:ILE:CD1 | 2.35 | 0.56 |
| 1:D:62:ARG:HB3 | 1:D:204:ALA:CB | 2.34 | 0.56 |
| 1:D:78:ASN:HB3 | 1:D:81:ASP:CG | 2.25 | 0.56 |
| 1:H:97:ALA:HB3 | 1:H:100:GLU:OE2 | 2.05 | 0.56 |
| 1:F:329:ILE:CD1 | 1:F:329:ILE:H | 2.07 | 0.56 |
| 1:E:201:VAL:H | 1:E:205:GLU:CD | 2.06 | 0.56 |
| 1:D:162:ASN:ND2 | 1:D:278:THR:HG22 | 2.18 | 0.56 |
| 1:G:34:ILE:HG12 | 1:G:67:LEU:HD23 | 1.86 | 0.56 |
| 1:D:109:PRO:HD2 | 1:D:161:HIS:CE1 | 2.40 | 0.56 |
| 1:F:225:ASN:O | 1:F:229:THR:HG22 | 2.06 | 0.56 |
| 1:F:238:LYS:HD3 | 1:F:239:SER:H | 1.69 | 0.56 |
| 1:E:345:ILE:HG22 | 1:E:349:LEU:HD12 | 1.87 | 0.56 |
| 1:G:250:ILE:O | 1:G:251:GLY:O | 2.23 | 0.56 |
| 1:G:123:MET:HA | 1:G:127:PHE:HD2 | 1.70 | 0.56 |
| 1:G:102:PRO:HB2 | 1:G:356:TRP:CZ3 | 2.40 | 0.56 |
| 1:G:105:LEU:HD22 | 1:G:105:LEU:H | 1.69 | 0.56 |
| 1:G:374:CYS:O | 1:G:375:PHE:HB3 | 2.04 | 0.56 |
| 1:E:186:THR:O | 1:E:189:LEU:HB2 | 2.05 | 0.56 |
| 1:D:226:GLU:HA | 1:D:229:THR:CG2 | 2.35 | 0.56 |
| 1:G:220:ALA:CB | 1:G:226:GLU:HG3 | 2.33 | 0.56 |
| 1:G:183:ARG:O | 1:G:186:THR:HB | 2.05 | 0.56 |
| 1:H:272:ALA:HB1 | 1:H:277:THR:CG2 | 2.35 | 0.56 |
| 1:D:258:PRO:HG3 | 1:D:306:TYR:CE2 | 2.39 | 0.56 |
| 1:D:273:GLY:O | 1:D:277:THR:N | 2.32 | 0.56 |
| 1:F:78:ASN:HB3 | 1:F:81:ASP:CG | 2.25 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:314:GLN:HE22 | 1:E:327:ILE:HG12 | 1.70 | 0.56 |
| 1:E:185:LEU:HD13 | 1:E:185:LEU:C | 2.26 | 0.56 |
| 1:G:153:LEU:HA | 1:G:161:HIS:O | 2.05 | 0.56 |
| 1:G:164:PRO:C | 1:G:165:ILE:HD12 | 2.25 | 0.56 |
| 1:E:349:LEU:HB3 | 1:E:352:PHE:CD2 | 2.41 | 0.56 |
| 1:G:305:MET:O | 1:G:306:TYR:C | 2.42 | 0.56 |
| 1:E:202:THR:HG23 | 1:E:203:THR:N | 2.20 | 0.56 |
| 1:D:201:VAL:H | 1:D:205:GLU:CD | 2.07 | 0.56 |
| 1:D:359:LYS:O | 1:D:360:GLN:HB3 | 2.05 | 0.56 |
| 1:H:34:ILE:HG12 | 1:H:67:LEU:HD23 | 1.87 | 0.56 |
| 1:F:97:ALA:HB3 | 1:F:100:GLU:OE2 | 2.05 | 0.56 |
| 1:G:259:GLU:CB | 1:G:263:GLN:HE22 | 1.99 | 0.56 |
| 1:E:227:MET:HG2 | 1:E:255:PHE:CE1 | 2.41 | 0.56 |
| 1:E:164:PRO:C | 1:E:165:ILE:HD12 | 2.24 | 0.56 |
| 1:H:43:VAL:HG13 | 1:H:44:MET:N | 2.20 | 0.56 |
| 1:E:220:ALA:CB | 1:E:226:GLU:HG3 | 2.33 | 0.56 |
| 1:H:359:LYS:O | 1:H:360:GLN:HB3 | 2.04 | 0.56 |
| 1:E:162:ASN:ND2 | 1:E:278:THR:HG22 | 2.15 | 0.56 |
| 1:E:242:LEU:HD12 | 1:E:242:LEU:C | 2.26 | 0.56 |
| 1:D:289:ILE:O | 1:D:289:ILE:HG23 | 2.06 | 0.56 |
| 1:H:5:THR:OG1 | 1:H:102:PRO:HD2 | 2.05 | 0.56 |
| 1:E:20:GLY:HA3 | 1:E:340:TRP:CZ2 | 2.40 | 0.56 |
| 1:D:136:ILE:HD12 | 1:D:139:VAL:H | 1.71 | 0.56 |
| 1:G:5:THR:OG1 | 1:G:102:PRO:HD2 | 2.05 | 0.56 |
| 1:H:257:CYS:SG | 1:H:258:PRO:CD | 2.94 | 0.56 |
| 1:D:221:LEU:N | 1:D:221:LEU:HD12 | 2.20 | 0.56 |
| 1:D:314:GLN:HE22 | 1:D:327:ILE:HG12 | 1.70 | 0.56 |
| 1:E:34:ILE:HG12 | 1:E:67:LEU:HD23 | 1.86 | 0.56 |
| 1:H:163:VAL:HG13 | 1:H:165:ILE:CD1 | 2.35 | 0.56 |
| 1:H:164:PRO:C | 1:H:165:ILE:HD12 | 2.26 | 0.56 |
| 1:D:102:PRO:HB2 | 1:D:356:TRP:CZ3 | 2.41 | 0.56 |
| 1:D:345:ILE:O | 1:D:349:LEU:HB2 | 2.06 | 0.56 |
| 1:E:109:PRO:CG | 1:E:136:ILE:HG12 | 2.32 | 0.56 |
| 1:F:216:LEU:HD13 | 1:F:250:ILE:CG1 | 2.36 | 0.56 |
| 1:F:222:ASP:O | 1:F:224:GLU:N | 2.39 | 0.56 |
| 1:F:5:THR:OG1 | 1:F:102:PRO:HD2 | 2.05 | 0.56 |
| 1:D:227:MET:HG2 | 1:D:255:PHE:CE1 | 2.40 | 0.56 |
| 1:D:325:MET:SD | 1:F:244:ASP:CG | 2.84 | 0.56 |
| 1:H:314:GLN:HE22 | 1:H:327:ILE:HG12 | 1.70 | 0.56 |
| 1:D:5:THR:OG1 | 1:D:102:PRO:HD2 | 2.05 | 0.56 |
| 1:F:201:VAL:H | 1:F:205:GLU:CD | 2.08 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:79:TRP:CZ2 | 1:G:118:LYS:HB3 | 2.41 | 0.56 |
| 1:D:183:ARG:O | 1:D:186:THR:HB | 2.05 | 0.56 |
| 1:D:186:THR:O | 1:D:189:LEU:HB2 | 2.05 | 0.56 |
| 1:G:314:GLN:HE22 | 1:G:327:ILE:HG12 | 1.70 | 0.56 |
| 1:F:314:GLN:HE22 | 1:F:327:ILE:HG12 | 1.70 | 0.56 |
| 1:E:284:LYS:HA | 1:E:284:LYS:HE2 | 1.88 | 0.56 |
| 1:F:263:GLN:C | 1:F:265:SER:H | 2.09 | 0.56 |
| 1:E:355:MET:HE2 | 1:E:356:TRP:HE1 | 1.69 | 0.56 |
| 1:F:183:ARG:O | 1:F:186:THR:HB | 2.06 | 0.56 |
| 1:G:238:LYS:HZ2 | 1:G:254:ARG:HH22 | 1.54 | 0.56 |
| 1:H:123:MET:O | 1:H:127:PHE:HB2 | 2.06 | 0.56 |
| 1:H:357:ILE:CD1 | 1:H:370:VAL:HG23 | 2.36 | 0.56 |
| 1:G:339:VAL:HG23 | 1:G:340:TRP:N | 2.21 | 0.56 |
| 1:D:20:GLY:HA3 | 1:D:340:TRP:CZ2 | 2.41 | 0.56 |
| 1:H:253:GLU:H | 1:H:253:GLU:CD | 2.09 | 0.56 |
| 1:G:317:ILE:HD13 | 1:G:317:ILE:N | 2.19 | 0.56 |
| 1:E:173:HIS:CE1 | 1:F:268:GLY:HA3 | 2.41 | 0.56 |
| 1:F:305:MET:O | 1:F:306:TYR:C | 2.44 | 0.56 |
| 1:F:102:PRO:HB2 | 1:F:356:TRP:CZ3 | 2.41 | 0.56 |
| 1:D:36:GLY:O | 1:D:65:LEU:HD11 | 2.06 | 0.56 |
| 1:H:202:THR:HG23 | 1:H:203:THR:N | 2.21 | 0.56 |
| 1:E:222:ASP:O | 1:E:224:GLU:N | 2.38 | 0.56 |
| 1:H:136:ILE:HD12 | 1:H:139:VAL:H | 1.70 | 0.55 |
| 1:H:317:ILE:N | 1:H:317:ILE:HD13 | 2.22 | 0.55 |
| 1:D:202:THR:HG23 | 1:D:203:THR:N | 2.21 | 0.55 |
| 1:G:122:ILE:HG22 | 1:G:123:MET:HE2 | 1.88 | 0.55 |
| 1:D:220:ALA:CB | 1:D:226:GLU:HG3 | 2.36 | 0.55 |
| 1:G:222:ASP:O | 1:G:224:GLU:N | 2.38 | 0.55 |
| 1:G:272:ALA:HB1 | 1:G:277:THR:CG2 | 2.35 | 0.55 |
| 1:D:62:ARG:HE | 1:D:208:ILE:HD11 | 1.71 | 0.55 |
| 1:E:76:ILE:N | 1:E:115:ASN:HD21 | 1.96 | 0.55 |
| 1:E:76:ILE:HG21 | 1:E:79:TRP:CE3 | 2.41 | 0.55 |
| 1:G:345:ILE:O | 1:G:349:LEU:HB2 | 2.06 | 0.55 |
| 1:D:216:LEU:HD13 | 1:D:250:ILE:CG1 | 2.36 | 0.55 |
| 1:E:339:VAL:HG23 | 1:E:340:TRP:N | 2.21 | 0.55 |
| 1:F:320:LEU:HD12 | 1:F:321:ALA:H | 1.70 | 0.55 |
| 1:D:253:GLU:H | 1:D:253:GLU:CD | 2.10 | 0.55 |
| 1:H:110:LEU:CB | 1:H:177:ARG:HG3 | 2.33 | 0.55 |
| 1:F:153:LEU:HA | 1:F:161:HIS:O | 2.06 | 0.55 |
| 1:E:221:LEU:HD23 | 1:E:315:LYS:HD3 | 1.88 | 0.55 |
| 1:G:67:LEU:HD12 | 1:G:67:LEU:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:253:GLU:CD | 1:E:253:GLU:H | 2.10 | 0.55 |
| 1:F:210:ARG:O | 1:F:211:ASP:CB | 2.54 | 0.55 |
| 1:E:238:LYS:HZ3 | 1:E:254:ARG:HH22 | 1.54 | 0.55 |
| 1:G:173:HIS:CE1 | 1:H:268:GLY:HA3 | 2.41 | 0.55 |
| 1:D:272:ALA:HB1 | 1:D:277:THR:CG2 | 2.36 | 0.55 |
| 1:H:78:ASN:HB3 | 1:H:81:ASP:CG | 2.27 | 0.55 |
| 1:G:221:LEU:HD23 | 1:G:315:LYS:HD3 | 1.89 | 0.55 |
| 1:F:227:MET:HG2 | 1:F:255:PHE:CE1 | 2.42 | 0.55 |
| 1:H:210:ARG:O | 1:H:211:ASP:HB3 | 2.05 | 0.55 |
| 1:D:286:ASP:HB3 | 1:D:289:ILE:CG2 | 2.36 | 0.55 |
| 1:E:286:ASP:HB3 | 1:E:289:ILE:CG2 | 2.36 | 0.55 |
| 1:H:345:ILE:O | 1:H:349:LEU:HB2 | 2.05 | 0.55 |
| 1:E:78:ASN:HB3 | 1:E:81:ASP:CG | 2.26 | 0.55 |
| 1:F:20:GLY:HA3 | 1:F:340:TRP:CZ2 | 2.41 | 0.55 |
| 1:G:109:PRO:HD2 | 1:G:161:HIS:CE1 | 2.40 | 0.55 |
| 1:F:350:SER:C | 1:F:352:PHE:N | 2.57 | 0.55 |
| 1:H:227:MET:HG2 | 1:H:255:PHE:CE1 | 2.42 | 0.55 |
| 1:F:91:TYR:O | 1:F:92:ASN:HB3 | 2.07 | 0.55 |
| 1:D:339:VAL:HG23 | 1:D:340:TRP:N | 2.22 | 0.55 |
| 1:E:352:PHE:HZ | 1:G:47:MET:HE1 | 1.71 | 0.55 |
| 1:F:163:VAL:HG13 | 1:F:165:ILE:CD1 | 2.36 | 0.55 |
| 1:F:79:TRP:CZ2 | 1:F:118:LYS:HB3 | 2.42 | 0.55 |
| 1:G:241:GLU:OE1 | 1:G:247:VAL:HG22 | 2.07 | 0.55 |
| 1:E:219:VAL:HG23 | 1:E:220:ALA:N | 2.22 | 0.55 |
| 1:G:242:LEU:C | 1:G:242:LEU:HD12 | 2.27 | 0.55 |
| 1:E:102:PRO:HB2 | 1:E:356:TRP:CZ3 | 2.42 | 0.55 |
| 1:F:317:ILE:N | 1:F:317:ILE:HD13 | 2.22 | 0.55 |
| 1:G:76:ILE:N | 1:G:115:ASN:HD21 | 1.96 | 0.55 |
| 1:G:123:MET:O | 1:G:127:PHE:HB2 | 2.07 | 0.55 |
| 1:G:98:PRO:HG3 | 1:G:127:PHE:CD1 | 2.41 | 0.55 |
| 1:H:267:ILE:HD13 | 1:H:267:ILE:O | 2.06 | 0.55 |
| 1:G:263:GLN:O | 1:G:263:GLN:HG2 | 2.07 | 0.55 |
| 1:D:263:GLN:C | 1:D:265:SER:H | 2.10 | 0.55 |
| 1:E:305:MET:O | 1:E:306:TYR:C | 2.44 | 0.55 |
| 1:D:123:MET:HA | 1:D:127:PHE:HD2 | 1.72 | 0.55 |
| 1:D:109:PRO:CG | 1:D:136:ILE:HG12 | 2.34 | 0.55 |
| 1:G:332:PRO:HB2 | 1:G:334:GLU:OE1 | 2.07 | 0.55 |
| 1:F:257:CYS:SG | 1:F:258:PRO:CD | 2.95 | 0.55 |
| 1:F:332:PRO:HB2 | 1:F:334:GLU:OE1 | 2.07 | 0.55 |
| 1:E:123:MET:O | 1:E:127:PHE:HB2 | 2.07 | 0.55 |
| 1:H:241:GLU:OE1 | 1:H:247:VAL:HG22 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:235:SER:HB2 | 1:G:236:LEU:HD13 | 1.89 | 0.55 |
| 1:G:20:GLY:HA3 | 1:G:340:TRP:HZ2 | 1.72 | 0.55 |
| 1:H:182:GLY:O | 1:H:185:LEU:HB3 | 2.06 | 0.55 |
| 1:D:345:ILE:HG22 | 1:D:349:LEU:HD12 | 1.89 | 0.54 |
| 1:E:216:LEU:HD13 | 1:E:250:ILE:CG1 | 2.35 | 0.54 |
| 1:D:181:ALA:HB3 | 1:D:184:ASP:OD1 | 2.06 | 0.54 |
| 1:F:221:LEU:HD23 | 1:F:315:LYS:HD3 | 1.88 | 0.54 |
| 1:D:185:LEU:C | 1:D:185:LEU:HD13 | 2.27 | 0.54 |
| 1:D:358:THR:H | 1:D:361:GLU:CD | 2.10 | 0.54 |
| 1:G:163:VAL:HG13 | 1:G:165:ILE:CD1 | 2.36 | 0.54 |
| 1:F:75:ILE:HA | 1:F:111:ASN:HD21 | 1.72 | 0.54 |
| 1:G:112:PRO:HA | 1:H:194:THR:O | 2.07 | 0.54 |
| 1:H:98:PRO:CB | 1:H:127:PHE:HB3 | 2.31 | 0.54 |
| 1:E:225:ASN:O | 1:E:229:THR:HG22 | 2.08 | 0.54 |
| 1:E:235:SER:HB2 | 1:E:236:LEU:HD13 | 1.89 | 0.54 |
| 1:E:325:MET:SD | 1:G:244:ASP:CG | 2.86 | 0.54 |
| 1:D:20:GLY:CA | 1:D:340:TRP:HZ2 | 2.21 | 0.54 |
| 1:E:304:THR:HG22 | 1:E:335:ARG:HD3 | 1.88 | 0.54 |
| 1:G:277:THR:HA | 1:G:280:ASN:ND2 | 2.23 | 0.54 |
| 1:G:201:VAL:H | 1:G:205:GLU:CD | 2.10 | 0.54 |
| 1:E:241:GLU:OE1 | 1:E:247:VAL:HG22 | 2.07 | 0.54 |
| 1:F:76:ILE:N | 1:F:115:ASN:HD21 | 1.93 | 0.54 |
| 1:H:221:LEU:CB | 1:H:315:LYS:HE2 | 2.38 | 0.54 |
| 1:F:186:THR:O | 1:F:189:LEU:HB2 | 2.07 | 0.54 |
| 1:H:201:VAL:H | 1:H:205:GLU:CD | 2.10 | 0.54 |
| 1:H:258:PRO:HA | 1:H:261:LEU:HD12 | 1.88 | 0.54 |
| 1:G:286:ASP:HB3 | 1:G:289:ILE:CG2 | 2.37 | 0.54 |
| 1:H:136:ILE:HD13 | 1:H:138:ALA:N | 2.22 | 0.54 |
| 1:D:369:ILE:HG13 | 1:D:372:ARG:NH2 | 2.23 | 0.54 |
| 1:F:123:MET:O | 1:F:127:PHE:HB2 | 2.08 | 0.54 |
| 1:D:122:ILE:HG22 | 1:D:123:MET:HE2 | 1.90 | 0.54 |
| 1:H:339:VAL:HG23 | 1:H:340:TRP:N | 2.21 | 0.54 |
| 1:H:108:ALA:HA | 1:H:137:GLN:HG2 | 1.89 | 0.54 |
| 1:D:317:ILE:HD13 | 1:D:317:ILE:N | 2.23 | 0.54 |
| 1:F:189:LEU:CD1 | 1:F:213:LYS:HB3 | 2.37 | 0.54 |
| 1:F:299:MET:HB3 | 1:F:304:THR:HG23 | 1.89 | 0.54 |
| 1:G:225:ASN:O | 1:G:229:THR:HG22 | 2.08 | 0.54 |
| 1:D:320:LEU:HD12 | 1:D:321:ALA:H | 1.73 | 0.54 |
| 1:G:253:GLU:CD | 1:G:253:GLU:H | 2.10 | 0.54 |
| 1:H:110:LEU:HB2 | 1:H:177:ARG:CG | 2.34 | 0.54 |
| 1:E:369:ILE:HG13 | 1:E:372:ARG:NH2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:109:PRO:HD2 | 1:F:161:HIS:CE1 | 2.43 | 0.54 |
| 1:E:185:LEU:O | 1:E:185:LEU:HD13 | 2.07 | 0.54 |
| 1:G:154:ASP:HA | 1:G:300:SER:O | 2.07 | 0.54 |
| 1:F:250:ILE:O | 1:F:251:GLY:O | 2.25 | 0.54 |
| 1:F:258:PRO:HA | 1:F:261:LEU:HD12 | 1.90 | 0.54 |
| 1:G:216:LEU:HD13 | 1:G:250:ILE:CG1 | 2.36 | 0.54 |
| 1:G:9:VAL:HG21 | 1:G:344:SER:HA | 1.90 | 0.54 |
| 1:D:257:CYS:SG | 1:D:258:PRO:CD | 2.96 | 0.54 |
| 1:F:339:VAL:HG23 | 1:F:340:TRP:N | 2.23 | 0.54 |
| 1:H:109:PRO:HD2 | 1:H:161:HIS:CE1 | 2.42 | 0.54 |
| 1:D:332:PRO:HB2 | 1:D:334:GLU:OE1 | 2.08 | 0.54 |
| 1:F:202:THR:HG23 | 1:F:203:THR:N | 2.23 | 0.54 |
| 1:G:79:TRP:HA | 1:G:79:TRP:HE3 | 1.72 | 0.54 |
| 1:F:122:ILE:HG22 | 1:F:123:MET:HE2 | 1.90 | 0.54 |
| 1:E:123:MET:HA | 1:E:127:PHE:HD2 | 1.72 | 0.54 |
| 1:D:350:SER:C | 1:D:352:PHE:N | 2.60 | 0.54 |
| 1:G:257:CYS:SG | 1:G:258:PRO:CD | 2.96 | 0.54 |
| 1:H:163:VAL:HG22 | 1:H:165:ILE:HD11 | 1.90 | 0.53 |
| 1:H:332:PRO:HB2 | 1:H:334:GLU:OE1 | 2.08 | 0.53 |
| 1:D:139:VAL:HG21 | 1:F:43:VAL:HG21 | 1.90 | 0.53 |
| 1:E:109:PRO:HD2 | 1:E:161:HIS:CE1 | 2.41 | 0.53 |
| 1:H:305:MET:O | 1:H:306:TYR:C | 2.45 | 0.53 |
| 1:D:221:LEU:HD23 | 1:D:315:LYS:HD3 | 1.90 | 0.53 |
| 1:G:91:TYR:O | 1:G:92:ASN:HB3 | 2.06 | 0.53 |
| 1:D:263:GLN:O | 1:D:263:GLN:HG2 | 2.07 | 0.53 |
| 1:F:173:HIS:CE1 | 1:G:268:GLY:HA3 | 2.42 | 0.53 |
| 1:G:202:THR:HG23 | 1:G:203:THR:N | 2.22 | 0.53 |
| 1:E:62:ARG:HE | 1:E:208:ILE:HD11 | 1.73 | 0.53 |
| 1:F:98:PRO:HG3 | 1:F:127:PHE:CD1 | 2.44 | 0.53 |
| 1:E:289:ILE:HG23 | 1:E:289:ILE:O | 2.06 | 0.53 |
| 1:F:258:PRO:O | 1:F:261:LEU:HD12 | 2.08 | 0.53 |
| 1:H:98:PRO:HG3 | 1:H:127:PHE:CD1 | 2.44 | 0.53 |
| 1:D:250:ILE:O | 1:D:251:GLY:O | 2.27 | 0.53 |
| 1:E:67:LEU:HD12 | 1:E:67:LEU:N | 2.24 | 0.53 |
| 1:H:299:MET:HB3 | 1:H:304:THR:HG23 | 1.89 | 0.53 |
| 1:E:277:THR:HA | 1:E:280:ASN:ND2 | 2.24 | 0.53 |
| 1:H:235:SER:HB2 | 1:H:236:LEU:HD13 | 1.89 | 0.53 |
| 1:G:181:ALA:HB3 | 1:G:184:ASP:OD1 | 2.09 | 0.53 |
| 1:G:189:LEU:CD1 | 1:G:213:LYS:HB3 | 2.36 | 0.53 |
| 1:F:320:LEU:HD12 | 1:F:321:ALA:N | 2.24 | 0.53 |
| 1:H:185:LEU:C | 1:H:185:LEU:HD13 | 2.28 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:358:THR:H | 1:E:361:GLU:CD | 2.10 | 0.53 |
| 1:E:263:GLN:C | 1:E:265:SER:H | 2.12 | 0.53 |
| 1:D:304:THR:HG22 | 1:D:335:ARG:HD3 | 1.90 | 0.53 |
| 1:F:277:THR:HA | 1:F:280:ASN:ND2 | 2.23 | 0.53 |
| 1:G:255:PHE:O | 1:G:258:PRO:HD2 | 2.08 | 0.53 |
| 1:F:112:PRO:HA | 1:G:194:THR:O | 2.08 | 0.53 |
| 1:E:7:ALA:O | 1:E:22:ALA:CA | 2.57 | 0.53 |
| 1:D:277:THR:HA | 1:D:280:ASN:ND2 | 2.23 | 0.53 |
| 1:H:349:LEU:HB3 | 1:H:352:PHE:CD2 | 2.43 | 0.53 |
| 1:G:78:ASN:HB3 | 1:G:81:ASP:CG | 2.27 | 0.53 |
| 1:G:284:LYS:HE2 | 1:G:284:LYS:HA | 1.90 | 0.53 |
| 1:E:317:ILE:HD13 | 1:E:317:ILE:N | 2.23 | 0.53 |
| 1:F:59:GLN:HE21 | 1:F:62:ARG:HH21 | 1.57 | 0.53 |
| 1:H:238:LYS:HZ3 | 1:H:254:ARG:HH22 | 1.54 | 0.53 |
| 1:E:108:ALA:HA | 1:E:137:GLN:HG2 | 1.91 | 0.53 |
| 1:E:20:GLY:CA | 1:E:340:TRP:HZ2 | 2.21 | 0.53 |
| 1:G:108:ALA:HA | 1:G:137:GLN:HG2 | 1.91 | 0.53 |
| 1:G:358:THR:H | 1:G:361:GLU:CD | 2.12 | 0.53 |
| 1:D:123:MET:O | 1:D:127:PHE:HB2 | 2.08 | 0.53 |
| 1:D:187:ASP:HA | 1:D:190:MET:HE3 | 1.91 | 0.53 |
| 1:F:7:ALA:O | 1:F:22:ALA:CA | 2.57 | 0.53 |
| 1:F:20:GLY:CA | 1:F:340:TRP:HZ2 | 2.22 | 0.53 |
| 1:F:185:LEU:HD13 | 1:F:185:LEU:C | 2.29 | 0.53 |
| 1:H:263:GLN:C | 1:H:265:SER:H | 2.12 | 0.53 |
| 1:G:263:GLN:C | 1:G:265:SER:H | 2.12 | 0.53 |
| 1:G:299:MET:HB3 | 1:G:304:THR:HG23 | 1.91 | 0.53 |
| 1:G:240:TYR:CE1 | 1:G:241:GLU:O | 2.62 | 0.53 |
| 1:H:9:VAL:HG21 | 1:H:344:SER:HA | 1.91 | 0.53 |
| 1:G:20:GLY:HA3 | 1:G:340:TRP:CZ2 | 2.44 | 0.53 |
| 1:G:336:LYS:HD2 | 1:G:336:LYS:O | 2.09 | 0.53 |
| 1:H:138:ALA:HB1 | 1:H:163:VAL:CG1 | 2.39 | 0.53 |
| 1:F:44:MET:CE | 1:F:45:VAL:H | 2.22 | 0.53 |
| 1:F:241:GLU:OE1 | 1:F:247:VAL:HG22 | 2.09 | 0.53 |
| 1:E:202:THR:CG2 | 1:E:205:GLU:HB2 | 2.34 | 0.53 |
| 1:D:66:THR:HG23 | 1:D:203:THR:CG2 | 2.29 | 0.53 |
| 1:H:79:TRP:HE3 | 1:H:79:TRP:HA | 1.74 | 0.53 |
| 1:G:369:ILE:HG13 | 1:G:372:ARG:NH2 | 2.24 | 0.53 |
| 1:E:229:THR:HG23 | 1:E:230:ALA:N | 2.24 | 0.53 |
| 1:F:253:GLU:H | 1:F:253:GLU:CD | 2.12 | 0.53 |
| 1:D:166:TYR:CD2 | 1:F:64:ILE:HG21 | 2.44 | 0.53 |
| 1:E:258:PRO:HG3 | 1:E:306:TYR:CE2 | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:122:ILE:HG22 | 1:H:123:MET:HE2 | 1.90 | 0.53 |
| 1:D:238:LYS:HZ2 | 1:D:254:ARG:NH2 | 2.07 | 0.53 |
| 1:D:169:TYR:HA | 1:F:42:GLY:CA | 2.36 | 0.52 |
| 1:D:76:ILE:N | 1:D:115:ASN:HD21 | 1.95 | 0.52 |
| 1:E:99:GLU:CG | 1:E:128:ASN:HB2 | 2.39 | 0.52 |
| 1:E:320:LEU:HD12 | 1:E:321:ALA:H | 1.74 | 0.52 |
| 1:H:185:LEU:O | 1:H:185:LEU:HD13 | 2.09 | 0.52 |
| 1:E:139:VAL:HG21 | 1:G:43:VAL:HG21 | 1.90 | 0.52 |
| 1:G:75:ILE:HA | 1:G:111:ASN:HD21 | 1.74 | 0.52 |
| 1:D:98:PRO:HG3 | 1:D:127:PHE:CD1 | 2.45 | 0.52 |
| 1:D:242:LEU:HD12 | 1:D:242:LEU:C | 2.30 | 0.52 |
| 1:E:139:VAL:HG22 | 1:G:43:VAL:HG11 | 1.91 | 0.52 |
| 1:E:299:MET:HB3 | 1:E:304:THR:HG23 | 1.90 | 0.52 |
| 1:H:44:MET:HE3 | 1:H:45:VAL:H | 1.74 | 0.52 |
| 1:H:44:MET:HE2 | 1:H:47:MET:HG2 | 1.92 | 0.52 |
| 1:D:79:TRP:HE3 | 1:D:79:TRP:HA | 1.73 | 0.52 |
| 1:H:222:ASP:O | 1:H:224:GLU:N | 2.43 | 0.52 |
| 1:D:108:ALA:HA | 1:D:137:GLN:HG2 | 1.92 | 0.52 |
| 1:D:302:GLY:C | 1:D:304:THR:N | 2.63 | 0.52 |
| 1:G:43:VAL:HG13 | 1:G:44:MET:N | 2.24 | 0.52 |
| 1:D:202:THR:CG2 | 1:D:205:GLU:HB2 | 2.36 | 0.52 |
| 1:E:112:PRO:HA | 1:F:194:THR:O | 2.09 | 0.52 |
| 1:D:258:PRO:HA | 1:D:261:LEU:HD12 | 1.90 | 0.52 |
| 1:F:235:SER:HB2 | 1:F:236:LEU:HD13 | 1.90 | 0.52 |
| 1:H:216:LEU:HD13 | 1:H:250:ILE:CG1 | 2.35 | 0.52 |
| 1:H:229:THR:HG23 | 1:H:230:ALA:N | 2.24 | 0.52 |
| 1:F:284:LYS:HE2 | 1:F:284:LYS:HA | 1.92 | 0.52 |
| 1:D:163:VAL:HG22 | 1:D:165:ILE:HD11 | 1.91 | 0.52 |
| 1:E:272:ALA:HB1 | 1:E:277:THR:HG21 | 1.91 | 0.52 |
| 1:F:349:LEU:HB3 | 1:F:352:PHE:CD2 | 2.43 | 0.52 |
| 1:F:355:MET:O | 1:F:373:LYS:HE3 | 2.10 | 0.52 |
| 1:H:238:LYS:HZ2 | 1:H:254:ARG:HH22 | 1.58 | 0.52 |
| 1:D:235:SER:HB2 | 1:D:236:LEU:HD13 | 1.90 | 0.52 |
| 1:H:350:SER:C | 1:H:352:PHE:N | 2.60 | 0.52 |
| 1:D:327:ILE:HD13 | 1:D:327:ILE:N | 2.24 | 0.52 |
| 1:F:34:ILE:C | 1:F:34:ILE:HD12 | 2.30 | 0.52 |
| 1:G:34:ILE:O | 1:G:35:VAL:HG13 | 2.10 | 0.52 |
| 1:H:67:LEU:HD12 | 1:H:67:LEU:N | 2.24 | 0.52 |
| 1:G:110:LEU:CB | 1:G:177:ARG:HG3 | 2.37 | 0.52 |
| 1:G:304:THR:HG22 | 1:G:335:ARG:HD3 | 1.91 | 0.52 |
| 1:F:267:ILE:O | 1:F:267:ILE:HD13 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:136:ILE:HD13 | 1:F:138:ALA:N | 2.24 | 0.52 |
| 1:E:198:TYR:HB3 | 1:E:200:PHE:HE1 | 1.74 | 0.52 |
| 1:H:358:THR:H | 1:H:361:GLU:CD | 2.13 | 0.52 |
| 1:H:20:GLY:HA3 | 1:H:340:TRP:HZ2 | 1.75 | 0.52 |
| 1:H:340:TRP:CE3 | 1:H:341:ILE:HD13 | 2.41 | 0.52 |
| 1:H:263:GLN:O | 1:H:263:GLN:HG2 | 2.10 | 0.52 |
| 1:D:153:LEU:HD13 | 1:D:313:MET:HE1 | 1.92 | 0.52 |
| 1:E:165:ILE:HG13 | 1:E:170:ALA:HB1 | 1.91 | 0.52 |
| 1:E:332:PRO:HB2 | 1:E:334:GLU:OE1 | 2.10 | 0.52 |
| 1:F:219:VAL:HG23 | 1:F:220:ALA:N | 2.24 | 0.52 |
| 1:F:273:GLY:N | 1:F:277:THR:HG23 | 2.19 | 0.52 |
| 1:G:202:THR:CG2 | 1:G:205:GLU:HB2 | 2.35 | 0.52 |
| 1:E:59:GLN:HE21 | 1:E:62:ARG:HH21 | 1.56 | 0.52 |
| 1:H:304:THR:HG22 | 1:H:335:ARG:HD3 | 1.91 | 0.52 |
| 1:E:350:SER:C | 1:E:352:PHE:N | 2.63 | 0.52 |
| 1:F:226:GLU:HA | 1:F:229:THR:CG2 | 2.39 | 0.52 |
| 1:G:227:MET:HG2 | 1:G:255:PHE:CE1 | 2.45 | 0.52 |
| 1:D:59:GLN:HE21 | 1:D:62:ARG:HH21 | 1.57 | 0.52 |
| 1:D:99:GLU:CG | 1:D:128:ASN:HB2 | 2.40 | 0.52 |
| 1:E:98:PRO:HG3 | 1:E:127:PHE:CD1 | 2.45 | 0.52 |
| 1:G:121:GLN:O | 1:G:125:GLU:HG2 | 2.09 | 0.52 |
| 1:G:355:MET:O | 1:G:373:LYS:HE3 | 2.10 | 0.52 |
| 1:H:210:ARG:O | 1:H:211:ASP:CB | 2.57 | 0.52 |
| 1:E:226:GLU:HA | 1:E:229:THR:CG2 | 2.40 | 0.52 |
| 1:E:9:VAL:HG21 | 1:E:344:SER:HA | 1.92 | 0.52 |
| 1:E:263:GLN:HG2 | 1:E:263:GLN:O | 2.10 | 0.52 |
| 1:E:257:CYS:SG | 1:E:258:PRO:CD | 2.98 | 0.52 |
| 1:F:272:ALA:HB1 | 1:F:277:THR:HG21 | 1.92 | 0.52 |
| 1:F:198:TYR:HB3 | 1:F:200:PHE:HE1 | 1.75 | 0.52 |
| 1:G:187:ASP:HA | 1:G:190:MET:HE3 | 1.92 | 0.52 |
| 1:D:99:GLU:O | 1:D:130:PRO:HB3 | 2.10 | 0.52 |
| 1:G:357:ILE:CD1 | 1:G:370:VAL:HG23 | 2.40 | 0.52 |
| 1:G:370:VAL:O | 1:G:374:CYS:SG | 2.68 | 0.52 |
| 1:D:189:LEU:CD1 | 1:D:213:LYS:HB3 | 2.39 | 0.52 |
| 1:H:102:PRO:HB2 | 1:H:356:TRP:HZ3 | 1.73 | 0.52 |
| 1:E:336:LYS:HD2 | 1:E:336:LYS:O | 2.10 | 0.52 |
| 1:G:302:GLY:C | 1:G:304:THR:N | 2.63 | 0.51 |
| 1:E:359:LYS:O | 1:E:360:GLN:HB3 | 2.09 | 0.51 |
| 1:D:219:VAL:O | 1:D:220:ALA:HB3 | 2.09 | 0.51 |
| 1:D:229:THR:HG23 | 1:D:230:ALA:N | 2.25 | 0.51 |
| 1:H:273:GLY:H | 1:H:277:THR:CG2 | 2.20 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:67:LEU:N | 1:F:67:LEU:HD12 | 2.24 | 0.51 |
| 1:F:336:LYS:O | 1:F:336:LYS:HD2 | 2.09 | 0.51 |
| 1:E:304:THR:CG2 | 1:E:335:ARG:HD3 | 2.39 | 0.51 |
| 1:F:166:TYR:CD2 | 1:H:64:ILE:HG21 | 2.45 | 0.51 |
| 1:G:219:VAL:O | 1:G:220:ALA:HB3 | 2.09 | 0.51 |
| 1:H:273:GLY:N | 1:H:277:THR:HG23 | 2.20 | 0.51 |
| 1:G:20:GLY:CA | 1:G:340:TRP:HZ2 | 2.22 | 0.51 |
| 1:F:358:THR:H | 1:F:361:GLU:CD | 2.12 | 0.51 |
| 1:H:153:LEU:HD13 | 1:H:313:MET:HE1 | 1.92 | 0.51 |
| 1:H:163:VAL:HG22 | 1:H:165:ILE:CD1 | 2.40 | 0.51 |
| 1:D:136:ILE:HD12 | 1:D:139:VAL:CG2 | 2.35 | 0.51 |
| 1:G:136:ILE:HD13 | 1:G:138:ALA:N | 2.26 | 0.51 |
| 1:F:79:TRP:HE3 | 1:F:79:TRP:HA | 1.75 | 0.51 |
| 1:E:79:TRP:HE3 | 1:E:79:TRP:HA | 1.74 | 0.51 |
| 1:D:75:ILE:HA | 1:D:111:ASN:HD21 | 1.74 | 0.51 |
| 1:H:189:LEU:CD1 | 1:H:213:LYS:HB3 | 2.38 | 0.51 |
| 1:E:189:LEU:CD1 | 1:E:213:LYS:HB3 | 2.38 | 0.51 |
| 1:G:229:THR:HG23 | 1:G:230:ALA:N | 2.25 | 0.51 |
| 1:H:286:ASP:HB3 | 1:H:289:ILE:CG2 | 2.38 | 0.51 |
| 1:D:185:LEU:HD13 | 1:D:185:LEU:O | 2.10 | 0.51 |
| 1:E:267:ILE:O | 1:E:267:ILE:HD13 | 2.10 | 0.51 |
| 1:E:345:ILE:O | 1:E:349:LEU:HB2 | 2.10 | 0.51 |
| 1:H:59:GLN:HE21 | 1:H:62:ARG:HH21 | 1.59 | 0.51 |
| 1:E:36:GLY:O | 1:E:65:LEU:HD11 | 2.10 | 0.51 |
| 1:H:79:TRP:CZ2 | 1:H:118:LYS:HB3 | 2.45 | 0.51 |
| 1:H:99:GLU:CG | 1:H:128:ASN:HB2 | 2.38 | 0.51 |
| 1:G:226:GLU:HA | 1:G:229:THR:CG2 | 2.41 | 0.51 |
| 1:D:304:THR:CG2 | 1:D:335:ARG:HD3 | 2.41 | 0.51 |
| 1:G:138:ALA:HB1 | 1:G:163:VAL:CG1 | 2.40 | 0.51 |
| 1:E:153:LEU:HD13 | 1:E:313:MET:HE1 | 1.92 | 0.51 |
| 1:F:165:ILE:HG13 | 1:F:170:ALA:HB1 | 1.93 | 0.51 |
| 1:F:304:THR:HG22 | 1:F:335:ARG:HD3 | 1.92 | 0.51 |
| 1:H:198:TYR:HB3 | 1:H:200:PHE:HE1 | 1.75 | 0.51 |
| 1:E:84:LYS:O | 1:E:87:HIS:HB3 | 2.11 | 0.51 |
| 1:D:67:LEU:N | 1:D:67:LEU:HD12 | 2.25 | 0.51 |
| 1:D:336:LYS:HD2 | 1:D:336:LYS:O | 2.10 | 0.51 |
| 1:E:163:VAL:HG22 | 1:E:165:ILE:HD11 | 1.92 | 0.51 |
| 1:E:166:TYR:CD2 | 1:G:64:ILE:HG21 | 2.45 | 0.51 |
| 1:H:20:GLY:HA3 | 1:H:340:TRP:CZ2 | 2.45 | 0.51 |
| 1:F:110:LEU:HB2 | 1:F:177:ARG:CG | 2.36 | 0.51 |
| 1:H:75:ILE:HA | 1:H:111:ASN:HD21 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:76:ILE:N | 1:H:115:ASN:HD21 | 1.96 | 0.51 |
| 1:H:7:ALA:O | 1:H:22:ALA:CA | 2.58 | 0.51 |
| 1:F:286:ASP:HB3 | 1:F:289:ILE:CG2 | 2.39 | 0.51 |
| 1:D:299:MET:HB3 | 1:D:304:THR:HG23 | 1.91 | 0.51 |
| 1:G:330:ILE:O | 1:G:332:PRO:HD3 | 2.10 | 0.51 |
| 1:E:153:LEU:HA | 1:E:161:HIS:O | 2.11 | 0.51 |
| 1:E:355:MET:O | 1:E:373:LYS:HE3 | 2.11 | 0.51 |
| 1:F:186:THR:HG22 | 1:F:190:MET:HE2 | 1.93 | 0.51 |
| 1:D:357:ILE:CD1 | 1:D:370:VAL:HG23 | 2.41 | 0.51 |
| 1:H:34:ILE:HD12 | 1:H:34:ILE:C | 2.31 | 0.51 |
| 1:E:192:ILE:HD12 | 1:E:253:GLU:HB3 | 1.93 | 0.51 |
| 1:G:258:PRO:HA | 1:G:261:LEU:HD12 | 1.93 | 0.51 |
| 1:E:122:ILE:HG22 | 1:E:123:MET:HE2 | 1.93 | 0.51 |
| 1:G:7:ALA:O | 1:G:22:ALA:CA | 2.59 | 0.51 |
| 1:F:242:LEU:HD12 | 1:F:242:LEU:C | 2.31 | 0.51 |
| 1:F:108:ALA:HA | 1:F:137:GLN:HG2 | 1.93 | 0.51 |
| 1:H:369:ILE:HG13 | 1:H:372:ARG:NH2 | 2.26 | 0.51 |
| 1:F:221:LEU:CB | 1:F:315:LYS:HE2 | 2.41 | 0.51 |
| 1:H:20:GLY:CA | 1:H:340:TRP:HZ2 | 2.23 | 0.51 |
| 1:F:325:MET:SD | 1:H:244:ASP:OD1 | 2.69 | 0.51 |
| 1:E:181:ALA:HB3 | 1:E:184:ASP:OD1 | 2.11 | 0.51 |
| 1:D:241:GLU:OE1 | 1:D:247:VAL:HG22 | 2.11 | 0.51 |
| 1:H:357:ILE:HD12 | 1:H:370:VAL:HG23 | 1.93 | 0.51 |
| 1:F:121:GLN:O | 1:F:125:GLU:HG2 | 2.11 | 0.51 |
| 1:G:44:MET:CE | 1:G:45:VAL:H | 2.24 | 0.50 |
| 1:E:75:ILE:HA | 1:E:111:ASN:HD21 | 1.75 | 0.50 |
| 1:G:102:PRO:HB2 | 1:G:356:TRP:HZ3 | 1.76 | 0.50 |
| 1:H:277:THR:HA | 1:H:280:ASN:ND2 | 2.25 | 0.50 |
| 1:D:91:TYR:O | 1:D:92:ASN:HB3 | 2.11 | 0.50 |
| 1:F:219:VAL:O | 1:F:220:ALA:HB3 | 2.11 | 0.50 |
| 1:F:229:THR:HG23 | 1:F:230:ALA:N | 2.25 | 0.50 |
| 1:G:273:GLY:N | 1:G:277:THR:HG23 | 2.20 | 0.50 |
| 1:G:59:GLN:HE21 | 1:G:62:ARG:HH21 | 1.58 | 0.50 |
| 1:F:111:ASN:CG | 1:F:112:PRO:HD2 | 2.32 | 0.50 |
| 1:F:66:THR:HG23 | 1:F:203:THR:CG2 | 2.30 | 0.50 |
| 1:G:349:LEU:HB3 | 1:G:352:PHE:CD2 | 2.46 | 0.50 |
| 1:H:120:THR:O | 1:H:124:PHE:HB2 | 2.12 | 0.50 |
| 1:G:153:LEU:HD13 | 1:G:313:MET:HE1 | 1.93 | 0.50 |
| 1:F:302:GLY:C | 1:F:304:THR:N | 2.63 | 0.50 |
| 1:G:198:TYR:HB3 | 1:G:200:PHE:HE1 | 1.76 | 0.50 |
| 1:D:198:TYR:HB3 | 1:D:200:PHE:HE1 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:357:ILE:CD1 | 1:E:370:VAL:HG23 | 2.41 | 0.50 |
| 1:D:7:ALA:O | 1:D:22:ALA:CA | 2.59 | 0.50 |
| 1:F:357:ILE:CD1 | 1:F:370:VAL:HG23 | 2.41 | 0.50 |
| 1:F:370:VAL:O | 1:F:374:CYS:SG | 2.70 | 0.50 |
| 1:E:221:LEU:CB | 1:E:315:LYS:HE2 | 2.40 | 0.50 |
| 1:F:78:ASN:HB3 | 1:F:81:ASP:OD1 | 2.11 | 0.50 |
| 1:G:185:LEU:HD13 | 1:G:185:LEU:C | 2.32 | 0.50 |
| 1:F:153:LEU:HD13 | 1:F:313:MET:HE1 | 1.94 | 0.50 |
| 1:F:369:ILE:HG13 | 1:F:372:ARG:NH2 | 2.27 | 0.50 |
| 1:G:273:GLY:H | 1:G:277:THR:CG2 | 2.19 | 0.50 |
| 1:H:202:THR:CG2 | 1:H:205:GLU:HB2 | 2.35 | 0.50 |
| 1:E:169:TYR:HA | 1:G:42:GLY:CA | 2.36 | 0.50 |
| 1:D:192:ILE:HD12 | 1:D:253:GLU:HB3 | 1.93 | 0.50 |
| 1:D:163:VAL:HG22 | 1:D:165:ILE:CD1 | 2.42 | 0.50 |
| 1:G:163:VAL:HG22 | 1:G:165:ILE:HD11 | 1.93 | 0.50 |
| 1:E:102:PRO:HB2 | 1:E:356:TRP:HZ3 | 1.76 | 0.50 |
| 1:F:139:VAL:HG21 | 1:H:43:VAL:HG21 | 1.94 | 0.50 |
| 1:H:111:ASN:CG | 1:H:112:PRO:HD2 | 2.32 | 0.50 |
| 1:F:120:THR:O | 1:F:124:PHE:HB2 | 2.12 | 0.50 |
| 1:F:340:TRP:CE3 | 1:F:341:ILE:HD13 | 2.42 | 0.50 |
| 1:D:323:SER:O | 1:D:324:THR:OG1 | 2.24 | 0.50 |
| 1:E:147:ARG:HH22 | 1:E:330:ILE:HD13 | 1.77 | 0.50 |
| 1:F:143:TYR:CE1 | 1:H:44:MET:SD | 3.04 | 0.50 |
| 1:F:202:THR:HG22 | 1:F:205:GLU:N | 2.17 | 0.50 |
| 1:D:112:PRO:HA | 1:E:194:THR:O | 2.11 | 0.50 |
| 1:H:71:ILE:HD12 | 1:H:76:ILE:CG1 | 2.38 | 0.50 |
| 1:G:272:ALA:HB1 | 1:G:277:THR:HG21 | 1.93 | 0.50 |
| 1:E:340:TRP:CE3 | 1:E:341:ILE:HD13 | 2.41 | 0.50 |
| 1:H:259:GLU:CB | 1:H:263:GLN:HE22 | 1.99 | 0.50 |
| 1:H:330:ILE:O | 1:H:332:PRO:HD3 | 2.12 | 0.50 |
| 1:G:163:VAL:O | 1:G:163:VAL:HG13 | 2.11 | 0.50 |
| 1:F:273:GLY:H | 1:F:277:THR:CG2 | 2.20 | 0.50 |
| 1:D:225:ASN:O | 1:D:229:THR:HG22 | 2.12 | 0.50 |
| 1:H:272:ALA:HB1 | 1:H:277:THR:HG21 | 1.93 | 0.50 |
| 1:D:78:ASN:HB3 | 1:D:81:ASP:OD1 | 2.12 | 0.50 |
| 1:D:320:LEU:HD12 | 1:D:321:ALA:N | 2.26 | 0.50 |
| 1:H:192:ILE:HD12 | 1:H:253:GLU:HB3 | 1.93 | 0.50 |
| 1:G:298:VAL:HG23 | 1:G:330:ILE:O | 2.12 | 0.50 |
| 1:E:302:GLY:C | 1:E:304:THR:N | 2.64 | 0.50 |
| 1:F:110:LEU:CB | 1:F:177:ARG:HG3 | 2.36 | 0.50 |
| 1:F:332:PRO:HB2 | 1:F:334:GLU:CD | 2.32 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:THR:HG22 | 1:E:205:GLU:N | 2.16 | 0.50 |
| 1:H:181:ALA:HB3 | 1:H:184:ASP:OD1 | 2.12 | 0.50 |
| 1:H:186:THR:O | 1:H:189:LEU:HB2 | 2.11 | 0.50 |
| 1:H:226:GLU:HA | 1:H:229:THR:CG2 | 2.41 | 0.50 |
| 1:D:272:ALA:HB1 | 1:D:277:THR:HG21 | 1.94 | 0.50 |
| 1:D:44:MET:HE2 | 1:D:45:VAL:H | 1.76 | 0.50 |
| 1:H:165:ILE:HG13 | 1:H:170:ALA:HB1 | 1.90 | 0.49 |
| 1:D:165:ILE:HG13 | 1:D:170:ALA:HB1 | 1.94 | 0.49 |
| 1:D:349:LEU:HB3 | 1:D:352:PHE:CD2 | 2.46 | 0.49 |
| 1:F:163:VAL:HG22 | 1:F:165:ILE:HD11 | 1.94 | 0.49 |
| 1:H:121:GLN:O | 1:H:125:GLU:HG2 | 2.11 | 0.49 |
| 1:G:186:THR:O | 1:G:189:LEU:HB2 | 2.12 | 0.49 |
| 1:D:110:LEU:HB2 | 1:D:177:ARG:CG | 2.35 | 0.49 |
| 1:D:136:ILE:HD13 | 1:D:138:ALA:N | 2.26 | 0.49 |
| 1:D:298:VAL:HG23 | 1:D:330:ILE:O | 2.12 | 0.49 |
| 1:E:258:PRO:HA | 1:E:261:LEU:HD12 | 1.94 | 0.49 |
| 1:G:44:MET:HE2 | 1:G:47:MET:HG2 | 1.93 | 0.49 |
| 1:E:111:ASN:CG | 1:E:112:PRO:HD2 | 2.32 | 0.49 |
| 1:H:370:VAL:O | 1:H:374:CYS:SG | 2.70 | 0.49 |
| 1:D:151:ILE:HG12 | 1:D:164:PRO:HA | 1.94 | 0.49 |
| 1:G:267:ILE:O | 1:G:267:ILE:HD13 | 2.11 | 0.49 |
| 1:G:62:ARG:HE | 1:G:208:ILE:HD11 | 1.77 | 0.49 |
| 1:G:357:ILE:HD12 | 1:G:370:VAL:HG23 | 1.94 | 0.49 |
| 1:E:219:VAL:O | 1:E:220:ALA:HB3 | 2.11 | 0.49 |
| 1:D:219:VAL:HG23 | 1:D:220:ALA:N | 2.26 | 0.49 |
| 1:G:202:THR:HG22 | 1:G:205:GLU:N | 2.17 | 0.49 |
| 1:H:140:LEU:HG | 1:H:343:GLY:HA2 | 1.94 | 0.49 |
| 1:D:143:TYR:CE1 | 1:F:44:MET:SD | 3.05 | 0.49 |
| 1:F:304:THR:CG2 | 1:F:335:ARG:HD3 | 2.43 | 0.49 |
| 1:E:250:ILE:O | 1:E:251:GLY:O | 2.30 | 0.49 |
| 1:F:202:THR:CG2 | 1:F:205:GLU:HB2 | 2.37 | 0.49 |
| 1:H:111:ASN:ND2 | 1:H:112:PRO:HD2 | 2.28 | 0.49 |
| 1:G:99:GLU:O | 1:G:130:PRO:HB3 | 2.11 | 0.49 |
| 1:G:88:HIS:O | 1:G:91:TYR:O | 2.31 | 0.49 |
| 1:G:340:TRP:CE3 | 1:G:341:ILE:HD13 | 2.42 | 0.49 |
| 1:D:121:GLN:O | 1:D:125:GLU:HG2 | 2.12 | 0.49 |
| 1:G:140:LEU:HG | 1:G:343:GLY:HA2 | 1.94 | 0.49 |
| 1:H:304:THR:CG2 | 1:H:335:ARG:HD3 | 2.43 | 0.49 |
| 1:D:163:VAL:O | 1:D:163:VAL:HG13 | 2.11 | 0.49 |
| 1:F:181:ALA:HB3 | 1:F:184:ASP:OD1 | 2.11 | 0.49 |
| 1:F:298:VAL:HG23 | 1:F:330:ILE:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:176:MET:O | 1:G:178:LEU:HD12 | 2.12 | 0.49 |
| 1:F:62:ARG:HE | 1:F:208:ILE:HD11 | 1.76 | 0.49 |
| 1:H:374:CYS:O | 1:H:375:PHE:HB3 | 2.13 | 0.49 |
| 1:D:84:LYS:O | 1:D:87:HIS:HB3 | 2.12 | 0.49 |
| 1:G:84:LYS:O | 1:G:87:HIS:HB3 | 2.12 | 0.49 |
| 1:G:320:LEU:HD12 | 1:G:321:ALA:H | 1.76 | 0.49 |
| 1:G:185:LEU:O | 1:G:185:LEU:HD13 | 2.12 | 0.49 |
| 1:D:355:MET:O | 1:D:373:LYS:HE3 | 2.13 | 0.49 |
| 1:G:332:PRO:HB2 | 1:G:334:GLU:CD | 2.32 | 0.49 |
| 1:E:143:TYR:CE1 | 1:G:44:MET:SD | 3.05 | 0.49 |
| 1:E:110:LEU:CB | 1:E:177:ARG:HG3 | 2.37 | 0.49 |
| 1:H:62:ARG:HE | 1:H:208:ILE:HD11 | 1.76 | 0.49 |
| 1:E:111:ASN:ND2 | 1:E:112:PRO:HD2 | 2.27 | 0.49 |
| 1:G:124:PHE:O | 1:G:128:ASN:HA | 2.13 | 0.49 |
| 1:D:273:GLY:N | 1:D:277:THR:HG23 | 2.21 | 0.49 |
| 1:F:88:HIS:O | 1:F:91:TYR:O | 2.31 | 0.49 |
| 1:D:34:ILE:HD12 | 1:D:34:ILE:C | 2.32 | 0.49 |
| 1:H:287:ILE:HG23 | 1:H:288:ASP:N | 2.27 | 0.49 |
| 1:H:153:LEU:HA | 1:H:161:HIS:O | 2.12 | 0.49 |
| 1:E:370:VAL:O | 1:E:374:CYS:SG | 2.71 | 0.49 |
| 1:D:370:VAL:O | 1:D:374:CYS:SG | 2.70 | 0.49 |
| 1:H:336:LYS:O | 1:H:336:LYS:HD2 | 2.12 | 0.49 |
| 1:D:372:ARG:O | 1:D:373:LYS:CB | 2.61 | 0.49 |
| 1:G:304:THR:CG2 | 1:G:335:ARG:HD3 | 2.43 | 0.49 |
| 1:F:138:ALA:HB1 | 1:F:163:VAL:CG1 | 2.43 | 0.49 |
| 1:D:202:THR:HG22 | 1:D:205:GLU:N | 2.18 | 0.49 |
| 1:G:245:GLY:O | 1:G:246:GLN:HG3 | 2.12 | 0.49 |
| 1:H:320:LEU:HD12 | 1:H:321:ALA:N | 2.28 | 0.49 |
| 1:E:353:GLN:N | 1:E:353:GLN:HE21 | 2.11 | 0.49 |
| 1:G:165:ILE:HG13 | 1:G:170:ALA:HB1 | 1.94 | 0.49 |
| 1:E:136:ILE:HD13 | 1:E:136:ILE:C | 2.33 | 0.49 |
| 1:H:202:THR:HG22 | 1:H:205:GLU:N | 2.18 | 0.49 |
| 1:G:120:THR:O | 1:G:124:PHE:HB2 | 2.13 | 0.49 |
| 1:D:212:ILE:HD12 | 1:D:240:TYR:CE1 | 2.48 | 0.49 |
| 1:D:221:LEU:CB | 1:D:315:LYS:HE2 | 2.41 | 0.49 |
| 1:G:221:LEU:CB | 1:G:315:LYS:HE2 | 2.42 | 0.49 |
| 1:G:327:ILE:N | 1:G:327:ILE:HD13 | 2.26 | 0.49 |
| 1:E:320:LEU:HD12 | 1:E:321:ALA:N | 2.27 | 0.49 |
| 1:H:327:ILE:N | 1:H:327:ILE:HD13 | 2.26 | 0.49 |
| 1:E:140:LEU:HG | 1:E:343:GLY:HA2 | 1.95 | 0.49 |
| 1:G:165:ILE:N | 1:G:165:ILE:HD12 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:227:MET:HG2 | 1:D:255:PHE:HE1 | 1.78 | 0.48 |
| 1:F:80:ASP:O | 1:F:83:GLU:HG2 | 2.13 | 0.48 |
| 1:D:34:ILE:O | 1:D:35:VAL:HG13 | 2.13 | 0.48 |
| 1:G:263:GLN:O | 1:G:263:GLN:CG | 2.61 | 0.48 |
| 1:H:332:PRO:HB2 | 1:H:334:GLU:CD | 2.33 | 0.48 |
| 1:D:102:PRO:HB2 | 1:D:356:TRP:HZ3 | 1.76 | 0.48 |
| 1:F:102:PRO:HB2 | 1:F:356:TRP:HZ3 | 1.76 | 0.48 |
| 1:H:44:MET:CE | 1:H:45:VAL:H | 2.25 | 0.48 |
| 1:D:357:ILE:HD12 | 1:D:370:VAL:HG23 | 1.95 | 0.48 |
| 1:H:120:THR:O | 1:H:124:PHE:CB | 2.61 | 0.48 |
| 1:E:23:GLY:HA2 | 1:E:344:SER:CB | 2.37 | 0.48 |
| 1:F:359:LYS:O | 1:F:360:GLN:CB | 2.61 | 0.48 |
| 1:H:70:PRO:HB2 | 1:H:82:MET:SD | 2.53 | 0.48 |
| 1:F:263:GLN:HG2 | 1:F:263:GLN:O | 2.13 | 0.48 |
| 1:D:147:ARG:HH22 | 1:D:330:ILE:HD13 | 1.77 | 0.48 |
| 1:E:273:GLY:H | 1:E:277:THR:CG2 | 2.17 | 0.48 |
| 1:E:163:VAL:HG22 | 1:E:165:ILE:CD1 | 2.43 | 0.48 |
| 1:E:330:ILE:O | 1:E:332:PRO:HD3 | 2.13 | 0.48 |
| 1:F:120:THR:O | 1:F:124:PHE:CB | 2.61 | 0.48 |
| 1:D:340:TRP:CE3 | 1:D:341:ILE:HD13 | 2.42 | 0.48 |
| 1:G:320:LEU:HD12 | 1:G:321:ALA:N | 2.28 | 0.48 |
| 1:F:100:GLU:OE2 | 1:F:100:GLU:N | 2.45 | 0.48 |
| 1:H:171:LEU:HD23 | 1:H:173:HIS:HB2 | 1.95 | 0.48 |
| 1:D:140:LEU:HG | 1:D:343:GLY:HA2 | 1.94 | 0.48 |
| 1:F:140:LEU:HG | 1:F:343:GLY:HA2 | 1.94 | 0.48 |
| 1:D:332:PRO:HB2 | 1:D:334:GLU:CD | 2.33 | 0.48 |
| 1:D:143:TYR:CE2 | 1:D:346:LEU:HB2 | 2.48 | 0.48 |
| 1:F:165:ILE:HD12 | 1:F:165:ILE:N | 2.28 | 0.48 |
| 1:H:219:VAL:HG23 | 1:H:220:ALA:N | 2.28 | 0.48 |
| 1:H:102:PRO:CB | 1:H:131:ALA:HB3 | 2.42 | 0.48 |
| 1:D:13:GLY:O | 1:D:14:SER:OG | 2.29 | 0.48 |
| 1:D:263:GLN:CG | 1:D:263:GLN:O | 2.61 | 0.48 |
| 1:E:298:VAL:HG23 | 1:E:330:ILE:O | 2.13 | 0.48 |
| 1:F:332:PRO:O | 1:F:335:ARG:HB3 | 2.14 | 0.48 |
| 1:G:219:VAL:HG23 | 1:G:220:ALA:N | 2.28 | 0.48 |
| 1:H:176:MET:O | 1:H:178:LEU:HD12 | 2.14 | 0.48 |
| 1:E:151:ILE:HG12 | 1:E:164:PRO:HA | 1.94 | 0.48 |
| 1:G:240:TYR:CG | 1:G:241:GLU:N | 2.82 | 0.48 |
| 1:H:212:ILE:HD12 | 1:H:240:TYR:CE1 | 2.48 | 0.48 |
| 1:H:355:MET:O | 1:H:373:LYS:HE3 | 2.12 | 0.48 |
| 1:E:78:ASN:HB3 | 1:E:81:ASP:OD1 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:166:TYR:O | 1:H:169:TYR:O | 2.32 | 0.48 |
| 1:D:165:ILE:N | 1:D:165:ILE:HD12 | 2.29 | 0.48 |
| 1:E:187:ASP:HA | 1:E:190:MET:HE3 | 1.95 | 0.48 |
| 1:H:84:LYS:O | 1:H:87:HIS:HB3 | 2.12 | 0.48 |
| 1:D:355:MET:HE2 | 1:D:356:TRP:NE1 | 2.28 | 0.48 |
| 1:E:332:PRO:O | 1:E:335:ARG:HB3 | 2.13 | 0.48 |
| 1:F:169:TYR:HA | 1:H:42:GLY:CA | 2.38 | 0.48 |
| 1:H:221:LEU:H | 1:H:221:LEU:CD1 | 2.25 | 0.48 |
| 1:F:327:ILE:N | 1:F:327:ILE:HD13 | 2.27 | 0.48 |
| 1:H:353:GLN:HE21 | 1:H:353:GLN:N | 2.11 | 0.48 |
| 1:H:138:ALA:CB | 1:H:163:VAL:HG11 | 2.44 | 0.48 |
| 1:D:138:ALA:HB1 | 1:D:163:VAL:CG1 | 2.44 | 0.48 |
| 1:F:240:TYR:CG | 1:F:241:GLU:N | 2.81 | 0.48 |
| 1:G:359:LYS:O | 1:G:360:GLN:CB | 2.62 | 0.48 |
| 1:F:99:GLU:CG | 1:F:128:ASN:HB2 | 2.40 | 0.48 |
| 1:G:100:GLU:OE2 | 1:G:100:GLU:N | 2.47 | 0.48 |
| 1:G:147:ARG:HH22 | 1:G:330:ILE:HD13 | 1.77 | 0.48 |
| 1:D:211:ASP:OD1 | 1:D:212:ILE:N | 2.47 | 0.48 |
| 1:D:80:ASP:O | 1:D:83:GLU:HG2 | 2.14 | 0.48 |
| 1:H:78:ASN:HB3 | 1:H:81:ASP:OD1 | 2.13 | 0.48 |
| 1:E:70:PRO:HB2 | 1:E:82:MET:SD | 2.53 | 0.48 |
| 1:F:84:LYS:O | 1:F:87:HIS:HB3 | 2.13 | 0.48 |
| 1:E:91:TYR:O | 1:E:92:ASN:HB3 | 2.13 | 0.48 |
| 1:D:369:ILE:HG13 | 1:D:372:ARG:HH22 | 1.79 | 0.47 |
| 1:E:176:MET:O | 1:E:178:LEU:HD12 | 2.14 | 0.47 |
| 1:G:163:VAL:HG22 | 1:G:165:ILE:CD1 | 2.44 | 0.47 |
| 1:E:143:TYR:CE2 | 1:E:346:LEU:HB2 | 2.49 | 0.47 |
| 1:D:111:ASN:CG | 1:D:112:PRO:HD2 | 2.35 | 0.47 |
| 1:F:151:ILE:HG12 | 1:F:164:PRO:HA | 1.97 | 0.47 |
| 1:E:240:TYR:CG | 1:E:241:GLU:N | 2.82 | 0.47 |
| 1:G:238:LYS:HZ2 | 1:G:254:ARG:HH12 | 1.61 | 0.47 |
| 1:G:111:ASN:CG | 1:G:112:PRO:HD2 | 2.34 | 0.47 |
| 1:G:355:MET:HE2 | 1:G:356:TRP:NE1 | 2.29 | 0.47 |
| 1:G:80:ASP:O | 1:G:83:GLU:HG2 | 2.14 | 0.47 |
| 1:H:355:MET:HE2 | 1:H:356:TRP:NE1 | 2.29 | 0.47 |
| 1:G:78:ASN:HB3 | 1:G:81:ASP:OD1 | 2.14 | 0.47 |
| 1:H:298:VAL:HG23 | 1:H:330:ILE:O | 2.13 | 0.47 |
| 1:D:102:PRO:CB | 1:D:131:ALA:HB3 | 2.43 | 0.47 |
| 1:E:110:LEU:HB2 | 1:E:177:ARG:CG | 2.37 | 0.47 |
| 1:H:80:ASP:O | 1:H:83:GLU:HG2 | 2.14 | 0.47 |
| 1:E:327:ILE:HD13 | 1:E:327:ILE:N | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:192:ILE:HD12 | 1:F:253:GLU:HB3 | 1.95 | 0.47 |
| 1:E:43:VAL:HG13 | 1:E:44:MET:N | 2.28 | 0.47 |
| 1:G:329:ILE:O | 1:G:330:ILE:C | 2.53 | 0.47 |
| 1:E:332:PRO:HB2 | 1:E:334:GLU:CD | 2.34 | 0.47 |
| 1:F:176:MET:O | 1:F:178:LEU:HD12 | 2.15 | 0.47 |
| 1:E:196:ARG:NH2 | 1:E:251:GLY:HA3 | 2.22 | 0.47 |
| 1:E:374:CYS:O | 1:E:375:PHE:HB3 | 2.14 | 0.47 |
| 1:G:102:PRO:CB | 1:G:131:ALA:HB3 | 2.43 | 0.47 |
| 1:H:186:THR:HG22 | 1:H:190:MET:HE2 | 1.95 | 0.47 |
| 1:G:23:GLY:HA2 | 1:G:344:SER:CB | 2.37 | 0.47 |
| 1:F:221:LEU:CD1 | 1:F:221:LEU:H | 2.26 | 0.47 |
| 1:D:44:MET:CE | 1:D:45:VAL:H | 2.27 | 0.47 |
| 1:F:147:ARG:HH22 | 1:F:330:ILE:HD13 | 1.77 | 0.47 |
| 1:E:339:VAL:HG23 | 1:E:340:TRP:H | 1.78 | 0.47 |
| 1:D:73:HIS:HA | 1:D:158:GLY:O | 2.15 | 0.47 |
| 1:F:259:GLU:CB | 1:F:263:GLN:HE22 | 2.01 | 0.47 |
| 1:D:8:LEU:N | 1:D:102:PRO:O | 2.45 | 0.47 |
| 1:D:334:GLU:H | 1:D:334:GLU:CD | 2.18 | 0.47 |
| 1:E:227:MET:HG2 | 1:E:255:PHE:HE1 | 1.78 | 0.47 |
| 1:G:138:ALA:CB | 1:G:163:VAL:HG11 | 2.45 | 0.47 |
| 1:E:165:ILE:N | 1:E:165:ILE:HD12 | 2.29 | 0.47 |
| 1:F:227:MET:HG2 | 1:F:255:PHE:HE1 | 1.79 | 0.47 |
| 1:F:139:VAL:HG22 | 1:H:43:VAL:HG11 | 1.95 | 0.47 |
| 1:H:238:LYS:HD3 | 1:H:239:SER:O | 2.14 | 0.47 |
| 1:H:361:GLU:HG3 | 1:H:361:GLU:H | 1.42 | 0.47 |
| 1:E:78:ASN:HD22 | 1:E:81:ASP:CG | 2.18 | 0.47 |
| 1:E:34:ILE:O | 1:E:35:VAL:HG13 | 2.15 | 0.47 |
| 1:H:287:ILE:CG2 | 1:H:288:ASP:N | 2.78 | 0.47 |
| 1:E:263:GLN:CG | 1:E:263:GLN:O | 2.63 | 0.47 |
| 1:D:329:ILE:N | 1:D:329:ILE:CD1 | 2.73 | 0.47 |
| 1:E:138:ALA:HB1 | 1:E:163:VAL:CG1 | 2.44 | 0.47 |
| 1:E:136:ILE:HD13 | 1:E:138:ALA:N | 2.29 | 0.47 |
| 1:E:171:LEU:HD23 | 1:E:173:HIS:HB2 | 1.97 | 0.47 |
| 1:F:330:ILE:O | 1:F:332:PRO:HD3 | 2.15 | 0.47 |
| 1:F:111:ASN:ND2 | 1:F:112:PRO:HD2 | 2.30 | 0.47 |
| 1:F:202:THR:HG23 | 1:F:204:ALA:H | 1.80 | 0.47 |
| 1:D:129:VAL:HG21 | 1:D:132:MET:CG | 2.40 | 0.47 |
| 1:G:120:THR:O | 1:G:124:PHE:CB | 2.62 | 0.47 |
| 1:G:99:GLU:CG | 1:G:128:ASN:HB2 | 2.43 | 0.47 |
| 1:F:357:ILE:HD12 | 1:F:370:VAL:HG23 | 1.96 | 0.47 |
| 1:D:325:MET:SD | 1:F:244:ASP:OD1 | 2.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:192:ILE:HD12 | 1:G:253:GLU:HB3 | 1.97 | 0.47 |
| 1:H:73:HIS:HA | 1:H:158:GLY:O | 2.15 | 0.47 |
| 1:F:136:ILE:C | 1:F:136:ILE:HD13 | 2.35 | 0.47 |
| 1:F:163:VAL:O | 1:F:163:VAL:HG13 | 2.15 | 0.47 |
| 1:F:163:VAL:HG22 | 1:F:165:ILE:CD1 | 2.45 | 0.47 |
| 1:G:211:ASP:HA | 1:G:214:GLU:HG3 | 1.96 | 0.47 |
| 1:G:238:LYS:HD3 | 1:G:239:SER:O | 2.15 | 0.47 |
| 1:E:120:THR:O | 1:E:124:PHE:HB2 | 2.15 | 0.47 |
| 1:H:124:PHE:O | 1:H:128:ASN:HA | 2.15 | 0.47 |
| 1:F:22:ALA:HB1 | 1:F:348:SER:HB2 | 1.97 | 0.47 |
| 1:D:176:MET:O | 1:D:178:LEU:HD12 | 2.14 | 0.47 |
| 1:G:34:ILE:C | 1:G:34:ILE:HD12 | 2.34 | 0.47 |
| 1:D:332:PRO:O | 1:D:335:ARG:HB3 | 2.15 | 0.47 |
| 1:E:139:VAL:CG2 | 1:G:43:VAL:HG11 | 2.45 | 0.47 |
| 1:H:320:LEU:HD12 | 1:H:321:ALA:H | 1.80 | 0.47 |
| 1:H:300:SER:HA | 1:H:335:ARG:HB2 | 1.97 | 0.47 |
| 1:G:147:ARG:CZ | 1:G:330:ILE:HD13 | 2.45 | 0.47 |
| 1:E:163:VAL:HG13 | 1:E:163:VAL:O | 2.15 | 0.47 |
| 1:E:357:ILE:HD12 | 1:E:370:VAL:HG23 | 1.96 | 0.47 |
| 1:H:211:ASP:OD1 | 1:H:212:ILE:N | 2.48 | 0.47 |
| 1:E:238:LYS:HZ2 | 1:E:254:ARG:HH12 | 1.63 | 0.47 |
| 1:D:7:ALA:N | 1:D:22:ALA:HB2 | 2.22 | 0.47 |
| 1:G:230:ALA:O | 1:G:233:SER:O | 2.33 | 0.47 |
| 1:E:325:MET:SD | 1:G:244:ASP:OD1 | 2.73 | 0.47 |
| 1:H:295:ALA:HB1 | 1:H:328:LYS:NZ | 2.30 | 0.47 |
| 1:H:25:ASP:O | 1:H:26:ALA:O | 2.33 | 0.47 |
| 1:F:171:LEU:HD23 | 1:F:173:HIS:HB2 | 1.97 | 0.46 |
| 1:E:202:THR:HG23 | 1:E:204:ALA:H | 1.79 | 0.46 |
| 1:H:54:VAL:HG11 | 1:H:88:HIS:CB | 2.45 | 0.46 |
| 1:H:100:GLU:N | 1:H:100:GLU:OE2 | 2.48 | 0.46 |
| 1:E:34:ILE:HD12 | 1:E:34:ILE:C | 2.35 | 0.46 |
| 1:D:192:ILE:HD12 | 1:D:253:GLU:CB | 2.45 | 0.46 |
| 1:D:70:PRO:HB2 | 1:D:82:MET:SD | 2.56 | 0.46 |
| 1:H:263:GLN:O | 1:H:263:GLN:CG | 2.62 | 0.46 |
| 1:H:138:ALA:CB | 1:H:163:VAL:CG1 | 2.94 | 0.46 |
| 1:G:334:GLU:CD | 1:G:334:GLU:H | 2.18 | 0.46 |
| 1:D:111:ASN:ND2 | 1:D:112:PRO:HD2 | 2.29 | 0.46 |
| 1:H:245:GLY:O | 1:H:246:GLN:HG3 | 2.16 | 0.46 |
| 1:D:374:CYS:O | 1:D:375:PHE:HB3 | 2.15 | 0.46 |
| 1:H:238:LYS:HZ2 | 1:H:254:ARG:HH12 | 1.62 | 0.46 |
| 1:G:339:VAL:HG23 | 1:G:340:TRP:H | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:34:ILE:O | 1:H:35:VAL:HG13 | 2.14 | 0.46 |
| 1:F:361:GLU:H | 1:F:361:GLU:HG3 | 1.40 | 0.46 |
| 1:H:147:ARG:HH22 | 1:H:330:ILE:HD13 | 1.78 | 0.46 |
| 1:F:211:ASP:HA | 1:F:214:GLU:HG3 | 1.95 | 0.46 |
| 1:F:329:ILE:O | 1:F:330:ILE:C | 2.54 | 0.46 |
| 1:D:211:ASP:HA | 1:D:214:GLU:HG3 | 1.97 | 0.46 |
| 1:D:178:LEU:H | 1:D:178:LEU:CD1 | 2.22 | 0.46 |
| 1:D:43:VAL:HG13 | 1:D:44:MET:N | 2.31 | 0.46 |
| 1:G:287:ILE:HG23 | 1:G:288:ASP:N | 2.29 | 0.46 |
| 1:G:353:GLN:HE21 | 1:G:353:GLN:N | 2.13 | 0.46 |
| 1:D:147:ARG:CZ | 1:D:330:ILE:HD13 | 2.45 | 0.46 |
| 1:E:372:ARG:O | 1:E:373:LYS:CB | 2.64 | 0.46 |
| 1:H:202:THR:HG23 | 1:H:204:ALA:H | 1.81 | 0.46 |
| 1:E:211:ASP:OD1 | 1:E:212:ILE:N | 2.48 | 0.46 |
| 1:E:113:LYS:HG2 | 1:E:117:GLU:CD | 2.36 | 0.46 |
| 1:D:240:TYR:CG | 1:D:241:GLU:N | 2.83 | 0.46 |
| 1:G:25:ASP:O | 1:G:26:ALA:O | 2.34 | 0.46 |
| 1:F:213:LYS:O | 1:F:217:CYS:HB3 | 2.16 | 0.46 |
| 1:F:143:TYR:CE2 | 1:F:346:LEU:HB2 | 2.50 | 0.46 |
| 1:E:211:ASP:HA | 1:E:214:GLU:HG3 | 1.98 | 0.46 |
| 1:F:75:ILE:HG12 | 1:F:111:ASN:OD1 | 2.15 | 0.46 |
| 1:G:111:ASN:ND2 | 1:G:112:PRO:HD2 | 2.30 | 0.46 |
| 1:E:121:GLN:O | 1:E:125:GLU:HG2 | 2.16 | 0.46 |
| 1:E:120:THR:O | 1:E:124:PHE:CB | 2.64 | 0.46 |
| 1:G:22:ALA:HB1 | 1:G:348:SER:HB2 | 1.98 | 0.46 |
| 1:F:124:PHE:O | 1:F:128:ASN:HA | 2.16 | 0.46 |
| 1:E:53:TYR:C | 1:E:54:VAL:HG22 | 2.36 | 0.46 |
| 1:H:323:SER:O | 1:H:324:THR:OG1 | 2.28 | 0.46 |
| 1:D:25:ASP:O | 1:D:26:ALA:O | 2.34 | 0.46 |
| 1:E:163:VAL:HG13 | 1:E:165:ILE:HD11 | 1.98 | 0.46 |
| 1:D:202:THR:HG23 | 1:D:204:ALA:H | 1.81 | 0.46 |
| 1:G:196:ARG:NH2 | 1:G:251:GLY:HA3 | 2.25 | 0.46 |
| 1:E:124:PHE:O | 1:E:128:ASN:HA | 2.16 | 0.46 |
| 1:H:219:VAL:O | 1:H:220:ALA:HB3 | 2.16 | 0.46 |
| 1:H:196:ARG:NH2 | 1:H:251:GLY:HA3 | 2.23 | 0.46 |
| 1:D:23:GLY:HA2 | 1:D:344:SER:CB | 2.38 | 0.46 |
| 1:F:99:GLU:O | 1:F:130:PRO:HB3 | 2.15 | 0.46 |
| 1:D:273:GLY:H | 1:D:277:THR:CG2 | 2.22 | 0.46 |
| 1:D:78:ASN:HD22 | 1:D:81:ASP:CG | 2.19 | 0.46 |
| 1:F:13:GLY:O | 1:F:14:SER:OG | 2.26 | 0.46 |
| 1:D:163:VAL:HG13 | 1:D:165:ILE:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:139:VAL:HG22 | 1:F:43:VAL:HG11 | 1.96 | 0.46 |
| 1:F:355:MET:HE2 | 1:F:356:TRP:NE1 | 2.31 | 0.46 |
| 1:G:117:GLU:OE2 | 1:G:371:HIS:HB2 | 2.16 | 0.46 |
| 1:F:104:LEU:HD12 | 1:F:133:TYR:O | 2.16 | 0.46 |
| 1:E:80:ASP:O | 1:E:83:GLU:HG2 | 2.16 | 0.46 |
| 1:H:91:TYR:O | 1:H:92:ASN:HB3 | 2.16 | 0.46 |
| 1:E:147:ARG:CZ | 1:E:330:ILE:HD13 | 2.46 | 0.46 |
| 1:D:124:PHE:O | 1:D:128:ASN:HA | 2.16 | 0.46 |
| 1:G:104:LEU:HD12 | 1:G:133:TYR:O | 2.15 | 0.46 |
| 1:G:287:ILE:CG2 | 1:G:288:ASP:N | 2.78 | 0.46 |
| 1:D:136:ILE:HD13 | 1:D:139:VAL:H | 1.80 | 0.46 |
| 1:F:230:ALA:O | 1:F:233:SER:O | 2.34 | 0.46 |
| 1:F:163:VAL:HG13 | 1:F:165:ILE:HD11 | 1.98 | 0.46 |
| 1:H:211:ASP:HA | 1:H:214:GLU:HG3 | 1.97 | 0.46 |
| 1:H:230:ALA:O | 1:H:233:SER:O | 2.34 | 0.46 |
| 1:H:359:LYS:O | 1:H:360:GLN:CB | 2.64 | 0.46 |
| 1:E:104:LEU:HD12 | 1:E:133:TYR:O | 2.15 | 0.46 |
| 1:G:54:VAL:HG11 | 1:G:88:HIS:CB | 2.46 | 0.46 |
| 1:E:100:GLU:N | 1:E:100:GLU:OE2 | 2.49 | 0.46 |
| 1:H:302:GLY:C | 1:H:304:THR:N | 2.63 | 0.45 |
| 1:G:11:ASP:CB | 1:G:18:LYS:HB2 | 2.46 | 0.45 |
| 1:G:332:PRO:O | 1:G:335:ARG:HB3 | 2.16 | 0.45 |
| 1:E:136:ILE:HD12 | 1:E:139:VAL:CG2 | 2.39 | 0.45 |
| 1:E:5:THR:OG1 | 1:E:101:HIS:HA | 2.16 | 0.45 |
| 1:F:238:LYS:HZ2 | 1:F:254:ARG:HH12 | 1.63 | 0.45 |
| 1:F:374:CYS:O | 1:F:375:PHE:HB3 | 2.17 | 0.45 |
| 1:H:227:MET:HG2 | 1:H:255:PHE:HE1 | 1.79 | 0.45 |
| 1:H:242:LEU:HG | 1:H:246:GLN:C | 2.37 | 0.45 |
| 1:E:54:VAL:HG11 | 1:E:88:HIS:CB | 2.47 | 0.45 |
| 1:F:34:ILE:O | 1:F:35:VAL:HG13 | 2.16 | 0.45 |
| 1:H:11:ASP:HB2 | 1:H:18:LYS:HB2 | 1.98 | 0.45 |
| 1:D:309:ILE:HA | 1:D:309:ILE:HD13 | 1.81 | 0.45 |
| 1:F:73:HIS:HA | 1:F:158:GLY:O | 2.16 | 0.45 |
| 1:D:5:THR:OG1 | 1:D:101:HIS:HA | 2.16 | 0.45 |
| 1:D:334:GLU:N | 1:D:334:GLU:OE2 | 2.47 | 0.45 |
| 1:F:8:LEU:HD12 | 1:F:21:PHE:HA | 1.98 | 0.45 |
| 1:D:52:SER:O | 1:D:53:TYR:CD1 | 2.69 | 0.45 |
| 1:E:75:ILE:HG12 | 1:E:111:ASN:OD1 | 2.15 | 0.45 |
| 1:E:105:LEU:HD22 | 1:E:105:LEU:N | 2.31 | 0.45 |
| 1:F:245:GLY:O | 1:F:246:GLN:HG3 | 2.17 | 0.45 |
| 1:D:339:VAL:HG23 | 1:D:340:TRP:H | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:192:ILE:HD12 | 1:E:253:GLU:CB | 2.46 | 0.45 |
| 1:F:353:GLN:HE21 | 1:F:353:GLN:N | 2.14 | 0.45 |
| 1:E:25:ASP:O | 1:E:26:ALA:O | 2.35 | 0.45 |
| 1:H:163:VAL:HG13 | 1:H:163:VAL:O | 2.16 | 0.45 |
| 1:H:329:ILE:O | 1:H:330:ILE:C | 2.55 | 0.45 |
| 1:G:138:ALA:CB | 1:G:163:VAL:CG1 | 2.94 | 0.45 |
| 1:E:147:ARG:NH2 | 1:E:330:ILE:HD13 | 2.32 | 0.45 |
| 1:F:209:VAL:C | 1:F:212:ILE:HG12 | 2.36 | 0.45 |
| 1:F:238:LYS:HD3 | 1:F:239:SER:O | 2.17 | 0.45 |
| 1:E:212:ILE:HD12 | 1:E:240:TYR:CE1 | 2.51 | 0.45 |
| 1:F:71:ILE:HD12 | 1:F:76:ILE:CG1 | 2.38 | 0.45 |
| 1:H:113:LYS:HG2 | 1:H:117:GLU:CD | 2.37 | 0.45 |
| 1:H:370:VAL:HG13 | 1:H:371:HIS:N | 2.31 | 0.45 |
| 1:G:221:LEU:CD1 | 1:G:221:LEU:H | 2.28 | 0.45 |
| 1:F:25:ASP:O | 1:F:26:ALA:O | 2.33 | 0.45 |
| 1:D:136:ILE:HD13 | 1:D:136:ILE:C | 2.37 | 0.45 |
| 1:E:71:ILE:HD12 | 1:E:76:ILE:CG1 | 2.38 | 0.45 |
| 1:E:99:GLU:O | 1:E:130:PRO:HB3 | 2.16 | 0.45 |
| 1:G:8:LEU:HD12 | 1:G:21:PHE:HA | 1.98 | 0.45 |
| 1:D:287:ILE:CG2 | 1:D:288:ASP:N | 2.79 | 0.45 |
| 1:G:70:PRO:HB2 | 1:G:82:MET:SD | 2.56 | 0.45 |
| 1:D:8:LEU:HD12 | 1:D:21:PHE:HA | 1.97 | 0.45 |
| 1:G:334:GLU:N | 1:G:334:GLU:OE2 | 2.47 | 0.45 |
| 1:H:99:GLU:O | 1:H:130:PRO:HB3 | 2.17 | 0.45 |
| 1:E:221:LEU:CD1 | 1:E:221:LEU:H | 2.22 | 0.45 |
| 1:F:325:MET:CE | 1:F:326:LYS:H | 2.29 | 0.45 |
| 1:D:275:HIS:H | 1:D:275:HIS:CD2 | 2.34 | 0.45 |
| 1:F:136:ILE:HD13 | 1:F:139:VAL:H | 1.82 | 0.45 |
| 1:F:346:LEU:HD11 | 1:F:355:MET:HE1 | 1.98 | 0.45 |
| 1:D:105:LEU:N | 1:D:105:LEU:HD22 | 2.30 | 0.45 |
| 1:G:121:GLN:HA | 1:G:125:GLU:HG2 | 1.97 | 0.45 |
| 1:H:176:MET:HE1 | 1:H:277:THR:C | 2.36 | 0.45 |
| 1:G:37:ARG:HB3 | 1:G:38:PRO:HD2 | 1.97 | 0.45 |
| 1:F:309:ILE:HA | 1:F:309:ILE:HD13 | 1.80 | 0.45 |
| 1:H:334:GLU:N | 1:H:334:GLU:OE2 | 2.48 | 0.45 |
| 1:D:330:ILE:O | 1:D:332:PRO:HD3 | 2.16 | 0.45 |
| 1:E:334:GLU:CD | 1:E:334:GLU:H | 2.20 | 0.45 |
| 1:H:8:LEU:HD12 | 1:H:21:PHE:HA | 1.99 | 0.45 |
| 1:D:11:ASP:HB2 | 1:D:18:LYS:HB2 | 1.98 | 0.45 |
| 1:E:92:ASN:ND2 | 1:E:93:GLU:HG3 | 2.32 | 0.45 |
| 1:F:92:ASN:ND2 | 1:F:93:GLU:HG3 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:192:ILE:HD12 | 1:H:253:GLU:CB | 2.46 | 0.45 |
| 1:D:140:LEU:N | 1:D:140:LEU:CD1 | 2.79 | 0.45 |
| 1:G:11:ASP:HB2 | 1:G:18:LYS:HB2 | 1.98 | 0.45 |
| 1:F:147:ARG:CZ | 1:F:330:ILE:HD13 | 2.45 | 0.45 |
| 1:E:200:PHE:HA | 1:E:205:GLU:OE1 | 2.17 | 0.45 |
| 1:G:211:ASP:OD1 | 1:G:212:ILE:N | 2.50 | 0.45 |
| 1:D:267:ILE:CG2 | 1:D:268:GLY:N | 2.79 | 0.45 |
| 1:D:287:ILE:HG23 | 1:D:288:ASP:N | 2.30 | 0.45 |
| 1:E:176:MET:HE1 | 1:E:277:THR:C | 2.37 | 0.45 |
| 1:F:61:LYS:CB | 1:F:64:ILE:HD11 | 2.47 | 0.45 |
| 1:G:147:ARG:NH2 | 1:G:330:ILE:HD13 | 2.31 | 0.45 |
| 1:F:139:VAL:CG2 | 1:H:43:VAL:HG11 | 2.47 | 0.45 |
| 1:D:53:TYR:C | 1:D:54:VAL:HG22 | 2.37 | 0.45 |
| 1:D:113:LYS:HG2 | 1:D:117:GLU:CD | 2.37 | 0.45 |
| 1:G:369:ILE:HG13 | 1:G:372:ARG:HH22 | 1.82 | 0.45 |
| 1:D:22:ALA:HB1 | 1:D:348:SER:HB2 | 1.99 | 0.45 |
| 1:G:171:LEU:HD23 | 1:G:173:HIS:HB2 | 1.99 | 0.45 |
| 1:E:44:MET:CE | 1:E:45:VAL:H | 2.30 | 0.45 |
| 1:H:334:GLU:H | 1:H:334:GLU:CD | 2.21 | 0.45 |
| 1:E:369:ILE:HG13 | 1:E:372:ARG:HH22 | 1.80 | 0.45 |
| 1:G:257:CYS:SG | 1:G:258:PRO:N | 2.90 | 0.45 |
| 1:F:166:TYR:HD2 | 1:H:64:ILE:HG21 | 1.82 | 0.45 |
| 1:H:121:GLN:HA | 1:H:125:GLU:HG2 | 1.98 | 0.45 |
| 1:F:78:ASN:HD22 | 1:F:81:ASP:CG | 2.20 | 0.45 |
| 1:F:70:PRO:HB2 | 1:F:82:MET:SD | 2.57 | 0.45 |
| 1:E:275:HIS:CD2 | 1:E:275:HIS:H | 2.35 | 0.45 |
| 1:D:171:LEU:HD23 | 1:D:173:HIS:HB2 | 2.00 | 0.44 |
| 1:G:300:SER:HA | 1:G:335:ARG:HB2 | 1.99 | 0.44 |
| 1:F:176:MET:HE1 | 1:F:277:THR:C | 2.37 | 0.44 |
| 1:F:334:GLU:CD | 1:F:334:GLU:H | 2.21 | 0.44 |
| 1:G:160:THR:OG1 | 1:G:178:LEU:HD13 | 2.18 | 0.44 |
| 1:D:117:GLU:OE2 | 1:D:371:HIS:HB2 | 2.17 | 0.44 |
| 1:F:23:GLY:HA2 | 1:F:344:SER:CB | 2.35 | 0.44 |
| 1:D:277:THR:HA | 1:D:280:ASN:HD22 | 1.82 | 0.44 |
| 1:G:242:LEU:HG | 1:G:246:GLN:C | 2.35 | 0.44 |
| 1:E:312:ARG:HA | 1:E:315:LYS:HE3 | 2.00 | 0.44 |
| 1:D:110:LEU:CB | 1:D:177:ARG:HG3 | 2.36 | 0.44 |
| 1:F:211:ASP:OD1 | 1:F:212:ILE:N | 2.51 | 0.44 |
| 1:E:250:ILE:H | 1:E:250:ILE:HD12 | 1.82 | 0.44 |
| 1:G:98:PRO:HG3 | 1:G:127:PHE:HD1 | 1.83 | 0.44 |
| 1:F:113:LYS:HG2 | 1:F:117:GLU:CD | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:289:ILE:HD13 | 1:G:289:ILE:C | 2.38 | 0.44 |
| 1:F:11:ASP:CB | 1:F:18:LYS:HB2 | 2.47 | 0.44 |
| 1:H:339:VAL:HG23 | 1:H:340:TRP:H | 1.79 | 0.44 |
| 1:G:1:ASP:O | 1:G:4:GLU:O | 2.34 | 0.44 |
| 1:H:136:ILE:HD13 | 1:H:139:VAL:H | 1.81 | 0.44 |
| 1:D:142:LEU:HD21 | 1:D:165:ILE:HB | 1.98 | 0.44 |
| 1:G:136:ILE:HD13 | 1:G:136:ILE:C | 2.37 | 0.44 |
| 1:G:142:LEU:HD21 | 1:G:165:ILE:HB | 1.98 | 0.44 |
| 1:H:66:THR:HA | 1:H:203:THR:OG1 | 2.18 | 0.44 |
| 1:G:212:ILE:HD12 | 1:G:240:TYR:CE1 | 2.52 | 0.44 |
| 1:H:23:GLY:HA2 | 1:H:344:SER:CB | 2.36 | 0.44 |
| 1:H:160:THR:OG1 | 1:H:178:LEU:HD13 | 2.18 | 0.44 |
| 1:D:11:ASP:CB | 1:D:18:LYS:HB2 | 2.47 | 0.44 |
| 1:H:326:LYS:HE3 | 1:H:327:ILE:N | 2.32 | 0.44 |
| 1:H:89:THR:O | 1:H:94:LEU:HG | 2.17 | 0.44 |
| 1:H:147:ARG:CZ | 1:H:330:ILE:HD13 | 2.45 | 0.44 |
| 1:H:332:PRO:O | 1:H:335:ARG:HB3 | 2.18 | 0.44 |
| 1:F:138:ALA:CB | 1:F:163:VAL:HG11 | 2.48 | 0.44 |
| 1:G:227:MET:HG2 | 1:G:255:PHE:HE1 | 1.81 | 0.44 |
| 1:H:61:LYS:CB | 1:H:64:ILE:HD11 | 2.48 | 0.44 |
| 1:F:370:VAL:HG13 | 1:F:371:HIS:N | 2.31 | 0.44 |
| 1:H:277:THR:O | 1:H:280:ASN:ND2 | 2.51 | 0.44 |
| 1:H:92:ASN:ND2 | 1:H:93:GLU:HG3 | 2.32 | 0.44 |
| 1:F:54:VAL:HG11 | 1:F:88:HIS:CB | 2.47 | 0.44 |
| 1:G:249:THR:HG23 | 1:G:249:THR:O | 2.18 | 0.44 |
| 1:H:151:ILE:HG12 | 1:H:164:PRO:HA | 2.00 | 0.44 |
| 1:D:147:ARG:NH2 | 1:D:330:ILE:HD13 | 2.32 | 0.44 |
| 1:E:349:LEU:HB3 | 1:E:352:PHE:HE2 | 1.82 | 0.44 |
| 1:E:121:GLN:HA | 1:E:125:GLU:HG2 | 1.99 | 0.44 |
| 1:D:359:LYS:O | 1:D:360:GLN:CB | 2.64 | 0.44 |
| 1:H:111:ASN:CG | 1:H:112:PRO:CD | 2.86 | 0.44 |
| 1:H:214:GLU:HG2 | 2:H:401:ADP:C2 | 2.53 | 0.44 |
| 1:H:117:GLU:OE2 | 1:H:371:HIS:HB2 | 2.17 | 0.44 |
| 1:F:129:VAL:HG21 | 1:F:132:MET:CG | 2.38 | 0.44 |
| 1:F:117:GLU:OE2 | 1:F:371:HIS:HB2 | 2.17 | 0.44 |
| 1:D:176:MET:HE1 | 1:D:277:THR:C | 2.38 | 0.44 |
| 1:D:188:TYR:O | 1:D:192:ILE:HG23 | 2.17 | 0.44 |
| 1:H:11:ASP:CB | 1:H:18:LYS:HB2 | 2.47 | 0.44 |
| 1:D:353:GLN:HE21 | 1:D:353:GLN:N | 2.16 | 0.44 |
| 1:F:334:GLU:N | 1:F:334:GLU:OE2 | 2.49 | 0.44 |
| 1:F:312:ARG:HA | 1:F:315:LYS:HE3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:277:THR:HA | 1:E:280:ASN:HD22 | 1.83 | 0.44 |
| 1:F:250:ILE:H | 1:F:250:ILE:HD12 | 1.82 | 0.44 |
| 1:F:214:GLU:HG2 | 2:F:401:ADP:C2 | 2.53 | 0.44 |
| 1:E:64:ILE:H | 1:E:64:ILE:HG13 | 1.55 | 0.44 |
| 1:G:124:PHE:CZ | 1:G:359:LYS:HA | 2.53 | 0.44 |
| 1:D:196:ARG:NH2 | 1:D:251:GLY:HA3 | 2.23 | 0.44 |
| 1:H:349:LEU:HB3 | 1:H:352:PHE:HE2 | 1.82 | 0.44 |
| 1:H:5:THR:OG1 | 1:H:101:HIS:HA | 2.17 | 0.44 |
| 1:G:53:TYR:C | 1:G:54:VAL:HG22 | 2.38 | 0.44 |
| 1:D:100:GLU:OE2 | 1:D:100:GLU:N | 2.50 | 0.44 |
| 1:D:361:GLU:O | 1:D:364:GLU:HG2 | 2.18 | 0.44 |
| 1:H:147:ARG:NH2 | 1:H:330:ILE:HD13 | 2.32 | 0.44 |
| 1:D:329:ILE:O | 1:D:330:ILE:C | 2.55 | 0.44 |
| 1:G:202:THR:HG23 | 1:G:204:ALA:H | 1.83 | 0.44 |
| 1:G:61:LYS:CB | 1:G:64:ILE:HD11 | 2.48 | 0.44 |
| 1:D:54:VAL:HG11 | 1:D:88:HIS:CB | 2.48 | 0.44 |
| 1:E:214:GLU:HG2 | 2:E:401:ADP:C2 | 2.53 | 0.44 |
| 1:G:71:ILE:HD12 | 1:G:76:ILE:CG1 | 2.40 | 0.44 |
| 1:D:325:MET:CE | 1:D:326:LYS:H | 2.31 | 0.44 |
| 1:G:73:HIS:HA | 1:G:158:GLY:O | 2.17 | 0.44 |
| 1:D:259:GLU:CB | 1:D:263:GLN:HE22 | 2.00 | 0.44 |
| 1:D:300:SER:HA | 1:D:335:ARG:HB2 | 2.00 | 0.44 |
| 1:E:138:ALA:CB | 1:E:163:VAL:HG11 | 2.48 | 0.44 |
| 1:F:277:THR:HA | 1:F:280:ASN:HD22 | 1.83 | 0.44 |
| 1:F:352:PHE:HZ | 1:H:47:MET:CE | 2.30 | 0.44 |
| 1:F:166:TYR:O | 1:F:169:TYR:O | 2.36 | 0.44 |
| 1:E:111:ASN:CG | 1:E:112:PRO:CD | 2.87 | 0.44 |
| 1:H:22:ALA:HB1 | 1:H:348:SER:HB2 | 2.00 | 0.44 |
| 1:F:105:LEU:HD22 | 1:F:105:LEU:N | 2.31 | 0.44 |
| 1:F:249:THR:HG23 | 1:F:249:THR:O | 2.16 | 0.44 |
| 1:H:275:HIS:CD2 | 1:H:275:HIS:H | 2.34 | 0.44 |
| 1:D:330:ILE:CG2 | 1:D:330:ILE:O | 2.64 | 0.43 |
| 1:G:110:LEU:HB2 | 1:G:177:ARG:CG | 2.37 | 0.43 |
| 1:E:346:LEU:HD11 | 1:E:355:MET:HE1 | 2.00 | 0.43 |
| 1:E:355:MET:HE2 | 1:E:356:TRP:NE1 | 2.31 | 0.43 |
| 1:F:212:ILE:HD12 | 1:F:240:TYR:CE1 | 2.53 | 0.43 |
| 1:F:280:ASN:OD1 | 1:F:281:SER:N | 2.50 | 0.43 |
| 1:G:176:MET:HE1 | 1:G:277:THR:CB | 2.38 | 0.43 |
| 1:F:121:GLN:HA | 1:F:125:GLU:HG2 | 2.00 | 0.43 |
| 1:G:213:LYS:O | 1:G:217:CYS:HB3 | 2.18 | 0.43 |
| 1:D:245:GLY:O | 1:D:246:GLN:HG3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:92:ASN:ND2 | 1:G:93:GLU:HG3 | 2.33 | 0.43 |
| 1:E:326:LYS:HE3 | 1:E:327:ILE:N | 2.33 | 0.43 |
| 1:H:163:VAL:HG13 | 1:H:165:ILE:HD11 | 2.00 | 0.43 |
| 1:D:163:VAL:CG2 | 1:D:165:ILE:HD11 | 2.48 | 0.43 |
| 1:G:136:ILE:HD13 | 1:G:139:VAL:H | 1.82 | 0.43 |
| 1:E:200:PHE:O | 1:E:201:VAL:HG13 | 2.18 | 0.43 |
| 1:E:76:ILE:CG2 | 1:E:79:TRP:H | 2.31 | 0.43 |
| 1:E:61:LYS:CB | 1:E:64:ILE:HD11 | 2.48 | 0.43 |
| 1:G:372:ARG:O | 1:G:373:LYS:CB | 2.65 | 0.43 |
| 1:H:206:ARG:HA | 1:H:209:VAL:HG12 | 2.00 | 0.43 |
| 1:H:240:TYR:CG | 1:H:241:GLU:N | 2.86 | 0.43 |
| 1:E:229:THR:HG23 | 1:E:230:ALA:H | 1.82 | 0.43 |
| 1:H:372:ARG:O | 1:H:373:LYS:CB | 2.65 | 0.43 |
| 1:G:78:ASN:HD22 | 1:G:81:ASP:CG | 2.22 | 0.43 |
| 1:D:92:ASN:ND2 | 1:D:93:GLU:HG3 | 2.32 | 0.43 |
| 1:H:138:ALA:HB1 | 1:H:163:VAL:HG12 | 2.00 | 0.43 |
| 1:H:163:VAL:CG2 | 1:H:165:ILE:HD11 | 2.47 | 0.43 |
| 1:F:147:ARG:NH2 | 1:F:330:ILE:HD13 | 2.32 | 0.43 |
| 1:E:209:VAL:C | 1:E:212:ILE:HG12 | 2.37 | 0.43 |
| 1:G:209:VAL:C | 1:G:212:ILE:HG12 | 2.38 | 0.43 |
| 1:G:75:ILE:HG12 | 1:G:111:ASN:OD1 | 2.17 | 0.43 |
| 1:G:5:THR:OG1 | 1:G:101:HIS:HA | 2.18 | 0.43 |
| 1:D:22:ALA:O | 1:D:23:GLY:C | 2.57 | 0.43 |
| 1:E:11:ASP:CB | 1:E:18:LYS:HB2 | 2.48 | 0.43 |
| 1:F:11:ASP:HB2 | 1:F:18:LYS:HB2 | 1.98 | 0.43 |
| 1:H:188:TYR:O | 1:H:192:ILE:HG23 | 2.18 | 0.43 |
| 1:E:287:ILE:HG23 | 1:E:288:ASP:N | 2.33 | 0.43 |
| 1:G:163:VAL:HG13 | 1:G:165:ILE:HD11 | 2.00 | 0.43 |
| 1:E:330:ILE:O | 1:E:330:ILE:CG2 | 2.65 | 0.43 |
| 1:F:369:ILE:HG13 | 1:F:372:ARG:HH22 | 1.83 | 0.43 |
| 1:E:166:TYR:HD2 | 1:G:64:ILE:HG21 | 1.83 | 0.43 |
| 1:H:52:SER:O | 1:H:53:TYR:CD1 | 2.71 | 0.43 |
| 1:D:75:ILE:HG12 | 1:D:111:ASN:OD1 | 2.18 | 0.43 |
| 1:G:105:LEU:N | 1:G:105:LEU:HD22 | 2.32 | 0.43 |
| 1:H:16:LEU:HD11 | 2:H:401:ADP:H5'2 | 2.01 | 0.43 |
| 1:F:11:ASP:O | 1:F:106:THR:HB | 2.18 | 0.43 |
| 1:H:312:ARG:HA | 1:H:315:LYS:HE3 | 2.00 | 0.43 |
| 1:F:279:TYR:O | 1:F:282:ILE:HG22 | 2.19 | 0.43 |
| 1:G:192:ILE:HD12 | 1:G:253:GLU:CB | 2.48 | 0.43 |
| 1:F:287:ILE:HG23 | 1:F:288:ASP:N | 2.32 | 0.43 |
| 1:F:95:ARG:CZ | 1:F:95:ARG:HB2 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:263:GLN:O | 1:F:263:GLN:CG | 2.66 | 0.43 |
| 1:H:142:LEU:HD21 | 1:H:165:ILE:HB | 2.01 | 0.43 |
| 1:D:173:HIS:NE2 | 1:E:267:ILE:O | 2.51 | 0.43 |
| 1:F:238:LYS:HZ2 | 1:F:254:ARG:NH2 | 2.13 | 0.43 |
| 1:G:277:THR:HA | 1:G:280:ASN:HD22 | 1.84 | 0.43 |
| 1:G:105:LEU:CD2 | 1:G:132:MET:HB2 | 2.42 | 0.43 |
| 1:E:213:LYS:O | 1:E:217:CYS:HB3 | 2.18 | 0.43 |
| 1:D:280:ASN:OD1 | 1:D:281:SER:N | 2.51 | 0.43 |
| 1:H:369:ILE:HG13 | 1:H:372:ARG:HH22 | 1.84 | 0.43 |
| 1:E:88:HIS:O | 1:E:91:TYR:O | 2.36 | 0.43 |
| 1:G:295:ALA:HB1 | 1:G:328:LYS:NZ | 2.33 | 0.43 |
| 1:D:361:GLU:HG3 | 1:D:361:GLU:H | 1.41 | 0.43 |
| 1:F:275:HIS:H | 1:F:275:HIS:CD2 | 2.35 | 0.43 |
| 1:D:332:PRO:HA | 1:D:333:PRO:HD3 | 1.89 | 0.43 |
| 1:E:267:ILE:CG2 | 1:E:268:GLY:N | 2.81 | 0.43 |
| 1:F:196:ARG:NH2 | 1:F:251:GLY:HA3 | 2.25 | 0.43 |
| 1:F:136:ILE:HD12 | 1:F:139:VAL:CG2 | 2.39 | 0.43 |
| 1:F:142:LEU:HD21 | 1:F:165:ILE:HB | 2.00 | 0.43 |
| 1:H:76:ILE:CG2 | 1:H:79:TRP:H | 2.32 | 0.43 |
| 1:G:370:VAL:HG13 | 1:G:371:HIS:N | 2.33 | 0.43 |
| 1:H:222:ASP:CG | 1:H:225:ASN:HB3 | 2.39 | 0.43 |
| 1:F:289:ILE:C | 1:F:289:ILE:HD13 | 2.38 | 0.43 |
| 1:H:78:ASN:HD22 | 1:H:81:ASP:CG | 2.21 | 0.43 |
| 1:G:312:ARG:HA | 1:G:315:LYS:HE3 | 2.01 | 0.43 |
| 1:E:249:THR:O | 1:E:249:THR:HG23 | 2.18 | 0.43 |
| 1:E:73:HIS:HA | 1:E:158:GLY:O | 2.18 | 0.43 |
| 1:H:136:ILE:HD13 | 1:H:136:ILE:C | 2.39 | 0.43 |
| 1:H:165:ILE:HD12 | 1:H:165:ILE:N | 2.34 | 0.43 |
| 1:D:138:ALA:CB | 1:D:163:VAL:HG11 | 2.49 | 0.43 |
| 1:E:329:ILE:O | 1:E:330:ILE:C | 2.56 | 0.43 |
| 1:E:334:GLU:OE2 | 1:E:334:GLU:N | 2.48 | 0.43 |
| 1:H:105:LEU:CD2 | 1:H:132:MET:HB2 | 2.45 | 0.43 |
| 1:F:242:LEU:HG | 1:F:246:GLN:C | 2.39 | 0.43 |
| 1:F:287:ILE:CG2 | 1:F:288:ASP:N | 2.81 | 0.43 |
| 1:E:347:ALA:HA | 1:E:356:TRP:HZ2 | 1.84 | 0.43 |
| 1:F:257:CYS:SG | 1:F:258:PRO:N | 2.91 | 0.43 |
| 1:G:267:ILE:CG2 | 1:G:268:GLY:N | 2.81 | 0.43 |
| 1:E:113:LYS:HG2 | 1:E:117:GLU:OE2 | 2.19 | 0.43 |
| 1:E:105:LEU:CD2 | 1:E:132:MET:HB2 | 2.44 | 0.43 |
| 1:E:64:ILE:CD1 | 1:E:65:LEU:N | 2.72 | 0.43 |
| 1:D:370:VAL:HG13 | 1:D:371:HIS:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:113:LYS:HG2 | 1:G:117:GLU:CD | 2.39 | 0.43 |
| 1:G:374:CYS:O | 1:G:375:PHE:CB | 2.67 | 0.43 |
| 1:G:22:ALA:O | 1:G:23:GLY:C | 2.57 | 0.43 |
| 1:H:267:ILE:CG2 | 1:H:268:GLY:N | 2.82 | 0.43 |
| 1:E:146:GLY:O | 1:E:147:ARG:HB2 | 2.19 | 0.43 |
| 1:F:5:THR:OG1 | 1:F:101:HIS:HA | 2.18 | 0.43 |
| 1:D:71:ILE:HD12 | 1:D:76:ILE:CG1 | 2.41 | 0.43 |
| 1:E:238:LYS:CD | 1:E:239:SER:H | 2.31 | 0.43 |
| 1:D:295:ALA:HB1 | 1:D:328:LYS:NZ | 2.34 | 0.43 |
| 1:F:53:TYR:C | 1:F:54:VAL:HG22 | 2.38 | 0.43 |
| 1:G:146:GLY:O | 1:G:147:ARG:HB2 | 2.19 | 0.43 |
| 1:F:138:ALA:CB | 1:F:163:VAL:CG1 | 2.97 | 0.43 |
| 1:D:120:THR:O | 1:D:124:PHE:HB2 | 2.19 | 0.43 |
| 1:E:325:MET:CE | 1:E:326:LYS:H | 2.31 | 0.43 |
| 1:E:279:TYR:O | 1:E:282:ILE:HG22 | 2.19 | 0.43 |
| 1:F:192:ILE:HD12 | 1:F:253:GLU:CB | 2.48 | 0.43 |
| 1:D:121:GLN:HA | 1:D:125:GLU:HG2 | 2.01 | 0.43 |
| 1:E:160:THR:OG1 | 1:E:178:LEU:HD13 | 2.19 | 0.42 |
| 1:E:273:GLY:N | 1:E:277:THR:HG23 | 2.20 | 0.42 |
| 1:F:44:MET:HE2 | 1:F:47:MET:HG2 | 2.00 | 0.42 |
| 1:F:172:PRO:HA | 1:F:175:ILE:CD1 | 2.49 | 0.42 |
| 1:G:64:ILE:H | 1:G:64:ILE:HG13 | 1.53 | 0.42 |
| 1:E:16:LEU:HD11 | 2:E:401:ADP:H5'2 | 2.01 | 0.42 |
| 1:H:75:ILE:HG12 | 1:H:111:ASN:OD1 | 2.18 | 0.42 |
| 1:H:14:SER:O | 1:H:71:ILE:HG23 | 2.19 | 0.42 |
| 1:F:22:ALA:O | 1:F:23:GLY:C | 2.57 | 0.42 |
| 1:F:105:LEU:CD2 | 1:F:132:MET:HB2 | 2.44 | 0.42 |
| 1:D:174:ALA:CB | 1:D:281:SER:HA | 2.49 | 0.42 |
| 1:E:11:ASP:HB2 | 1:E:18:LYS:HB2 | 2.00 | 0.42 |
| 1:G:275:HIS:H | 1:G:275:HIS:CD2 | 2.37 | 0.42 |
| 1:D:149:THR:HG23 | 1:D:166:TYR:HA | 2.01 | 0.42 |
| 1:G:121:GLN:HG3 | 1:G:362:TYR:OH | 2.19 | 0.42 |
| 1:E:22:ALA:O | 1:E:23:GLY:C | 2.57 | 0.42 |
| 1:D:242:LEU:HG | 1:D:246:GLN:C | 2.39 | 0.42 |
| 1:E:289:ILE:HD13 | 1:E:289:ILE:C | 2.40 | 0.42 |
| 1:H:6:THR:O | 1:H:102:PRO:HD2 | 2.20 | 0.42 |
| 1:E:287:ILE:CG2 | 1:E:288:ASP:N | 2.82 | 0.42 |
| 1:H:136:ILE:HD12 | 1:H:139:VAL:CG2 | 2.41 | 0.42 |
| 1:F:176:MET:HE1 | 1:F:277:THR:CB | 2.41 | 0.42 |
| 1:F:372:ARG:O | 1:F:373:LYS:CB | 2.65 | 0.42 |
| 1:D:61:LYS:CB | 1:D:64:ILE:HD11 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:200:PHE:HA | 1:F:205:GLU:OE1 | 2.19 | 0.42 |
| 1:G:238:LYS:HZ3 | 1:G:254:ARG:HH22 | 1.64 | 0.42 |
| 1:H:222:ASP:OD2 | 1:H:225:ASN:HB3 | 2.18 | 0.42 |
| 1:E:11:ASP:O | 1:E:106:THR:HB | 2.19 | 0.42 |
| 1:F:339:VAL:HG23 | 1:F:340:TRP:H | 1.82 | 0.42 |
| 1:D:139:VAL:HG11 | 1:F:43:VAL:HG21 | 2.01 | 0.42 |
| 1:F:44:MET:HE3 | 1:F:45:VAL:H | 1.83 | 0.42 |
| 1:G:154:ASP:O | 1:G:154:ASP:CG | 2.58 | 0.42 |
| 1:F:240:TYR:CZ | 1:F:241:GLU:O | 2.72 | 0.42 |
| 1:F:300:SER:HA | 1:F:335:ARG:HB2 | 2.02 | 0.42 |
| 1:G:200:PHE:HA | 1:G:205:GLU:OE1 | 2.19 | 0.42 |
| 1:E:206:ARG:HA | 1:E:209:VAL:HG12 | 2.02 | 0.42 |
| 1:E:14:SER:O | 1:E:71:ILE:HG23 | 2.19 | 0.42 |
| 1:H:209:VAL:C | 1:H:212:ILE:HG12 | 2.40 | 0.42 |
| 1:G:325:MET:CE | 1:G:326:LYS:H | 2.32 | 0.42 |
| 1:G:263:GLN:O | 1:G:265:SER:N | 2.52 | 0.42 |
| 1:D:138:ALA:CB | 1:D:163:VAL:CG1 | 2.98 | 0.42 |
| 1:G:136:ILE:HD12 | 1:G:139:VAL:CG2 | 2.40 | 0.42 |
| 1:E:370:VAL:HG13 | 1:E:371:HIS:N | 2.35 | 0.42 |
| 1:D:120:THR:O | 1:D:124:PHE:CB | 2.67 | 0.42 |
| 1:G:346:LEU:HD11 | 1:G:355:MET:HE1 | 2.02 | 0.42 |
| 1:E:236:LEU:O | 1:E:254:ARG:NH1 | 2.49 | 0.42 |
| 1:E:238:LYS:HD3 | 1:E:239:SER:O | 2.19 | 0.42 |
| 1:D:213:LYS:O | 1:D:217:CYS:HB3 | 2.20 | 0.42 |
| 1:E:323:SER:C | 1:E:324:THR:HG23 | 2.39 | 0.42 |
| 1:E:136:ILE:HD13 | 1:E:139:VAL:H | 1.84 | 0.42 |
| 1:F:222:ASP:CG | 1:F:225:ASN:HB3 | 2.40 | 0.42 |
| 1:F:224:GLU:C | 1:F:224:GLU:CD | 2.78 | 0.42 |
| 1:F:102:PRO:CB | 1:F:131:ALA:HB3 | 2.45 | 0.42 |
| 1:D:62:ARG:NE | 1:D:208:ILE:HD11 | 2.35 | 0.42 |
| 1:F:111:ASN:CG | 1:F:112:PRO:CD | 2.88 | 0.42 |
| 1:D:238:LYS:HB2 | 1:D:238:LYS:HE3 | 1.86 | 0.42 |
| 1:H:129:VAL:HG21 | 1:H:132:MET:CG | 2.39 | 0.42 |
| 1:F:11:ASP:HB3 | 1:F:18:LYS:H | 1.84 | 0.42 |
| 1:D:37:ARG:HB3 | 1:D:38:PRO:HD2 | 2.01 | 0.42 |
| 1:E:257:CYS:SG | 1:E:258:PRO:N | 2.93 | 0.42 |
| 1:E:305:MET:O | 1:E:306:TYR:O | 2.38 | 0.42 |
| 1:E:138:ALA:CB | 1:E:163:VAL:CG1 | 2.97 | 0.42 |
| 1:D:105:LEU:CD2 | 1:D:132:MET:HB2 | 2.45 | 0.42 |
| 1:D:209:VAL:C | 1:D:212:ILE:HG12 | 2.39 | 0.42 |
| 1:H:105:LEU:HD22 | 1:H:105:LEU:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:230:ALA:O | 1:D:233:SER:O | 2.37 | 0.42 |
| 1:D:95:ARG:HB2 | 1:D:95:ARG:CZ | 2.50 | 0.42 |
| 1:E:292:ASP:O | 1:E:296:ASN:HB2 | 2.20 | 0.42 |
| 1:E:147:ARG:HH22 | 1:E:330:ILE:HD12 | 1.85 | 0.42 |
| 1:E:300:SER:HA | 1:E:335:ARG:HB2 | 2.02 | 0.42 |
| 1:E:147:ARG:NH2 | 1:E:330:ILE:CD1 | 2.82 | 0.42 |
| 1:F:16:LEU:HD11 | 2:F:401:ADP:H5'2 | 2.02 | 0.42 |
| 1:F:147:ARG:NH2 | 1:F:330:ILE:CD1 | 2.82 | 0.42 |
| 1:F:347:ALA:HA | 1:F:356:TRP:HZ2 | 1.85 | 0.42 |
| 1:G:305:MET:O | 1:G:306:TYR:O | 2.38 | 0.42 |
| 1:G:111:ASN:CG | 1:G:112:PRO:CD | 2.88 | 0.42 |
| 1:G:358:THR:OG1 | 1:G:359:LYS:N | 2.53 | 0.42 |
| 1:E:22:ALA:HB1 | 1:E:348:SER:HB2 | 2.02 | 0.42 |
| 1:F:70:PRO:HG3 | 1:F:85:ILE:CD1 | 2.49 | 0.42 |
| 1:H:292:ASP:O | 1:H:296:ASN:HB2 | 2.19 | 0.42 |
| 1:G:13:GLY:O | 1:G:14:SER:OG | 2.33 | 0.42 |
| 1:G:147:ARG:HH22 | 1:G:330:ILE:HD12 | 1.82 | 0.42 |
| 1:G:332:PRO:HA | 1:G:333:PRO:HD3 | 1.87 | 0.42 |
| 1:G:280:ASN:OD1 | 1:G:281:SER:N | 2.53 | 0.42 |
| 1:E:149:THR:HG23 | 1:E:166:TYR:HA | 2.02 | 0.42 |
| 1:H:200:PHE:HA | 1:H:205:GLU:OE1 | 2.20 | 0.42 |
| 1:H:36:GLY:HA3 | 1:H:66:THR:O | 2.20 | 0.42 |
| 1:H:54:VAL:HG11 | 1:H:88:HIS:HB3 | 2.02 | 0.42 |
| 1:H:22:ALA:O | 1:H:23:GLY:C | 2.58 | 0.42 |
| 1:D:214:GLU:HG2 | 2:D:401:ADP:C2 | 2.55 | 0.42 |
| 1:H:361:GLU:O | 1:H:364:GLU:HG2 | 2.20 | 0.42 |
| 1:H:286:ASP:OD2 | 1:H:289:ILE:HG22 | 2.20 | 0.42 |
| 1:F:43:VAL:CG1 | 1:F:44:MET:N | 2.81 | 0.42 |
| 1:F:61:LYS:HB3 | 1:F:64:ILE:HD11 | 2.02 | 0.42 |
| 1:D:166:TYR:HD2 | 1:F:64:ILE:HG21 | 1.83 | 0.42 |
| 1:G:11:ASP:O | 1:G:106:THR:HB | 2.20 | 0.42 |
| 1:E:216:LEU:HD21 | 1:E:240:TYR:HB2 | 2.02 | 0.42 |
| 1:E:117:GLU:OE2 | 1:E:371:HIS:HB2 | 2.20 | 0.42 |
| 1:E:238:LYS:HZ2 | 1:E:254:ARG:HH22 | 1.63 | 0.42 |
| 1:G:286:ASP:OD2 | 1:G:289:ILE:HG22 | 2.20 | 0.42 |
| 1:H:143:TYR:CE2 | 1:H:346:LEU:HB2 | 2.54 | 0.42 |
| 1:D:91:TYR:O | 1:D:92:ASN:HB2 | 2.17 | 0.42 |
| 1:F:318:THR:OG1 | 1:F:327:ILE:HD11 | 2.20 | 0.42 |
| 1:H:146:GLY:O | 1:H:147:ARG:HB2 | 2.20 | 0.41 |
| 1:H:329:ILE:N | 1:H:329:ILE:CD1 | 2.72 | 0.41 |
| 1:E:280:ASN:OD1 | 1:E:281:SER:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:237:GLU:O | 1:G:250:ILE:CD1 | 2.68 | 0.41 |
| 1:D:76:ILE:CG2 | 1:D:79:TRP:H | 2.33 | 0.41 |
| 1:G:374:CYS:C | 1:G:375:PHE:HD2 | 2.24 | 0.41 |
| 1:D:238:LYS:HZ2 | 1:D:254:ARG:HH12 | 1.67 | 0.41 |
| 1:H:305:MET:O | 1:H:306:TYR:O | 2.38 | 0.41 |
| 1:H:87:HIS:CE1 | 1:H:91:TYR:HE2 | 2.37 | 0.41 |
| 1:E:70:PRO:HG3 | 1:E:85:ILE:CD1 | 2.50 | 0.41 |
| 1:G:188:TYR:O | 1:G:192:ILE:HG23 | 2.19 | 0.41 |
| 1:F:188:TYR:O | 1:F:192:ILE:HG23 | 2.20 | 0.41 |
| 1:G:151:ILE:HG12 | 1:G:164:PRO:HA | 2.01 | 0.41 |
| 1:F:76:ILE:CG2 | 1:F:79:TRP:H | 2.34 | 0.41 |
| 1:G:216:LEU:HD21 | 1:G:240:TYR:HB2 | 2.03 | 0.41 |
| 1:E:129:VAL:HG21 | 1:E:132:MET:CG | 2.39 | 0.41 |
| 1:H:121:GLN:HG3 | 1:H:362:TYR:OH | 2.20 | 0.41 |
| 1:F:22:ALA:HB1 | 1:F:348:SER:CB | 2.49 | 0.41 |
| 1:D:229:THR:HG23 | 1:D:230:ALA:H | 1.85 | 0.41 |
| 1:D:160:THR:OG1 | 1:D:178:LEU:HD13 | 2.21 | 0.41 |
| 1:E:245:GLY:O | 1:E:246:GLN:HG3 | 2.21 | 0.41 |
| 1:H:104:LEU:HD12 | 1:H:133:TYR:O | 2.20 | 0.41 |
| 1:H:325:MET:CE | 1:H:326:LYS:H | 2.33 | 0.41 |
| 1:H:140:LEU:N | 1:H:140:LEU:CD1 | 2.84 | 0.41 |
| 1:G:309:ILE:HD13 | 1:G:309:ILE:HA | 1.82 | 0.41 |
| 1:G:250:ILE:HD12 | 1:G:250:ILE:H | 1.85 | 0.41 |
| 1:H:358:THR:OG1 | 1:H:359:LYS:N | 2.52 | 0.41 |
| 1:D:104:LEU:HD12 | 1:D:133:TYR:O | 2.20 | 0.41 |
| 1:F:18:LYS:CD | 1:F:30:VAL:HG13 | 2.51 | 0.41 |
| 1:E:31:PHE:CD1 | 1:E:31:PHE:N | 2.88 | 0.41 |
| 1:D:249:THR:HG23 | 1:D:249:THR:O | 2.21 | 0.41 |
| 1:E:163:VAL:CG2 | 1:E:165:ILE:HD11 | 2.51 | 0.41 |
| 1:F:267:ILE:CG2 | 1:F:268:GLY:N | 2.83 | 0.41 |
| 1:F:352:PHE:CZ | 1:H:47:MET:CE | 3.03 | 0.41 |
| 1:G:277:THR:O | 1:G:280:ASN:ND2 | 2.54 | 0.41 |
| 1:D:200:PHE:O | 1:D:201:VAL:HG13 | 2.21 | 0.41 |
| 1:G:16:LEU:HD11 | 2:G:401:ADP:H5'2 | 2.02 | 0.41 |
| 1:D:216:LEU:HD21 | 1:D:240:TYR:HB2 | 2.02 | 0.41 |
| 1:D:250:ILE:HD12 | 1:D:250:ILE:H | 1.86 | 0.41 |
| 1:D:257:CYS:SG | 1:D:258:PRO:N | 2.92 | 0.41 |
| 1:H:315:LYS:HB2 | 1:H:315:LYS:HZ1 | 1.85 | 0.41 |
| 1:E:295:ALA:HB1 | 1:E:328:LYS:NZ | 2.35 | 0.41 |
| 1:H:279:TYR:O | 1:H:282:ILE:HG22 | 2.21 | 0.41 |
| 1:H:309:ILE:HA | 1:H:309:ILE:HD13 | 1.80 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:TYR:O | 1:D:169:TYR:O | 2.39 | 0.41 |
| 1:G:174:ALA:CB | 1:G:281:SER:HA | 2.50 | 0.41 |
| 1:H:43:VAL:CG1 | 1:H:44:MET:N | 2.81 | 0.41 |
| 1:D:53:TYR:O | 1:D:54:VAL:CG2 | 2.69 | 0.41 |
| 1:G:206:ARG:HA | 1:G:209:VAL:HG12 | 2.03 | 0.41 |
| 1:D:111:ASN:CG | 1:D:112:PRO:CD | 2.89 | 0.41 |
| 1:D:124:PHE:CZ | 1:D:359:LYS:HA | 2.55 | 0.41 |
| 1:H:79:TRP:HH2 | 1:H:119:MET:HB2 | 1.85 | 0.41 |
| 1:D:150:GLY:HA3 | 1:D:296:ASN:HB3 | 2.03 | 0.41 |
| 1:G:163:VAL:CG2 | 1:G:165:ILE:HD11 | 2.51 | 0.41 |
| 1:D:64:ILE:HG13 | 1:D:64:ILE:H | 1.56 | 0.41 |
| 1:H:200:PHE:O | 1:H:201:VAL:HG13 | 2.21 | 0.41 |
| 1:G:238:LYS:HZ2 | 1:G:254:ARG:NH2 | 2.19 | 0.41 |
| 1:H:280:ASN:OD1 | 1:H:281:SER:N | 2.53 | 0.41 |
| 1:E:286:ASP:OD2 | 1:E:289:ILE:HG22 | 2.21 | 0.41 |
| 1:D:325:MET:SD | 1:F:244:ASP:OD2 | 2.79 | 0.41 |
| 1:D:279:TYR:O | 1:D:282:ILE:HG22 | 2.21 | 0.41 |
| 1:H:18:LYS:CD | 1:H:30:VAL:HG13 | 2.50 | 0.41 |
| 1:D:146:GLY:O | 1:D:147:ARG:HB2 | 2.21 | 0.41 |
| 1:E:173:HIS:NE2 | 1:F:267:ILE:O | 2.54 | 0.41 |
| 1:E:242:LEU:HG | 1:E:246:GLN:C | 2.40 | 0.41 |
| 1:H:346:LEU:HD11 | 1:H:355:MET:CE | 2.51 | 0.41 |
| 1:D:312:ARG:HA | 1:D:315:LYS:HE3 | 2.02 | 0.41 |
| 1:D:323:SER:C | 1:D:324:THR:HG23 | 2.41 | 0.41 |
| 1:G:138:ALA:HB1 | 1:G:163:VAL:HG12 | 2.03 | 0.41 |
| 1:E:352:PHE:HZ | 1:G:47:MET:CE | 2.34 | 0.41 |
| 1:D:36:GLY:HA3 | 1:D:66:THR:O | 2.20 | 0.41 |
| 1:E:124:PHE:CZ | 1:E:359:LYS:HA | 2.56 | 0.41 |
| 1:H:213:LYS:O | 1:H:217:CYS:HB3 | 2.20 | 0.41 |
| 1:E:238:LYS:CG | 1:E:239:SER:N | 2.83 | 0.41 |
| 1:D:16:LEU:HD11 | 2:D:401:ADP:H5'2 | 2.03 | 0.41 |
| 1:D:206:ARG:HA | 1:D:209:VAL:HG12 | 2.03 | 0.41 |
| 1:D:326:LYS:HE3 | 1:D:327:ILE:N | 2.35 | 0.41 |
| 1:G:326:LYS:HE3 | 1:G:327:ILE:N | 2.36 | 0.41 |
| 1:H:107:GLU:C | 1:H:137:GLN:HE21 | 2.24 | 0.41 |
| 1:H:154:ASP:CG | 1:H:154:ASP:O | 2.57 | 0.41 |
| 1:E:102:PRO:CB | 1:E:131:ALA:HB3 | 2.46 | 0.41 |
| 1:G:36:GLY:HA3 | 1:G:66:THR:O | 2.21 | 0.41 |
| 1:G:214:GLU:HG2 | 2:G:401:ADP:C2 | 2.56 | 0.41 |
| 1:G:76:ILE:CG2 | 1:G:79:TRP:H | 2.34 | 0.41 |
| 1:E:359:LYS:O | 1:E:360:GLN:CB | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:374:CYS:C | 1:D:375:PHE:HD2 | 2.24 | 0.41 |
| 1:G:143:TYR:CE2 | 1:G:346:LEU:HB2 | 2.56 | 0.41 |
| 1:H:216:LEU:HD21 | 1:H:240:TYR:HB2 | 2.03 | 0.41 |
| 1:F:121:GLN:HG3 | 1:F:362:TYR:OH | 2.21 | 0.41 |
| 1:E:242:LEU:CD2 | 1:E:246:GLN:HB2 | 2.42 | 0.41 |
| 1:D:286:ASP:OD2 | 1:D:289:ILE:HG22 | 2.21 | 0.41 |
| 1:F:325:MET:SD | 1:H:244:ASP:OD2 | 2.79 | 0.41 |
| 1:E:323:SER:O | 1:E:324:THR:OG1 | 2.24 | 0.41 |
| 1:G:108:ALA:HA | 1:G:109:PRO:HD3 | 1.93 | 0.41 |
| 1:E:6:THR:O | 1:E:102:PRO:HD2 | 2.21 | 0.41 |
| 1:F:237:GLU:O | 1:F:250:ILE:CD1 | 2.69 | 0.41 |
| 1:F:146:GLY:O | 1:F:147:ARG:HB2 | 2.21 | 0.41 |
| 1:F:6:THR:O | 1:F:102:PRO:HD2 | 2.21 | 0.41 |
| 1:G:118:LYS:O | 1:G:122:ILE:HG12 | 2.21 | 0.41 |
| 1:G:8:LEU:N | 1:G:102:PRO:O | 2.47 | 0.41 |
| 1:H:277:THR:HA | 1:H:280:ASN:HD22 | 1.84 | 0.41 |
| 1:D:286:ASP:OD2 | 1:D:288:ASP:HB3 | 2.21 | 0.41 |
| 1:H:286:ASP:CB | 1:H:289:ILE:HG22 | 2.46 | 0.41 |
| 1:D:325:MET:HE2 | 1:D:326:LYS:H | 1.85 | 0.41 |
| 1:F:325:MET:HE2 | 1:F:326:LYS:H | 1.85 | 0.41 |
| 1:E:95:ARG:HB2 | 1:E:95:ARG:CZ | 2.50 | 0.41 |
| 1:E:55:GLY:O | 1:E:58:ALA:N | 2.54 | 0.41 |
| 1:D:147:ARG:NH2 | 1:D:330:ILE:CD1 | 2.82 | 0.40 |
| 1:F:222:ASP:OD2 | 1:F:225:ASN:HB3 | 2.21 | 0.40 |
| 1:G:43:VAL:CG1 | 1:G:44:MET:N | 2.85 | 0.40 |
| 1:F:8:LEU:N | 1:F:102:PRO:O | 2.47 | 0.40 |
| 1:G:160:THR:CG2 | 1:G:178:LEU:HD13 | 2.52 | 0.40 |
| 1:H:53:TYR:C | 1:H:54:VAL:HG22 | 2.41 | 0.40 |
| 1:E:121:GLN:HG3 | 1:E:362:TYR:OH | 2.21 | 0.40 |
| 1:D:113:LYS:HG2 | 1:D:117:GLU:OE2 | 2.20 | 0.40 |
| 1:H:118:LYS:O | 1:H:122:ILE:HG12 | 2.20 | 0.40 |
| 1:D:238:LYS:CG | 1:D:239:SER:N | 2.85 | 0.40 |
| 1:G:229:THR:HG23 | 1:G:230:ALA:H | 1.86 | 0.40 |
| 1:E:8:LEU:HD12 | 1:E:21:PHE:HA | 2.02 | 0.40 |
| 1:D:221:LEU:CD1 | 1:D:221:LEU:H | 2.26 | 0.40 |
| 1:F:29:ALA:HB3 | 1:F:93:GLU:HB3 | 2.03 | 0.40 |
| 1:E:188:TYR:O | 1:E:192:ILE:HG23 | 2.20 | 0.40 |
| 1:H:290:ARG:HB3 | 1:H:290:ARG:HE | 1.69 | 0.40 |
| 1:F:37:ARG:HB3 | 1:F:38:PRO:HD2 | 2.03 | 0.40 |
| 1:H:172:PRO:HA | 1:H:175:ILE:CD1 | 2.50 | 0.40 |
| 1:D:169:TYR:CD2 | 1:F:40:HIS:O | 2.75 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:18:LYS:CD | 1:G:30:VAL:HG13 | 2.52 | 0.40 |
| 1:G:334:GLU:C | 1:G:335:ARG:O | 2.59 | 0.40 |
| 1:F:206:ARG:HA | 1:F:209:VAL:HG12 | 2.03 | 0.40 |
| 1:F:250:ILE:H | 1:F:250:ILE:CD1 | 2.33 | 0.40 |
| 1:D:66:THR:HA | 1:D:203:THR:OG1 | 2.21 | 0.40 |
| 1:F:66:THR:HA | 1:F:203:THR:OG1 | 2.21 | 0.40 |
| 1:H:123:MET:HA | 1:H:127:PHE:CD2 | 2.54 | 0.40 |
| 1:G:369:ILE:CG2 | 1:G:370:VAL:N | 2.83 | 0.40 |
| 1:H:237:GLU:O | 1:H:250:ILE:CD1 | 2.69 | 0.40 |
| 1:H:289:ILE:C | 1:H:289:ILE:HD13 | 2.41 | 0.40 |
| 1:H:70:PRO:HG3 | 1:H:85:ILE:CD1 | 2.51 | 0.40 |
| 1:G:54:VAL:HG11 | 1:G:88:HIS:HB3 | 2.03 | 0.40 |
| 1:E:361:GLU:O | 1:E:364:GLU:HG2 | 2.21 | 0.40 |
| 1:G:95:ARG:HB2 | 1:G:95:ARG:CZ | 2.51 | 0.40 |
| 1:F:263:GLN:C | 1:F:265:SER:N | 2.75 | 0.40 |
| 1:F:229:THR:HG23 | 1:F:230:ALA:H | 1.87 | 0.40 |
| 1:F:273:GLY:C | 1:F:277:THR:HG23 | 2.41 | 0.40 |
| 1:F:213:LYS:HD2 | 1:F:306:TYR:OH | 2.22 | 0.40 |
| 1:F:110:LEU:HD12 | 1:F:177:ARG:CG | 2.51 | 0.40 |
| 1:H:374:CYS:C | 1:H:375:PHE:HD2 | 2.25 | 0.40 |
| 1:D:308:GLY:HA2 | 1:D:311:ASP:OD2 | 2.22 | 0.40 |
| 1:F:113:LYS:HG2 | 1:F:117:GLU:OE2 | 2.21 | 0.40 |
| 1:D:277:THR:O | 1:D:280:ASN:ND2 | 2.55 | 0.40 |
| 1:D:11:ASP:O | 1:D:106:THR:HB | 2.20 | 0.40 |
| 1:D:18:LYS:CD | 1:D:30:VAL:HG13 | 2.51 | 0.40 |
| 1:D:326:LYS:HG3 | 1:D:328:LYS:NZ | 2.37 | 0.40 |
| 1:F:89:THR:O | 1:F:94:LEU:HG | 2.21 | 0.40 |
| 1:F:329:ILE:N | 1:F:329:ILE:CD1 | 2.76 | 0.40 |
| 1:F:123:MET:HA | 1:F:127:PHE:CD2 | 2.54 | 0.40 |
| 1:E:223:PHE:O | 1:E:226:GLU:HB2 | 2.22 | 0.40 |
| 1:G:22:ALA:HB1 | 1:G:348:SER:CB | 2.51 | 0.40 |
| 1:F:286:ASP:OD2 | 1:F:289:ILE:HG22 | 2.22 | 0.40 |
| 1:H:29:ALA:HB3 | 1:H:93:GLU:HB3 | 2.03 | 0.40 |
| 1:E:326:LYS:HG3 | 1:E:328:LYS:NZ | 2.37 | 0.40 |
| 1:E:224:GLU:C | 1:E:224:GLU:CD | 2.80 | 0.40 |
| 1:F:336:LYS:HE2 | 1:F:337:TYR:CZ | 2.55 | 0.40 |
| 1:D:31:PHE:N | 1:D:31:PHE:CD1 | 2.90 | 0.40 |
| 1:H:108:ALA:HA | 1:H:109:PRO:HD3 | 1.93 | 0.40 |
| 1:H:110:LEU:HD11 | 1:H:175:ILE:CB | 2.50 | 0.40 |
| 1:D:139:VAL:CG2 | 1:F:43:VAL:HG11 | 2.51 | 0.40 |
| 1:D:147:ARG:HH22 | 1:D:330:ILE:HD12 | 1.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:142:LEU:HD21 | 1:E:165:ILE:HB | 2.02 | 0.40 |
| 1:F:79:TRP:HH2 | 1:F:119:MET:HB2 | 1.86 | 0.40 |
| 1:H:250:ILE:H | 1:H:250:ILE:HD12 | 1.87 | 0.40 |
| 1:H:124:PHE:CZ | 1:H:359:LYS:HA | 2.56 | 0.40 |
| 1:F:124:PHE:CZ | 1:F:359:LYS:HA | 2.56 | 0.40 |
| 1:F:374:CYS:C | 1:F:375:PHE:HD2 | 2.24 | 0.40 |
| 1:H:257:CYS:SG | 1:H:258:PRO:N | 2.94 | 0.40 |
| 1:F:326:LYS:HE3 | 1:F:327:ILE:N | 2.35 | 0.40 |
| 1:H:353:GLN:NE2 | 1:H:353:GLN:N | 2.70 | 0.40 |
| 1:H:55:GLY:O | 1:H:58:ALA:N | 2.54 | 0.40 |
| 1:F:31:PHE:HB2 | 1:F:56:ASP:OD1 | 2.21 | 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 | D | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 | 26 |
| 1 | E | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 | 26 |
| 1 | F | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 | 26 |
| 1 | G | 373/377 (99%) | 327 (88%) | 24 (6%) | 22 (6%) | 2 | 27 |
| 1 | H | 373/377 (99%) | 327 (88%) | 24 (6%) | 22 (6%) | 2 | 27 |
| All | All | 1865/1885 (99%) | 1632 (88%) | 120 (6%) | 113 (6%) | 4 | 26 |

All (113) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 92 | ASN |
| 1 | D | 144 | ALA |
| 1 | D | 223 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 235 | SER |
| 1 | D | 351 | THR |
| 1 | E | 92 | ASN |
| 1 | E | 144 | ALA |
| 1 | E | 223 | PHE |
| 1 | E | 235 | SER |
| 1 | E | 351 | THR |
| 1 | F | 92 | ASN |
| 1 | F | 144 | ALA |
| 1 | F | 223 | PHE |
| 1 | F | 235 | SER |
| 1 | F | 251 | GLY |
| 1 | F | 351 | THR |
| 1 | G | 92 | ASN |
| 1 | G | 144 | ALA |
| 1 | G | 223 | PHE |
| 1 | G | 235 | SER |
| 1 | G | 351 | THR |
| 1 | H | 92 | ASN |
| 1 | H | 144 | ALA |
| 1 | H | 223 | PHE |
| 1 | H | 235 | SER |
| 1 | H | 351 | THR |
| 1 | D | 22 | ALA |
| 1 | D | 23 | GLY |
| 1 | D | 35 | VAL |
| 1 | D | 201 | VAL |
| 1 | D | 211 | ASP |
| 1 | D | 251 | GLY |
| 1 | D | 303 | THR |
| 1 | D | 335 | ARG |
| 1 | D | 350 | SER |
| 1 | E | 14 | SER |
| 1 | E | 22 | ALA |
| 1 | E | 23 | GLY |
| 1 | E | 35 | VAL |
| 1 | E | 201 | VAL |
| 1 | E | 211 | ASP |
| 1 | E | 251 | GLY |
| 1 | E | 303 | THR |
| 1 | E | 350 | SER |
| 1 | F | 14 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 22 | ALA |
| 1 | F | 23 | GLY |
| 1 | F | 35 | VAL |
| 1 | F | 201 | VAL |
| 1 | F | 211 | ASP |
| 1 | F | 303 | THR |
| 1 | F | 335 | ARG |
| 1 | F | 350 | SER |
| 1 | G | 22 | ALA |
| 1 | G | 23 | GLY |
| 1 | G | 35 | VAL |
| 1 | G | 201 | VAL |
| 1 | G | 211 | ASP |
| 1 | G | 251 | GLY |
| 1 | G | 303 | THR |
| 1 | G | 350 | SER |
| 1 | H | 22 | ALA |
| 1 | H | 23 | GLY |
| 1 | H | 35 | VAL |
| 1 | H | 201 | VAL |
| 1 | H | 211 | ASP |
| 1 | H | 251 | GLY |
| 1 | H | 303 | THR |
| 1 | H | 335 | ARG |
| 1 | H | 350 | SER |
| 1 | D | 14 | SER |
| 1 | D | 79 | TRP |
| 1 | E | 79 | TRP |
| 1 | E | 335 | ARG |
| 1 | F | 79 | TRP |
| 1 | G | 14 | SER |
| 1 | G | 335 | ARG |
| 1 | H | 14 | SER |
| 1 | H | 79 | TRP |
| 1 | H | 360 | GLN |
| 1 | D | 360 | GLN |
| 1 | F | 26 | ALA |
| 1 | F | 360 | GLN |
| 1 | G | 26 | ALA |
| 1 | G | 79 | TRP |
| 1 | G | 360 | GLN |
| 1 | D | 26 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 264 | PRO |
| 1 | E | 26 | ALA |
| 1 | E | 217 | CYS |
| 1 | E | 243 | PRO |
| 1 | E | 264 | PRO |
| 1 | E | 360 | GLN |
| 1 | F | 264 | PRO |
| 1 | G | 243 | PRO |
| 1 | G | 264 | PRO |
| 1 | H | 26 | ALA |
| 1 | H | 243 | PRO |
| 1 | H | 264 | PRO |
| 1 | D | 243 | PRO |
| 1 | D | 306 | TYR |
| 1 | E | 306 | TYR |
| 1 | F | 306 | TYR |
| 1 | G | 306 | TYR |
| 1 | H | 306 | TYR |
| 1 | G | 330 | ILE |
| 1 | H | 330 | ILE |
| 1 | D | 158 | GLY |
| 1 | D | 330 | ILE |
| 1 | F | 158 | GLY |
| 1 | F | 330 | ILE |
| 1 | E | 330 | ILE |
| 1 | F | 243 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | D | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 | 29 |
| 1 | E | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 | 29 |
| 1 | F | 318/320 (99%) | 274 (86%) | 44 (14%) | 4 | 28 |
| 1 | G | 318/320 (99%) | 274 (86%) | 44 (14%) | 4 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | H | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 | 29 |
| All | All | 1590/1600 (99%) | 1373 (86%) | 217 (14%) | 9 | 29 |

All (217) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 3 | ASP |
| 1 | D | 10 | CYS |
| 1 | D | 31 | PHE |
| 1 | D | 45 | VAL |
| 1 | D | 49 | GLN |
| 1 | D | 66 | THR |
| 1 | D | 79 | TRP |
| 1 | D | 105 | LEU |
| 1 | D | 106 | THR |
| 1 | D | 118 | LYS |
| 1 | D | 134 | VAL |
| 1 | D | 136 | ILE |
| 1 | D | 147 | ARG |
| 1 | D | 160 | THR |
| 1 | D | 171 | LEU |
| 1 | D | 176 | MET |
| 1 | D | 178 | LEU |
| 1 | D | 201 | VAL |
| 1 | D | 202 | THR |
| 1 | D | 216 | LEU |
| 1 | D | 217 | CYS |
| 1 | D | 227 | MET |
| 1 | D | 236 | LEU |
| 1 | D | 238 | LYS |
| 1 | D | 242 | LEU |
| 1 | D | 250 | ILE |
| 1 | D | 253 | GLU |
| 1 | D | 257 | CYS |
| 1 | D | 265 | SER |
| 1 | D | 267 | ILE |
| 1 | D | 289 | ILE |
| 1 | D | 306 | TYR |
| 1 | D | 313 | MET |
| 1 | D | 320 | LEU |
| 1 | D | 326 | LYS |
| 1 | D | 327 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 329 | ILE |
| 1 | D | 336 | LYS |
| 1 | D | 349 | LEU |
| 1 | D | 351 | THR |
| 1 | D | 361 | GLU |
| 1 | D | 371 | HIS |
| 1 | D | 373 | LYS |
| 1 | E | 3 | ASP |
| 1 | E | 10 | CYS |
| 1 | E | 31 | PHE |
| 1 | E | 45 | VAL |
| 1 | E | 49 | GLN |
| 1 | E | 66 | THR |
| 1 | E | 79 | TRP |
| 1 | E | 105 | LEU |
| 1 | E | 106 | THR |
| 1 | E | 118 | LYS |
| 1 | E | 134 | VAL |
| 1 | E | 136 | ILE |
| 1 | E | 147 | ARG |
| 1 | E | 160 | THR |
| 1 | E | 171 | LEU |
| 1 | E | 176 | MET |
| 1 | E | 178 | LEU |
| 1 | E | 201 | VAL |
| 1 | E | 202 | THR |
| 1 | E | 216 | LEU |
| 1 | E | 217 | CYS |
| 1 | E | 227 | MET |
| 1 | E | 236 | LEU |
| 1 | E | 238 | LYS |
| 1 | E | 242 | LEU |
| 1 | E | 250 | ILE |
| 1 | E | 253 | GLU |
| 1 | E | 257 | CYS |
| 1 | E | 265 | SER |
| 1 | E | 267 | ILE |
| 1 | E | 289 | ILE |
| 1 | E | 306 | TYR |
| 1 | E | 313 | MET |
| 1 | E | 320 | LEU |
| 1 | E | 326 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 327 | ILE |
| 1 | E | 329 | ILE |
| 1 | E | 336 | LYS |
| 1 | E | 349 | LEU |
| 1 | E | 351 | THR |
| 1 | E | 361 | GLU |
| 1 | E | 371 | HIS |
| 1 | E | 373 | LYS |
| 1 | F | 3 | ASP |
| 1 | F | 10 | CYS |
| 1 | F | 31 | PHE |
| 1 | F | 45 | VAL |
| 1 | F | 49 | GLN |
| 1 | F | 66 | THR |
| 1 | F | 79 | TRP |
| 1 | F | 105 | LEU |
| 1 | F | 106 | THR |
| 1 | F | 118 | LYS |
| 1 | F | 134 | VAL |
| 1 | F | 136 | ILE |
| 1 | F | 147 | ARG |
| 1 | F | 160 | THR |
| 1 | F | 171 | LEU |
| 1 | F | 176 | MET |
| 1 | F | 178 | LEU |
| 1 | F | 201 | VAL |
| 1 | F | 202 | THR |
| 1 | F | 216 | LEU |
| 1 | F | 217 | CYS |
| 1 | F | 227 | MET |
| 1 | F | 236 | LEU |
| 1 | F | 238 | LYS |
| 1 | F | 242 | LEU |
| 1 | F | 250 | ILE |
| 1 | F | 253 | GLU |
| 1 | F | 257 | CYS |
| 1 | F | 259 | GLU |
| 1 | F | 265 | SER |
| 1 | F | 267 | ILE |
| 1 | F | 289 | ILE |
| 1 | F | 306 | TYR |
| 1 | F | 313 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 320 | LEU |
| 1 | F | 326 | LYS |
| 1 | F | 327 | ILE |
| 1 | F | 329 | ILE |
| 1 | F | 336 | LYS |
| 1 | F | 349 | LEU |
| 1 | F | 351 | THR |
| 1 | F | 361 | GLU |
| 1 | F | 371 | HIS |
| 1 | F | 373 | LYS |
| 1 | G | 3 | ASP |
| 1 | G | 5 | THR |
| 1 | G | 10 | CYS |
| 1 | G | 31 | PHE |
| 1 | G | 45 | VAL |
| 1 | G | 49 | GLN |
| 1 | G | 66 | THR |
| 1 | G | 79 | TRP |
| 1 | G | 105 | LEU |
| 1 | G | 106 | THR |
| 1 | G | 118 | LYS |
| 1 | G | 134 | VAL |
| 1 | G | 136 | ILE |
| 1 | G | 147 | ARG |
| 1 | G | 160 | THR |
| 1 | G | 171 | LEU |
| 1 | G | 176 | MET |
| 1 | G | 178 | LEU |
| 1 | G | 201 | VAL |
| 1 | G | 202 | THR |
| 1 | G | 216 | LEU |
| 1 | G | 217 | CYS |
| 1 | G | 227 | MET |
| 1 | G | 236 | LEU |
| 1 | G | 238 | LYS |
| 1 | G | 242 | LEU |
| 1 | G | 250 | ILE |
| 1 | G | 253 | GLU |
| 1 | G | 257 | CYS |
| 1 | G | 265 | SER |
| 1 | G | 267 | ILE |
| 1 | G | 289 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 306 | TYR |
| 1 | G | 313 | MET |
| 1 | G | 320 | LEU |
| 1 | G | 326 | LYS |
| 1 | G | 327 | ILE |
| 1 | G | 329 | ILE |
| 1 | G | 336 | LYS |
| 1 | G | 349 | LEU |
| 1 | G | 351 | THR |
| 1 | G | 361 | GLU |
| 1 | G | 371 | HIS |
| 1 | G | 373 | LYS |
| 1 | H | 3 | ASP |
| 1 | H | 10 | CYS |
| 1 | H | 31 | PHE |
| 1 | H | 45 | VAL |
| 1 | H | 49 | GLN |
| 1 | H | 66 | THR |
| 1 | H | 79 | TRP |
| 1 | H | 105 | LEU |
| 1 | H | 106 | THR |
| 1 | H | 118 | LYS |
| 1 | H | 134 | VAL |
| 1 | H | 136 | ILE |
| 1 | H | 147 | ARG |
| 1 | H | 160 | THR |
| 1 | H | 171 | LEU |
| 1 | H | 176 | MET |
| 1 | H | 178 | LEU |
| 1 | H | 201 | VAL |
| 1 | H | 202 | THR |
| 1 | H | 216 | LEU |
| 1 | H | 217 | CYS |
| 1 | H | 227 | MET |
| 1 | H | 236 | LEU |
| 1 | H | 238 | LYS |
| 1 | H | 242 | LEU |
| 1 | H | 250 | ILE |
| 1 | H | 253 | GLU |
| 1 | H | 257 | CYS |
| 1 | H | 265 | SER |
| 1 | H | 267 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 289 | ILE |
| 1 | H | 306 | TYR |
| 1 | H | 313 | MET |
| 1 | H | 320 | LEU |
| 1 | H | 326 | LYS |
| 1 | H | 327 | ILE |
| 1 | H | 329 | ILE |
| 1 | H | 336 | LYS |
| 1 | H | 349 | LEU |
| 1 | H | 351 | THR |
| 1 | H | 361 | GLU |
| 1 | H | 371 | HIS |
| 1 | H | 373 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 12 | ASN |
| 1 | D | 59 | GLN |
| 1 | D | 78 | ASN |
| 1 | D | 87 | HIS |
| 1 | D | 92 | ASN |
| 1 | D | 115 | ASN |
| 1 | D | 137 | GLN |
| 1 | D | 162 | ASN |
| 1 | D | 263 | GLN |
| 1 | D | 275 | HIS |
| 1 | D | 296 | ASN |
| 1 | D | 353 | GLN |
| 1 | E | 12 | ASN |
| 1 | E | 59 | GLN |
| 1 | E | 78 | ASN |
| 1 | E | 87 | HIS |
| 1 | E | 92 | ASN |
| 1 | E | 115 | ASN |
| 1 | E | 137 | GLN |
| 1 | E | 162 | ASN |
| 1 | E | 263 | GLN |
| 1 | E | 275 | HIS |
| 1 | E | 296 | ASN |
| 1 | E | 353 | GLN |
| 1 | F | 12 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 59 | GLN |
| 1 | F | 78 | ASN |
| 1 | F | 87 | HIS |
| 1 | F | 92 | ASN |
| 1 | F | 115 | ASN |
| 1 | F | 137 | GLN |
| 1 | F | 162 | ASN |
| 1 | F | 263 | GLN |
| 1 | F | 275 | HIS |
| 1 | F | 296 | ASN |
| 1 | F | 353 | GLN |
| 1 | F | 354 | GLN |
| 1 | G | 12 | ASN |
| 1 | G | 59 | GLN |
| 1 | G | 78 | ASN |
| 1 | G | 87 | HIS |
| 1 | G | 92 | ASN |
| 1 | G | 115 | ASN |
| 1 | G | 137 | GLN |
| 1 | G | 162 | ASN |
| 1 | G | 263 | GLN |
| 1 | G | 275 | HIS |
| 1 | G | 296 | ASN |
| 1 | G | 297 | ASN |
| 1 | G | 353 | GLN |
| 1 | H | 12 | ASN |
| 1 | H | 59 | GLN |
| 1 | H | 78 | ASN |
| 1 | H | 87 | HIS |
| 1 | H | 92 | ASN |
| 1 | H | 115 | ASN |
| 1 | H | 137 | GLN |
| 1 | H | 162 | ASN |
| 1 | H | 263 | GLN |
| 1 | H | 275 | HIS |
| 1 | H | 296 | ASN |
| 1 | H | 353 | 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | ADP | D | 401 | 3 | 24,29,29 | 1.36 | 3 (12%) | 23,45,45 | 3.11 | 1 (4%) |
| 2 | ADP | E | 401 | 3 | 24,29,29 | 1.45 | 4 (16%) | 23,45,45 | 2.99 | 1 (4%) |
| 2 | ADP | F | 401 | 3 | 24,29,29 | 1.40 | 6 (25%) | 23,45,45 | 3.17 | 1 (4%) |
| 2 | ADP | G | 401 | 3 | 24,29,29 | 1.53 | 4 (16%) | 23,45,45 | 2.77 | 1 (4%) |
| 2 | ADP | H | 401 | 3 | 24,29,29 | 1.39 | 4 (16%) | 23,45,45 | 3.12 | 1 (4%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | ADP | D | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | E | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | G | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | F | 401 | ADP | C5-N7 | -2.24 | 1.31 | 1.39 |
| 2 | D | 401 | ADP | C5-N7 | -2.20 | 1.31 | 1.39 |
| 2 | H | 401 | ADP | C5-N7 | -2.19 | 1.31 | 1.39 |
| 2 | F | 401 | ADP | PB-O2B | 2.00 | 1.61 | 1.54 |
| 2 | G | 401 | ADP | C5'-C4' | 2.07 | 1.58 | 1.51 |
| 2 | F | 401 | ADP | C4-N3 | 2.08 | 1.38 | 1.35 |
| 2 | F | 401 | ADP | C5'-C4' | 2.10 | 1.58 | 1.51 |
| 2 | E | 401 | ADP | C5'-C4' | 2.14 | 1.58 | 1.51 |
| 2 | H | 401 | ADP | C4-N3 | 2.16 | 1.38 | 1.35 |
| 2 | F | 401 | ADP | C2-N3 | 2.51 | 1.36 | 1.32 |
| 2 | H | 401 | ADP | C2-N3 | 2.57 | 1.36 | 1.32 |
| 2 | D | 401 | ADP | O4'-C1' | 2.65 | 1.45 | 1.41 |
| 2 | G | 401 | ADP | O4'-C1' | 2.71 | 1.45 | 1.41 |
| 2 | E | 401 | ADP | C4-N3 | 2.78 | 1.39 | 1.35 |
| 2 | D | 401 | ADP | C2-N3 | 2.81 | 1.37 | 1.32 |
| 2 | E | 401 | ADP | C2-N3 | 2.83 | 1.37 | 1.32 |
| 2 | F | 401 | ADP | O4'-C1' | 2.85 | 1.45 | 1.41 |
| 2 | E | 401 | ADP | O4'-C1' | 2.94 | 1.45 | 1.41 |
| 2 | H | 401 | ADP | O4'-C1' | 3.06 | 1.45 | 1.41 |
| 2 | G | 401 | ADP | C2-N3 | 3.24 | 1.37 | 1.32 |
| 2 | G | 401 | ADP | C4-N3 | 3.38 | 1.40 | 1.35 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 2 | F | 401 | ADP | N3-C2-N1 | -14.64 | 117.37 | 128.87 |
| 2 | D | 401 | ADP | N3-C2-N1 | -14.42 | 117.55 | 128.87 |
| 2 | H | 401 | ADP | N3-C2-N1 | -14.39 | 117.57 | 128.87 |
| 2 | E | 401 | ADP | N3-C2-N1 | -13.78 | 118.05 | 128.87 |
| 2 | G | 401 | ADP | N3-C2-N1 | -12.56 | 119.01 | 128.87 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | D | 401 | ADP | 2 | 0 |
| 2 | E | 401 | ADP | 2 | 0 |
| 2 | F | 401 | ADP | 2 | 0 |
| 2 | G | 401 | ADP | 2 | 0 |
| 2 | H | 401 | ADP | 2 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.