



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:39 am BST

PDB ID : 1FFX
Title : TUBULIN:STATHMIN-LIKE DOMAIN COMPLEX
Authors : Gigant, B.; Martin-Barbey, C.; Knossow, M.
Deposited on : 2000-07-26
Resolution : 3.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

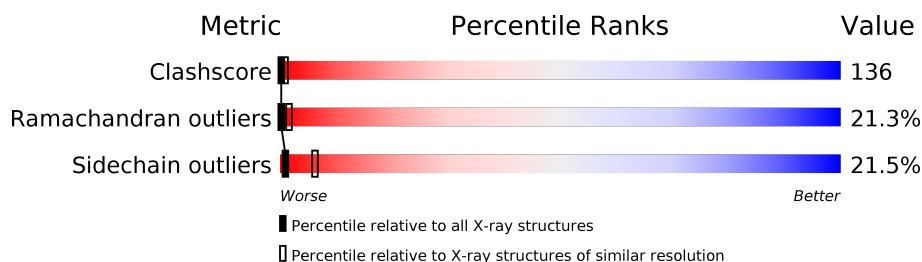
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 1085 (4.22-3.70) |
| Ramachandran outliers | 138981 | 1047 (4.22-3.70) |
| Sidechain outliers | 138945 | 1039 (4.22-3.70) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 451 | <div> <div>9%</div> <div>53%</div> <div>27%</div> <div>• 6%</div> </div> |
| 1 | C | 451 | <div> <div>9%</div> <div>55%</div> <div>25%</div> <div>• 6%</div> </div> |
| 2 | B | 445 | <div> <div>6%</div> <div>57%</div> <div>25%</div> <div>5%</div> <div>8%</div> </div> |
| 2 | D | 445 | <div> <div>6%</div> <div>56%</div> <div>24%</div> <div>6%</div> <div>8%</div> </div> |
| 3 | E | 91 | <div> <div>32%</div> <div>68%</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | GDP | D | 503 | - | - | X | - |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13568 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PROTEIN (TUBULIN).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 423 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3295 | 2082 | 559 | 632 | 22 | | | |
| 1 | C | 423 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3295 | 2082 | 559 | 632 | 22 | | | |

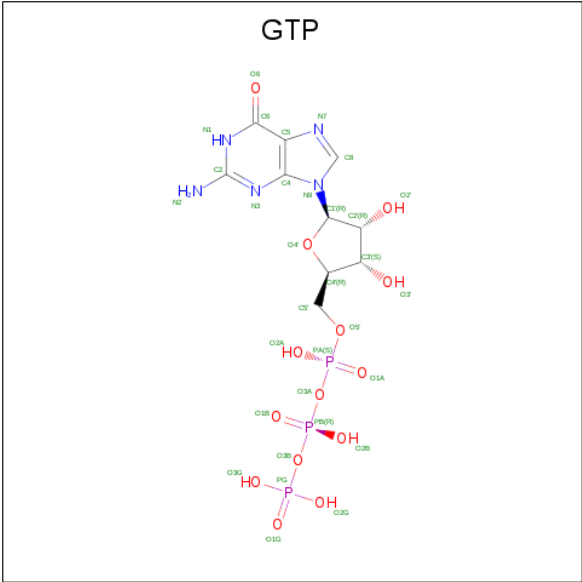
- Molecule 2 is a protein called PROTEIN (TUBULIN).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 410 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3201 | 2014 | 550 | 611 | 26 | | | |
| 2 | D | 410 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3201 | 2014 | 550 | 611 | 26 | | | |

- Molecule 3 is a protein called PROTEIN (STATHMIN-LIKE DOMAIN OF RB3).

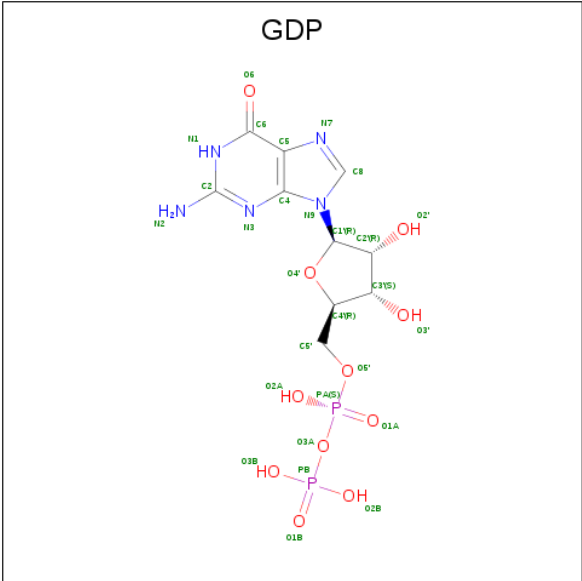
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 3 | E | 91 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 273 | 91 | 92 | | | |

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | | |
| 4 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | | |

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | | |

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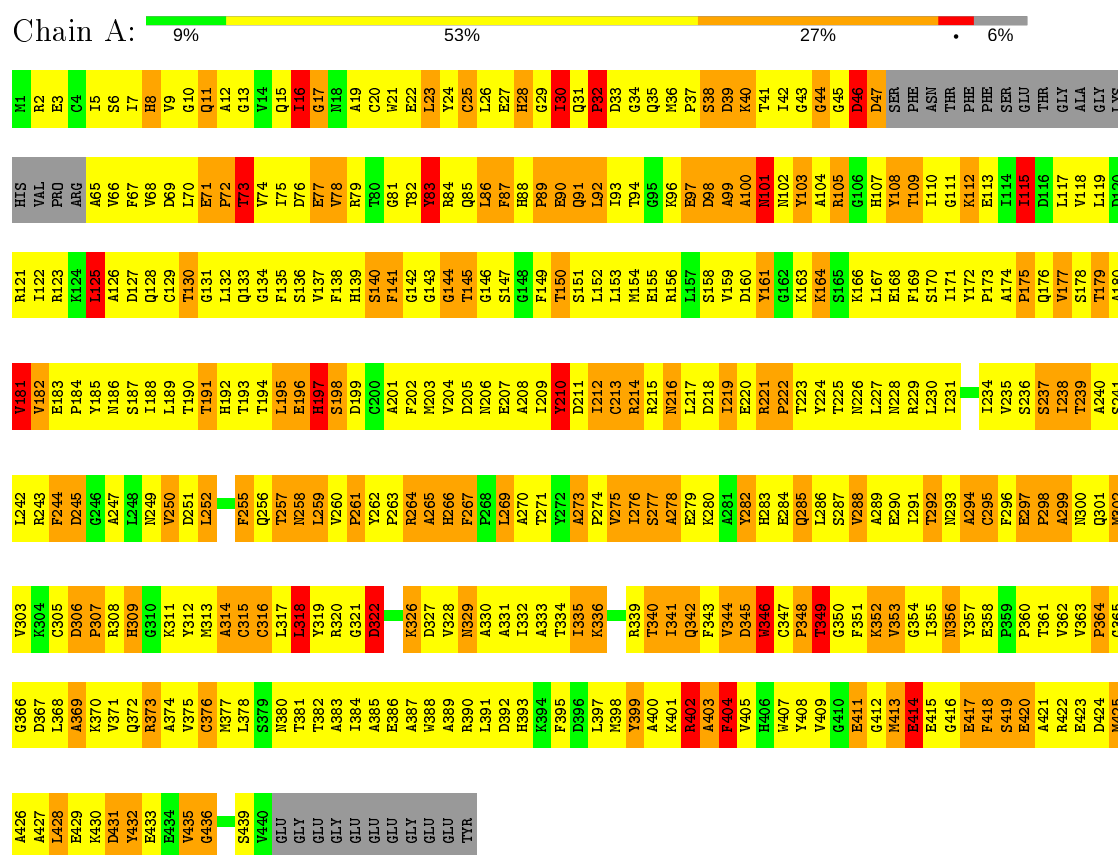
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | | |

3 Residue-property plots

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

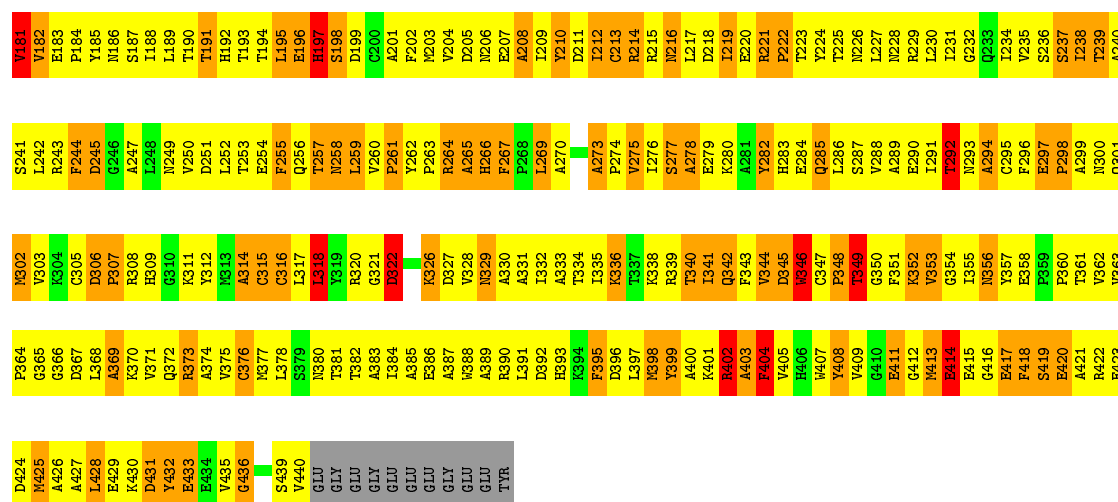
Note EDS was not executed.

• Molecule 1: PROTEIN (TUBULIN)

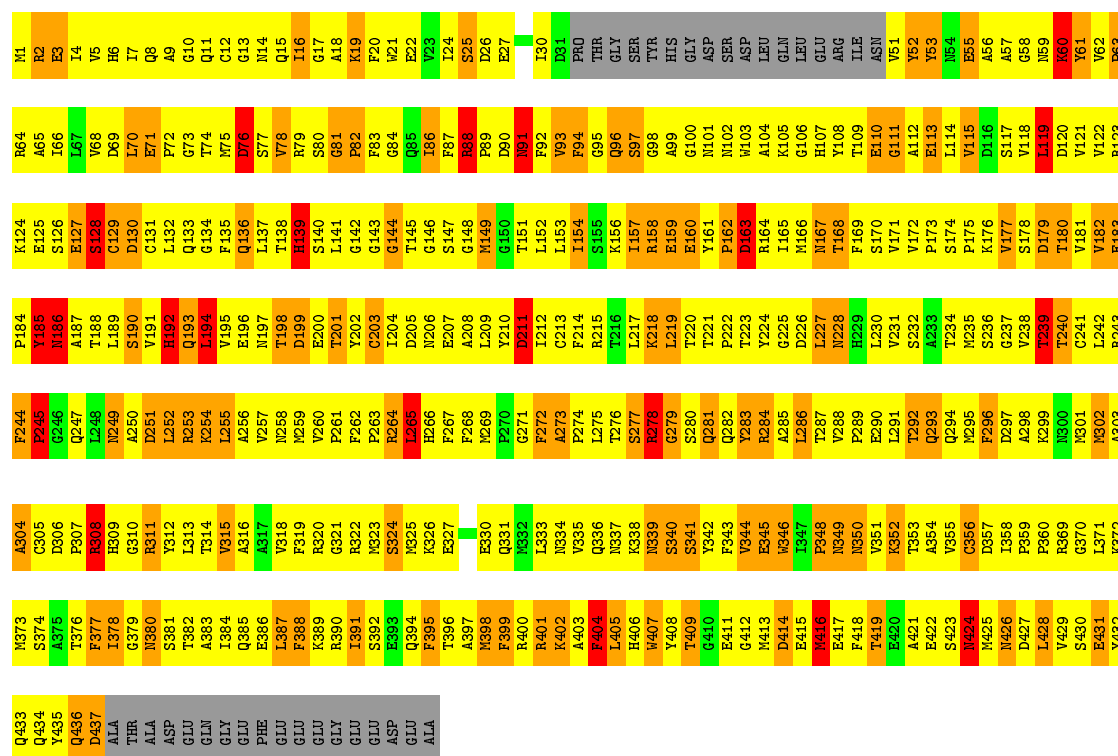


• Molecule 1: PROTEIN (TUBULIN)

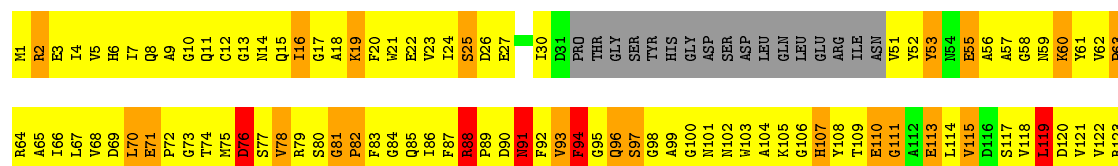




• Molecule 2: PROTEIN (TUBULIN)



• Molecule 2: PROTEIN (TUBULIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | P 65 | Depositor |
| Cell constants a, b, c, α , β , γ | 328.50 Å 328.50 Å 54.40 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 7.00 – 3.95 | Depositor |
| % Data completeness (in resolution range) | 94.3 (7.00-3.95) | Depositor |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | 0.06 | Depositor |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.267 , 0.367 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 13568 | wwPDB-VP |
| Average B, all atoms (Å ²) | 67.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.59 | 0/3367 | 0.86 | 5/4570 (0.1%) |
| 1 | C | 0.56 | 0/3367 | 0.84 | 5/4570 (0.1%) |
| 2 | B | 0.56 | 0/3270 | 0.82 | 1/4428 (0.0%) |
| 2 | D | 0.58 | 0/3270 | 0.84 | 0/4428 |
| All | All | 0.57 | 0/13274 | 0.84 | 11/17996 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 2 |
| 2 | B | 0 | 1 |
| 2 | D | 0 | 1 |
| All | All | 0 | 5 |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 417 | GLU | N-CA-C | -5.93 | 94.99 | 111.00 |
| 1 | C | 318 | LEU | CA-CB-CG | 5.91 | 128.90 | 115.30 |
| 1 | A | 417 | GLU | N-CA-C | -5.77 | 95.43 | 111.00 |
| 1 | A | 318 | LEU | CA-CB-CG | 5.63 | 128.26 | 115.30 |
| 1 | A | 294 | ALA | N-CA-C | -5.38 | 96.46 | 111.00 |
| 1 | C | 294 | ALA | N-CA-C | -5.33 | 96.61 | 111.00 |
| 2 | B | 356 | CYS | N-CA-C | 5.20 | 125.05 | 111.00 |
| 1 | A | 44 | GLY | N-CA-C | -5.15 | 100.23 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 81 | GLY | N-CA-C | -5.13 | 100.27 | 113.10 |
| 1 | C | 43 | GLY | N-CA-C | -5.05 | 100.47 | 113.10 |
| 1 | A | 81 | GLY | N-CA-C | -5.04 | 100.49 | 113.10 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 108 | TYR | Sidechain |
| 2 | B | 61 | TYR | Sidechain |
| 1 | C | 108 | TYR | Sidechain |
| 1 | C | 210 | TYR | Sidechain |
| 2 | D | 312 | TYR | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3295 | 0 | 3202 | 883 | 0 |
| 1 | C | 3295 | 0 | 3202 | 910 | 0 |
| 2 | B | 3201 | 0 | 3091 | 916 | 0 |
| 2 | D | 3201 | 0 | 3091 | 883 | 0 |
| 3 | E | 456 | 0 | 103 | 79 | 0 |
| 4 | A | 32 | 0 | 12 | 4 | 0 |
| 4 | C | 32 | 0 | 12 | 8 | 0 |
| 5 | B | 28 | 0 | 12 | 5 | 0 |
| 5 | D | 28 | 0 | 12 | 9 | 0 |
| All | All | 13568 | 0 | 12737 | 3585 | 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 136.

All (3585) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:175:PRO:HD2 | 2:B:207:GLU:HB2 | 1.23 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:158:ARG:HD3 | 2:D:197:ASN:ND2 | 1.63 | 1.14 |
| 1:A:214:ARG:HH21 | 1:A:220:GLU:HA | 1.04 | 1.14 |
| 2:D:311:ARG:HH21 | 2:D:437:ASP:HB2 | 1.03 | 1.13 |
| 2:B:179:ASP:HA | 1:C:352:LYS:HE2 | 1.20 | 1.12 |
| 1:C:222:PRO:HB2 | 1:C:227:LEU:HD11 | 1.31 | 1.12 |
| 1:C:175:PRO:HD2 | 1:C:207:GLU:HB2 | 1.16 | 1.12 |
| 2:D:175:PRO:HD2 | 2:D:207:GLU:HB2 | 1.26 | 1.12 |
| 1:C:214:ARG:HH21 | 1:C:220:GLU:HA | 0.99 | 1.12 |
| 2:B:92:PHE:HE1 | 2:B:118:VAL:HA | 0.96 | 1.12 |
| 1:C:419:SER:HA | 1:C:422:ARG:HD3 | 1.22 | 1.12 |
| 2:D:278:ARG:HA | 2:D:278:ARG:HH11 | 0.96 | 1.12 |
| 1:A:222:PRO:HB2 | 1:A:227:LEU:HD11 | 1.31 | 1.11 |
| 1:A:102:ASN:HB2 | 1:A:105:ARG:HB2 | 1.31 | 1.11 |
| 1:A:70:LEU:HD12 | 1:A:145:THR:HA | 1.26 | 1.11 |
| 2:B:92:PHE:CE1 | 2:B:118:VAL:HA | 1.85 | 1.10 |
| 2:D:92:PHE:HE1 | 2:D:118:VAL:HA | 0.98 | 1.10 |
| 1:A:419:SER:HA | 1:A:422:ARG:HD3 | 1.20 | 1.09 |
| 1:A:175:PRO:HD2 | 1:A:207:GLU:HB2 | 1.09 | 1.08 |
| 1:C:70:LEU:HD12 | 1:C:145:THR:HA | 1.22 | 1.08 |
| 2:B:311:ARG:HH21 | 2:B:437:ASP:HB2 | 1.04 | 1.08 |
| 1:C:306:ASP:OD1 | 1:C:308:ARG:HB3 | 1.54 | 1.08 |
| 2:D:92:PHE:CE1 | 2:D:118:VAL:HA | 1.88 | 1.08 |
| 1:C:102:ASN:HB2 | 1:C:105:ARG:HB2 | 1.33 | 1.08 |
| 2:B:206:ASN:HD22 | 2:B:227:LEU:HD21 | 1.19 | 1.07 |
| 2:B:213:CYS:HB3 | 2:B:219:LEU:HD12 | 1.32 | 1.07 |
| 2:B:2:ARG:HG3 | 2:B:133:GLN:NE2 | 1.70 | 1.06 |
| 1:C:316:CYS:HB2 | 1:C:352:LYS:HB3 | 1.33 | 1.06 |
| 2:D:192:HIS:HA | 2:D:195:VAL:HG22 | 1.34 | 1.06 |
| 1:A:133:GLN:H | 1:A:164:LYS:HD3 | 1.12 | 1.06 |
| 2:D:240:THR:O | 2:D:243:ARG:HB2 | 1.56 | 1.06 |
| 1:A:383:ALA:O | 1:A:386:GLU:HG2 | 1.55 | 1.05 |
| 2:B:190:SER:HB2 | 2:B:425:MET:HG3 | 1.35 | 1.05 |
| 2:B:191:VAL:HG21 | 2:B:421:ALA:HB1 | 1.38 | 1.05 |
| 2:D:158:ARG:HG3 | 2:D:159:GLU:H | 1.16 | 1.05 |
| 2:D:213:CYS:HB3 | 2:D:219:LEU:HD12 | 1.37 | 1.04 |
| 1:A:306:ASP:OD1 | 1:A:308:ARG:HB3 | 1.57 | 1.04 |
| 1:A:7:ILE:HG22 | 1:A:66:VAL:HB | 1.37 | 1.04 |
| 2:B:178:SER:O | 2:B:182:VAL:HB | 1.57 | 1.04 |
| 1:C:7:ILE:HG22 | 1:C:66:VAL:HB | 1.33 | 1.04 |
| 2:B:192:HIS:HA | 2:B:195:VAL:HG22 | 1.36 | 1.04 |
| 2:B:278:ARG:NH1 | 2:B:278:ARG:HA | 1.72 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:278:ARG:HH11 | 2:B:278:ARG:HA | 0.91 | 1.03 |
| 2:D:2:ARG:HG3 | 2:D:133:GLN:NE2 | 1.73 | 1.03 |
| 2:B:158:ARG:HD3 | 2:B:197:ASN:ND2 | 1.74 | 1.03 |
| 1:A:409:VAL:HA | 1:A:414:GLU:OE1 | 1.57 | 1.02 |
| 2:D:178:SER:O | 2:D:182:VAL:HB | 1.56 | 1.02 |
| 2:B:264:ARG:HH21 | 2:B:428:LEU:HD12 | 1.22 | 1.02 |
| 1:A:141:PHE:HE2 | 1:A:172:TYR:HA | 1.23 | 1.02 |
| 2:B:158:ARG:HG3 | 2:B:159:GLU:H | 1.22 | 1.01 |
| 1:C:133:GLN:H | 1:C:164:LYS:HD3 | 1.19 | 1.01 |
| 1:A:88:HIS:HB3 | 1:A:91:GLN:NE2 | 1.75 | 1.01 |
| 1:C:9:VAL:HG12 | 1:C:68:VAL:HG13 | 1.43 | 1.01 |
| 1:A:413:MET:SD | 3:E:15:UNK:HA | 2.01 | 1.00 |
| 1:A:9:VAL:HG12 | 1:A:68:VAL:HG13 | 1.44 | 1.00 |
| 2:B:240:THR:O | 2:B:243:ARG:HB2 | 1.62 | 1.00 |
| 1:C:93:ILE:HD13 | 1:C:118:VAL:HG22 | 1.43 | 0.99 |
| 1:A:242:LEU:HD21 | 1:A:318:LEU:HD21 | 1.43 | 0.99 |
| 2:B:322:ARG:HG2 | 2:B:357:ASP:HA | 1.45 | 0.99 |
| 2:D:278:ARG:HA | 2:D:278:ARG:NH1 | 1.76 | 0.99 |
| 2:D:264:ARG:HH21 | 2:D:428:LEU:HD12 | 1.25 | 0.99 |
| 1:C:11:GLN:HG3 | 1:C:74:VAL:HG21 | 1.45 | 0.98 |
| 2:D:191:VAL:HG21 | 2:D:421:ALA:HB1 | 1.42 | 0.98 |
| 2:D:206:ASN:HD22 | 2:D:227:LEU:HD21 | 1.26 | 0.98 |
| 1:A:316:CYS:HB2 | 1:A:352:LYS:HB3 | 1.41 | 0.98 |
| 2:B:220:THR:HB | 1:C:326:LYS:HD2 | 1.43 | 0.98 |
| 1:A:387:ALA:HA | 1:A:390:ARG:HD3 | 1.45 | 0.98 |
| 2:D:190:SER:HB2 | 2:D:425:MET:HG3 | 1.44 | 0.98 |
| 2:B:196:GLU:O | 2:B:198:THR:HG22 | 1.64 | 0.97 |
| 1:C:387:ALA:HA | 1:C:390:ARG:HD3 | 1.46 | 0.97 |
| 2:B:77:SER:HA | 2:B:80:SER:HB3 | 1.46 | 0.97 |
| 1:A:102:ASN:HB2 | 1:A:105:ARG:CB | 1.95 | 0.97 |
| 1:A:115:ILE:HD11 | 1:A:156:ARG:HG3 | 1.47 | 0.97 |
| 1:C:141:PHE:HE2 | 1:C:172:TYR:HA | 1.27 | 0.97 |
| 1:A:11:GLN:HG3 | 1:A:74:VAL:HG21 | 1.45 | 0.97 |
| 1:C:88:HIS:HB3 | 1:C:91:GLN:NE2 | 1.80 | 0.97 |
| 1:C:115:ILE:HD11 | 1:C:156:ARG:HG3 | 1.47 | 0.96 |
| 2:D:158:ARG:HB2 | 2:D:197:ASN:HB2 | 1.47 | 0.96 |
| 1:A:69:ASP:HB3 | 1:A:75:ILE:HG21 | 1.46 | 0.96 |
| 2:B:132:LEU:HB3 | 2:B:164:ARG:NH2 | 1.80 | 0.96 |
| 1:A:322:ASP:H | 1:A:357:TYR:HA | 1.30 | 0.96 |
| 1:C:166:LYS:HE3 | 1:C:198:SER:H | 1.31 | 0.96 |
| 1:C:409:VAL:HA | 1:C:414:GLU:OE1 | 1.64 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:91:ASN:HD22 | 2:D:91:ASN:H | 1.10 | 0.96 |
| 1:A:237:SER:HA | 1:A:241:SER:HB2 | 1.48 | 0.96 |
| 2:B:278:ARG:CA | 2:B:278:ARG:HH11 | 1.79 | 0.95 |
| 1:C:214:ARG:NH2 | 1:C:220:GLU:HA | 1.80 | 0.95 |
| 2:B:91:ASN:HD22 | 2:B:91:ASN:H | 1.05 | 0.95 |
| 1:C:185:TYR:HA | 1:C:188:ILE:HD11 | 1.48 | 0.95 |
| 2:B:223:THR:HG22 | 2:B:226:ASP:OD2 | 1.66 | 0.95 |
| 1:C:386:GLU:HG3 | 1:C:387:ALA:H | 1.32 | 0.95 |
| 2:D:8:GLN:HG2 | 2:D:14:ASN:HD22 | 1.30 | 0.95 |
| 1:C:102:ASN:HB2 | 1:C:105:ARG:CB | 1.97 | 0.95 |
| 1:A:214:ARG:NH2 | 1:A:220:GLU:HA | 1.81 | 0.94 |
| 1:C:362:VAL:HG13 | 1:C:367:ASP:HB2 | 1.49 | 0.94 |
| 1:A:311:LYS:HD3 | 1:A:344:VAL:HG13 | 1.48 | 0.94 |
| 2:D:322:ARG:HG2 | 2:D:357:ASP:HA | 1.45 | 0.94 |
| 2:D:196:GLU:O | 2:D:198:THR:HG22 | 1.66 | 0.94 |
| 2:D:77:SER:HA | 2:D:80:SER:HB3 | 1.48 | 0.94 |
| 1:A:93:ILE:HD13 | 1:A:118:VAL:HG22 | 1.48 | 0.94 |
| 2:B:407:TRP:HZ2 | 1:C:256:GLN:HB2 | 1.30 | 0.94 |
| 1:A:79:ARG:HD3 | 1:A:89:PRO:HB3 | 1.50 | 0.93 |
| 2:D:218:LYS:HZ3 | 2:D:278:ARG:N | 1.65 | 0.93 |
| 1:A:175:PRO:CD | 1:A:207:GLU:HB2 | 1.97 | 0.93 |
| 2:D:263:PRO:C | 2:D:265:LEU:H | 1.68 | 0.93 |
| 1:C:322:ASP:H | 1:C:357:TYR:HA | 1.32 | 0.93 |
| 1:A:409:VAL:HG22 | 1:A:414:GLU:HG3 | 1.51 | 0.93 |
| 1:C:102:ASN:HD21 | 2:D:257:VAL:HG11 | 1.33 | 0.93 |
| 1:A:398:MET:SD | 2:B:348:PRO:HD2 | 2.09 | 0.93 |
| 2:B:218:LYS:HZ3 | 2:B:278:ARG:H | 0.96 | 0.92 |
| 1:A:322:ASP:N | 1:A:357:TYR:HA | 1.84 | 0.92 |
| 1:C:383:ALA:O | 1:C:386:GLU:HG2 | 1.68 | 0.92 |
| 1:C:87:PHE:HE2 | 1:C:92:LEU:HD21 | 1.34 | 0.92 |
| 1:C:322:ASP:N | 1:C:357:TYR:HA | 1.84 | 0.92 |
| 2:B:158:ARG:HB2 | 2:B:197:ASN:HB2 | 1.51 | 0.92 |
| 1:A:102:ASN:HD21 | 2:B:257:VAL:HG11 | 1.31 | 0.92 |
| 1:A:386:GLU:HG3 | 1:A:387:ALA:H | 1.33 | 0.92 |
| 1:C:409:VAL:HG22 | 1:C:414:GLU:CG | 2.00 | 0.92 |
| 2:D:311:ARG:NH2 | 2:D:437:ASP:HB2 | 1.83 | 0.92 |
| 1:C:137:VAL:HG11 | 1:C:154:MET:HE2 | 1.51 | 0.92 |
| 1:C:175:PRO:C | 1:C:177:VAL:H | 1.65 | 0.92 |
| 2:D:132:LEU:HB3 | 2:D:164:ARG:NH2 | 1.84 | 0.91 |
| 1:C:237:SER:HA | 1:C:241:SER:HB2 | 1.49 | 0.91 |
| 2:D:218:LYS:HZ3 | 2:D:278:ARG:H | 0.91 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:VAL:HG13 | 1:A:367:ASP:HB2 | 1.50 | 0.91 |
| 1:C:409:VAL:HG22 | 1:C:414:GLU:HG3 | 1.50 | 0.91 |
| 2:D:284:ARG:O | 2:D:287:THR:HG23 | 1.71 | 0.91 |
| 1:A:137:VAL:HG11 | 1:A:154:MET:HE2 | 1.50 | 0.91 |
| 2:B:194:LEU:HD23 | 2:B:195:VAL:HG13 | 1.52 | 0.91 |
| 1:A:409:VAL:HG22 | 1:A:414:GLU:CG | 2.01 | 0.91 |
| 2:B:8:GLN:HG2 | 2:B:14:ASN:HD22 | 1.32 | 0.91 |
| 1:A:398:MET:HG3 | 1:A:399:TYR:HD1 | 1.33 | 0.91 |
| 1:C:335:ILE:HG13 | 1:C:336:LYS:H | 1.32 | 0.91 |
| 1:A:175:PRO:C | 1:A:177:VAL:H | 1.70 | 0.90 |
| 2:D:194:LEU:HD23 | 2:D:195:VAL:HG13 | 1.50 | 0.90 |
| 2:B:218:LYS:HZ3 | 2:B:278:ARG:N | 1.70 | 0.90 |
| 2:B:263:PRO:C | 2:B:265:LEU:H | 1.64 | 0.90 |
| 1:A:166:LYS:HE3 | 1:A:198:SER:H | 1.35 | 0.90 |
| 2:D:262:PHE:HB3 | 2:D:263:PRO:HD2 | 1.53 | 0.90 |
| 1:A:223:THR:HB | 1:A:226:ASN:OD1 | 1.71 | 0.90 |
| 2:B:2:ARG:NE | 2:B:243:ARG:HD2 | 1.86 | 0.90 |
| 2:D:278:ARG:N | 2:D:278:ARG:HD2 | 1.84 | 0.90 |
| 1:A:402:ARG:HD2 | 2:B:346:TRP:CZ3 | 2.07 | 0.90 |
| 2:B:286:LEU:HD12 | 2:B:373:MET:HB2 | 1.54 | 0.90 |
| 2:B:59:ASN:HB2 | 2:B:64:ARG:NE | 1.86 | 0.90 |
| 1:C:398:MET:SD | 2:D:348:PRO:HD2 | 2.11 | 0.90 |
| 2:B:278:ARG:N | 2:B:278:ARG:HD2 | 1.83 | 0.90 |
| 2:D:70:LEU:HG | 2:D:99:ALA:HB3 | 1.53 | 0.89 |
| 2:D:121:VAL:HA | 2:D:124:LYS:HG2 | 1.54 | 0.89 |
| 2:B:311:ARG:NH2 | 2:B:437:ASP:HB2 | 1.88 | 0.89 |
| 2:B:96:GLN:HE22 | 1:C:130:THR:HG22 | 1.35 | 0.89 |
| 1:A:335:ILE:HG13 | 1:A:336:LYS:H | 1.36 | 0.89 |
| 1:A:243:ARG:HH12 | 1:A:250:VAL:HG13 | 1.38 | 0.88 |
| 1:C:2:ARG:NH2 | 1:C:133:GLN:HE22 | 1.70 | 0.88 |
| 2:B:321:GLY:HA2 | 2:B:359:PRO:HB3 | 1.53 | 0.88 |
| 1:A:166:LYS:NZ | 1:A:197:HIS:HB2 | 1.88 | 0.88 |
| 1:A:9:VAL:HG12 | 1:A:68:VAL:CG1 | 2.03 | 0.88 |
| 1:C:79:ARG:HD3 | 1:C:89:PRO:HB3 | 1.55 | 0.88 |
| 1:A:16:ILE:HG22 | 1:A:17:GLY:N | 1.87 | 0.88 |
| 1:A:418:PHE:N | 1:A:418:PHE:HD2 | 1.72 | 0.88 |
| 1:C:242:LEU:HD21 | 1:C:318:LEU:HD21 | 1.52 | 0.88 |
| 2:D:51:VAL:HG23 | 2:D:53:TYR:H | 1.38 | 0.88 |
| 1:C:31:GLN:HB3 | 1:C:32:PRO:HD2 | 1.56 | 0.88 |
| 1:C:69:ASP:OD1 | 1:C:70:LEU:N | 2.05 | 0.88 |
| 2:B:133:GLN:NE2 | 2:B:252:LEU:HB3 | 1.87 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:261:PRO:HG2 | 1:C:380:ASN:HD21 | 1.39 | 0.88 |
| 1:A:107:HIS:HD1 | 1:A:151:SER:HB2 | 1.37 | 0.88 |
| 2:D:278:ARG:HH11 | 2:D:278:ARG:CA | 1.84 | 0.88 |
| 1:A:287:SER:H | 1:A:290:GLU:CD | 1.77 | 0.87 |
| 2:B:284:ARG:O | 2:B:287:THR:HG23 | 1.73 | 0.87 |
| 1:A:186:ASN:ND2 | 1:A:391:LEU:HD11 | 1.90 | 0.87 |
| 1:C:175:PRO:CD | 1:C:207:GLU:HB2 | 2.04 | 0.87 |
| 2:D:339:ASN:HB3 | 2:D:342:TYR:HD1 | 1.37 | 0.87 |
| 1:C:186:ASN:ND2 | 1:C:391:LEU:HD11 | 1.90 | 0.87 |
| 1:C:206:ASN:HB3 | 1:C:210:TYR:CE2 | 2.10 | 0.87 |
| 1:C:398:MET:HG3 | 1:C:399:TYR:HD1 | 1.38 | 0.87 |
| 1:A:216:ASN:HD22 | 1:A:275:VAL:HG12 | 1.38 | 0.87 |
| 1:A:409:VAL:HG13 | 1:A:414:GLU:OE2 | 1.75 | 0.87 |
| 1:A:144:GLY:N | 1:A:147:SER:HB3 | 1.89 | 0.87 |
| 1:A:261:PRO:HG2 | 1:A:380:ASN:HD21 | 1.38 | 0.87 |
| 1:A:320:ARG:HB3 | 1:A:374:ALA:HB3 | 1.56 | 0.87 |
| 2:B:176:LYS:HD2 | 2:B:210:TYR:CZ | 2.10 | 0.87 |
| 1:C:243:ARG:HH12 | 1:C:250:VAL:HG13 | 1.39 | 0.86 |
| 1:C:27:GLU:HG3 | 1:C:28:HIS:H | 1.40 | 0.86 |
| 2:B:396:THR:HG23 | 2:B:400:ARG:HD3 | 1.54 | 0.86 |
| 2:D:396:THR:HG23 | 2:D:400:ARG:HD3 | 1.57 | 0.86 |
| 2:D:223:THR:HG22 | 2:D:226:ASP:OD2 | 1.76 | 0.86 |
| 2:D:88:ARG:HB2 | 2:D:89:PRO:HD3 | 1.56 | 0.86 |
| 1:A:322:ASP:H | 1:A:357:TYR:CA | 1.88 | 0.86 |
| 2:B:339:ASN:HB3 | 2:B:342:TYR:HD1 | 1.40 | 0.86 |
| 2:B:311:ARG:HB2 | 2:B:344:VAL:H | 1.40 | 0.86 |
| 2:B:88:ARG:HB2 | 2:B:89:PRO:HD3 | 1.55 | 0.86 |
| 1:A:166:LYS:HZ2 | 1:A:197:HIS:HB2 | 1.38 | 0.86 |
| 2:D:358:ILE:H | 2:D:358:ILE:HD12 | 1.40 | 0.86 |
| 1:C:87:PHE:CE2 | 1:C:92:LEU:HD21 | 2.10 | 0.86 |
| 2:D:321:GLY:HA2 | 2:D:359:PRO:HB3 | 1.58 | 0.86 |
| 1:C:418:PHE:HD2 | 1:C:418:PHE:N | 1.73 | 0.86 |
| 2:B:223:THR:HG22 | 2:B:226:ASP:CG | 1.97 | 0.86 |
| 1:C:362:VAL:HG21 | 1:C:370:LYS:HA | 1.57 | 0.85 |
| 2:D:142:GLY:HA2 | 2:D:185:TYR:HB3 | 1.57 | 0.85 |
| 1:A:31:GLN:HB3 | 1:A:32:PRO:HD2 | 1.58 | 0.85 |
| 1:C:409:VAL:HG13 | 1:C:414:GLU:OE2 | 1.75 | 0.85 |
| 1:C:223:THR:HB | 1:C:226:ASN:OD1 | 1.76 | 0.85 |
| 1:C:322:ASP:H | 1:C:357:TYR:CA | 1.88 | 0.85 |
| 1:A:138:PHE:HZ | 1:A:235:VAL:HG11 | 1.37 | 0.85 |
| 1:C:190:THR:HA | 1:C:193:THR:HG22 | 1.58 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:332:ILE:HD11 | 1:A:353:VAL:HG21 | 1.58 | 0.85 |
| 1:C:102:ASN:O | 1:C:104:ALA:N | 2.09 | 0.85 |
| 1:C:344:VAL:HG11 | 1:C:346:TRP:NE1 | 1.91 | 0.85 |
| 2:D:103:TRP:HE1 | 2:D:189:LEU:HD21 | 1.40 | 0.85 |
| 2:D:344:VAL:HB | 2:D:346:TRP:NE1 | 1.91 | 0.85 |
| 2:D:59:ASN:HB2 | 2:D:64:ARG:NE | 1.90 | 0.85 |
| 3:E:35:UNK:C | 3:E:37:UNK:N | 2.35 | 0.85 |
| 1:C:386:GLU:HG3 | 1:C:387:ALA:N | 1.90 | 0.85 |
| 2:B:19:LYS:HZ1 | 2:B:82:PRO:HG3 | 1.42 | 0.85 |
| 2:D:158:ARG:HG3 | 2:D:159:GLU:N | 1.91 | 0.85 |
| 2:B:141:LEU:HB3 | 2:B:186:ASN:HB3 | 1.57 | 0.84 |
| 2:B:91:ASN:N | 2:B:91:ASN:HD22 | 1.75 | 0.84 |
| 2:B:132:LEU:HB3 | 2:B:164:ARG:HH21 | 1.35 | 0.84 |
| 1:C:214:ARG:HA | 1:C:218:ASP:O | 1.77 | 0.84 |
| 2:D:286:LEU:HD12 | 2:D:373:MET:HB2 | 1.58 | 0.84 |
| 1:A:362:VAL:HB | 1:A:370:LYS:HG2 | 1.59 | 0.84 |
| 1:C:206:ASN:HD22 | 1:C:210:TYR:HE2 | 1.21 | 0.84 |
| 1:C:418:PHE:CD2 | 1:C:418:PHE:N | 2.45 | 0.84 |
| 2:D:176:LYS:HD2 | 2:D:210:TYR:CZ | 2.13 | 0.84 |
| 2:B:133:GLN:HE21 | 2:B:252:LEU:HB3 | 1.41 | 0.84 |
| 2:B:51:VAL:HG23 | 2:B:53:TYR:H | 1.42 | 0.84 |
| 1:C:166:LYS:NZ | 1:C:197:HIS:HB2 | 1.91 | 0.84 |
| 2:D:13:GLY:O | 2:D:16:ILE:HG23 | 1.76 | 0.84 |
| 1:A:2:ARG:NH2 | 1:A:133:GLN:HE22 | 1.76 | 0.84 |
| 1:C:216:ASN:HD22 | 1:C:275:VAL:HG12 | 1.42 | 0.84 |
| 1:C:320:ARG:HB3 | 1:C:374:ALA:HB3 | 1.60 | 0.84 |
| 1:A:206:ASN:HB3 | 1:A:210:TYR:CE2 | 2.11 | 0.84 |
| 1:A:362:VAL:HG21 | 1:A:370:LYS:HA | 1.59 | 0.84 |
| 1:C:138:PHE:HZ | 1:C:235:VAL:HG11 | 1.41 | 0.84 |
| 2:D:12:CYS:HB3 | 5:D:503:GDP:C8 | 2.12 | 0.84 |
| 1:C:362:VAL:HB | 1:C:370:LYS:HG2 | 1.58 | 0.84 |
| 2:D:213:CYS:HA | 2:D:217:LEU:HD23 | 1.58 | 0.84 |
| 2:B:103:TRP:HE1 | 2:B:189:LEU:HD21 | 1.42 | 0.83 |
| 1:C:241:SER:HA | 1:C:320:ARG:NH2 | 1.92 | 0.83 |
| 1:C:284:GLU:HG2 | 1:C:285:GLN:HE21 | 1.41 | 0.83 |
| 2:B:121:VAL:HA | 2:B:124:LYS:HG2 | 1.57 | 0.83 |
| 2:D:58:GLY:C | 2:D:64:ARG:HE | 1.81 | 0.83 |
| 2:D:141:LEU:HB3 | 2:D:186:ASN:HB3 | 1.61 | 0.83 |
| 1:A:402:ARG:HG2 | 1:A:403:ALA:H | 1.43 | 0.83 |
| 1:C:69:ASP:HB3 | 1:C:75:ILE:HG21 | 1.60 | 0.83 |
| 2:D:19:LYS:NZ | 2:D:82:PRO:HG3 | 1.93 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:27:GLU:HG3 | 1:A:28:HIS:H | 1.43 | 0.83 |
| 2:B:264:ARG:HH21 | 2:B:428:LEU:CD1 | 1.92 | 0.83 |
| 2:B:109:THR:HG21 | 2:B:411:GLU:HG2 | 1.61 | 0.83 |
| 2:D:2:ARG:NE | 2:D:243:ARG:HD2 | 1.93 | 0.83 |
| 2:B:192:HIS:C | 2:B:194:LEU:H | 1.82 | 0.83 |
| 2:D:3:GLU:OE2 | 2:D:130:ASP:HB3 | 1.79 | 0.83 |
| 2:D:92:PHE:HE1 | 2:D:118:VAL:CA | 1.88 | 0.83 |
| 1:A:100:ALA:HB1 | 1:A:105:ARG:O | 1.78 | 0.82 |
| 1:A:350:GLY:C | 1:A:351:PHE:HD1 | 1.82 | 0.82 |
| 1:A:92:LEU:N | 1:A:92:LEU:HD12 | 1.94 | 0.82 |
| 2:D:132:LEU:HB3 | 2:D:164:ARG:HH21 | 1.42 | 0.82 |
| 2:D:311:ARG:HB2 | 2:D:344:VAL:H | 1.43 | 0.82 |
| 2:D:311:ARG:HG3 | 2:D:344:VAL:HA | 1.61 | 0.82 |
| 1:A:284:GLU:HG2 | 1:A:285:GLN:HE21 | 1.42 | 0.82 |
| 2:B:398:MET:O | 2:B:400:ARG:N | 2.12 | 0.82 |
| 1:C:9:VAL:HG12 | 1:C:68:VAL:CG1 | 2.08 | 0.82 |
| 3:E:42:UNK:C | 3:E:44:UNK:N | 2.41 | 0.82 |
| 1:A:339:ARG:C | 1:A:339:ARG:HD2 | 1.98 | 0.82 |
| 1:A:88:HIS:HB3 | 1:A:91:GLN:HE22 | 1.45 | 0.82 |
| 2:B:175:PRO:HD2 | 2:B:207:GLU:CB | 2.09 | 0.82 |
| 1:A:102:ASN:O | 1:A:104:ALA:N | 2.12 | 0.82 |
| 1:A:190:THR:HA | 1:A:193:THR:HG22 | 1.60 | 0.82 |
| 1:A:212:ILE:HG13 | 1:A:213:CYS:N | 1.94 | 0.82 |
| 1:A:373:ARG:HB3 | 1:A:373:ARG:HH11 | 1.45 | 0.82 |
| 2:B:189:LEU:C | 2:B:191:VAL:H | 1.83 | 0.82 |
| 1:C:208:ALA:O | 1:C:211:ASP:HB2 | 1.80 | 0.82 |
| 2:D:109:THR:O | 2:D:111:GLY:N | 2.13 | 0.82 |
| 2:D:189:LEU:C | 2:D:191:VAL:H | 1.83 | 0.82 |
| 2:D:313:LEU:HA | 2:D:344:VAL:HG11 | 1.60 | 0.82 |
| 1:A:206:ASN:HD22 | 1:A:210:TYR:HE2 | 1.26 | 0.82 |
| 2:B:358:ILE:H | 2:B:358:ILE:HD12 | 1.44 | 0.82 |
| 2:B:58:GLY:C | 2:B:64:ARG:HE | 1.83 | 0.82 |
| 2:D:59:ASN:HA | 2:D:64:ARG:HH21 | 1.45 | 0.82 |
| 1:C:287:SER:H | 1:C:290:GLU:CD | 1.82 | 0.81 |
| 2:D:287:THR:HB | 2:D:289:PRO:HD2 | 1.61 | 0.81 |
| 1:A:418:PHE:N | 1:A:418:PHE:CD2 | 2.45 | 0.81 |
| 2:B:19:LYS:NZ | 2:B:82:PRO:HG3 | 1.96 | 0.81 |
| 2:B:96:GLN:HE22 | 1:C:130:THR:CG2 | 1.94 | 0.81 |
| 2:D:103:TRP:NE1 | 2:D:189:LEU:HD21 | 1.95 | 0.81 |
| 2:B:102:ASN:HD22 | 2:B:105:LYS:HG3 | 1.45 | 0.81 |
| 1:C:417:GLU:HB3 | 1:C:418:PHE:CD2 | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:175:PRO:HD2 | 2:D:207:GLU:CB | 2.10 | 0.81 |
| 1:C:258:ASN:HD22 | 1:C:258:ASN:N | 1.78 | 0.81 |
| 2:D:143:GLY:O | 2:D:145:THR:N | 2.11 | 0.81 |
| 1:A:115:ILE:HD13 | 1:A:115:ILE:O | 1.80 | 0.81 |
| 1:A:386:GLU:HG3 | 1:A:387:ALA:N | 1.93 | 0.81 |
| 1:C:115:ILE:HD13 | 1:C:115:ILE:O | 1.81 | 0.81 |
| 1:C:388:TRP:CH2 | 1:C:428:LEU:HD13 | 2.15 | 0.81 |
| 2:D:109:THR:HG21 | 2:D:411:GLU:HG2 | 1.63 | 0.81 |
| 1:A:107:HIS:ND1 | 1:A:151:SER:HB2 | 1.96 | 0.81 |
| 2:B:179:ASP:HA | 1:C:352:LYS:CE | 2.09 | 0.81 |
| 1:C:409:VAL:HG13 | 1:C:414:GLU:CD | 2.01 | 0.81 |
| 2:D:218:LYS:NZ | 2:D:278:ARG:H | 1.77 | 0.81 |
| 3:E:48:UNK:O | 3:E:50:UNK:N | 2.13 | 0.81 |
| 1:C:402:ARG:HD2 | 2:D:346:TRP:CZ3 | 2.15 | 0.81 |
| 2:B:287:THR:HB | 2:B:289:PRO:HD2 | 1.63 | 0.80 |
| 1:A:417:GLU:HB3 | 1:A:418:PHE:CD2 | 2.16 | 0.80 |
| 2:B:109:THR:O | 2:B:111:GLY:N | 2.14 | 0.80 |
| 2:D:184:PRO:HB2 | 2:D:399:PHE:CE1 | 2.17 | 0.80 |
| 2:D:311:ARG:HH21 | 2:D:437:ASP:CB | 1.91 | 0.80 |
| 2:D:390:ARG:O | 2:D:392:SER:N | 2.13 | 0.80 |
| 3:E:61:UNK:O | 3:E:63:UNK:N | 2.14 | 0.80 |
| 2:B:262:PHE:HB3 | 2:B:263:PRO:HD2 | 1.61 | 0.80 |
| 1:C:373:ARG:HH11 | 1:C:373:ARG:HB3 | 1.46 | 0.80 |
| 2:D:264:ARG:HH11 | 2:D:264:ARG:HG3 | 1.47 | 0.80 |
| 1:A:104:ALA:HA | 1:A:108:TYR:HD2 | 1.46 | 0.80 |
| 1:A:174:ALA:O | 1:A:177:VAL:N | 2.15 | 0.80 |
| 2:D:168:THR:OG1 | 2:D:201:THR:HB | 1.82 | 0.80 |
| 2:D:286:LEU:HG | 2:D:373:MET:HE3 | 1.62 | 0.80 |
| 2:B:401:ARG:NH1 | 1:C:440:VAL:HA | 1.95 | 0.80 |
| 2:B:115:VAL:HG11 | 2:B:156:LYS:HZ2 | 1.46 | 0.80 |
| 2:D:335:VAL:HA | 2:D:338:LYS:CB | 2.12 | 0.80 |
| 1:A:388:TRP:CH2 | 1:A:428:LEU:HD13 | 2.16 | 0.80 |
| 2:B:286:LEU:O | 2:B:286:LEU:HG | 1.79 | 0.80 |
| 1:C:291:ILE:HD12 | 1:C:373:ARG:HG3 | 1.63 | 0.80 |
| 2:D:133:GLN:NE2 | 2:D:252:LEU:HB3 | 1.97 | 0.80 |
| 2:B:142:GLY:HA2 | 2:B:185:TYR:HB3 | 1.61 | 0.80 |
| 2:D:12:CYS:HB2 | 5:D:503:GDP:O2A | 1.81 | 0.80 |
| 3:E:21:UNK:O | 3:E:24:UNK:N | 2.15 | 0.80 |
| 2:D:285:ALA:O | 2:D:286:LEU:HD23 | 1.82 | 0.80 |
| 2:D:387:LEU:O | 2:D:387:LEU:HD23 | 1.81 | 0.80 |
| 1:A:133:GLN:N | 1:A:164:LYS:HD3 | 1.94 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:103:TRP:NE1 | 2:B:189:LEU:HD21 | 1.96 | 0.79 |
| 2:D:218:LYS:HZ1 | 2:D:278:ARG:HB2 | 1.46 | 0.79 |
| 2:D:391:ILE:HD12 | 2:D:391:ILE:H | 1.47 | 0.79 |
| 2:B:335:VAL:HA | 2:B:338:LYS:HB3 | 1.63 | 0.79 |
| 1:C:16:ILE:HG22 | 1:C:17:GLY:N | 1.96 | 0.79 |
| 3:E:31:UNK:HA | 3:E:34:UNK:CB | 2.13 | 0.79 |
| 2:B:59:ASN:HA | 2:B:64:ARG:HH21 | 1.47 | 0.79 |
| 1:A:180:ALA:C | 1:A:182:VAL:H | 1.86 | 0.79 |
| 1:C:212:ILE:HG13 | 1:C:213:CYS:N | 1.95 | 0.79 |
| 1:A:419:SER:HA | 1:A:422:ARG:CD | 2.10 | 0.79 |
| 2:B:335:VAL:HA | 2:B:338:LYS:CB | 2.13 | 0.79 |
| 1:C:311:LYS:HD3 | 1:C:344:VAL:HG13 | 1.62 | 0.79 |
| 2:D:102:ASN:HD22 | 2:D:105:LYS:HG3 | 1.47 | 0.79 |
| 1:C:339:ARG:HD2 | 1:C:339:ARG:C | 2.03 | 0.79 |
| 2:D:353:THR:HG22 | 2:D:354:ALA:N | 1.96 | 0.79 |
| 2:B:102:ASN:ND2 | 2:B:105:LYS:HG3 | 1.98 | 0.79 |
| 2:D:179:ASP:HB3 | 2:D:181:VAL:HG12 | 1.63 | 0.79 |
| 2:B:70:LEU:HG | 2:B:99:ALA:HB3 | 1.62 | 0.79 |
| 1:C:335:ILE:HG13 | 1:C:336:LYS:N | 1.97 | 0.79 |
| 1:A:417:GLU:HB3 | 1:A:418:PHE:CE2 | 2.18 | 0.79 |
| 2:B:179:ASP:HB3 | 2:B:181:VAL:HG12 | 1.65 | 0.79 |
| 2:B:182:VAL:O | 2:B:182:VAL:HG12 | 1.81 | 0.79 |
| 1:C:417:GLU:HB3 | 1:C:418:PHE:CE2 | 2.17 | 0.79 |
| 1:C:92:LEU:HD12 | 1:C:92:LEU:N | 1.97 | 0.79 |
| 1:A:388:TRP:HH2 | 1:A:428:LEU:HD13 | 1.47 | 0.79 |
| 2:D:322:ARG:HE | 2:D:357:ASP:HB3 | 1.46 | 0.78 |
| 2:D:274:PRO:HB2 | 2:D:371:LEU:HD12 | 1.65 | 0.78 |
| 1:A:185:TYR:HA | 1:A:188:ILE:HD11 | 1.63 | 0.78 |
| 1:A:196:GLU:O | 1:A:197:HIS:HB3 | 1.82 | 0.78 |
| 1:A:344:VAL:HG11 | 1:A:346:TRP:NE1 | 1.98 | 0.78 |
| 2:D:205:ASP:HB2 | 2:D:387:LEU:HD11 | 1.62 | 0.78 |
| 1:C:175:PRO:C | 1:C:177:VAL:N | 2.36 | 0.78 |
| 1:C:227:LEU:O | 1:C:231:ILE:HG12 | 1.84 | 0.78 |
| 2:D:91:ASN:HD22 | 2:D:91:ASN:N | 1.77 | 0.78 |
| 2:B:217:LEU:HG | 2:B:218:LYS:N | 1.98 | 0.78 |
| 1:C:107:HIS:HD1 | 1:C:151:SER:HB2 | 1.49 | 0.78 |
| 1:C:362:VAL:HG13 | 1:C:367:ASP:CB | 2.13 | 0.78 |
| 1:C:371:VAL:HG12 | 1:C:373:ARG:H | 1.48 | 0.78 |
| 2:D:2:ARG:HG3 | 2:D:133:GLN:HE21 | 1.48 | 0.78 |
| 3:E:31:UNK:O | 3:E:34:UNK:N | 2.17 | 0.78 |
| 1:C:144:GLY:N | 1:C:147:SER:HB3 | 1.99 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:223:THR:HG22 | 2:D:226:ASP:CG | 2.03 | 0.78 |
| 1:A:33:ASP:HA | 1:A:36:MET:HB3 | 1.66 | 0.78 |
| 2:B:285:ALA:O | 2:B:286:LEU:HD23 | 1.84 | 0.78 |
| 1:A:30:ILE:HG13 | 1:A:31:GLN:N | 1.97 | 0.78 |
| 1:C:282:TYR:N | 1:C:282:TYR:CD2 | 2.50 | 0.78 |
| 1:C:234:ILE:HD13 | 1:C:302:MET:SD | 2.24 | 0.78 |
| 2:D:292:THR:HG21 | 2:D:331:GLN:HB3 | 1.66 | 0.78 |
| 2:B:179:ASP:HB2 | 2:B:182:VAL:HG23 | 1.63 | 0.78 |
| 1:C:402:ARG:HG2 | 1:C:403:ALA:H | 1.46 | 0.78 |
| 1:C:388:TRP:HH2 | 1:C:428:LEU:HD13 | 1.49 | 0.78 |
| 2:D:102:ASN:ND2 | 2:D:105:LYS:HG3 | 1.99 | 0.78 |
| 2:D:244:PHE:HB2 | 2:D:245:PRO:HD2 | 1.66 | 0.78 |
| 2:B:158:ARG:HG3 | 2:B:159:GLU:N | 1.98 | 0.77 |
| 2:B:87:PHE:O | 2:B:87:PHE:HD1 | 1.67 | 0.77 |
| 1:C:104:ALA:HA | 1:C:108:TYR:HD2 | 1.48 | 0.77 |
| 1:C:212:ILE:HD11 | 1:C:230:LEU:HD21 | 1.65 | 0.77 |
| 2:D:288:VAL:HG11 | 2:D:327:GLU:OE1 | 1.84 | 0.77 |
| 2:D:339:ASN:HB3 | 2:D:342:TYR:CD1 | 2.19 | 0.77 |
| 3:E:35:UNK:O | 3:E:37:UNK:N | 2.18 | 0.77 |
| 2:B:402:LYS:HE3 | 1:C:440:VAL:HB | 1.65 | 0.77 |
| 2:B:213:CYS:HA | 2:B:217:LEU:HD23 | 1.67 | 0.77 |
| 2:D:274:PRO:HB2 | 2:D:371:LEU:CD1 | 2.15 | 0.77 |
| 1:C:413:MET:HG3 | 3:E:66:UNK:CB | 2.14 | 0.77 |
| 1:C:298:PRO:O | 1:C:301:GLN:HG3 | 1.85 | 0.77 |
| 2:D:179:ASP:CB | 2:D:182:VAL:H | 1.98 | 0.77 |
| 1:A:413:MET:CE | 1:A:413:MET:H | 1.97 | 0.77 |
| 1:C:133:GLN:N | 1:C:164:LYS:HD3 | 1.99 | 0.77 |
| 1:C:322:ASP:CA | 1:C:357:TYR:HA | 2.15 | 0.77 |
| 1:A:69:ASP:OD1 | 1:A:70:LEU:N | 2.17 | 0.77 |
| 2:B:4:ILE:O | 2:B:58:GLY:HA2 | 1.84 | 0.77 |
| 2:D:183:GLU:C | 2:D:185:TYR:H | 1.88 | 0.77 |
| 2:D:305:CYS:SG | 2:D:387:LEU:HB2 | 2.24 | 0.77 |
| 3:E:73:UNK:O | 3:E:75:UNK:N | 2.17 | 0.77 |
| 1:A:102:ASN:CB | 1:A:105:ARG:HB2 | 2.14 | 0.77 |
| 2:B:344:VAL:HB | 2:B:346:TRP:NE1 | 2.00 | 0.77 |
| 1:A:258:ASN:HD22 | 1:A:258:ASN:N | 1.82 | 0.77 |
| 2:B:172:VAL:HG13 | 2:B:173:PRO:HD2 | 1.67 | 0.77 |
| 2:B:313:LEU:HA | 2:B:344:VAL:HG11 | 1.66 | 0.77 |
| 1:C:419:SER:HA | 1:C:422:ARG:CD | 2.11 | 0.77 |
| 2:D:230:LEU:H | 2:D:230:LEU:HD12 | 1.48 | 0.77 |
| 1:C:322:ASP:HA | 1:C:357:TYR:HD1 | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:19:LYS:HZ1 | 2:D:82:PRO:HG3 | 1.48 | 0.77 |
| 1:C:180:ALA:C | 1:C:182:VAL:H | 1.84 | 0.76 |
| 1:A:402:ARG:CG | 1:A:403:ALA:H | 1.98 | 0.76 |
| 2:B:175:PRO:CD | 2:B:207:GLU:HB2 | 2.12 | 0.76 |
| 2:B:266:HIS:ND1 | 2:B:432:TYR:CZ | 2.53 | 0.76 |
| 2:B:311:ARG:HG3 | 2:B:344:VAL:HA | 1.65 | 0.76 |
| 1:C:151:SER:HB3 | 1:C:192:HIS:CE1 | 2.20 | 0.76 |
| 1:C:33:ASP:HA | 1:C:36:MET:HB3 | 1.66 | 0.76 |
| 2:B:264:ARG:NH2 | 2:B:428:LEU:HD12 | 1.99 | 0.76 |
| 2:D:264:ARG:HH21 | 2:D:428:LEU:CD1 | 1.98 | 0.76 |
| 1:A:164:LYS:HZ2 | 1:A:164:LYS:N | 1.83 | 0.76 |
| 1:A:414:GLU:HG2 | 1:A:415:GLU:H | 1.50 | 0.76 |
| 2:B:149:MET:HA | 2:B:149:MET:HE3 | 1.68 | 0.76 |
| 2:B:262:PHE:O | 2:B:265:LEU:HA | 1.85 | 0.76 |
| 2:B:184:PRO:HB2 | 2:B:399:PHE:CE1 | 2.20 | 0.76 |
| 2:D:115:VAL:HG11 | 2:D:156:LYS:NZ | 2.00 | 0.76 |
| 3:E:42:UNK:O | 3:E:44:UNK:N | 2.18 | 0.76 |
| 1:A:371:VAL:HG12 | 1:A:373:ARG:H | 1.50 | 0.76 |
| 1:C:388:TRP:CZ3 | 1:C:428:LEU:HD22 | 2.21 | 0.76 |
| 2:D:180:THR:HB | 2:D:404:PHE:CE1 | 2.19 | 0.76 |
| 2:D:19:LYS:HA | 2:D:22:GLU:CD | 2.06 | 0.76 |
| 2:B:407:TRP:CZ2 | 1:C:256:GLN:HB2 | 2.19 | 0.76 |
| 2:D:303:ALA:HB1 | 2:D:387:LEU:CD1 | 2.14 | 0.76 |
| 1:A:227:LEU:O | 1:A:231:ILE:HG12 | 1.86 | 0.76 |
| 1:A:243:ARG:HH12 | 1:A:250:VAL:CG1 | 1.99 | 0.76 |
| 2:B:91:ASN:ND2 | 2:B:91:ASN:H | 1.82 | 0.76 |
| 1:C:311:LYS:HD2 | 1:C:436:GLY:HA2 | 1.66 | 0.76 |
| 1:C:88:HIS:HB3 | 1:C:91:GLN:HE22 | 1.48 | 0.76 |
| 2:D:194:LEU:CD2 | 2:D:195:VAL:HG13 | 2.16 | 0.76 |
| 2:D:202:TYR:CE1 | 2:D:378:ILE:HD12 | 2.20 | 0.76 |
| 2:D:175:PRO:CD | 2:D:207:GLU:HB2 | 2.12 | 0.76 |
| 1:A:98:ASP:OD1 | 2:B:1:MET:HB3 | 1.85 | 0.76 |
| 2:B:401:ARG:HH11 | 1:C:440:VAL:HA | 1.48 | 0.76 |
| 1:C:269:LEU:HD12 | 1:C:270:ALA:N | 2.00 | 0.76 |
| 2:D:94:PHE:HB2 | 2:D:114:LEU:HD13 | 1.68 | 0.76 |
| 1:A:398:MET:HG3 | 1:A:399:TYR:CD1 | 2.21 | 0.76 |
| 1:A:409:VAL:HG13 | 1:A:414:GLU:CD | 2.06 | 0.76 |
| 1:C:97:GLU:O | 1:C:99:ALA:N | 2.17 | 0.76 |
| 2:D:286:LEU:HA | 2:D:290:GLU:OE2 | 1.84 | 0.76 |
| 2:D:335:VAL:HA | 2:D:338:LYS:HB3 | 1.67 | 0.76 |
| 1:A:398:MET:HB3 | 2:B:346:TRP:O | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:385:GLN:HE21 | 2:B:433:GLN:HE21 | 1.31 | 0.76 |
| 2:B:390:ARG:O | 2:B:392:SER:N | 2.17 | 0.76 |
| 1:C:174:ALA:O | 1:C:177:VAL:N | 2.19 | 0.76 |
| 1:C:256:GLN:HB3 | 1:C:260:VAL:HB | 1.68 | 0.76 |
| 1:C:89:PRO:O | 1:C:90:GLU:HB2 | 1.85 | 0.76 |
| 2:D:182:VAL:HG12 | 2:D:182:VAL:O | 1.85 | 0.76 |
| 2:D:390:ARG:C | 2:D:392:SER:H | 1.88 | 0.76 |
| 1:A:115:ILE:HG13 | 1:A:152:LEU:CD2 | 2.16 | 0.75 |
| 2:D:344:VAL:HB | 2:D:346:TRP:CE2 | 2.21 | 0.75 |
| 2:D:91:ASN:ND2 | 2:D:91:ASN:H | 1.84 | 0.75 |
| 2:B:179:ASP:CB | 2:B:182:VAL:H | 1.99 | 0.75 |
| 2:B:244:PHE:HB2 | 2:B:245:PRO:HD2 | 1.65 | 0.75 |
| 2:B:273:ALA:HB2 | 2:B:295:MET:HB2 | 1.67 | 0.75 |
| 2:D:70:LEU:HG | 2:D:99:ALA:CB | 2.15 | 0.75 |
| 2:D:87:PHE:O | 2:D:87:PHE:HD1 | 1.67 | 0.75 |
| 1:A:151:SER:HB3 | 1:A:192:HIS:CE1 | 2.22 | 0.75 |
| 2:B:115:VAL:HG11 | 2:B:156:LYS:NZ | 2.01 | 0.75 |
| 2:B:205:ASP:HB2 | 2:B:387:LEU:HD11 | 1.69 | 0.75 |
| 2:B:407:TRP:CE3 | 2:B:407:TRP:HA | 2.20 | 0.75 |
| 2:D:158:ARG:CG | 2:D:159:GLU:H | 1.98 | 0.75 |
| 3:E:63:UNK:C | 3:E:65:UNK:H | 1.94 | 0.75 |
| 2:B:100:GLY:HA3 | 1:C:254:GLU:OE1 | 1.86 | 0.75 |
| 1:C:340:THR:OG1 | 1:C:341:ILE:HD12 | 1.86 | 0.75 |
| 1:C:398:MET:HB3 | 2:D:346:TRP:O | 1.87 | 0.75 |
| 3:E:54:UNK:C | 3:E:56:UNK:N | 2.48 | 0.75 |
| 1:A:234:ILE:HD13 | 1:A:302:MET:SD | 2.25 | 0.75 |
| 2:D:21:TRP:CZ2 | 2:D:65:ALA:HB2 | 2.22 | 0.75 |
| 1:A:208:ALA:O | 1:A:211:ASP:HB2 | 1.87 | 0.75 |
| 2:B:218:LYS:HZ1 | 2:B:278:ARG:HB2 | 1.50 | 0.75 |
| 2:D:174:SER:OG | 2:D:176:LYS:HG3 | 1.87 | 0.75 |
| 2:D:196:GLU:OE2 | 2:D:196:GLU:HA | 1.86 | 0.75 |
| 1:A:145:THR:O | 1:A:149:PHE:HB3 | 1.87 | 0.75 |
| 1:A:348:PRO:O | 1:A:350:GLY:N | 2.19 | 0.75 |
| 1:A:141:PHE:CE2 | 1:A:172:TYR:HA | 2.15 | 0.75 |
| 2:B:292:THR:HG21 | 2:B:331:GLN:HB3 | 1.69 | 0.75 |
| 1:A:322:ASP:CA | 1:A:357:TYR:HA | 2.17 | 0.74 |
| 2:B:8:GLN:HG2 | 2:B:14:ASN:ND2 | 2.02 | 0.74 |
| 2:B:92:PHE:HE1 | 2:B:118:VAL:CA | 1.89 | 0.74 |
| 1:C:276:ILE:HG12 | 1:C:282:TYR:CD2 | 2.22 | 0.74 |
| 2:B:179:ASP:CA | 1:C:352:LYS:HE2 | 2.11 | 0.74 |
| 1:A:335:ILE:HG13 | 1:A:336:LYS:N | 2.01 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:PRO:HG3 | 1:A:399:TYR:CZ | 2.22 | 0.74 |
| 1:A:39:ASP:CG | 1:A:40:LYS:H | 1.88 | 0.74 |
| 2:B:143:GLY:O | 2:B:145:THR:N | 2.18 | 0.74 |
| 1:C:107:HIS:ND1 | 1:C:151:SER:HB2 | 2.01 | 0.74 |
| 2:B:220:THR:HB | 1:C:326:LYS:CD | 2.17 | 0.74 |
| 2:B:274:PRO:HB2 | 2:B:371:LEU:CD1 | 2.16 | 0.74 |
| 2:B:387:LEU:HD23 | 2:B:387:LEU:O | 1.86 | 0.74 |
| 2:D:241:CYS:O | 2:D:243:ARG:HG2 | 1.87 | 0.74 |
| 2:D:385:GLN:HE21 | 2:D:433:GLN:HE21 | 1.35 | 0.74 |
| 2:B:286:LEU:HG | 2:B:373:MET:HE3 | 1.69 | 0.74 |
| 1:C:172:TYR:HB3 | 1:C:205:ASP:CA | 2.18 | 0.74 |
| 1:C:177:VAL:HB | 2:D:349:ASN:ND2 | 2.02 | 0.74 |
| 1:C:289:ALA:HA | 1:C:292:THR:CG2 | 2.17 | 0.74 |
| 1:C:350:GLY:C | 1:C:351:PHE:HD1 | 1.90 | 0.74 |
| 2:D:192:HIS:C | 2:D:194:LEU:H | 1.89 | 0.74 |
| 1:A:269:LEU:HD12 | 1:A:270:ALA:N | 2.03 | 0.74 |
| 1:A:282:TYR:CD2 | 1:A:282:TYR:N | 2.51 | 0.74 |
| 2:B:385:GLN:HE21 | 2:B:433:GLN:NE2 | 1.85 | 0.74 |
| 1:A:214:ARG:HA | 1:A:218:ASP:O | 1.86 | 0.74 |
| 2:B:179:ASP:C | 2:B:181:VAL:H | 1.88 | 0.74 |
| 1:C:166:LYS:HZ2 | 1:C:197:HIS:HB2 | 1.51 | 0.74 |
| 1:A:77:GLU:HB3 | 1:A:83:TYR:CD2 | 2.23 | 0.74 |
| 1:C:10:GLY:O | 1:C:13:GLY:N | 2.19 | 0.74 |
| 1:C:196:GLU:O | 1:C:197:HIS:HB3 | 1.84 | 0.74 |
| 1:C:209:ILE:HG23 | 1:C:213:CYS:HB2 | 1.70 | 0.74 |
| 2:B:163:ASP:OD2 | 2:B:164:ARG:HD3 | 1.87 | 0.74 |
| 2:B:176:LYS:HD2 | 2:B:210:TYR:CE2 | 2.22 | 0.74 |
| 2:B:322:ARG:HE | 2:B:357:ASP:HB3 | 1.53 | 0.74 |
| 2:B:407:TRP:HZ2 | 1:C:256:GLN:CB | 2.01 | 0.74 |
| 2:D:70:LEU:HD11 | 2:D:110:GLU:O | 1.88 | 0.74 |
| 1:A:291:ILE:HG21 | 1:A:375:VAL:CG2 | 2.18 | 0.74 |
| 1:C:101:ASN:OD1 | 2:D:254:LYS:HD3 | 1.86 | 0.74 |
| 2:D:179:ASP:C | 2:D:181:VAL:H | 1.90 | 0.74 |
| 1:C:172:TYR:HB3 | 1:C:205:ASP:HA | 1.70 | 0.74 |
| 1:C:183:GLU:N | 1:C:184:PRO:HD2 | 2.03 | 0.74 |
| 2:D:80:SER:C | 2:D:82:PRO:HD2 | 2.07 | 0.74 |
| 2:B:94:PHE:HB2 | 2:B:114:LEU:HD13 | 1.69 | 0.73 |
| 1:A:209:ILE:C | 1:A:211:ASP:H | 1.90 | 0.73 |
| 2:D:371:LEU:HB3 | 2:D:373:MET:O | 1.86 | 0.73 |
| 2:B:145:THR:HB | 5:B:501:GDP:O2B | 1.88 | 0.73 |
| 2:B:385:GLN:NE2 | 2:B:433:GLN:HG2 | 2.03 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:179:ASP:HB2 | 2:D:182:VAL:H | 1.53 | 0.73 |
| 2:B:123:ARG:NH2 | 2:B:160:GLU:HG3 | 2.03 | 0.73 |
| 2:B:13:GLY:O | 2:B:16:ILE:HG23 | 1.88 | 0.73 |
| 2:B:166:MET:HE3 | 2:B:197:ASN:HB3 | 1.69 | 0.73 |
| 1:C:115:ILE:HG13 | 1:C:152:LEU:CD2 | 2.18 | 0.73 |
| 2:D:1:MET:O | 2:D:3:GLU:N | 2.19 | 0.73 |
| 1:A:190:THR:O | 1:A:192:HIS:N | 2.22 | 0.73 |
| 1:A:175:PRO:C | 1:A:177:VAL:N | 2.39 | 0.73 |
| 1:A:238:ILE:HG22 | 1:A:239:THR:N | 2.03 | 0.73 |
| 1:A:385:ALA:HB2 | 1:A:432:TYR:HD2 | 1.53 | 0.73 |
| 2:B:339:ASN:HB3 | 2:B:342:TYR:CD1 | 2.23 | 0.73 |
| 2:B:77:SER:HA | 2:B:80:SER:CB | 2.18 | 0.73 |
| 1:C:262:TYR:HB3 | 1:C:263:PRO:HD2 | 1.70 | 0.73 |
| 2:D:142:GLY:CA | 2:D:185:TYR:HB3 | 2.18 | 0.73 |
| 2:D:343:PHE:O | 2:D:345:GLU:N | 2.21 | 0.73 |
| 2:D:394:GLN:O | 2:D:398:MET:HB3 | 1.87 | 0.73 |
| 2:B:168:THR:OG1 | 2:B:201:THR:HB | 1.88 | 0.73 |
| 1:C:132:LEU:HB3 | 1:C:164:LYS:HD3 | 1.71 | 0.73 |
| 2:D:407:TRP:HA | 2:D:407:TRP:CE3 | 2.22 | 0.73 |
| 2:B:390:ARG:C | 2:B:392:SER:H | 1.92 | 0.73 |
| 2:D:191:VAL:HG12 | 2:D:191:VAL:O | 1.87 | 0.73 |
| 1:A:27:GLU:HG3 | 1:A:28:HIS:ND1 | 2.04 | 0.73 |
| 1:A:298:PRO:O | 1:A:301:GLN:HG3 | 1.89 | 0.73 |
| 1:A:414:GLU:HB2 | 1:A:417:GLU:HB2 | 1.71 | 0.73 |
| 2:B:206:ASN:HD22 | 2:B:227:LEU:CD2 | 2.01 | 0.73 |
| 2:B:288:VAL:HG11 | 2:B:327:GLU:OE1 | 1.88 | 0.73 |
| 2:D:179:ASP:HB2 | 2:D:182:VAL:HG23 | 1.71 | 0.73 |
| 2:D:77:SER:HA | 2:D:80:SER:CB | 2.19 | 0.73 |
| 1:A:267:PHE:CD1 | 1:A:267:PHE:N | 2.57 | 0.73 |
| 1:A:322:ASP:HA | 1:A:357:TYR:HD1 | 1.54 | 0.73 |
| 2:B:402:LYS:HG3 | 1:C:440:VAL:HG12 | 1.70 | 0.73 |
| 2:D:385:GLN:NE2 | 2:D:433:GLN:HG2 | 2.04 | 0.73 |
| 2:D:77:SER:CA | 2:D:80:SER:HB3 | 2.19 | 0.73 |
| 1:A:115:ILE:HG13 | 1:A:152:LEU:HD21 | 1.70 | 0.72 |
| 1:A:194:THR:O | 1:A:197:HIS:O | 2.06 | 0.72 |
| 2:B:407:TRP:HE3 | 2:B:407:TRP:HA | 1.54 | 0.72 |
| 1:C:194:THR:O | 1:C:197:HIS:O | 2.07 | 0.72 |
| 1:C:322:ASP:HA | 1:C:357:TYR:HA | 1.71 | 0.72 |
| 2:D:115:VAL:HG11 | 2:D:156:LYS:HZ2 | 1.52 | 0.72 |
| 2:D:18:ALA:C | 2:D:20:PHE:H | 1.92 | 0.72 |
| 2:B:190:SER:CB | 2:B:425:MET:HG3 | 2.16 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:322:ASP:H | 1:C:357:TYR:C | 1.92 | 0.72 |
| 2:D:263:PRO:C | 2:D:265:LEU:N | 2.42 | 0.72 |
| 2:D:286:LEU:O | 2:D:286:LEU:HG | 1.89 | 0.72 |
| 3:E:25:UNK:C | 3:E:27:UNK:N | 2.49 | 0.72 |
| 2:B:266:HIS:HA | 2:B:432:TYR:OH | 1.89 | 0.72 |
| 1:C:100:ALA:HB1 | 1:C:105:ARG:HD2 | 1.70 | 0.72 |
| 1:C:70:LEU:HD12 | 1:C:145:THR:CA | 2.12 | 0.72 |
| 1:A:215:ARG:HH22 | 1:A:300:ASN:ND2 | 1.87 | 0.72 |
| 2:B:16:ILE:HB | 2:B:228:ASN:HD21 | 1.53 | 0.72 |
| 1:C:267:PHE:CD1 | 1:C:267:PHE:N | 2.55 | 0.72 |
| 1:A:202:PHE:HE1 | 1:A:378:LEU:HD22 | 1.55 | 0.72 |
| 2:B:158:ARG:CG | 2:B:159:GLU:H | 1.99 | 0.72 |
| 2:B:2:ARG:HH11 | 2:B:251:ASP:HA | 1.54 | 0.72 |
| 2:B:4:ILE:O | 2:B:64:ARG:HD2 | 1.89 | 0.72 |
| 2:D:18:ALA:O | 2:D:20:PHE:N | 2.21 | 0.72 |
| 1:A:345:ASP:O | 1:A:347:CYS:N | 2.23 | 0.72 |
| 2:B:133:GLN:NE2 | 2:B:252:LEU:H | 1.87 | 0.72 |
| 2:B:274:PRO:HB2 | 2:B:371:LEU:HD12 | 1.70 | 0.72 |
| 2:B:77:SER:CA | 2:B:80:SER:HB3 | 2.20 | 0.72 |
| 2:D:176:LYS:HD2 | 2:D:210:TYR:CE2 | 2.25 | 0.72 |
| 2:D:308:ARG:NH2 | 2:D:342:TYR:CD1 | 2.56 | 0.72 |
| 2:B:353:THR:HG22 | 2:B:354:ALA:N | 2.04 | 0.72 |
| 1:C:263:PRO:O | 1:C:265:ALA:N | 2.22 | 0.72 |
| 2:D:132:LEU:HD22 | 2:D:164:ARG:HG3 | 1.72 | 0.72 |
| 2:D:331:GLN:O | 2:D:334:ASN:HB3 | 1.89 | 0.72 |
| 2:B:158:ARG:O | 2:B:160:GLU:N | 2.22 | 0.72 |
| 1:C:285:GLN:OE1 | 1:C:372:GLN:HG2 | 1.90 | 0.72 |
| 1:C:44:GLY:C | 1:C:46:ASP:H | 1.92 | 0.72 |
| 2:D:158:ARG:CA | 2:D:197:ASN:HD22 | 2.02 | 0.72 |
| 1:A:289:ALA:HA | 1:A:292:THR:CG2 | 2.20 | 0.72 |
| 1:A:97:GLU:O | 1:A:99:ALA:N | 2.22 | 0.72 |
| 2:B:394:GLN:O | 2:B:398:MET:HB3 | 1.89 | 0.72 |
| 2:D:194:LEU:HD11 | 2:D:428:LEU:HD11 | 1.72 | 0.72 |
| 2:D:273:ALA:HB2 | 2:D:295:MET:HB2 | 1.70 | 0.72 |
| 2:D:353:THR:CG2 | 2:D:354:ALA:N | 2.52 | 0.72 |
| 2:B:138:THR:O | 2:B:139:HIS:HB3 | 1.90 | 0.72 |
| 2:B:194:LEU:CD2 | 2:B:195:VAL:HG13 | 2.19 | 0.72 |
| 2:B:286:LEU:HA | 2:B:290:GLU:OE2 | 1.89 | 0.72 |
| 1:C:39:ASP:CG | 1:C:40:LYS:H | 1.91 | 0.72 |
| 2:B:92:PHE:CE1 | 2:B:118:VAL:CA | 2.70 | 0.71 |
| 2:D:16:ILE:HB | 2:D:228:ASN:HD21 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:194:THR:O | 1:C:197:HIS:N | 2.22 | 0.71 |
| 1:C:348:PRO:O | 1:C:350:GLY:N | 2.23 | 0.71 |
| 2:D:396:THR:HG23 | 2:D:400:ARG:CD | 2.19 | 0.71 |
| 1:A:256:GLN:HB3 | 1:A:260:VAL:HB | 1.71 | 0.71 |
| 2:B:422:GLU:O | 2:B:426:ASN:HB2 | 1.90 | 0.71 |
| 1:A:291:ILE:HG21 | 1:A:375:VAL:HG21 | 1.73 | 0.71 |
| 2:B:263:PRO:C | 2:B:265:LEU:N | 2.39 | 0.71 |
| 1:C:139:HIS:HB3 | 1:C:170:SER:HA | 1.72 | 0.71 |
| 1:C:402:ARG:CG | 1:C:403:ALA:H | 2.03 | 0.71 |
| 3:E:58:UNK:O | 3:E:61:UNK:N | 2.24 | 0.71 |
| 1:A:109:THR:HG21 | 1:A:411:GLU:OE2 | 1.90 | 0.71 |
| 1:A:362:VAL:HG13 | 1:A:367:ASP:CB | 2.19 | 0.71 |
| 1:A:194:THR:O | 1:A:197:HIS:N | 2.22 | 0.71 |
| 1:A:414:GLU:HG2 | 1:A:415:GLU:N | 2.04 | 0.71 |
| 2:B:196:GLU:OE2 | 2:B:196:GLU:HA | 1.91 | 0.71 |
| 2:B:398:MET:C | 2:B:400:ARG:H | 1.94 | 0.71 |
| 1:C:109:THR:HG21 | 1:C:411:GLU:OE2 | 1.90 | 0.71 |
| 2:D:322:ARG:NE | 2:D:357:ASP:HB3 | 2.05 | 0.71 |
| 1:C:70:LEU:CD1 | 1:C:145:THR:HA | 2.13 | 0.71 |
| 1:C:427:ALA:O | 1:C:430:LYS:HB3 | 1.90 | 0.71 |
| 2:D:158:ARG:CB | 2:D:197:ASN:HD22 | 2.02 | 0.71 |
| 2:D:158:ARG:HA | 2:D:197:ASN:HD22 | 1.54 | 0.71 |
| 1:A:243:ARG:CZ | 1:A:243:ARG:HA | 2.21 | 0.71 |
| 1:A:31:GLN:O | 1:A:33:ASP:N | 2.23 | 0.71 |
| 2:B:142:GLY:CA | 2:B:185:TYR:HB3 | 2.20 | 0.71 |
| 2:B:343:PHE:O | 2:B:345:GLU:N | 2.24 | 0.71 |
| 2:D:22:GLU:OE1 | 2:D:82:PRO:HB2 | 1.91 | 0.71 |
| 2:D:266:HIS:HA | 2:D:432:TYR:OH | 1.91 | 0.71 |
| 1:A:78:VAL:HG11 | 1:A:87:PHE:HE2 | 1.54 | 0.71 |
| 2:D:427:ASP:O | 2:D:429:VAL:N | 2.24 | 0.71 |
| 2:D:4:ILE:O | 2:D:58:GLY:HA2 | 1.91 | 0.71 |
| 1:A:215:ARG:HH22 | 1:A:300:ASN:HD21 | 1.39 | 0.70 |
| 1:A:414:GLU:CB | 1:A:417:GLU:HB2 | 2.21 | 0.70 |
| 2:B:430:SER:O | 2:B:434:GLN:HG3 | 1.90 | 0.70 |
| 1:C:175:PRO:O | 1:C:177:VAL:HG23 | 1.91 | 0.70 |
| 2:D:163:ASP:OD2 | 2:D:164:ARG:HD3 | 1.91 | 0.70 |
| 1:A:322:ASP:HA | 1:A:357:TYR:HA | 1.73 | 0.70 |
| 1:A:26:LEU:HG | 1:A:361:THR:CB | 2.21 | 0.70 |
| 2:B:87:PHE:O | 2:B:90:ASP:OD1 | 2.08 | 0.70 |
| 1:C:264:ARG:O | 1:C:266:HIS:N | 2.24 | 0.70 |
| 1:C:284:GLU:HG2 | 1:C:285:GLN:NE2 | 2.04 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:8:HIS:CD2 | 1:A:17:GLY:HA3 | 2.27 | 0.70 |
| 1:C:153:LEU:O | 1:C:156:ARG:HB2 | 1.90 | 0.70 |
| 1:C:171:ILE:HD12 | 1:C:171:ILE:N | 2.06 | 0.70 |
| 1:C:418:PHE:O | 1:C:420:GLU:N | 2.23 | 0.70 |
| 1:A:332:ILE:CD1 | 1:A:353:VAL:HG21 | 2.21 | 0.70 |
| 2:B:191:VAL:HG12 | 2:B:191:VAL:O | 1.90 | 0.70 |
| 2:B:206:ASN:ND2 | 2:B:227:LEU:HD21 | 2.01 | 0.70 |
| 2:B:405:LEU:HD13 | 2:B:406:HIS:N | 2.06 | 0.70 |
| 1:C:398:MET:HG3 | 1:C:399:TYR:CD1 | 2.25 | 0.70 |
| 2:D:255:LEU:CD2 | 2:D:259:MET:HG3 | 2.21 | 0.70 |
| 1:A:340:THR:OG1 | 1:A:341:ILE:HD12 | 1.90 | 0.70 |
| 1:A:399:TYR:HH | 1:A:408:TYR:HE2 | 1.37 | 0.70 |
| 1:C:98:ASP:OD1 | 2:D:1:MET:HB3 | 1.91 | 0.70 |
| 3:E:19:UNK:O | 3:E:21:UNK:N | 2.24 | 0.70 |
| 1:A:16:ILE:HD12 | 1:A:171:ILE:HD11 | 1.73 | 0.70 |
| 2:B:22:GLU:OE1 | 2:B:82:PRO:HB2 | 1.90 | 0.70 |
| 2:B:230:LEU:H | 2:B:230:LEU:HD12 | 1.55 | 0.70 |
| 1:C:7:ILE:HD12 | 1:C:153:LEU:HD21 | 1.74 | 0.70 |
| 1:A:209:ILE:HG23 | 1:A:213:CYS:HB2 | 1.73 | 0.70 |
| 1:A:350:GLY:O | 1:A:351:PHE:HD1 | 1.74 | 0.70 |
| 1:C:102:ASN:CB | 1:C:105:ARG:HB2 | 2.16 | 0.70 |
| 1:C:5:ILE:HD12 | 1:C:125:LEU:HD22 | 1.74 | 0.70 |
| 1:C:115:ILE:HG13 | 1:C:152:LEU:HD21 | 1.73 | 0.70 |
| 1:C:362:VAL:HG21 | 1:C:369:ALA:O | 1.92 | 0.70 |
| 2:D:51:VAL:HG23 | 2:D:53:TYR:N | 2.07 | 0.70 |
| 1:A:418:PHE:O | 1:A:420:GLU:N | 2.25 | 0.70 |
| 2:B:391:ILE:HD12 | 2:B:391:ILE:N | 2.07 | 0.70 |
| 2:D:133:GLN:HE21 | 2:D:252:LEU:HB3 | 1.54 | 0.70 |
| 2:D:71:GLU:HB2 | 2:D:72:PRO:HD2 | 1.74 | 0.70 |
| 1:A:7:ILE:HG21 | 1:A:122:ILE:HD11 | 1.73 | 0.70 |
| 1:A:134:GLY:H | 1:A:164:LYS:CG | 2.04 | 0.70 |
| 2:B:158:ARG:HA | 2:B:197:ASN:HD22 | 1.54 | 0.70 |
| 2:B:241:CYS:O | 2:B:243:ARG:HG2 | 1.92 | 0.70 |
| 2:B:55:GLU:HB2 | 2:B:244:PHE:HA | 1.73 | 0.70 |
| 3:E:19:UNK:C | 3:E:21:UNK:N | 2.54 | 0.70 |
| 1:A:177:VAL:HB | 2:B:349:ASN:ND2 | 2.06 | 0.70 |
| 1:C:195:LEU:HB3 | 1:C:196:GLU:OE2 | 1.90 | 0.70 |
| 1:C:78:VAL:C | 1:C:82:THR:HA | 2.13 | 0.70 |
| 2:D:385:GLN:HE21 | 2:D:433:GLN:NE2 | 1.90 | 0.70 |
| 1:A:322:ASP:H | 1:A:357:TYR:C | 1.94 | 0.69 |
| 1:C:7:ILE:HG21 | 1:C:122:ILE:HD11 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:77:GLU:HB3 | 1:C:83:TYR:CD2 | 2.26 | 0.69 |
| 1:C:190:THR:O | 1:C:192:HIS:N | 2.25 | 0.69 |
| 1:C:220:GLU:OE2 | 2:D:326:LYS:HD3 | 1.92 | 0.69 |
| 1:C:184:PRO:HG3 | 1:C:399:TYR:CZ | 2.28 | 0.69 |
| 2:D:391:ILE:N | 2:D:391:ILE:HD12 | 2.07 | 0.69 |
| 2:D:264:ARG:NH2 | 2:D:428:LEU:HD12 | 2.03 | 0.69 |
| 1:A:280:LYS:O | 1:A:282:TYR:CE2 | 2.45 | 0.69 |
| 1:A:284:GLU:HG2 | 1:A:285:GLN:NE2 | 2.07 | 0.69 |
| 1:A:89:PRO:O | 1:A:90:GLU:HB2 | 1.90 | 0.69 |
| 1:C:291:ILE:HG21 | 1:C:375:VAL:CG2 | 2.22 | 0.69 |
| 1:A:205:ASP:OD2 | 1:A:207:GLU:HB3 | 1.92 | 0.69 |
| 1:A:11:GLN:HB3 | 4:A:500:GTP:O2A | 1.91 | 0.69 |
| 2:B:133:GLN:HE21 | 2:B:252:LEU:CB | 2.05 | 0.69 |
| 2:D:183:GLU:O | 2:D:185:TYR:N | 2.24 | 0.69 |
| 2:D:218:LYS:NZ | 2:D:278:ARG:HB2 | 2.07 | 0.69 |
| 2:D:59:ASN:HB2 | 2:D:64:ARG:CZ | 2.22 | 0.69 |
| 1:A:78:VAL:O | 1:A:82:THR:HG23 | 1.92 | 0.69 |
| 1:C:414:GLU:HG2 | 1:C:415:GLU:H | 1.58 | 0.69 |
| 2:D:262:PHE:O | 2:D:265:LEU:HA | 1.93 | 0.69 |
| 2:D:218:LYS:NZ | 2:D:278:ARG:N | 2.39 | 0.69 |
| 2:D:138:THR:O | 2:D:139:HIS:HB3 | 1.91 | 0.69 |
| 2:B:345:GLU:O | 2:B:345:GLU:HG2 | 1.92 | 0.69 |
| 1:C:31:GLN:CB | 1:C:32:PRO:HD2 | 2.23 | 0.69 |
| 2:D:396:THR:CG2 | 2:D:400:ARG:HD3 | 2.23 | 0.69 |
| 2:D:416:MET:C | 2:D:418:PHE:H | 1.95 | 0.69 |
| 1:A:78:VAL:HG11 | 1:A:92:LEU:HD21 | 1.73 | 0.69 |
| 2:B:255:LEU:CD2 | 2:B:259:MET:HG3 | 2.22 | 0.69 |
| 2:B:218:LYS:NZ | 2:B:278:ARG:H | 1.83 | 0.69 |
| 1:C:100:ALA:HB1 | 1:C:105:ARG:O | 1.92 | 0.69 |
| 1:C:205:ASP:OD2 | 1:C:207:GLU:HB3 | 1.93 | 0.69 |
| 1:C:30:ILE:HG13 | 1:C:31:GLN:N | 2.07 | 0.69 |
| 1:C:78:VAL:O | 1:C:82:THR:HG23 | 1.91 | 0.69 |
| 2:D:259:MET:HE1 | 2:D:316:ALA:N | 2.08 | 0.69 |
| 2:D:59:ASN:CG | 2:D:60:LYS:H | 1.95 | 0.69 |
| 1:A:154:MET:SD | 1:A:197:HIS:CD2 | 2.86 | 0.69 |
| 1:A:276:ILE:HD12 | 1:A:277:SER:N | 2.07 | 0.69 |
| 1:A:86:LEU:CD2 | 1:A:89:PRO:HD3 | 2.23 | 0.69 |
| 1:C:202:PHE:HE1 | 1:C:378:LEU:HD22 | 1.57 | 0.69 |
| 1:C:287:SER:N | 1:C:290:GLU:HB2 | 2.07 | 0.69 |
| 2:B:183:GLU:C | 2:B:185:TYR:H | 1.95 | 0.69 |
| 2:B:274:PRO:HA | 2:B:294:GLN:NE2 | 2.08 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:269:LEU:C | 1:C:269:LEU:HD12 | 2.13 | 0.69 |
| 2:D:422:GLU:O | 2:D:426:ASN:HB2 | 1.93 | 0.69 |
| 1:A:191:THR:CB | 1:A:421:ALA:HB1 | 2.23 | 0.69 |
| 2:B:179:ASP:C | 2:B:181:VAL:N | 2.45 | 0.69 |
| 2:B:320:ARG:HG2 | 2:B:320:ARG:HH11 | 1.58 | 0.69 |
| 1:C:171:ILE:HD12 | 1:C:171:ILE:H | 1.56 | 0.69 |
| 2:D:123:ARG:NH2 | 2:D:160:GLU:HG3 | 2.08 | 0.69 |
| 3:E:17:UNK:C | 3:E:19:UNK:N | 2.48 | 0.69 |
| 1:A:413:MET:O | 1:A:414:GLU:HB3 | 1.92 | 0.68 |
| 2:B:333:LEU:HG | 2:B:337:ASN:ND2 | 2.08 | 0.68 |
| 1:C:286:LEU:HA | 1:C:290:GLU:OE1 | 1.93 | 0.68 |
| 2:D:105:LYS:HA | 2:D:109:THR:OG1 | 1.93 | 0.68 |
| 3:E:71:UNK:O | 3:E:73:UNK:N | 2.27 | 0.68 |
| 2:B:132:LEU:HD22 | 2:B:164:ARG:HG3 | 1.75 | 0.68 |
| 1:C:258:ASN:ND2 | 1:C:258:ASN:N | 2.39 | 0.68 |
| 2:D:247:GLN:HB2 | 2:D:355:VAL:O | 1.92 | 0.68 |
| 2:D:92:PHE:CE1 | 2:D:118:VAL:CA | 2.71 | 0.68 |
| 1:A:259:LEU:HD21 | 1:A:378:LEU:HB3 | 1.74 | 0.68 |
| 2:B:296:PHE:HA | 2:B:377:PHE:HE2 | 1.59 | 0.68 |
| 2:B:344:VAL:HB | 2:B:346:TRP:CE2 | 2.28 | 0.68 |
| 2:B:416:MET:C | 2:B:418:PHE:H | 1.96 | 0.68 |
| 1:A:10:GLY:O | 1:A:13:GLY:N | 2.26 | 0.68 |
| 2:B:111:GLY:C | 2:B:113:GLU:H | 1.94 | 0.68 |
| 1:C:209:ILE:C | 1:C:211:ASP:H | 1.95 | 0.68 |
| 1:C:414:GLU:CB | 1:C:417:GLU:HB2 | 2.24 | 0.68 |
| 2:D:313:LEU:HA | 2:D:344:VAL:CG1 | 2.23 | 0.68 |
| 2:D:407:TRP:HE3 | 2:D:407:TRP:HA | 1.56 | 0.68 |
| 1:A:330:ALA:O | 1:A:334:THR:HG23 | 1.93 | 0.68 |
| 1:A:75:ILE:HG12 | 1:A:75:ILE:O | 1.92 | 0.68 |
| 2:B:175:PRO:O | 2:B:177:VAL:HG23 | 1.93 | 0.68 |
| 2:D:430:SER:O | 2:D:434:GLN:HG3 | 1.93 | 0.68 |
| 1:A:103:TYR:N | 1:A:185:TYR:HE1 | 1.92 | 0.68 |
| 1:A:172:TYR:HB3 | 1:A:205:ASP:CA | 2.24 | 0.68 |
| 1:A:311:LYS:HD3 | 1:A:344:VAL:HG22 | 1.75 | 0.68 |
| 2:B:21:TRP:CZ2 | 2:B:65:ALA:HB2 | 2.29 | 0.68 |
| 2:B:391:ILE:HD12 | 2:B:391:ILE:H | 1.57 | 0.68 |
| 2:D:175:PRO:O | 2:D:177:VAL:HG23 | 1.93 | 0.68 |
| 1:A:305:CYS:SG | 1:A:306:ASP:N | 2.65 | 0.68 |
| 2:B:109:THR:HG21 | 2:B:411:GLU:CG | 2.24 | 0.68 |
| 2:B:102:ASN:HB3 | 2:B:105:LYS:HD2 | 1.74 | 0.68 |
| 1:C:433:GLU:OE1 | 1:C:433:GLU:HA | 1.92 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:126:SER:OG | 2:D:127:GLU:N | 2.26 | 0.68 |
| 2:D:71:GLU:HB2 | 2:D:72:PRO:CD | 2.24 | 0.68 |
| 1:A:153:LEU:O | 1:A:156:ARG:HB2 | 1.93 | 0.68 |
| 1:A:134:GLY:H | 1:A:164:LYS:HG2 | 1.58 | 0.68 |
| 1:A:171:ILE:N | 1:A:171:ILE:HD12 | 2.08 | 0.68 |
| 1:A:172:TYR:HB3 | 1:A:205:ASP:HA | 1.75 | 0.68 |
| 1:A:258:ASN:O | 1:A:259:LEU:HB2 | 1.93 | 0.68 |
| 2:B:51:VAL:HG23 | 2:B:53:TYR:N | 2.08 | 0.68 |
| 1:C:145:THR:O | 1:C:149:PHE:HB3 | 1.93 | 0.68 |
| 1:C:215:ARG:HH22 | 1:C:300:ASN:ND2 | 1.91 | 0.68 |
| 2:D:55:GLU:HB2 | 2:D:244:PHE:HA | 1.75 | 0.68 |
| 1:A:321:GLY:HA2 | 1:A:357:TYR:O | 1.94 | 0.68 |
| 2:B:163:ASP:CG | 2:B:164:ARG:N | 2.47 | 0.68 |
| 1:C:147:SER:O | 1:C:189:LEU:HD23 | 1.93 | 0.68 |
| 2:D:179:ASP:C | 2:D:181:VAL:N | 2.47 | 0.68 |
| 1:A:104:ALA:HA | 1:A:108:TYR:CD2 | 2.28 | 0.67 |
| 2:B:5:VAL:HB | 2:B:135:PHE:CD2 | 2.29 | 0.67 |
| 1:C:31:GLN:O | 1:C:33:ASP:N | 2.28 | 0.67 |
| 1:C:414:GLU:HB2 | 1:C:417:GLU:HB2 | 1.76 | 0.67 |
| 2:D:16:ILE:HD12 | 2:D:231:VAL:HG11 | 1.76 | 0.67 |
| 2:D:405:LEU:HD13 | 2:D:406:HIS:N | 2.09 | 0.67 |
| 3:E:50:UNK:O | 3:E:52:UNK:N | 2.27 | 0.67 |
| 1:A:139:HIS:CD2 | 1:A:150:THR:HG21 | 2.29 | 0.67 |
| 1:A:412:GLY:O | 1:A:414:GLU:OE1 | 2.12 | 0.67 |
| 1:A:427:ALA:O | 1:A:430:LYS:HB3 | 1.93 | 0.67 |
| 2:B:398:MET:N | 2:B:401:ARG:HB2 | 2.09 | 0.67 |
| 2:D:104:ALA:O | 2:D:108:TYR:HB2 | 1.94 | 0.67 |
| 2:B:102:ASN:HD21 | 2:B:104:ALA:HB3 | 1.58 | 0.67 |
| 2:B:174:SER:OG | 2:B:176:LYS:HG3 | 1.94 | 0.67 |
| 2:B:221:THR:OG1 | 1:C:326:LYS:HB2 | 1.94 | 0.67 |
| 1:A:413:MET:HE2 | 1:A:413:MET:H | 1.58 | 0.67 |
| 1:A:311:LYS:HD2 | 1:A:436:GLY:HA2 | 1.76 | 0.67 |
| 2:D:353:THR:CG2 | 2:D:354:ALA:H | 2.08 | 0.67 |
| 2:D:8:GLN:HG2 | 2:D:14:ASN:ND2 | 2.06 | 0.67 |
| 2:B:237:GLY:O | 2:B:376:THR:HG21 | 1.95 | 0.67 |
| 2:B:263:PRO:O | 2:B:265:LEU:N | 2.27 | 0.67 |
| 2:B:331:GLN:O | 2:B:334:ASN:HB3 | 1.95 | 0.67 |
| 1:C:287:SER:OG | 1:C:290:GLU:N | 2.28 | 0.67 |
| 2:B:179:ASP:HB2 | 2:B:182:VAL:H | 1.58 | 0.67 |
| 1:C:213:CYS:SG | 1:C:217:LEU:HD23 | 2.34 | 0.67 |
| 2:D:217:LEU:HG | 2:D:218:LYS:N | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:3:GLU:OE2 | 2:B:130:ASP:HB3 | 1.93 | 0.67 |
| 1:C:264:ARG:O | 1:C:266:HIS:ND1 | 2.28 | 0.67 |
| 1:C:280:LYS:O | 1:C:282:TYR:CE2 | 2.47 | 0.67 |
| 1:C:404:PHE:HD1 | 1:C:404:PHE:H | 1.42 | 0.67 |
| 1:C:414:GLU:HG2 | 1:C:415:GLU:N | 2.09 | 0.67 |
| 2:D:122:VAL:O | 2:D:126:SER:N | 2.26 | 0.67 |
| 2:D:174:SER:HB2 | 2:D:207:GLU:N | 2.10 | 0.67 |
| 1:A:287:SER:OG | 1:A:290:GLU:HG3 | 1.94 | 0.67 |
| 1:A:44:GLY:C | 1:A:46:ASP:H | 1.97 | 0.67 |
| 2:D:205:ASP:OD2 | 2:D:207:GLU:HB3 | 1.95 | 0.67 |
| 2:D:266:HIS:HB2 | 2:D:380:ASN:OD1 | 1.95 | 0.67 |
| 1:C:177:VAL:HB | 2:D:349:ASN:CG | 2.15 | 0.67 |
| 2:D:386:GLU:C | 2:D:388:PHE:H | 1.98 | 0.67 |
| 1:A:237:SER:CA | 1:A:241:SER:HB2 | 2.23 | 0.67 |
| 1:A:88:HIS:CB | 1:A:91:GLN:HE22 | 2.08 | 0.67 |
| 2:B:264:ARG:HH22 | 2:B:431:GLU:HG3 | 1.60 | 0.67 |
| 2:B:92:PHE:CD1 | 2:B:118:VAL:HG22 | 2.30 | 0.67 |
| 1:C:141:PHE:CE2 | 1:C:172:TYR:HA | 2.19 | 0.67 |
| 1:C:291:ILE:CD1 | 1:C:373:ARG:HG3 | 2.24 | 0.67 |
| 1:C:180:ALA:C | 1:C:182:VAL:N | 2.48 | 0.67 |
| 1:A:413:MET:SD | 1:A:413:MET:N | 2.68 | 0.66 |
| 1:C:210:TYR:CE2 | 1:C:227:LEU:HD23 | 2.30 | 0.66 |
| 2:D:255:LEU:HD23 | 2:D:259:MET:CG | 2.25 | 0.66 |
| 2:D:87:PHE:O | 2:D:87:PHE:CD1 | 2.48 | 0.66 |
| 1:A:70:LEU:CD1 | 1:A:145:THR:HA | 2.17 | 0.66 |
| 1:A:164:LYS:HZ3 | 1:A:164:LYS:HB2 | 1.59 | 0.66 |
| 1:A:189:LEU:HD13 | 1:A:193:THR:HG21 | 1.77 | 0.66 |
| 2:B:305:CYS:SG | 2:B:387:LEU:HB2 | 2.35 | 0.66 |
| 2:D:62:VAL:HG23 | 2:D:62:VAL:O | 1.94 | 0.66 |
| 2:D:4:ILE:O | 2:D:64:ARG:HD2 | 1.95 | 0.66 |
| 1:A:355:ILE:HD12 | 1:A:355:ILE:N | 2.10 | 0.66 |
| 2:B:70:LEU:HG | 2:B:99:ALA:CB | 2.24 | 0.66 |
| 1:A:365:GLY:O | 1:A:368:LEU:CD1 | 2.43 | 0.66 |
| 2:B:87:PHE:O | 2:B:87:PHE:CD1 | 2.48 | 0.66 |
| 1:C:189:LEU:HD13 | 1:C:193:THR:HG21 | 1.77 | 0.66 |
| 1:C:386:GLU:CG | 1:C:387:ALA:H | 2.07 | 0.66 |
| 2:D:350:ASN:HD22 | 2:D:351:VAL:HG23 | 1.60 | 0.66 |
| 1:A:306:ASP:C | 1:A:308:ARG:H | 1.98 | 0.66 |
| 2:B:19:LYS:HA | 2:B:22:GLU:CD | 2.16 | 0.66 |
| 1:C:273:ALA:HB2 | 1:C:295:CYS:HB2 | 1.76 | 0.66 |
| 1:C:306:ASP:C | 1:C:308:ARG:H | 1.99 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:5:VAL:HB | 2:D:135:PHE:CD2 | 2.30 | 0.66 |
| 1:A:242:LEU:O | 1:A:243:ARG:NH1 | 2.28 | 0.66 |
| 1:A:287:SER:OG | 1:A:290:GLU:N | 2.28 | 0.66 |
| 2:B:16:ILE:HD12 | 2:B:231:VAL:HG11 | 1.77 | 0.66 |
| 2:B:255:LEU:HD23 | 2:B:259:MET:HG3 | 1.78 | 0.66 |
| 2:B:386:GLU:C | 2:B:388:PHE:H | 1.99 | 0.66 |
| 2:B:402:LYS:HE3 | 1:C:440:VAL:CB | 2.24 | 0.66 |
| 1:A:8:HIS:N | 1:A:8:HIS:ND1 | 2.43 | 0.66 |
| 2:B:102:ASN:O | 2:B:105:LYS:HB2 | 1.96 | 0.66 |
| 2:B:353:THR:CG2 | 2:B:354:ALA:N | 2.58 | 0.66 |
| 1:C:242:LEU:HB3 | 1:C:250:VAL:HG11 | 1.78 | 0.66 |
| 2:D:320:ARG:HG2 | 2:D:320:ARG:HH11 | 1.59 | 0.66 |
| 3:E:48:UNK:O | 3:E:49:UNK:C | 2.44 | 0.66 |
| 1:A:371:VAL:HG12 | 1:A:372:GLN:N | 2.11 | 0.66 |
| 1:A:78:VAL:C | 1:A:82:THR:HA | 2.15 | 0.66 |
| 2:B:111:GLY:C | 2:B:113:GLU:N | 2.47 | 0.66 |
| 2:B:118:VAL:C | 2:B:120:ASP:H | 1.97 | 0.66 |
| 1:C:371:VAL:HG12 | 1:C:373:ARG:N | 2.11 | 0.66 |
| 2:D:149:MET:HA | 2:D:149:MET:HE3 | 1.78 | 0.66 |
| 3:E:25:UNK:O | 3:E:29:UNK:N | 2.29 | 0.66 |
| 1:A:261:PRO:CG | 1:A:380:ASN:HD21 | 2.09 | 0.66 |
| 1:A:286:LEU:HA | 1:A:290:GLU:OE1 | 1.96 | 0.66 |
| 2:B:126:SER:OG | 2:B:127:GLU:N | 2.28 | 0.66 |
| 1:C:172:TYR:HB3 | 1:C:205:ASP:N | 2.11 | 0.66 |
| 1:C:7:ILE:HG22 | 1:C:66:VAL:CB | 2.18 | 0.66 |
| 1:A:195:LEU:HB3 | 1:A:196:GLU:OE2 | 1.95 | 0.66 |
| 1:A:262:TYR:HB3 | 1:A:263:PRO:HD2 | 1.77 | 0.66 |
| 1:A:422:ARG:O | 1:A:426:ALA:HB2 | 1.96 | 0.66 |
| 1:C:206:ASN:ND2 | 1:C:210:TYR:HE2 | 1.93 | 0.66 |
| 1:A:276:ILE:HG12 | 1:A:282:TYR:CD2 | 2.32 | 0.65 |
| 2:D:118:VAL:C | 2:D:120:ASP:H | 1.99 | 0.65 |
| 2:D:203:CYS:SG | 2:D:384:ILE:HD11 | 2.36 | 0.65 |
| 1:A:144:GLY:O | 1:A:146:GLY:N | 2.29 | 0.65 |
| 2:B:1:MET:O | 2:B:3:GLU:N | 2.26 | 0.65 |
| 1:C:217:LEU:HD11 | 1:C:368:LEU:HD22 | 1.79 | 0.65 |
| 1:C:217:LEU:O | 1:C:219:ILE:HG13 | 1.97 | 0.65 |
| 1:C:407:TRP:C | 1:C:409:VAL:H | 1.97 | 0.65 |
| 2:D:133:GLN:NE2 | 2:D:252:LEU:H | 1.93 | 0.65 |
| 2:D:296:PHE:HA | 2:D:377:PHE:HE2 | 1.61 | 0.65 |
| 1:A:231:ILE:O | 1:A:235:VAL:HG23 | 1.96 | 0.65 |
| 1:A:363:VAL:HG13 | 1:A:367:ASP:OD2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:ALA:C | 2:B:20:PHE:H | 2.00 | 0.65 |
| 2:B:58:GLY:O | 2:B:64:ARG:NE | 2.30 | 0.65 |
| 1:C:134:GLY:H | 1:C:164:LYS:CG | 2.09 | 0.65 |
| 1:C:151:SER:HB3 | 1:C:192:HIS:NE2 | 2.12 | 0.65 |
| 1:C:422:ARG:O | 1:C:426:ALA:HB2 | 1.97 | 0.65 |
| 2:D:167:ASN:HA | 2:D:200:GLU:O | 1.96 | 0.65 |
| 2:D:335:VAL:HA | 2:D:338:LYS:HB2 | 1.79 | 0.65 |
| 1:A:206:ASN:HB3 | 1:A:210:TYR:HE2 | 1.58 | 0.65 |
| 2:B:311:ARG:HB2 | 2:B:344:VAL:N | 2.10 | 0.65 |
| 1:C:413:MET:O | 1:C:414:GLU:HB3 | 1.96 | 0.65 |
| 2:D:278:ARG:H | 2:D:278:ARG:HD2 | 1.59 | 0.65 |
| 2:D:303:ALA:HB1 | 2:D:387:LEU:HD13 | 1.78 | 0.65 |
| 2:D:5:VAL:HA | 2:D:64:ARG:CD | 2.26 | 0.65 |
| 2:D:92:PHE:CD1 | 2:D:118:VAL:HG22 | 2.31 | 0.65 |
| 1:A:388:TRP:CZ3 | 1:A:428:LEU:HD22 | 2.31 | 0.65 |
| 2:B:218:LYS:NZ | 2:B:278:ARG:HB2 | 2.11 | 0.65 |
| 2:B:255:LEU:HD23 | 2:B:259:MET:CG | 2.27 | 0.65 |
| 1:A:174:ALA:O | 1:A:176:GLN:N | 2.29 | 0.65 |
| 1:A:186:ASN:ND2 | 1:A:391:LEU:HD21 | 2.10 | 0.65 |
| 1:A:286:LEU:O | 1:A:373:ARG:HD2 | 1.97 | 0.65 |
| 2:B:247:GLN:HB2 | 2:B:355:VAL:O | 1.97 | 0.65 |
| 2:B:264:ARG:HH11 | 2:B:264:ARG:HG3 | 1.60 | 0.65 |
| 1:C:330:ALA:O | 1:C:334:THR:HG23 | 1.96 | 0.65 |
| 2:D:227:LEU:HD23 | 2:D:227:LEU:O | 1.96 | 0.65 |
| 2:D:59:ASN:CG | 2:D:60:LYS:N | 2.50 | 0.65 |
| 1:A:247:ALA:O | 1:A:249:ASN:ND2 | 2.30 | 0.65 |
| 1:A:287:SER:C | 1:A:289:ALA:H | 1.98 | 0.65 |
| 2:B:392:SER:HB2 | 2:B:426:ASN:ND2 | 2.11 | 0.65 |
| 1:C:12:ALA:HB3 | 1:C:140:SER:CB | 2.27 | 0.65 |
| 1:C:143:GLY:O | 1:C:144:GLY:O | 2.13 | 0.65 |
| 1:C:209:ILE:N | 1:C:209:ILE:HD12 | 2.11 | 0.65 |
| 2:D:274:PRO:HA | 2:D:294:GLN:NE2 | 2.11 | 0.65 |
| 1:A:177:VAL:HB | 2:B:349:ASN:CG | 2.17 | 0.65 |
| 1:A:264:ARG:O | 1:A:266:HIS:N | 2.30 | 0.65 |
| 2:B:169:PHE:CD2 | 2:B:235:MET:SD | 2.90 | 0.65 |
| 1:C:186:ASN:HD22 | 1:C:391:LEU:HD11 | 1.60 | 0.65 |
| 1:C:412:GLY:O | 1:C:414:GLU:OE1 | 2.15 | 0.65 |
| 2:D:158:ARG:HB2 | 2:D:197:ASN:HD22 | 1.61 | 0.65 |
| 3:E:73:UNK:C | 3:E:75:UNK:H | 2.10 | 0.65 |
| 1:A:183:GLU:N | 1:A:184:PRO:HD2 | 2.12 | 0.65 |
| 1:A:258:ASN:ND2 | 1:A:258:ASN:N | 2.43 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:139:HIS:CD2 | 2:B:139:HIS:C | 2.69 | 0.65 |
| 2:B:287:THR:OG1 | 2:B:290:GLU:HB2 | 1.97 | 0.65 |
| 2:D:163:ASP:CG | 2:D:164:ARG:N | 2.50 | 0.65 |
| 2:D:209:LEU:HB3 | 2:D:227:LEU:HG | 1.79 | 0.65 |
| 2:D:398:MET:N | 2:D:401:ARG:HB2 | 2.12 | 0.65 |
| 1:A:133:GLN:HA | 1:A:164:LYS:HG3 | 1.79 | 0.65 |
| 2:B:122:VAL:O | 2:B:126:SER:N | 2.27 | 0.65 |
| 2:B:339:ASN:C | 2:B:341:SER:H | 2.00 | 0.65 |
| 1:C:144:GLY:O | 1:C:146:GLY:N | 2.30 | 0.65 |
| 2:D:172:VAL:HG13 | 2:D:173:PRO:HD2 | 1.78 | 0.65 |
| 2:D:183:GLU:C | 2:D:185:TYR:N | 2.47 | 0.65 |
| 1:A:311:LYS:HD3 | 1:A:344:VAL:CG1 | 2.23 | 0.64 |
| 1:A:407:TRP:C | 1:A:409:VAL:H | 2.00 | 0.64 |
| 2:B:205:ASP:OD2 | 2:B:207:GLU:HB3 | 1.96 | 0.64 |
| 1:C:133:GLN:HA | 1:C:164:LYS:HG3 | 1.79 | 0.64 |
| 1:C:8:HIS:N | 1:C:8:HIS:ND1 | 2.44 | 0.64 |
| 1:A:180:ALA:C | 1:A:182:VAL:N | 2.51 | 0.64 |
| 1:C:362:VAL:CG1 | 1:C:367:ASP:HB2 | 2.26 | 0.64 |
| 2:D:137:LEU:HD23 | 2:D:154:ILE:HD11 | 1.80 | 0.64 |
| 2:D:5:VAL:HA | 2:D:64:ARG:HD2 | 1.79 | 0.64 |
| 1:A:277:SER:O | 1:A:278:ALA:HB2 | 1.97 | 0.64 |
| 2:B:107:HIS:HD2 | 2:B:151:THR:HG23 | 1.62 | 0.64 |
| 2:B:158:ARG:CA | 2:B:197:ASN:HD22 | 2.09 | 0.64 |
| 2:B:59:ASN:CG | 2:B:60:LYS:H | 1.99 | 0.64 |
| 1:C:100:ALA:CB | 1:C:105:ARG:HD2 | 2.27 | 0.64 |
| 2:B:96:GLN:NE2 | 1:C:130:THR:HG22 | 2.11 | 0.64 |
| 1:C:360:PRO:HB3 | 1:C:374:ALA:HB2 | 1.79 | 0.64 |
| 1:A:183:GLU:HB2 | 1:A:184:PRO:CD | 2.27 | 0.64 |
| 1:A:78:VAL:HG11 | 1:A:87:PHE:CE2 | 2.32 | 0.64 |
| 2:B:278:ARG:HD2 | 2:B:278:ARG:H | 1.59 | 0.64 |
| 1:C:138:PHE:CZ | 1:C:235:VAL:HG11 | 2.30 | 0.64 |
| 1:A:138:PHE:CZ | 1:A:235:VAL:HG11 | 2.26 | 0.64 |
| 1:A:292:THR:HA | 1:A:295:CYS:HB3 | 1.80 | 0.64 |
| 1:A:285:GLN:OE1 | 1:A:372:GLN:HG2 | 1.96 | 0.64 |
| 1:A:433:GLU:HA | 1:A:433:GLU:OE1 | 1.97 | 0.64 |
| 2:B:133:GLN:HE22 | 2:B:252:LEU:H | 1.43 | 0.64 |
| 2:B:51:VAL:C | 2:B:53:TYR:H | 2.00 | 0.64 |
| 2:B:71:GLU:HB2 | 2:B:72:PRO:CD | 2.27 | 0.64 |
| 1:C:267:PHE:N | 1:C:267:PHE:HD1 | 1.94 | 0.64 |
| 1:C:203:MET:SD | 1:C:388:TRP:CD1 | 2.91 | 0.64 |
| 2:D:288:VAL:N | 2:D:289:PRO:HD2 | 2.12 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:SER:O | 1:A:189:LEU:HD23 | 1.97 | 0.64 |
| 1:A:16:ILE:HG22 | 1:A:17:GLY:H | 1.62 | 0.64 |
| 1:A:191:THR:HB | 1:A:421:ALA:HB1 | 1.79 | 0.64 |
| 2:B:192:HIS:O | 2:B:194:LEU:N | 2.30 | 0.64 |
| 2:B:2:ARG:HG3 | 2:B:133:GLN:HE21 | 1.58 | 0.64 |
| 1:C:191:THR:CB | 1:C:421:ALA:HB1 | 2.27 | 0.64 |
| 2:D:255:LEU:HD23 | 2:D:259:MET:HG3 | 1.80 | 0.64 |
| 1:A:287:SER:N | 1:A:290:GLU:HB2 | 2.13 | 0.64 |
| 1:A:350:GLY:O | 1:A:351:PHE:CD1 | 2.50 | 0.64 |
| 1:A:77:GLU:O | 1:A:83:TYR:HB2 | 1.97 | 0.64 |
| 1:A:86:LEU:HD22 | 1:A:89:PRO:HD3 | 1.79 | 0.64 |
| 2:B:183:GLU:HB3 | 2:B:184:PRO:CD | 2.26 | 0.64 |
| 2:B:339:ASN:O | 2:B:341:SER:N | 2.30 | 0.64 |
| 2:D:386:GLU:O | 2:D:388:PHE:N | 2.31 | 0.64 |
| 1:A:111:GLY:O | 1:A:113:GLU:N | 2.31 | 0.64 |
| 1:A:276:ILE:O | 1:A:369:ALA:HB3 | 1.98 | 0.64 |
| 1:A:87:PHE:HE2 | 1:A:92:LEU:HD21 | 1.60 | 0.64 |
| 1:C:160:ASP:O | 1:C:161:TYR:CD1 | 2.50 | 0.64 |
| 2:D:311:ARG:HB2 | 2:D:344:VAL:N | 2.12 | 0.64 |
| 2:D:377:PHE:O | 2:D:378:ILE:HG12 | 1.98 | 0.64 |
| 2:D:184:PRO:HB2 | 2:D:399:PHE:CZ | 2.32 | 0.64 |
| 2:D:92:PHE:HD1 | 2:D:118:VAL:HG22 | 1.61 | 0.64 |
| 1:C:331:ALA:HA | 1:C:334:THR:OG1 | 1.98 | 0.64 |
| 1:C:172:TYR:CE2 | 1:C:391:LEU:HD22 | 2.32 | 0.64 |
| 2:D:111:GLY:C | 2:D:113:GLU:H | 1.99 | 0.64 |
| 2:D:129:CYS:O | 2:D:130:ASP:O | 2.15 | 0.64 |
| 2:D:391:ILE:CD1 | 2:D:391:ILE:H | 2.10 | 0.64 |
| 2:D:59:ASN:ND2 | 2:D:60:LYS:N | 2.45 | 0.64 |
| 2:B:123:ARG:CZ | 2:B:160:GLU:OE2 | 2.45 | 0.64 |
| 2:B:385:GLN:NE2 | 2:B:433:GLN:HE21 | 1.96 | 0.64 |
| 2:B:80:SER:C | 2:B:82:PRO:HD2 | 2.18 | 0.64 |
| 1:C:104:ALA:HA | 1:C:108:TYR:CD2 | 2.31 | 0.64 |
| 2:D:385:GLN:HG2 | 2:D:433:GLN:HE21 | 1.62 | 0.64 |
| 1:A:186:ASN:HD22 | 1:A:391:LEU:HD11 | 1.63 | 0.63 |
| 2:B:371:LEU:HB3 | 2:B:373:MET:O | 1.97 | 0.63 |
| 2:B:427:ASP:O | 2:B:429:VAL:N | 2.31 | 0.63 |
| 2:B:59:ASN:HB2 | 2:B:64:ARG:CZ | 2.28 | 0.63 |
| 1:C:27:GLU:CG | 1:C:28:HIS:H | 2.10 | 0.63 |
| 2:D:140:SER:OG | 2:D:171:VAL:HB | 1.99 | 0.63 |
| 1:A:5:ILE:HD12 | 1:A:125:LEU:HD22 | 1.80 | 0.63 |
| 2:B:16:ILE:HG12 | 2:B:17:GLY:N | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:320:ARG:N | 2:B:374:SER:O | 2.29 | 0.63 |
| 1:C:287:SER:C | 1:C:289:ALA:H | 2.00 | 0.63 |
| 1:C:363:VAL:H | 1:C:367:ASP:HB2 | 1.61 | 0.63 |
| 2:D:102:ASN:HD22 | 2:D:105:LYS:CG | 2.11 | 0.63 |
| 2:D:345:GLU:O | 2:D:345:GLU:HG2 | 1.96 | 0.63 |
| 1:A:158:SER:HB3 | 1:A:166:LYS:NZ | 2.13 | 0.63 |
| 1:A:217:LEU:O | 1:A:219:ILE:HG13 | 1.99 | 0.63 |
| 1:A:259:LEU:HD11 | 1:A:378:LEU:HD13 | 1.79 | 0.63 |
| 1:A:307:PRO:HB3 | 1:A:381:THR:HG21 | 1.80 | 0.63 |
| 2:B:104:ALA:O | 2:B:108:TYR:HB2 | 1.98 | 0.63 |
| 2:B:140:SER:OG | 2:B:171:VAL:HB | 1.98 | 0.63 |
| 1:C:215:ARG:HH22 | 1:C:300:ASN:HD21 | 1.45 | 0.63 |
| 1:C:75:ILE:HG12 | 1:C:75:ILE:O | 1.97 | 0.63 |
| 1:C:101:ASN:CG | 2:D:254:LYS:HD3 | 2.17 | 0.63 |
| 2:D:287:THR:OG1 | 2:D:290:GLU:HB2 | 1.98 | 0.63 |
| 1:A:241:SER:HA | 1:A:320:ARG:NH2 | 2.13 | 0.63 |
| 1:A:263:PRO:O | 1:A:265:ALA:N | 2.28 | 0.63 |
| 1:A:217:LEU:HD11 | 1:A:368:LEU:HD22 | 1.81 | 0.63 |
| 1:A:43:GLY:O | 1:A:47:ASP:CG | 2.37 | 0.63 |
| 1:A:87:PHE:N | 1:A:87:PHE:CD2 | 2.63 | 0.63 |
| 2:B:137:LEU:HD23 | 2:B:154:ILE:HD11 | 1.80 | 0.63 |
| 2:B:174:SER:HB2 | 2:B:207:GLU:N | 2.12 | 0.63 |
| 2:B:357:ASP:HB3 | 2:B:358:ILE:HD12 | 1.81 | 0.63 |
| 1:C:404:PHE:HD1 | 1:C:404:PHE:N | 1.95 | 0.63 |
| 2:D:158:ARG:O | 2:D:160:GLU:N | 2.31 | 0.63 |
| 2:B:288:VAL:N | 2:B:289:PRO:HD2 | 2.14 | 0.63 |
| 1:C:243:ARG:CZ | 1:C:243:ARG:HA | 2.28 | 0.63 |
| 1:C:355:ILE:N | 1:C:355:ILE:HD12 | 2.13 | 0.63 |
| 1:C:404:PHE:CD1 | 1:C:404:PHE:N | 2.67 | 0.63 |
| 1:A:215:ARG:NH2 | 1:A:216:ASN:OD1 | 2.32 | 0.63 |
| 1:A:256:GLN:HA | 1:A:260:VAL:HG23 | 1.81 | 0.63 |
| 2:B:385:GLN:HG2 | 2:B:433:GLN:HE21 | 1.62 | 0.63 |
| 1:C:78:VAL:HG11 | 1:C:92:LEU:HD21 | 1.80 | 0.63 |
| 2:D:339:ASN:C | 2:D:341:SER:H | 2.01 | 0.63 |
| 2:D:5:VAL:HB | 2:D:135:PHE:HD2 | 1.62 | 0.63 |
| 1:A:72:PRO:HB3 | 1:A:94:THR:OG1 | 1.98 | 0.63 |
| 2:B:390:ARG:C | 2:B:392:SER:N | 2.53 | 0.63 |
| 1:C:243:ARG:HH12 | 1:C:250:VAL:CG1 | 2.11 | 0.63 |
| 2:D:158:ARG:HD3 | 2:D:197:ASN:CG | 2.18 | 0.63 |
| 1:A:311:LYS:CG | 1:A:344:VAL:HG22 | 2.28 | 0.63 |
| 1:A:291:ILE:HD12 | 1:A:373:ARG:HG3 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:399:PHE:CE2 | 2:B:404:PHE:HB3 | 2.34 | 0.63 |
| 2:B:71:GLU:HB2 | 2:B:72:PRO:HD2 | 1.79 | 0.63 |
| 1:C:206:ASN:HB3 | 1:C:210:TYR:HE2 | 1.61 | 0.63 |
| 1:C:373:ARG:NH1 | 1:C:373:ARG:HB3 | 2.12 | 0.63 |
| 1:C:385:ALA:HB2 | 1:C:432:TYR:HD2 | 1.63 | 0.63 |
| 2:D:107:HIS:CD2 | 2:D:151:THR:HG23 | 2.33 | 0.63 |
| 1:A:172:TYR:HB3 | 1:A:205:ASP:N | 2.14 | 0.62 |
| 1:C:93:ILE:HD13 | 1:C:118:VAL:CG2 | 2.26 | 0.62 |
| 2:D:215:ARG:HA | 2:D:215:ARG:NE | 2.13 | 0.62 |
| 2:D:286:LEU:HD13 | 2:D:371:LEU:O | 1.99 | 0.62 |
| 2:D:391:ILE:O | 2:D:425:MET:HE1 | 1.98 | 0.62 |
| 1:A:362:VAL:HG21 | 1:A:369:ALA:O | 1.98 | 0.62 |
| 1:A:70:LEU:HD12 | 1:A:145:THR:CA | 2.17 | 0.62 |
| 1:A:102:ASN:ND2 | 2:B:257:VAL:HG11 | 2.09 | 0.62 |
| 2:B:417:GLU:O | 2:B:417:GLU:HG3 | 1.98 | 0.62 |
| 1:C:156:ARG:O | 1:C:159:VAL:HB | 2.00 | 0.62 |
| 2:D:107:HIS:HD2 | 2:D:151:THR:HG23 | 1.64 | 0.62 |
| 2:D:264:ARG:HG3 | 2:D:264:ARG:NH1 | 2.12 | 0.62 |
| 2:D:398:MET:O | 2:D:400:ARG:N | 2.32 | 0.62 |
| 1:A:160:ASP:O | 1:A:161:TYR:CD1 | 2.52 | 0.62 |
| 1:A:171:ILE:HD12 | 1:A:171:ILE:H | 1.62 | 0.62 |
| 2:B:292:THR:HG23 | 2:B:319:PHE:HZ | 1.63 | 0.62 |
| 2:D:258:ASN:OD1 | 2:D:352:LYS:NZ | 2.29 | 0.62 |
| 3:E:35:UNK:O | 3:E:39:UNK:N | 2.32 | 0.62 |
| 1:A:293:ASN:O | 1:A:297:GLU:OE1 | 2.17 | 0.62 |
| 2:B:267:PHE:HB2 | 2:B:384:ILE:HD13 | 1.80 | 0.62 |
| 3:E:75:UNK:O | 3:E:76:UNK:C | 2.47 | 0.62 |
| 1:A:258:ASN:O | 1:A:259:LEU:CB | 2.48 | 0.62 |
| 1:A:280:LYS:O | 1:A:282:TYR:HE2 | 1.82 | 0.62 |
| 2:B:165:ILE:HD13 | 2:B:199:ASP:OD1 | 1.99 | 0.62 |
| 2:B:192:HIS:C | 2:B:194:LEU:N | 2.49 | 0.62 |
| 2:B:241:CYS:C | 2:B:243:ARG:N | 2.48 | 0.62 |
| 2:B:292:THR:HG23 | 2:B:319:PHE:CZ | 2.35 | 0.62 |
| 2:B:396:THR:CG2 | 2:B:400:ARG:HD3 | 2.28 | 0.62 |
| 2:B:62:VAL:O | 2:B:62:VAL:HG23 | 1.99 | 0.62 |
| 1:C:154:MET:SD | 1:C:197:HIS:CD2 | 2.93 | 0.62 |
| 1:C:307:PRO:HB3 | 1:C:381:THR:HG21 | 1.81 | 0.62 |
| 2:D:166:MET:HE3 | 2:D:197:ASN:HB3 | 1.82 | 0.62 |
| 2:D:267:PHE:HB2 | 2:D:384:ILE:HD13 | 1.81 | 0.62 |
| 2:D:385:GLN:HG2 | 2:D:433:GLN:NE2 | 2.13 | 0.62 |
| 1:A:156:ARG:O | 1:A:159:VAL:HB | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:132:LEU:O | 2:B:132:LEU:HD23 | 2.00 | 0.62 |
| 2:B:123:ARG:NE | 2:B:160:GLU:OE2 | 2.32 | 0.62 |
| 2:D:191:VAL:CG1 | 2:D:421:ALA:HA | 2.29 | 0.62 |
| 1:A:373:ARG:HB3 | 1:A:373:ARG:NH1 | 2.15 | 0.62 |
| 2:B:130:ASP:OD2 | 2:B:131:CYS:N | 2.32 | 0.62 |
| 2:B:215:ARG:NE | 2:B:215:ARG:HA | 2.13 | 0.62 |
| 1:C:407:TRP:CZ2 | 2:D:256:ALA:O | 2.53 | 0.62 |
| 2:D:282:GLN:HA | 2:D:285:ALA:HB2 | 1.80 | 0.62 |
| 1:A:267:PHE:HD1 | 1:A:267:PHE:N | 1.96 | 0.62 |
| 1:A:344:VAL:HG11 | 1:A:346:TRP:HE1 | 1.63 | 0.62 |
| 2:B:218:LYS:O | 2:B:219:LEU:HB2 | 2.00 | 0.62 |
| 2:B:2:ARG:HE | 2:B:243:ARG:HD2 | 1.64 | 0.62 |
| 1:C:27:GLU:HG3 | 1:C:28:HIS:ND1 | 2.14 | 0.62 |
| 1:C:311:LYS:HD3 | 1:C:344:VAL:HG22 | 1.80 | 0.62 |
| 1:C:331:ALA:C | 1:C:333:ALA:N | 2.51 | 0.62 |
| 1:C:344:VAL:HG12 | 1:C:345:ASP:N | 2.15 | 0.62 |
| 1:C:291:ILE:HG21 | 1:C:375:VAL:HG21 | 1.82 | 0.62 |
| 2:D:24:ILE:HG22 | 2:D:24:ILE:O | 1.98 | 0.62 |
| 2:D:333:LEU:HG | 2:D:337:ASN:ND2 | 2.15 | 0.62 |
| 2:D:348:PRO:O | 2:D:349:ASN:HB3 | 2.00 | 0.62 |
| 2:D:2:ARG:O | 2:D:57:ALA:HB1 | 1.99 | 0.62 |
| 1:A:132:LEU:HB3 | 1:A:164:LYS:HD3 | 1.80 | 0.62 |
| 1:A:407:TRP:CZ2 | 2:B:256:ALA:O | 2.53 | 0.62 |
| 2:B:102:ASN:ND2 | 2:B:105:LYS:H | 1.98 | 0.62 |
| 2:B:105:LYS:HA | 2:B:109:THR:OG1 | 1.99 | 0.62 |
| 2:B:153:LEU:O | 2:B:157:ILE:N | 2.33 | 0.62 |
| 2:B:344:VAL:HG23 | 2:B:345:GLU:N | 2.15 | 0.62 |
| 2:B:58:GLY:C | 2:B:64:ARG:NE | 2.52 | 0.62 |
| 2:D:149:MET:CE | 2:D:149:MET:HA | 2.29 | 0.62 |
| 2:D:206:ASN:ND2 | 2:D:227:LEU:HD21 | 2.07 | 0.62 |
| 1:A:181:VAL:HG13 | 1:A:408:TYR:OH | 2.00 | 0.62 |
| 1:A:365:GLY:O | 1:A:368:LEU:HD11 | 2.00 | 0.62 |
| 2:B:163:ASP:CG | 2:B:164:ARG:H | 2.03 | 0.62 |
| 1:C:345:ASP:O | 1:C:347:CYS:N | 2.31 | 0.62 |
| 2:D:158:ARG:HA | 2:D:197:ASN:ND2 | 2.15 | 0.62 |
| 2:D:2:ARG:HH11 | 2:D:251:ASP:HA | 1.64 | 0.62 |
| 3:E:58:UNK:O | 3:E:60:UNK:N | 2.33 | 0.62 |
| 2:B:280:SER:O | 2:B:282:GLN:HG2 | 1.99 | 0.61 |
| 2:B:385:GLN:HG2 | 2:B:433:GLN:NE2 | 2.14 | 0.61 |
| 1:C:191:THR:HB | 1:C:421:ALA:HB1 | 1.79 | 0.61 |
| 1:C:242:LEU:O | 1:C:243:ARG:NH1 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:267:PHE:H | 1:C:267:PHE:HD1 | 1.45 | 0.61 |
| 1:C:344:VAL:HG11 | 1:C:346:TRP:HE1 | 1.63 | 0.61 |
| 2:D:358:ILE:CD1 | 2:D:358:ILE:H | 2.13 | 0.61 |
| 1:A:210:TYR:CE2 | 1:A:227:LEU:HD23 | 2.34 | 0.61 |
| 1:A:317:LEU:HD23 | 1:A:377:MET:CB | 2.30 | 0.61 |
| 2:B:22:GLU:OE2 | 2:B:22:GLU:N | 2.33 | 0.61 |
| 1:C:362:VAL:CG2 | 1:C:370:LYS:HA | 2.28 | 0.61 |
| 2:D:280:SER:O | 2:D:282:GLN:HG2 | 2.00 | 0.61 |
| 1:A:413:MET:SD | 3:E:15:UNK:CA | 2.83 | 0.61 |
| 2:B:326:LYS:O | 2:B:330:GLU:HG3 | 2.00 | 0.61 |
| 1:C:139:HIS:CD2 | 1:C:150:THR:HG21 | 2.34 | 0.61 |
| 1:C:238:ILE:HG22 | 1:C:239:THR:N | 2.15 | 0.61 |
| 2:D:123:ARG:NE | 2:D:160:GLU:OE2 | 2.32 | 0.61 |
| 1:A:175:PRO:O | 1:A:177:VAL:HG23 | 2.00 | 0.61 |
| 2:B:5:VAL:HB | 2:B:135:PHE:HD2 | 1.65 | 0.61 |
| 2:B:241:CYS:SG | 2:B:320:ARG:NH1 | 2.73 | 0.61 |
| 2:B:218:LYS:NZ | 2:B:278:ARG:N | 2.46 | 0.61 |
| 1:C:2:ARG:NH2 | 1:C:133:GLN:NE2 | 2.46 | 0.61 |
| 1:C:414:GLU:CD | 1:C:414:GLU:N | 2.54 | 0.61 |
| 1:C:86:LEU:CD2 | 1:C:89:PRO:HD3 | 2.29 | 0.61 |
| 2:D:237:GLY:O | 2:D:376:THR:HG21 | 2.01 | 0.61 |
| 3:E:4:UNK:O | 3:E:6:UNK:N | 2.33 | 0.61 |
| 1:A:362:VAL:CG2 | 1:A:370:LYS:HA | 2.31 | 0.61 |
| 2:B:353:THR:CG2 | 2:B:354:ALA:H | 2.14 | 0.61 |
| 2:B:396:THR:HG23 | 2:B:400:ARG:CD | 2.27 | 0.61 |
| 1:C:258:ASN:HD22 | 1:C:258:ASN:H | 1.48 | 0.61 |
| 2:D:264:ARG:HH22 | 2:D:431:GLU:HG3 | 1.64 | 0.61 |
| 2:D:316:ALA:HB3 | 2:D:378:ILE:HB | 1.82 | 0.61 |
| 1:A:88:HIS:N | 1:A:91:GLN:OE1 | 2.33 | 0.61 |
| 2:B:191:VAL:HG13 | 2:B:421:ALA:HA | 1.83 | 0.61 |
| 2:B:2:ARG:NH1 | 2:B:251:ASP:HA | 2.15 | 0.61 |
| 2:B:312:TYR:HA | 2:B:381:SER:HA | 1.81 | 0.61 |
| 2:B:59:ASN:CG | 2:B:60:LYS:N | 2.54 | 0.61 |
| 2:D:287:THR:O | 2:D:290:GLU:HB3 | 2.01 | 0.61 |
| 1:A:398:MET:O | 1:A:400:ALA:N | 2.34 | 0.61 |
| 2:B:102:ASN:HD22 | 2:B:105:LYS:CG | 2.13 | 0.61 |
| 2:B:404:PHE:HD2 | 2:B:404:PHE:O | 1.83 | 0.61 |
| 1:C:164:LYS:N | 1:C:164:LYS:HZ1 | 1.98 | 0.61 |
| 1:C:78:VAL:O | 1:C:82:THR:HA | 2.01 | 0.61 |
| 2:D:51:VAL:C | 2:D:53:TYR:H | 2.03 | 0.61 |
| 1:A:139:HIS:NE2 | 1:A:150:THR:HG21 | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:92:PHE:HD1 | 2:B:118:VAL:HG22 | 1.63 | 0.61 |
| 1:C:101:ASN:OD1 | 2:D:254:LYS:NZ | 2.30 | 0.61 |
| 1:C:171:ILE:CG2 | 1:C:206:ASN:OD1 | 2.48 | 0.61 |
| 1:C:258:ASN:ND2 | 1:C:258:ASN:H | 1.99 | 0.61 |
| 1:C:65:ALA:O | 1:C:91:GLN:HB2 | 2.01 | 0.61 |
| 1:C:72:PRO:HB3 | 1:C:94:THR:OG1 | 2.01 | 0.61 |
| 2:D:94:PHE:HB2 | 2:D:114:LEU:CD1 | 2.31 | 0.61 |
| 1:A:103:TYR:CG | 1:A:188:ILE:HD13 | 2.36 | 0.61 |
| 1:A:101:ASN:O | 1:A:185:TYR:OH | 2.19 | 0.61 |
| 1:A:27:GLU:CG | 1:A:28:HIS:H | 2.12 | 0.61 |
| 1:A:321:GLY:N | 1:A:356:ASN:O | 2.34 | 0.61 |
| 2:B:223:THR:N | 2:B:226:ASP:OD2 | 2.30 | 0.61 |
| 1:C:188:ILE:HG22 | 1:C:417:GLU:O | 2.01 | 0.61 |
| 1:C:259:LEU:HD21 | 1:C:378:LEU:HB3 | 1.81 | 0.61 |
| 1:C:393:HIS:C | 1:C:395:PHE:H | 2.03 | 0.61 |
| 2:D:261:PRO:HB2 | 2:D:262:PHE:CD1 | 2.36 | 0.61 |
| 2:D:60:LYS:NZ | 2:D:60:LYS:N | 2.49 | 0.61 |
| 1:A:137:VAL:CG1 | 1:A:154:MET:HE2 | 2.29 | 0.61 |
| 2:B:140:SER:CB | 2:B:171:VAL:HB | 2.31 | 0.61 |
| 2:B:189:LEU:C | 2:B:191:VAL:N | 2.55 | 0.61 |
| 1:C:164:LYS:HZ2 | 1:C:164:LYS:HB2 | 1.66 | 0.61 |
| 2:D:5:VAL:HG22 | 2:D:64:ARG:HD3 | 1.83 | 0.61 |
| 3:E:35:UNK:HA | 3:E:38:UNK:CB | 2.31 | 0.61 |
| 3:E:50:UNK:C | 3:E:52:UNK:N | 2.62 | 0.61 |
| 1:A:143:GLY:O | 1:A:144:GLY:O | 2.18 | 0.60 |
| 1:A:103:TYR:HB2 | 1:A:185:TYR:CD1 | 2.36 | 0.60 |
| 1:A:242:LEU:HB3 | 1:A:250:VAL:HG11 | 1.83 | 0.60 |
| 1:A:354:GLY:C | 1:A:355:ILE:HD12 | 2.21 | 0.60 |
| 2:B:311:ARG:HG3 | 2:B:311:ARG:HH11 | 1.65 | 0.60 |
| 2:B:59:ASN:HB2 | 2:B:64:ARG:HE | 1.63 | 0.60 |
| 1:C:221:ARG:H | 1:C:221:ARG:CD | 2.13 | 0.60 |
| 2:D:350:ASN:ND2 | 2:D:351:VAL:HG23 | 2.16 | 0.60 |
| 2:D:296:PHE:HA | 2:D:377:PHE:CE2 | 2.35 | 0.60 |
| 2:D:385:GLN:HE21 | 2:D:433:GLN:HG2 | 1.65 | 0.60 |
| 1:A:282:TYR:HD2 | 1:A:282:TYR:N | 1.98 | 0.60 |
| 1:A:283:HIS:O | 1:A:284:GLU:HB3 | 2.00 | 0.60 |
| 2:B:321:GLY:CA | 2:B:359:PRO:HB3 | 2.27 | 0.60 |
| 2:B:286:LEU:HD13 | 2:B:371:LEU:O | 2.00 | 0.60 |
| 2:B:380:ASN:C | 2:B:380:ASN:HD22 | 2.05 | 0.60 |
| 2:B:66:ILE:O | 2:B:66:ILE:HG12 | 2.01 | 0.60 |
| 2:B:75:MET:O | 2:B:76:ASP:C | 2.39 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:118:VAL:O | 2:D:120:ASP:N | 2.32 | 0.60 |
| 2:D:153:LEU:O | 2:D:157:ILE:N | 2.34 | 0.60 |
| 2:D:163:ASP:CG | 2:D:164:ARG:H | 2.04 | 0.60 |
| 2:D:307:PRO:C | 2:D:309:HIS:H | 2.04 | 0.60 |
| 2:D:109:THR:HG21 | 2:D:411:GLU:CG | 2.30 | 0.60 |
| 1:A:318:LEU:HB2 | 1:A:376:CYS:O | 2.01 | 0.60 |
| 2:B:134:GLY:HA3 | 2:B:165:ILE:O | 2.02 | 0.60 |
| 2:B:287:THR:O | 2:B:290:GLU:HB3 | 2.01 | 0.60 |
| 2:B:308:ARG:NH2 | 2:B:342:TYR:CD1 | 2.61 | 0.60 |
| 2:B:348:PRO:O | 2:B:349:ASN:HB3 | 2.01 | 0.60 |
| 1:C:90:GLU:O | 1:C:121:ARG:NH1 | 2.34 | 0.60 |
| 1:C:126:ALA:HB1 | 1:C:132:LEU:HD11 | 1.83 | 0.60 |
| 1:C:16:ILE:HD12 | 1:C:171:ILE:HD11 | 1.83 | 0.60 |
| 1:C:183:GLU:HB2 | 1:C:184:PRO:CD | 2.30 | 0.60 |
| 1:C:185:TYR:O | 1:C:188:ILE:HD12 | 2.01 | 0.60 |
| 1:A:7:ILE:HG22 | 1:A:66:VAL:CB | 2.23 | 0.60 |
| 2:B:118:VAL:O | 2:B:120:ASP:N | 2.28 | 0.60 |
| 2:B:149:MET:O | 2:B:152:LEU:HB3 | 2.01 | 0.60 |
| 1:C:158:SER:HB3 | 1:C:166:LYS:NZ | 2.17 | 0.60 |
| 2:D:265:LEU:O | 2:D:266:HIS:ND1 | 2.34 | 0.60 |
| 2:D:312:TYR:HA | 2:D:381:SER:HA | 1.83 | 0.60 |
| 1:A:222:PRO:CB | 1:A:227:LEU:HD11 | 2.19 | 0.60 |
| 1:A:257:THR:OG1 | 1:A:258:ASN:ND2 | 2.35 | 0.60 |
| 2:B:2:ARG:CG | 2:B:133:GLN:NE2 | 2.58 | 0.60 |
| 1:C:276:ILE:O | 1:C:369:ALA:HB3 | 2.01 | 0.60 |
| 2:D:191:VAL:HG13 | 2:D:421:ALA:HA | 1.82 | 0.60 |
| 1:A:175:PRO:HD2 | 1:A:207:GLU:CB | 2.05 | 0.60 |
| 1:A:269:LEU:HD21 | 1:A:301:GLN:NE2 | 2.17 | 0.60 |
| 2:B:11:GLN:HG3 | 2:B:15:GLN:NE2 | 2.17 | 0.60 |
| 2:B:107:HIS:CD2 | 2:B:151:THR:HG23 | 2.35 | 0.60 |
| 2:B:184:PRO:HB2 | 2:B:399:PHE:CZ | 2.35 | 0.60 |
| 2:B:191:VAL:CG1 | 2:B:421:ALA:HA | 2.30 | 0.60 |
| 1:C:332:ILE:HD11 | 1:C:353:VAL:HG21 | 1.84 | 0.60 |
| 2:D:339:ASN:O | 2:D:341:SER:N | 2.34 | 0.60 |
| 2:D:399:PHE:CE2 | 2:D:404:PHE:HB3 | 2.37 | 0.60 |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:N | 2.17 | 0.60 |
| 2:B:296:PHE:HA | 2:B:377:PHE:CE2 | 2.36 | 0.60 |
| 1:C:139:HIS:NE2 | 1:C:150:THR:HG21 | 2.16 | 0.60 |
| 1:C:197:HIS:NE2 | 1:C:198:SER:HB3 | 2.17 | 0.60 |
| 1:C:21:TRP:HA | 1:C:24:TYR:HB2 | 1.82 | 0.60 |
| 1:C:371:VAL:HG12 | 1:C:372:GLN:N | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:305:CYS:SG | 1:C:384:ILE:HA | 2.42 | 0.60 |
| 1:C:9:VAL:HA | 1:C:68:VAL:O | 2.02 | 0.60 |
| 1:C:77:GLU:O | 1:C:83:TYR:HB2 | 2.02 | 0.60 |
| 2:D:111:GLY:C | 2:D:113:GLU:N | 2.53 | 0.60 |
| 2:D:139:HIS:C | 2:D:139:HIS:CD2 | 2.75 | 0.60 |
| 1:A:23:LEU:C | 1:A:25:CYS:H | 2.05 | 0.60 |
| 1:A:291:ILE:HG22 | 1:A:292:THR:N | 2.17 | 0.60 |
| 1:A:220:GLU:OE2 | 2:B:326:LYS:HD3 | 2.01 | 0.60 |
| 1:C:280:LYS:O | 1:C:282:TYR:HE2 | 1.84 | 0.60 |
| 2:D:159:GLU:OE2 | 3:E:82:UNK:CB | 2.50 | 0.60 |
| 1:A:215:ARG:NH2 | 1:A:300:ASN:HD21 | 1.99 | 0.60 |
| 1:A:31:GLN:CB | 1:A:32:PRO:HD2 | 2.27 | 0.60 |
| 1:A:360:PRO:HB3 | 1:A:374:ALA:HB2 | 1.83 | 0.60 |
| 1:A:69:ASP:OD1 | 1:A:71:GLU:HG3 | 2.02 | 0.60 |
| 1:A:9:VAL:HG21 | 1:A:150:THR:HB | 1.84 | 0.60 |
| 2:B:132:LEU:C | 2:B:132:LEU:HD23 | 2.22 | 0.60 |
| 2:B:311:ARG:HH11 | 2:B:344:VAL:HA | 1.67 | 0.60 |
| 1:C:209:ILE:H | 1:C:209:ILE:HD12 | 1.65 | 0.60 |
| 1:C:26:LEU:HG | 1:C:361:THR:CB | 2.32 | 0.60 |
| 1:C:287:SER:OG | 1:C:290:GLU:HG3 | 2.02 | 0.60 |
| 1:C:354:GLY:C | 1:C:355:ILE:HD12 | 2.22 | 0.60 |
| 2:D:102:ASN:HB3 | 2:D:105:LYS:HB2 | 1.83 | 0.60 |
| 2:D:102:ASN:ND2 | 2:D:105:LYS:H | 1.99 | 0.60 |
| 2:D:239:THR:O | 2:D:241:CYS:O | 2.20 | 0.60 |
| 2:D:398:MET:C | 2:D:400:ARG:H | 2.05 | 0.60 |
| 1:A:100:ALA:HA | 1:A:105:ARG:HD2 | 1.83 | 0.60 |
| 2:B:194:LEU:HD11 | 2:B:428:LEU:HD11 | 1.84 | 0.60 |
| 1:C:332:ILE:CD1 | 1:C:353:VAL:HG21 | 2.31 | 0.60 |
| 1:C:46:ASP:N | 1:C:46:ASP:OD2 | 2.34 | 0.60 |
| 3:E:83:UNK:C | 3:E:85:UNK:N | 2.63 | 0.60 |
| 1:A:69:ASP:HB3 | 1:A:75:ILE:CG2 | 2.26 | 0.59 |
| 2:B:266:HIS:HB2 | 2:B:380:ASN:OD1 | 2.02 | 0.59 |
| 2:B:60:LYS:N | 2:B:60:LYS:NZ | 2.50 | 0.59 |
| 1:C:329:ASN:HA | 1:C:332:ILE:HB | 1.83 | 0.59 |
| 2:D:102:ASN:O | 2:D:105:LYS:HB2 | 2.01 | 0.59 |
| 2:D:127:GLU:O | 2:D:128:SER:C | 2.40 | 0.59 |
| 2:D:166:MET:HG3 | 2:D:167:ASN:N | 2.16 | 0.59 |
| 2:D:240:THR:C | 2:D:243:ARG:HB2 | 2.22 | 0.59 |
| 2:D:263:PRO:O | 2:D:265:LEU:N | 2.33 | 0.59 |
| 2:D:380:ASN:HD22 | 2:D:380:ASN:C | 2.05 | 0.59 |
| 2:D:58:GLY:C | 2:D:64:ARG:NE | 2.55 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:243:ARG:HH12 | 2:B:252:LEU:HD12 | 1.67 | 0.59 |
| 2:B:350:ASN:HD22 | 2:B:351:VAL:HG23 | 1.68 | 0.59 |
| 2:B:322:ARG:NE | 2:B:357:ASP:HB3 | 2.17 | 0.59 |
| 2:B:303:ALA:HB1 | 2:B:387:LEU:CD1 | 2.32 | 0.59 |
| 1:C:264:ARG:NH2 | 1:C:424:ASP:OD1 | 2.35 | 0.59 |
| 1:C:321:GLY:HA2 | 1:C:357:TYR:O | 2.02 | 0.59 |
| 1:C:423:GLU:O | 1:C:427:ALA:N | 2.28 | 0.59 |
| 1:C:433:GLU:C | 1:C:435:VAL:H | 2.04 | 0.59 |
| 1:C:9:VAL:HG23 | 1:C:9:VAL:O | 2.01 | 0.59 |
| 2:D:218:LYS:HZ2 | 2:D:277:SER:HB3 | 1.67 | 0.59 |
| 1:A:182:VAL:CG1 | 1:A:183:GLU:N | 2.65 | 0.59 |
| 1:A:209:ILE:C | 1:A:211:ASP:N | 2.51 | 0.59 |
| 1:A:77:GLU:O | 1:A:83:TYR:CB | 2.50 | 0.59 |
| 2:B:259:MET:HE1 | 2:B:316:ALA:N | 2.16 | 0.59 |
| 1:C:209:ILE:C | 1:C:211:ASP:N | 2.55 | 0.59 |
| 2:D:99:ALA:HA | 2:D:105:LYS:HD3 | 1.83 | 0.59 |
| 2:D:390:ARG:C | 2:D:392:SER:N | 2.51 | 0.59 |
| 2:D:266:HIS:ND1 | 2:D:432:TYR:CZ | 2.70 | 0.59 |
| 2:D:58:GLY:O | 2:D:64:ARG:NE | 2.34 | 0.59 |
| 1:A:238:ILE:N | 1:A:241:SER:HB3 | 2.18 | 0.59 |
| 1:A:395:PHE:CD1 | 1:A:395:PHE:C | 2.75 | 0.59 |
| 1:A:44:GLY:HA3 | 1:A:47:ASP:HA | 1.84 | 0.59 |
| 2:B:416:MET:C | 2:B:418:PHE:N | 2.56 | 0.59 |
| 2:B:12:CYS:HB3 | 5:B:501:GDP:C8 | 2.37 | 0.59 |
| 1:C:237:SER:CA | 1:C:241:SER:HB2 | 2.28 | 0.59 |
| 1:C:395:PHE:CD1 | 1:C:395:PHE:C | 2.75 | 0.59 |
| 1:C:413:MET:H | 1:C:413:MET:CE | 2.15 | 0.59 |
| 1:C:86:LEU:HD22 | 1:C:89:PRO:HD3 | 1.84 | 0.59 |
| 2:D:141:LEU:HB3 | 2:D:186:ASN:CB | 2.32 | 0.59 |
| 2:D:75:MET:O | 2:D:76:ASP:C | 2.40 | 0.59 |
| 2:D:87:PHE:O | 2:D:90:ASP:OD1 | 2.19 | 0.59 |
| 1:A:68:VAL:HG21 | 1:A:118:VAL:HG21 | 1.83 | 0.59 |
| 1:A:87:PHE:CE2 | 1:A:92:LEU:HD21 | 2.38 | 0.59 |
| 2:B:102:ASN:HD22 | 2:B:105:LYS:N | 2.01 | 0.59 |
| 2:B:247:GLN:HG2 | 2:B:325:MET:SD | 2.42 | 0.59 |
| 2:B:391:ILE:CD1 | 2:B:391:ILE:H | 2.15 | 0.59 |
| 1:C:196:GLU:N | 1:C:196:GLU:CD | 2.55 | 0.59 |
| 1:C:261:PRO:CG | 1:C:380:ASN:HD21 | 2.13 | 0.59 |
| 2:D:66:ILE:HG12 | 2:D:66:ILE:O | 2.02 | 0.59 |
| 2:B:202:TYR:CE1 | 2:B:378:ILE:HD12 | 2.38 | 0.59 |
| 2:B:79:ARG:HA | 2:B:84:GLY:HA2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:94:PHE:HB2 | 2:B:114:LEU:CD1 | 2.33 | 0.59 |
| 1:C:413:MET:C | 1:C:414:GLU:OE1 | 2.41 | 0.59 |
| 2:D:169:PHE:CD2 | 2:D:235:MET:SD | 2.95 | 0.59 |
| 2:D:276:THR:HG21 | 2:D:281:GLN:HB3 | 1.84 | 0.59 |
| 2:D:312:TYR:CD2 | 2:D:381:SER:HB2 | 2.37 | 0.59 |
| 2:D:396:THR:HA | 2:D:400:ARG:HB3 | 1.83 | 0.59 |
| 1:A:101:ASN:OD1 | 2:B:254:LYS:HD3 | 2.02 | 0.59 |
| 1:A:345:ASP:C | 1:A:347:CYS:H | 2.06 | 0.59 |
| 2:B:18:ALA:O | 2:B:22:GLU:OE2 | 2.20 | 0.59 |
| 2:B:239:THR:O | 2:B:241:CYS:O | 2.19 | 0.59 |
| 2:B:2:ARG:HG3 | 2:B:133:GLN:CD | 2.21 | 0.59 |
| 1:C:258:ASN:O | 1:C:259:LEU:HB2 | 2.02 | 0.59 |
| 2:D:308:ARG:NH2 | 2:D:342:TYR:HB2 | 2.17 | 0.59 |
| 2:D:404:PHE:O | 2:D:404:PHE:HD2 | 1.85 | 0.59 |
| 3:E:67:UNK:O | 3:E:71:UNK:N | 2.35 | 0.59 |
| 2:B:181:VAL:O | 2:B:183:GLU:N | 2.35 | 0.59 |
| 2:B:2:ARG:NE | 2:B:243:ARG:CD | 2.64 | 0.59 |
| 2:B:253:ARG:HG3 | 2:B:253:ARG:NH1 | 2.17 | 0.59 |
| 2:B:307:PRO:C | 2:B:309:HIS:H | 2.06 | 0.59 |
| 2:B:395:PHE:HB3 | 2:B:422:GLU:OE1 | 2.03 | 0.59 |
| 1:C:103:TYR:N | 1:C:185:TYR:HE1 | 2.01 | 0.59 |
| 1:C:416:GLY:C | 1:C:418:PHE:N | 2.55 | 0.59 |
| 3:E:37:UNK:O | 3:E:38:UNK:C | 2.49 | 0.59 |
| 3:E:54:UNK:O | 3:E:56:UNK:N | 2.35 | 0.59 |
| 1:A:171:ILE:CG2 | 1:A:206:ASN:OD1 | 2.50 | 0.59 |
| 2:B:18:ALA:O | 2:B:20:PHE:N | 2.35 | 0.59 |
| 2:B:241:CYS:C | 2:B:243:ARG:H | 2.04 | 0.59 |
| 2:B:261:PRO:HB2 | 2:B:262:PHE:CD1 | 2.38 | 0.59 |
| 2:B:80:SER:OG | 2:B:81:GLY:N | 2.34 | 0.59 |
| 1:C:69:ASP:OD2 | 1:C:74:VAL:CG1 | 2.50 | 0.59 |
| 2:D:428:LEU:O | 2:D:432:TYR:HB2 | 2.03 | 0.59 |
| 1:A:183:GLU:HB2 | 1:A:184:PRO:HD3 | 1.85 | 0.58 |
| 2:B:385:GLN:OE1 | 2:B:429:VAL:HA | 2.03 | 0.58 |
| 2:B:75:MET:O | 2:B:76:ASP:O | 2.21 | 0.58 |
| 2:D:102:ASN:HB3 | 2:D:105:LYS:HD2 | 1.83 | 0.58 |
| 2:D:179:ASP:HB3 | 2:D:181:VAL:H | 1.66 | 0.58 |
| 2:D:51:VAL:N | 2:D:245:PRO:HB2 | 2.18 | 0.58 |
| 2:D:416:MET:C | 2:D:418:PHE:N | 2.56 | 0.58 |
| 1:A:269:LEU:C | 1:A:269:LEU:HD12 | 2.23 | 0.58 |
| 1:A:389:ALA:O | 1:A:392:ASP:HB3 | 2.03 | 0.58 |
| 1:C:286:LEU:O | 1:C:373:ARG:HD2 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:19:LYS:HA | 2:D:22:GLU:OE2 | 2.02 | 0.58 |
| 2:D:241:CYS:C | 2:D:243:ARG:N | 2.49 | 0.58 |
| 2:D:251:ASP:CG | 2:D:252:LEU:N | 2.56 | 0.58 |
| 2:B:179:ASP:HB2 | 2:B:182:VAL:CG2 | 2.33 | 0.58 |
| 2:B:197:ASN:O | 2:B:198:THR:HB | 2.02 | 0.58 |
| 2:B:200:GLU:CG | 2:B:268:PHE:CE2 | 2.86 | 0.58 |
| 1:C:217:LEU:HD23 | 1:C:219:ILE:CD1 | 2.33 | 0.58 |
| 1:C:256:GLN:O | 1:C:258:ASN:N | 2.36 | 0.58 |
| 1:A:241:SER:HB3 | 1:A:242:LEU:HD12 | 1.85 | 0.58 |
| 1:A:419:SER:O | 1:A:422:ARG:HG2 | 2.02 | 0.58 |
| 1:A:423:GLU:O | 1:A:427:ALA:N | 2.29 | 0.58 |
| 2:B:123:ARG:C | 2:B:125:GLU:H | 2.06 | 0.58 |
| 2:B:308:ARG:NH2 | 2:B:342:TYR:HB2 | 2.19 | 0.58 |
| 2:D:123:ARG:C | 2:D:125:GLU:H | 2.06 | 0.58 |
| 2:D:134:GLY:HA3 | 2:D:165:ILE:O | 2.03 | 0.58 |
| 2:D:9:ALA:HA | 2:D:68:VAL:O | 2.02 | 0.58 |
| 1:A:23:LEU:O | 1:A:26:LEU:HD12 | 2.03 | 0.58 |
| 1:A:26:LEU:HG | 1:A:361:THR:OG1 | 2.04 | 0.58 |
| 2:B:289:PRO:HB2 | 2:B:331:GLN:HE21 | 1.68 | 0.58 |
| 2:B:395:PHE:HD2 | 2:B:422:GLU:OE1 | 1.86 | 0.58 |
| 2:B:5:VAL:HA | 2:B:64:ARG:CD | 2.33 | 0.58 |
| 1:C:231:ILE:O | 1:C:235:VAL:HG23 | 2.04 | 0.58 |
| 2:D:307:PRO:O | 2:D:309:HIS:N | 2.36 | 0.58 |
| 2:D:321:GLY:CA | 2:D:359:PRO:HB3 | 2.32 | 0.58 |
| 3:E:66:UNK:O | 3:E:69:UNK:N | 2.37 | 0.58 |
| 1:A:186:ASN:O | 1:A:189:LEU:HB3 | 2.03 | 0.58 |
| 2:B:183:GLU:C | 2:B:185:TYR:N | 2.54 | 0.58 |
| 2:B:413:MET:SD | 2:B:417:GLU:HG2 | 2.43 | 0.58 |
| 2:D:12:CYS:HB2 | 5:D:503:GDP:PA | 2.43 | 0.58 |
| 1:A:38:SER:O | 1:A:39:ASP:HB3 | 2.04 | 0.58 |
| 2:B:158:ARG:HD3 | 2:B:197:ASN:CG | 2.23 | 0.58 |
| 2:B:198:THR:O | 2:B:200:GLU:N | 2.37 | 0.58 |
| 1:C:160:ASP:O | 1:C:161:TYR:CG | 2.57 | 0.58 |
| 2:D:409:THR:HA | 2:D:412:GLY:O | 2.03 | 0.58 |
| 3:E:58:UNK:C | 3:E:60:UNK:N | 2.66 | 0.58 |
| 1:A:371:VAL:HG12 | 1:A:373:ARG:N | 2.17 | 0.58 |
| 1:A:409:VAL:C | 1:A:411:GLU:H | 2.07 | 0.58 |
| 2:B:79:ARG:HA | 2:B:84:GLY:CA | 2.34 | 0.58 |
| 1:C:143:GLY:H | 1:C:147:SER:CB | 2.17 | 0.58 |
| 1:C:256:GLN:C | 1:C:258:ASN:N | 2.57 | 0.58 |
| 2:D:183:GLU:HB3 | 2:D:184:PRO:CD | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:165:ILE:HG13 | 2:D:253:ARG:HG3 | 1.86 | 0.58 |
| 1:A:402:ARG:HD2 | 2:B:346:TRP:CE3 | 2.38 | 0.58 |
| 2:B:282:GLN:HA | 2:B:285:ALA:HB2 | 1.86 | 0.58 |
| 1:C:259:LEU:HD11 | 1:C:378:LEU:HD13 | 1.85 | 0.58 |
| 1:C:36:MET:HA | 1:C:36:MET:CE | 2.34 | 0.58 |
| 2:D:196:GLU:O | 2:D:197:ASN:C | 2.39 | 0.58 |
| 2:D:80:SER:OG | 2:D:81:GLY:N | 2.36 | 0.58 |
| 1:A:7:ILE:HD12 | 1:A:153:LEU:HD21 | 1.85 | 0.58 |
| 2:B:107:HIS:HA | 2:B:152:LEU:HD22 | 1.86 | 0.58 |
| 2:B:391:ILE:O | 2:B:425:MET:HE1 | 2.03 | 0.58 |
| 1:C:103:TYR:HB2 | 1:C:185:TYR:CD1 | 2.38 | 0.58 |
| 2:D:192:HIS:C | 2:D:194:LEU:N | 2.56 | 0.58 |
| 2:D:405:LEU:HD22 | 2:D:405:LEU:C | 2.24 | 0.58 |
| 2:D:59:ASN:OD1 | 2:D:60:LYS:HD2 | 2.04 | 0.58 |
| 1:A:132:LEU:O | 1:A:133:GLN:HB2 | 2.04 | 0.57 |
| 2:B:102:ASN:ND2 | 2:B:105:LYS:N | 2.52 | 0.57 |
| 2:B:251:ASP:CG | 2:B:252:LEU:N | 2.55 | 0.57 |
| 2:B:258:ASN:OD1 | 2:B:352:LYS:NZ | 2.34 | 0.57 |
| 2:B:276:THR:HB | 2:B:281:GLN:OE1 | 2.03 | 0.57 |
| 2:B:386:GLU:O | 2:B:388:PHE:N | 2.34 | 0.57 |
| 1:C:215:ARG:NH2 | 1:C:216:ASN:OD1 | 2.37 | 0.57 |
| 1:C:336:LYS:HA | 1:C:336:LYS:HE2 | 1.85 | 0.57 |
| 2:D:187:ALA:HB2 | 2:D:391:ILE:HG22 | 1.85 | 0.57 |
| 2:D:247:GLN:HG2 | 2:D:325:MET:SD | 2.43 | 0.57 |
| 3:E:17:UNK:O | 3:E:19:UNK:N | 2.35 | 0.57 |
| 1:A:88:HIS:HB3 | 1:A:91:GLN:CD | 2.24 | 0.57 |
| 2:B:114:LEU:O | 2:B:117:SER:N | 2.36 | 0.57 |
| 2:B:158:ARG:HA | 2:B:197:ASN:ND2 | 2.19 | 0.57 |
| 2:B:335:VAL:HA | 2:B:338:LYS:HB2 | 1.86 | 0.57 |
| 1:C:317:LEU:HD23 | 1:C:377:MET:CB | 2.34 | 0.57 |
| 2:D:140:SER:CB | 2:D:171:VAL:HB | 2.34 | 0.57 |
| 2:D:289:PRO:HB2 | 2:D:331:GLN:HE21 | 1.69 | 0.57 |
| 1:A:363:VAL:H | 1:A:367:ASP:HB2 | 1.69 | 0.57 |
| 1:A:393:HIS:C | 1:A:395:PHE:H | 2.06 | 0.57 |
| 1:A:9:VAL:O | 1:A:9:VAL:HG23 | 2.03 | 0.57 |
| 2:B:167:ASN:HA | 2:B:200:GLU:O | 2.04 | 0.57 |
| 2:B:313:LEU:HA | 2:B:344:VAL:CG1 | 2.32 | 0.57 |
| 2:B:316:ALA:HB3 | 2:B:378:ILE:HB | 1.86 | 0.57 |
| 1:C:183:GLU:HB2 | 1:C:184:PRO:HD3 | 1.85 | 0.57 |
| 1:C:363:VAL:HG13 | 1:C:367:ASP:OD2 | 2.05 | 0.57 |
| 2:D:123:ARG:CZ | 2:D:160:GLU:OE2 | 2.53 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:339:ARG:HD2 | 1:A:340:THR:N | 2.19 | 0.57 |
| 1:A:404:PHE:CD1 | 1:A:404:PHE:N | 2.73 | 0.57 |
| 1:A:46:ASP:N | 1:A:46:ASP:OD2 | 2.37 | 0.57 |
| 1:A:93:ILE:HD13 | 1:A:118:VAL:HA | 1.86 | 0.57 |
| 2:B:102:ASN:C | 2:B:185:TYR:OH | 2.43 | 0.57 |
| 1:C:77:GLU:O | 1:C:83:TYR:CB | 2.53 | 0.57 |
| 2:D:7:ILE:HB | 2:D:137:LEU:HA | 1.86 | 0.57 |
| 2:D:276:THR:HB | 2:D:281:GLN:OE1 | 2.04 | 0.57 |
| 3:E:35:UNK:O | 3:E:38:UNK:N | 2.36 | 0.57 |
| 1:A:236:SER:O | 1:A:238:ILE:N | 2.31 | 0.57 |
| 1:A:387:ALA:HA | 1:A:390:ARG:CD | 2.29 | 0.57 |
| 2:B:132:LEU:HB3 | 2:B:164:ARG:CZ | 2.34 | 0.57 |
| 2:B:196:GLU:O | 2:B:197:ASN:C | 2.43 | 0.57 |
| 2:B:59:ASN:N | 2:B:64:ARG:HE | 2.01 | 0.57 |
| 2:B:59:ASN:OD1 | 2:B:60:LYS:HD2 | 2.05 | 0.57 |
| 1:C:286:LEU:HB2 | 1:C:291:ILE:HG13 | 1.86 | 0.57 |
| 1:C:409:VAL:C | 1:C:411:GLU:H | 2.05 | 0.57 |
| 2:D:311:ARG:HG3 | 2:D:311:ARG:HH11 | 1.70 | 0.57 |
| 1:A:229:ARG:HG3 | 1:A:229:ARG:HH11 | 1.69 | 0.57 |
| 1:A:311:LYS:HB2 | 1:A:344:VAL:HG22 | 1.87 | 0.57 |
| 1:A:404:PHE:N | 1:A:404:PHE:HD1 | 2.01 | 0.57 |
| 1:C:123:ARG:HA | 1:C:161:TYR:OH | 2.05 | 0.57 |
| 1:C:409:VAL:O | 1:C:412:GLY:O | 2.22 | 0.57 |
| 2:D:417:GLU:O | 2:D:417:GLU:HG3 | 2.04 | 0.57 |
| 1:A:209:ILE:N | 1:A:209:ILE:HD12 | 2.19 | 0.57 |
| 1:A:206:ASN:ND2 | 1:A:210:TYR:HE2 | 1.98 | 0.57 |
| 1:A:244:PHE:O | 1:A:245:ASP:C | 2.41 | 0.57 |
| 1:A:336:LYS:HA | 1:A:336:LYS:HE2 | 1.86 | 0.57 |
| 2:B:409:THR:HG23 | 2:B:414:ASP:HA | 1.86 | 0.57 |
| 1:C:134:GLY:H | 1:C:164:LYS:HG2 | 1.69 | 0.57 |
| 1:C:292:THR:HA | 1:C:295:CYS:HB3 | 1.86 | 0.57 |
| 1:C:401:LYS:O | 1:C:402:ARG:HB3 | 2.05 | 0.57 |
| 1:C:82:THR:HG22 | 1:C:83:TYR:H | 1.70 | 0.57 |
| 1:C:87:PHE:CD2 | 1:C:87:PHE:N | 2.64 | 0.57 |
| 2:D:154:ILE:C | 2:D:156:LYS:H | 2.08 | 0.57 |
| 2:D:292:THR:HG23 | 2:D:319:PHE:HZ | 1.70 | 0.57 |
| 1:A:371:VAL:HG12 | 1:A:372:GLN:H | 1.69 | 0.57 |
| 2:B:223:THR:HG23 | 2:B:225:GLY:N | 2.20 | 0.57 |
| 2:B:395:PHE:HE2 | 2:B:418:PHE:O | 1.88 | 0.57 |
| 1:C:142:GLY:O | 1:C:182:VAL:HG23 | 2.04 | 0.57 |
| 1:C:101:ASN:O | 1:C:185:TYR:OH | 2.22 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:206:ASN:HD22 | 2:D:227:LEU:CD2 | 2.09 | 0.57 |
| 2:D:215:ARG:CZ | 2:D:215:ARG:HA | 2.35 | 0.57 |
| 1:C:102:ASN:ND2 | 2:D:257:VAL:HG11 | 2.12 | 0.57 |
| 1:A:155:GLU:O | 1:A:159:VAL:HG23 | 2.04 | 0.57 |
| 1:A:164:LYS:NZ | 1:A:164:LYS:HB2 | 2.19 | 0.57 |
| 1:A:291:ILE:CD1 | 1:A:373:ARG:HG3 | 2.34 | 0.57 |
| 1:A:386:GLU:CG | 1:A:387:ALA:H | 2.13 | 0.57 |
| 1:A:401:LYS:O | 1:A:402:ARG:CB | 2.53 | 0.57 |
| 2:B:311:ARG:HH21 | 2:B:437:ASP:CB | 1.97 | 0.57 |
| 1:C:111:GLY:O | 1:C:113:GLU:N | 2.37 | 0.57 |
| 1:C:220:GLU:HB3 | 1:C:221:ARG:NE | 2.20 | 0.57 |
| 1:C:35:GLN:OE1 | 1:C:88:HIS:NE2 | 2.38 | 0.57 |
| 1:C:78:VAL:HG11 | 1:C:87:PHE:HE2 | 1.69 | 0.57 |
| 2:D:282:GLN:O | 2:D:284:ARG:N | 2.38 | 0.57 |
| 2:D:391:ILE:O | 2:D:391:ILE:HG22 | 2.05 | 0.57 |
| 2:D:416:MET:O | 2:D:417:GLU:HB3 | 2.04 | 0.57 |
| 1:A:139:HIS:HB3 | 1:A:170:SER:HA | 1.87 | 0.57 |
| 1:A:196:GLU:CD | 1:A:196:GLU:N | 2.58 | 0.57 |
| 1:A:267:PHE:H | 1:A:267:PHE:HD1 | 1.53 | 0.57 |
| 1:A:284:GLU:O | 1:A:285:GLN:HG3 | 2.05 | 0.57 |
| 1:A:417:GLU:HB3 | 1:A:418:PHE:HD2 | 1.68 | 0.57 |
| 2:B:102:ASN:HB3 | 2:B:105:LYS:HB2 | 1.86 | 0.57 |
| 2:B:149:MET:CE | 2:B:149:MET:HA | 2.34 | 0.57 |
| 2:B:163:ASP:OD1 | 2:B:164:ARG:HG2 | 2.05 | 0.57 |
| 2:B:21:TRP:CZ3 | 2:B:63:PRO:HB3 | 2.39 | 0.57 |
| 2:B:9:ALA:HA | 2:B:68:VAL:O | 2.04 | 0.57 |
| 1:C:143:GLY:H | 1:C:147:SER:HB2 | 1.70 | 0.57 |
| 1:C:182:VAL:O | 1:C:183:GLU:C | 2.43 | 0.57 |
| 2:D:133:GLN:OE1 | 2:D:133:GLN:HA | 2.05 | 0.57 |
| 2:D:198:THR:O | 2:D:200:GLU:N | 2.37 | 0.57 |
| 1:A:264:ARG:NH2 | 1:A:424:ASP:OD1 | 2.38 | 0.56 |
| 1:A:386:GLU:C | 1:A:388:TRP:H | 2.06 | 0.56 |
| 2:B:350:ASN:ND2 | 2:B:351:VAL:HG23 | 2.19 | 0.56 |
| 1:C:193:THR:HG23 | 1:C:193:THR:O | 2.05 | 0.56 |
| 1:C:293:ASN:O | 1:C:297:GLU:OE1 | 2.23 | 0.56 |
| 2:D:162:PRO:O | 2:D:163:ASP:C | 2.43 | 0.56 |
| 1:A:209:ILE:O | 1:A:211:ASP:N | 2.38 | 0.56 |
| 1:A:69:ASP:OD2 | 1:A:74:VAL:CG1 | 2.52 | 0.56 |
| 1:A:8:HIS:HD2 | 1:A:17:GLY:HA3 | 1.68 | 0.56 |
| 2:B:139:HIS:HD2 | 2:B:139:HIS:O | 1.88 | 0.56 |
| 1:C:137:VAL:HG21 | 1:C:154:MET:SD | 2.45 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:SER:C | 1:C:238:ILE:H | 2.08 | 0.56 |
| 1:C:8:HIS:CD2 | 1:C:17:GLY:HA3 | 2.41 | 0.56 |
| 2:D:333:LEU:O | 2:D:337:ASN:N | 2.38 | 0.56 |
| 2:D:339:ASN:C | 2:D:341:SER:N | 2.58 | 0.56 |
| 1:A:7:ILE:CG1 | 1:A:137:VAL:HG22 | 2.35 | 0.56 |
| 1:A:401:LYS:O | 1:A:402:ARG:HB3 | 2.05 | 0.56 |
| 2:B:120:ASP:O | 2:B:124:LYS:HE3 | 2.06 | 0.56 |
| 2:B:416:MET:O | 2:B:417:GLU:HB3 | 2.06 | 0.56 |
| 1:C:137:VAL:CG1 | 1:C:154:MET:HE2 | 2.30 | 0.56 |
| 1:C:23:LEU:O | 1:C:26:LEU:HD12 | 2.06 | 0.56 |
| 1:C:399:TYR:HH | 1:C:408:TYR:HE2 | 1.52 | 0.56 |
| 2:D:130:ASP:OD2 | 2:D:131:CYS:N | 2.38 | 0.56 |
| 2:D:218:LYS:O | 2:D:219:LEU:HB2 | 2.04 | 0.56 |
| 2:D:69:ASP:CB | 2:D:74:THR:HG23 | 2.35 | 0.56 |
| 2:B:200:GLU:CG | 2:B:268:PHE:HE2 | 2.19 | 0.56 |
| 1:C:257:THR:OG1 | 1:C:258:ASN:ND2 | 2.39 | 0.56 |
| 2:D:263:PRO:HG2 | 2:D:264:ARG:H | 1.71 | 0.56 |
| 1:A:188:ILE:HG22 | 1:A:417:GLU:O | 2.04 | 0.56 |
| 2:B:103:TRP:O | 2:B:105:LYS:O | 2.23 | 0.56 |
| 2:B:2:ARG:NH2 | 2:B:243:ARG:HA | 2.20 | 0.56 |
| 1:C:331:ALA:C | 1:C:333:ALA:H | 2.08 | 0.56 |
| 2:D:194:LEU:CD1 | 2:D:428:LEU:HD21 | 2.35 | 0.56 |
| 2:D:223:THR:N | 2:D:226:ASP:OD2 | 2.33 | 0.56 |
| 2:D:385:GLN:NE2 | 2:D:433:GLN:HE21 | 2.01 | 0.56 |
| 2:D:419:THR:O | 2:D:423:SER:N | 2.39 | 0.56 |
| 3:E:10:UNK:HA | 3:E:13:UNK:CB | 2.36 | 0.56 |
| 1:A:256:GLN:C | 1:A:258:ASN:N | 2.58 | 0.56 |
| 1:A:286:LEU:HB2 | 1:A:291:ILE:HG13 | 1.88 | 0.56 |
| 1:A:402:ARG:CG | 1:A:403:ALA:N | 2.68 | 0.56 |
| 1:A:433:GLU:C | 1:A:435:VAL:H | 2.07 | 0.56 |
| 2:B:307:PRO:O | 2:B:309:HIS:N | 2.38 | 0.56 |
| 2:B:312:TYR:CD2 | 2:B:381:SER:HB2 | 2.40 | 0.56 |
| 1:C:282:TYR:N | 1:C:282:TYR:HD2 | 2.00 | 0.56 |
| 1:C:423:GLU:O | 1:C:426:ALA:HB3 | 2.04 | 0.56 |
| 2:D:98:GLY:N | 2:D:110:GLU:OE1 | 2.38 | 0.56 |
| 2:D:133:GLN:HE21 | 2:D:252:LEU:CB | 2.18 | 0.56 |
| 3:E:46:UNK:C | 3:E:48:UNK:N | 2.62 | 0.56 |
| 1:A:209:ILE:HG12 | 1:A:231:ILE:HD11 | 1.88 | 0.56 |
| 1:A:329:ASN:HA | 1:A:332:ILE:HB | 1.87 | 0.56 |
| 2:B:141:LEU:HB3 | 2:B:186:ASN:CB | 2.30 | 0.56 |
| 2:B:183:GLU:O | 2:B:185:TYR:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:389:ALA:O | 1:C:392:ASP:HB3 | 2.06 | 0.56 |
| 1:C:398:MET:O | 1:C:400:ALA:N | 2.38 | 0.56 |
| 2:D:132:LEU:HD23 | 2:D:132:LEU:C | 2.26 | 0.56 |
| 2:D:151:THR:HG21 | 2:D:189:LEU:CD2 | 2.36 | 0.56 |
| 2:D:241:CYS:C | 2:D:243:ARG:H | 2.07 | 0.56 |
| 3:E:57:UNK:O | 3:E:58:UNK:C | 2.53 | 0.56 |
| 1:A:184:PRO:HG3 | 1:A:399:TYR:CE1 | 2.41 | 0.56 |
| 1:A:311:LYS:CD | 1:A:344:VAL:HG22 | 2.36 | 0.56 |
| 1:A:36:MET:HA | 1:A:36:MET:CE | 2.36 | 0.56 |
| 1:A:86:LEU:CD1 | 1:A:89:PRO:HD3 | 2.35 | 0.56 |
| 2:B:161:TYR:O | 2:B:162:PRO:C | 2.42 | 0.56 |
| 2:B:226:ASP:C | 2:B:228:ASN:H | 2.08 | 0.56 |
| 2:B:240:THR:C | 2:B:243:ARG:HB2 | 2.26 | 0.56 |
| 1:C:115:ILE:O | 1:C:119:LEU:HB2 | 2.05 | 0.56 |
| 1:C:174:ALA:O | 1:C:176:GLN:N | 2.39 | 0.56 |
| 1:C:185:TYR:CE1 | 1:C:408:TYR:HE1 | 2.22 | 0.56 |
| 1:C:288:VAL:HA | 1:C:373:ARG:HD3 | 1.86 | 0.56 |
| 1:C:401:LYS:O | 1:C:402:ARG:CB | 2.53 | 0.56 |
| 1:C:399:TYR:OH | 1:C:408:TYR:HE2 | 1.89 | 0.56 |
| 2:D:158:ARG:CZ | 2:D:197:ASN:HA | 2.36 | 0.56 |
| 1:A:195:LEU:C | 1:A:197:HIS:H | 2.09 | 0.56 |
| 1:A:213:CYS:SG | 1:A:217:LEU:HD23 | 2.46 | 0.56 |
| 1:A:316:CYS:SG | 1:A:316:CYS:O | 2.64 | 0.56 |
| 2:B:398:MET:C | 2:B:400:ARG:N | 2.57 | 0.56 |
| 1:C:387:ALA:HA | 1:C:390:ARG:CD | 2.30 | 0.56 |
| 1:C:69:ASP:HB3 | 1:C:75:ILE:CG2 | 2.35 | 0.56 |
| 2:D:133:GLN:HG3 | 2:D:252:LEU:HD22 | 1.87 | 0.56 |
| 2:D:372:LYS:O | 2:D:373:MET:HG3 | 2.06 | 0.56 |
| 1:A:102:ASN:HD21 | 2:B:257:VAL:CG1 | 2.12 | 0.56 |
| 1:A:151:SER:HB3 | 1:A:192:HIS:NE2 | 2.20 | 0.56 |
| 1:A:189:LEU:CD1 | 1:A:193:THR:HG21 | 2.35 | 0.56 |
| 1:A:243:ARG:NH1 | 1:A:250:VAL:HG13 | 2.16 | 0.56 |
| 1:A:350:GLY:C | 1:A:351:PHE:CD1 | 2.72 | 0.56 |
| 1:A:385:ALA:HB2 | 1:A:432:TYR:CD2 | 2.39 | 0.56 |
| 1:A:78:VAL:O | 1:A:82:THR:HA | 2.05 | 0.56 |
| 2:B:151:THR:HG21 | 2:B:189:LEU:CD2 | 2.36 | 0.56 |
| 1:C:102:ASN:HD21 | 2:D:257:VAL:CG1 | 2.14 | 0.56 |
| 1:C:182:VAL:CG1 | 1:C:183:GLU:N | 2.68 | 0.56 |
| 1:C:258:ASN:O | 1:C:259:LEU:CB | 2.54 | 0.56 |
| 1:C:289:ALA:HA | 1:C:292:THR:HG22 | 1.87 | 0.56 |
| 2:D:51:VAL:N | 2:D:245:PRO:HG2 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:273:ALA:O | 2:D:275:LEU:N | 2.37 | 0.56 |
| 2:D:292:THR:HG23 | 2:D:319:PHE:CZ | 2.41 | 0.56 |
| 2:D:88:ARG:HA | 2:D:88:ARG:HH11 | 1.70 | 0.56 |
| 1:A:143:GLY:H | 1:A:147:SER:CB | 2.19 | 0.56 |
| 1:A:362:VAL:CG1 | 1:A:367:ASP:HB2 | 2.29 | 0.56 |
| 1:A:69:ASP:OD2 | 1:A:74:VAL:HG12 | 2.05 | 0.56 |
| 2:D:132:LEU:HD23 | 2:D:132:LEU:O | 2.05 | 0.56 |
| 2:D:198:THR:C | 2:D:200:GLU:N | 2.59 | 0.56 |
| 2:D:165:ILE:HG13 | 2:D:253:ARG:CG | 2.36 | 0.56 |
| 2:D:320:ARG:N | 2:D:374:SER:O | 2.33 | 0.56 |
| 2:D:59:ASN:CB | 2:D:64:ARG:HB2 | 2.35 | 0.56 |
| 1:A:16:ILE:O | 1:A:19:ALA:N | 2.30 | 0.55 |
| 1:A:26:LEU:HD12 | 1:A:26:LEU:H | 1.71 | 0.55 |
| 1:A:393:HIS:O | 1:A:397:LEU:HB2 | 2.06 | 0.55 |
| 1:A:404:PHE:HD1 | 1:A:404:PHE:H | 1.54 | 0.55 |
| 2:B:3:GLU:OE2 | 2:B:128:SER:O | 2.24 | 0.55 |
| 2:B:241:CYS:O | 2:B:243:ARG:N | 2.39 | 0.55 |
| 1:C:140:SER:HB3 | 1:C:171:ILE:HD13 | 1.86 | 0.55 |
| 1:C:229:ARG:HH11 | 1:C:229:ARG:HG3 | 1.72 | 0.55 |
| 1:C:413:MET:SD | 3:E:66:UNK:C | 2.94 | 0.55 |
| 2:D:149:MET:O | 2:D:152:LEU:HB3 | 2.06 | 0.55 |
| 2:D:192:HIS:CA | 2:D:195:VAL:HG22 | 2.23 | 0.55 |
| 1:A:112:LYS:NZ | 3:E:12:UNK:CB | 2.69 | 0.55 |
| 1:A:234:ILE:CD1 | 1:A:302:MET:SD | 2.94 | 0.55 |
| 2:B:132:LEU:HD22 | 2:B:164:ARG:NE | 2.22 | 0.55 |
| 2:B:59:ASN:ND2 | 2:B:60:LYS:N | 2.54 | 0.55 |
| 1:C:166:LYS:HE3 | 1:C:198:SER:N | 2.12 | 0.55 |
| 1:C:238:ILE:N | 1:C:241:SER:HB3 | 2.21 | 0.55 |
| 1:C:247:ALA:O | 1:C:249:ASN:ND2 | 2.39 | 0.55 |
| 1:C:287:SER:C | 1:C:289:ALA:N | 2.59 | 0.55 |
| 2:D:12:CYS:HB3 | 5:D:503:GDP:N7 | 2.21 | 0.55 |
| 2:D:59:ASN:HB3 | 2:D:64:ARG:HB2 | 1.87 | 0.55 |
| 2:D:69:ASP:HB2 | 2:D:74:THR:HG23 | 1.87 | 0.55 |
| 2:D:93:VAL:HG23 | 2:D:94:PHE:N | 2.21 | 0.55 |
| 1:A:12:ALA:HB3 | 1:A:140:SER:CB | 2.36 | 0.55 |
| 2:B:97:SER:OG | 2:B:98:GLY:N | 2.39 | 0.55 |
| 1:C:142:GLY:O | 1:C:182:VAL:CG2 | 2.55 | 0.55 |
| 1:C:88:HIS:N | 1:C:91:GLN:OE1 | 2.39 | 0.55 |
| 2:D:97:SER:OG | 2:D:98:GLY:N | 2.38 | 0.55 |
| 1:A:143:GLY:H | 1:A:147:SER:HB2 | 1.71 | 0.55 |
| 1:A:154:MET:CE | 1:A:197:HIS:NE2 | 2.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:273:ALA:HB2 | 1:A:295:CYS:HA | 1.89 | 0.55 |
| 2:B:99:ALA:HA | 2:B:105:LYS:HD3 | 1.89 | 0.55 |
| 2:B:169:PHE:CG | 2:B:235:MET:SD | 2.99 | 0.55 |
| 2:B:272:PHE:HD1 | 2:B:275:LEU:HD23 | 1.71 | 0.55 |
| 1:C:186:ASN:O | 1:C:189:LEU:HB3 | 2.06 | 0.55 |
| 1:C:284:GLU:O | 1:C:285:GLN:HG3 | 2.06 | 0.55 |
| 2:D:102:ASN:HD21 | 2:D:104:ALA:HB3 | 1.71 | 0.55 |
| 2:D:395:PHE:HE2 | 2:D:418:PHE:O | 1.90 | 0.55 |
| 3:E:31:UNK:O | 3:E:32:UNK:C | 2.51 | 0.55 |
| 1:A:75:ILE:CG1 | 1:A:75:ILE:O | 2.54 | 0.55 |
| 1:C:100:ALA:CA | 1:C:105:ARG:HD2 | 2.36 | 0.55 |
| 1:C:2:ARG:HH22 | 1:C:133:GLN:HE22 | 1.54 | 0.55 |
| 2:D:274:PRO:HG3 | 2:D:374:SER:CB | 2.37 | 0.55 |
| 1:A:103:TYR:H | 1:A:185:TYR:HE1 | 1.54 | 0.55 |
| 1:A:258:ASN:H | 1:A:258:ASN:ND2 | 2.03 | 0.55 |
| 1:A:409:VAL:O | 1:A:412:GLY:O | 2.25 | 0.55 |
| 2:B:51:VAL:HG22 | 2:B:245:PRO:CG | 2.36 | 0.55 |
| 1:C:171:ILE:H | 1:C:171:ILE:CD1 | 2.20 | 0.55 |
| 1:C:386:GLU:C | 1:C:388:TRP:H | 2.10 | 0.55 |
| 1:C:96:LYS:O | 1:C:98:ASP:N | 2.39 | 0.55 |
| 2:D:338:LYS:O | 2:D:340:SER:N | 2.34 | 0.55 |
| 2:D:357:ASP:HB3 | 2:D:358:ILE:HD12 | 1.88 | 0.55 |
| 2:D:21:TRP:CZ3 | 2:D:63:PRO:HB3 | 2.41 | 0.55 |
| 1:A:139:HIS:CG | 1:A:140:SER:H | 2.23 | 0.55 |
| 1:A:218:ASP:CG | 1:A:219:ILE:H | 2.09 | 0.55 |
| 1:A:236:SER:C | 1:A:238:ILE:H | 2.09 | 0.55 |
| 2:B:158:ARG:CB | 2:B:197:ASN:HD22 | 2.19 | 0.55 |
| 2:B:191:VAL:HG22 | 2:B:421:ALA:O | 2.07 | 0.55 |
| 1:C:222:PRO:CB | 1:C:227:LEU:HD11 | 2.20 | 0.55 |
| 1:C:417:GLU:HB3 | 1:C:418:PHE:HD2 | 1.67 | 0.55 |
| 2:D:189:LEU:C | 2:D:191:VAL:N | 2.55 | 0.55 |
| 2:D:59:ASN:N | 2:D:64:ARG:HE | 2.04 | 0.55 |
| 2:B:320:ARG:HB2 | 2:B:374:SER:OG | 2.07 | 0.55 |
| 2:B:345:GLU:O | 2:B:345:GLU:CG | 2.55 | 0.55 |
| 1:C:427:ALA:HA | 1:C:430:LYS:HB2 | 1.88 | 0.55 |
| 1:C:72:PRO:HG3 | 1:C:96:LYS:HA | 1.89 | 0.55 |
| 1:C:88:HIS:HB3 | 1:C:91:GLN:CD | 2.26 | 0.55 |
| 2:D:120:ASP:O | 2:D:124:LYS:HE3 | 2.06 | 0.55 |
| 1:A:107:HIS:CE1 | 1:A:151:SER:HB2 | 2.41 | 0.55 |
| 1:A:197:HIS:NE2 | 1:A:198:SER:HB3 | 2.22 | 0.55 |
| 2:B:10:GLY:CA | 2:B:146:GLY:HA3 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:227:LEU:O | 2:B:227:LEU:HD23 | 2.06 | 0.55 |
| 2:B:133:GLN:HG3 | 2:B:252:LEU:HD22 | 1.88 | 0.55 |
| 2:B:264:ARG:NH2 | 2:B:431:GLU:HG3 | 2.20 | 0.55 |
| 2:B:180:THR:HB | 2:B:404:PHE:CE1 | 2.42 | 0.55 |
| 2:B:194:LEU:CD1 | 2:B:428:LEU:HD21 | 2.37 | 0.55 |
| 1:C:217:LEU:O | 1:C:217:LEU:HG | 2.06 | 0.55 |
| 1:C:286:LEU:HD12 | 1:C:291:ILE:HG12 | 1.89 | 0.55 |
| 2:D:230:LEU:H | 2:D:230:LEU:CD1 | 2.19 | 0.55 |
| 2:D:277:SER:O | 2:D:278:ARG:O | 2.25 | 0.55 |
| 1:A:259:LEU:HD21 | 1:A:378:LEU:CB | 2.37 | 0.55 |
| 1:A:331:ALA:HA | 1:A:334:THR:OG1 | 2.07 | 0.55 |
| 2:B:12:CYS:HB2 | 5:B:501:GDP:O1A | 2.07 | 0.55 |
| 2:B:132:LEU:HD11 | 2:B:135:PHE:CZ | 2.42 | 0.55 |
| 2:B:226:ASP:O | 2:B:228:ASN:N | 2.37 | 0.55 |
| 2:B:284:ARG:O | 2:B:287:THR:N | 2.40 | 0.55 |
| 2:D:242:LEU:O | 2:D:243:ARG:HD3 | 2.07 | 0.55 |
| 2:D:395:PHE:HB3 | 2:D:422:GLU:OE1 | 2.07 | 0.55 |
| 2:D:59:ASN:HA | 2:D:60:LYS:HZ3 | 1.71 | 0.55 |
| 1:A:287:SER:C | 1:A:289:ALA:N | 2.60 | 0.54 |
| 2:B:223:THR:HG23 | 2:B:225:GLY:CA | 2.36 | 0.54 |
| 2:B:263:PRO:HG2 | 2:B:264:ARG:H | 1.72 | 0.54 |
| 1:C:119:LEU:HD22 | 1:C:156:ARG:NE | 2.21 | 0.54 |
| 1:C:236:SER:O | 1:C:238:ILE:N | 2.34 | 0.54 |
| 1:C:318:LEU:HB2 | 1:C:376:CYS:O | 2.07 | 0.54 |
| 1:C:11:GLN:NE2 | 4:C:502:GTP:O2A | 2.40 | 0.54 |
| 2:D:107:HIS:HA | 2:D:152:LEU:HD22 | 1.88 | 0.54 |
| 2:D:133:GLN:HE22 | 2:D:252:LEU:H | 1.54 | 0.54 |
| 2:D:200:GLU:CG | 2:D:268:PHE:CE2 | 2.90 | 0.54 |
| 2:D:243:ARG:HH12 | 2:D:252:LEU:HD12 | 1.72 | 0.54 |
| 2:D:306:ASP:HB3 | 2:D:309:HIS:CD2 | 2.42 | 0.54 |
| 2:D:395:PHE:HD2 | 2:D:422:GLU:OE1 | 1.89 | 0.54 |
| 1:A:317:LEU:HD23 | 1:A:377:MET:HB3 | 1.88 | 0.54 |
| 1:A:399:TYR:OH | 1:A:408:TYR:HE2 | 1.90 | 0.54 |
| 2:B:218:LYS:O | 2:B:219:LEU:CB | 2.55 | 0.54 |
| 1:C:100:ALA:HA | 1:C:105:ARG:HD2 | 1.89 | 0.54 |
| 1:C:110:ILE:O | 1:C:111:GLY:C | 2.45 | 0.54 |
| 1:C:175:PRO:HD2 | 1:C:207:GLU:CB | 2.11 | 0.54 |
| 1:C:71:GLU:O | 1:C:73:THR:N | 2.40 | 0.54 |
| 2:D:288:VAL:N | 2:D:289:PRO:CD | 2.70 | 0.54 |
| 2:D:297:ASP:OD1 | 2:D:298:ALA:N | 2.40 | 0.54 |
| 1:A:103:TYR:O | 1:A:104:ALA:C | 2.45 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:427:ALA:HA | 1:A:430:LYS:HB2 | 1.89 | 0.54 |
| 2:B:218:LYS:HZ2 | 2:B:277:SER:HB3 | 1.72 | 0.54 |
| 2:B:377:PHE:O | 2:B:378:ILE:HG12 | 2.07 | 0.54 |
| 1:C:189:LEU:CD1 | 1:C:193:THR:HG21 | 2.37 | 0.54 |
| 1:C:316:CYS:SG | 1:C:316:CYS:O | 2.65 | 0.54 |
| 1:C:344:VAL:CG1 | 1:C:346:TRP:NE1 | 2.69 | 0.54 |
| 2:D:168:THR:OG1 | 2:D:201:THR:CB | 2.54 | 0.54 |
| 2:D:22:GLU:OE2 | 2:D:22:GLU:N | 2.41 | 0.54 |
| 2:D:428:LEU:HD12 | 2:D:428:LEU:H | 1.73 | 0.54 |
| 1:A:137:VAL:O | 1:A:168:GLU:HA | 2.07 | 0.54 |
| 2:B:394:GLN:O | 2:B:398:MET:CB | 2.56 | 0.54 |
| 2:B:60:LYS:HZ2 | 2:B:60:LYS:N | 2.04 | 0.54 |
| 2:B:59:ASN:CB | 2:B:64:ARG:HB2 | 2.37 | 0.54 |
| 1:C:209:ILE:CD1 | 1:C:209:ILE:H | 2.20 | 0.54 |
| 1:C:345:ASP:C | 1:C:347:CYS:H | 2.10 | 0.54 |
| 2:D:102:ASN:HD22 | 2:D:105:LYS:N | 2.05 | 0.54 |
| 2:D:114:LEU:O | 2:D:117:SER:N | 2.40 | 0.54 |
| 2:D:132:LEU:HD11 | 2:D:135:PHE:CE2 | 2.41 | 0.54 |
| 2:D:102:ASN:C | 2:D:185:TYR:OH | 2.46 | 0.54 |
| 2:D:189:LEU:O | 2:D:191:VAL:N | 2.38 | 0.54 |
| 2:D:303:ALA:O | 2:D:387:LEU:HD12 | 2.08 | 0.54 |
| 1:A:190:THR:HG21 | 1:A:425:MET:SD | 2.47 | 0.54 |
| 2:B:215:ARG:CZ | 2:B:215:ARG:HA | 2.37 | 0.54 |
| 2:B:378:ILE:HG22 | 2:B:378:ILE:O | 2.06 | 0.54 |
| 2:B:428:LEU:CD1 | 2:B:428:LEU:H | 2.20 | 0.54 |
| 2:B:437:ASP:N | 2:B:437:ASP:OD2 | 2.39 | 0.54 |
| 1:C:314:ALA:O | 1:C:315:CYS:CB | 2.56 | 0.54 |
| 1:C:419:SER:O | 1:C:422:ARG:N | 2.41 | 0.54 |
| 2:D:192:HIS:O | 2:D:194:LEU:N | 2.36 | 0.54 |
| 2:D:2:ARG:NH1 | 2:D:251:ASP:HA | 2.23 | 0.54 |
| 2:D:344:VAL:HG23 | 2:D:345:GLU:N | 2.21 | 0.54 |
| 1:A:389:ALA:CB | 1:A:429:GLU:OE2 | 2.55 | 0.54 |
| 1:C:134:GLY:H | 1:C:164:LYS:HG3 | 1.72 | 0.54 |
| 1:C:12:ALA:HB3 | 1:C:140:SER:OG | 2.07 | 0.54 |
| 1:C:169:PHE:HE1 | 1:C:238:ILE:HD12 | 1.73 | 0.54 |
| 1:C:26:LEU:H | 1:C:26:LEU:HD12 | 1.73 | 0.54 |
| 1:C:184:PRO:HG3 | 1:C:399:TYR:CE1 | 2.43 | 0.54 |
| 2:D:409:THR:HG23 | 2:D:414:ASP:HA | 1.89 | 0.54 |
| 2:D:5:VAL:HG12 | 2:D:5:VAL:O | 2.06 | 0.54 |
| 3:E:71:UNK:C | 3:E:73:UNK:N | 2.70 | 0.54 |
| 1:A:273:ALA:HB2 | 1:A:295:CYS:CA | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:209:LEU:HB3 | 2:B:227:LEU:HG | 1.89 | 0.54 |
| 2:B:98:GLY:N | 2:B:110:GLU:OE1 | 2.40 | 0.54 |
| 1:C:244:PHE:O | 1:C:245:ASP:C | 2.46 | 0.54 |
| 1:C:9:VAL:HG21 | 1:C:150:THR:CG2 | 2.38 | 0.54 |
| 2:D:132:LEU:HD11 | 2:D:135:PHE:CZ | 2.42 | 0.54 |
| 2:D:148:GLY:HA2 | 2:D:151:THR:HG22 | 1.89 | 0.54 |
| 1:A:123:ARG:HG2 | 1:A:161:TYR:OH | 2.08 | 0.54 |
| 1:A:242:LEU:HG | 1:A:318:LEU:HD11 | 1.89 | 0.54 |
| 1:A:331:ALA:C | 1:A:333:ALA:N | 2.58 | 0.54 |
| 1:A:93:ILE:HD13 | 1:A:118:VAL:CG2 | 2.29 | 0.54 |
| 2:B:187:ALA:HB2 | 2:B:391:ILE:HG22 | 1.88 | 0.54 |
| 1:C:177:VAL:HG11 | 2:D:349:ASN:HB3 | 1.90 | 0.54 |
| 1:C:238:ILE:O | 1:C:239:THR:C | 2.47 | 0.54 |
| 1:C:322:ASP:N | 1:C:357:TYR:O | 2.38 | 0.54 |
| 1:C:5:ILE:O | 1:C:135:PHE:HA | 2.07 | 0.54 |
| 1:C:78:VAL:HG11 | 1:C:87:PHE:CE2 | 2.42 | 0.54 |
| 2:D:129:CYS:O | 2:D:130:ASP:C | 2.46 | 0.54 |
| 2:D:385:GLN:OE1 | 2:D:429:VAL:HA | 2.08 | 0.54 |
| 1:A:103:TYR:HB2 | 1:A:185:TYR:HD1 | 1.72 | 0.54 |
| 1:A:322:ASP:N | 1:A:357:TYR:O | 2.38 | 0.54 |
| 2:B:60:LYS:NZ | 2:B:60:LYS:H | 2.06 | 0.54 |
| 2:B:69:ASP:HB2 | 2:B:74:THR:HG23 | 1.90 | 0.54 |
| 1:C:139:HIS:CG | 1:C:140:SER:H | 2.26 | 0.54 |
| 1:C:195:LEU:C | 1:C:197:HIS:H | 2.11 | 0.54 |
| 1:C:23:LEU:C | 1:C:25:CYS:H | 2.11 | 0.54 |
| 1:C:256:GLN:HA | 1:C:260:VAL:HG23 | 1.88 | 0.54 |
| 2:D:102:ASN:ND2 | 2:D:105:LYS:N | 2.55 | 0.54 |
| 2:D:2:ARG:HG3 | 2:D:133:GLN:CD | 2.26 | 0.54 |
| 2:D:371:LEU:O | 2:D:372:LYS:HB2 | 2.07 | 0.54 |
| 1:A:163:LYS:C | 1:A:164:LYS:HZ2 | 2.10 | 0.54 |
| 1:A:169:PHE:HE1 | 1:A:238:ILE:HD12 | 1.73 | 0.54 |
| 2:B:179:ASP:HB3 | 2:B:181:VAL:CG1 | 2.37 | 0.54 |
| 2:B:288:VAL:N | 2:B:289:PRO:CD | 2.71 | 0.54 |
| 2:B:331:GLN:OE1 | 2:B:331:GLN:HA | 2.08 | 0.54 |
| 1:C:241:SER:HB3 | 1:C:242:LEU:HD12 | 1.90 | 0.54 |
| 1:A:182:VAL:HG12 | 1:A:183:GLU:N | 2.23 | 0.53 |
| 1:A:190:THR:CG2 | 1:A:425:MET:HG2 | 2.38 | 0.53 |
| 1:A:35:GLN:OE1 | 1:A:88:HIS:NE2 | 2.41 | 0.53 |
| 2:B:344:VAL:CG2 | 2:B:345:GLU:N | 2.71 | 0.53 |
| 2:B:51:VAL:C | 2:B:53:TYR:N | 2.61 | 0.53 |
| 1:C:186:ASN:ND2 | 1:C:391:LEU:HD21 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:395:PHE:C | 1:C:397:LEU:N | 2.61 | 0.53 |
| 2:D:191:VAL:O | 2:D:191:VAL:CG1 | 2.55 | 0.53 |
| 2:D:223:THR:O | 2:D:226:ASP:N | 2.39 | 0.53 |
| 1:C:242:LEU:HB3 | 1:C:250:VAL:CG1 | 2.38 | 0.53 |
| 1:C:420:GLU:OE1 | 1:C:420:GLU:C | 2.46 | 0.53 |
| 1:C:86:LEU:CD1 | 1:C:89:PRO:HD3 | 2.38 | 0.53 |
| 1:C:92:LEU:CD1 | 1:C:92:LEU:N | 2.71 | 0.53 |
| 2:D:398:MET:SD | 2:D:399:PHE:CD2 | 3.01 | 0.53 |
| 1:A:16:ILE:CG2 | 1:A:17:GLY:N | 2.59 | 0.53 |
| 1:A:193:THR:O | 1:A:193:THR:HG23 | 2.07 | 0.53 |
| 1:A:405:VAL:O | 1:A:409:VAL:HG23 | 2.08 | 0.53 |
| 1:A:87:PHE:H | 1:A:87:PHE:HD2 | 1.54 | 0.53 |
| 2:B:130:ASP:OD2 | 2:B:130:ASP:C | 2.46 | 0.53 |
| 2:B:189:LEU:O | 2:B:191:VAL:N | 2.39 | 0.53 |
| 1:C:214:ARG:CA | 1:C:218:ASP:O | 2.53 | 0.53 |
| 1:C:242:LEU:HG | 1:C:318:LEU:HD11 | 1.89 | 0.53 |
| 2:D:308:ARG:NH2 | 2:D:342:TYR:CG | 2.76 | 0.53 |
| 1:A:408:TYR:O | 1:A:414:GLU:HG3 | 2.08 | 0.53 |
| 2:B:174:SER:OG | 2:B:207:GLU:HA | 2.09 | 0.53 |
| 2:B:204:ILE:HG21 | 2:B:209:LEU:HD11 | 1.89 | 0.53 |
| 1:A:183:GLU:OE2 | 2:B:348:PRO:HB2 | 2.09 | 0.53 |
| 2:B:371:LEU:O | 2:B:372:LYS:HB2 | 2.08 | 0.53 |
| 1:C:24:TYR:HA | 1:C:26:LEU:HD12 | 1.91 | 0.53 |
| 2:D:102:ASN:HD22 | 2:D:105:LYS:CB | 2.20 | 0.53 |
| 2:D:17:GLY:O | 2:D:20:PHE:HB3 | 2.07 | 0.53 |
| 2:D:283:TYR:O | 2:D:290:GLU:OE1 | 2.25 | 0.53 |
| 2:D:315:VAL:HG23 | 2:D:351:VAL:HG22 | 1.90 | 0.53 |
| 2:D:51:VAL:HG22 | 2:D:245:PRO:CG | 2.38 | 0.53 |
| 1:A:220:GLU:HB3 | 1:A:221:ARG:NE | 2.23 | 0.53 |
| 1:A:275:VAL:HG12 | 1:A:275:VAL:O | 2.09 | 0.53 |
| 1:A:273:ALA:HB2 | 1:A:295:CYS:HB2 | 1.91 | 0.53 |
| 1:A:82:THR:O | 1:A:83:TYR:HB2 | 2.09 | 0.53 |
| 2:B:284:ARG:O | 2:B:285:ALA:C | 2.47 | 0.53 |
| 2:B:274:PRO:HA | 2:B:294:GLN:CD | 2.28 | 0.53 |
| 2:B:297:ASP:OD1 | 2:B:298:ALA:N | 2.42 | 0.53 |
| 1:C:82:THR:O | 1:C:83:TYR:HB2 | 2.07 | 0.53 |
| 2:D:206:ASN:HD21 | 5:D:503:GDP:N2 | 2.06 | 0.53 |
| 1:A:331:ALA:O | 1:A:335:ILE:HG23 | 2.08 | 0.53 |
| 1:A:305:CYS:SG | 1:A:384:ILE:HA | 2.49 | 0.53 |
| 1:A:65:ALA:O | 1:A:91:GLN:HB2 | 2.08 | 0.53 |
| 1:A:92:LEU:N | 1:A:92:LEU:CD1 | 2.70 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:185:TYR:O | 2:B:188:THR:HG22 | 2.08 | 0.53 |
| 2:B:387:LEU:O | 2:B:387:LEU:CD2 | 2.56 | 0.53 |
| 1:C:217:LEU:HD23 | 1:C:219:ILE:HD12 | 1.89 | 0.53 |
| 1:C:238:ILE:O | 1:C:242:LEU:HD12 | 2.09 | 0.53 |
| 1:C:305:CYS:SG | 1:C:306:ASP:N | 2.77 | 0.53 |
| 2:D:179:ASP:HB2 | 2:D:182:VAL:CG2 | 2.38 | 0.53 |
| 2:D:274:PRO:HA | 2:D:294:GLN:CD | 2.29 | 0.53 |
| 1:A:271:THR:HG23 | 1:A:300:ASN:O | 2.08 | 0.53 |
| 2:B:223:THR:O | 2:B:226:ASP:N | 2.41 | 0.53 |
| 2:B:274:PRO:HG3 | 2:B:374:SER:CB | 2.38 | 0.53 |
| 2:B:209:LEU:HD21 | 2:B:302:MET:HG3 | 1.89 | 0.53 |
| 2:B:358:ILE:H | 2:B:358:ILE:CD1 | 2.18 | 0.53 |
| 2:B:88:ARG:CB | 2:B:89:PRO:HD3 | 2.32 | 0.53 |
| 1:C:181:VAL:HG22 | 1:C:408:TYR:OH | 2.09 | 0.53 |
| 1:C:184:PRO:HA | 1:C:395:PHE:HD2 | 1.74 | 0.53 |
| 1:C:333:ALA:O | 1:C:334:THR:C | 2.47 | 0.53 |
| 2:D:223:THR:HG23 | 2:D:225:GLY:CA | 2.39 | 0.53 |
| 2:D:226:ASP:C | 2:D:228:ASN:H | 2.12 | 0.53 |
| 2:D:241:CYS:O | 2:D:243:ARG:N | 2.42 | 0.53 |
| 2:B:59:ASN:HA | 2:B:60:LYS:HZ3 | 1.73 | 0.53 |
| 1:C:339:ARG:HD2 | 1:C:340:THR:N | 2.24 | 0.53 |
| 2:D:322:ARG:HG2 | 2:D:357:ASP:CA | 2.30 | 0.53 |
| 2:D:345:GLU:O | 2:D:345:GLU:CG | 2.57 | 0.53 |
| 2:D:79:ARG:HA | 2:D:84:GLY:HA2 | 1.90 | 0.53 |
| 1:A:216:ASN:HB3 | 1:A:275:VAL:CG1 | 2.39 | 0.53 |
| 2:B:6:HIS:O | 2:B:66:ILE:HG22 | 2.09 | 0.53 |
| 1:C:206:ASN:O | 1:C:210:TYR:HD2 | 1.92 | 0.53 |
| 1:C:285:GLN:C | 1:C:286:LEU:HD23 | 2.29 | 0.53 |
| 2:D:200:GLU:CG | 2:D:268:PHE:HE2 | 2.22 | 0.53 |
| 2:D:282:GLN:C | 2:D:285:ALA:H | 2.12 | 0.53 |
| 2:D:392:SER:HB2 | 2:D:426:ASN:ND2 | 2.24 | 0.53 |
| 2:D:190:SER:CB | 2:D:425:MET:HG3 | 2.28 | 0.53 |
| 1:A:341:ILE:HG22 | 1:A:342:GLN:N | 2.23 | 0.53 |
| 2:B:111:GLY:O | 2:B:114:LEU:N | 2.42 | 0.53 |
| 2:B:306:ASP:HB3 | 2:B:309:HIS:CD2 | 2.44 | 0.53 |
| 2:B:311:ARG:HG3 | 2:B:311:ARG:NH1 | 2.23 | 0.53 |
| 2:B:385:GLN:HE21 | 2:B:433:GLN:HG2 | 1.72 | 0.53 |
| 2:B:403:ALA:HB1 | 2:B:405:LEU:HD12 | 1.90 | 0.53 |
| 2:B:191:VAL:CG2 | 2:B:421:ALA:HB1 | 2.25 | 0.53 |
| 2:B:91:ASN:N | 2:B:91:ASN:ND2 | 2.49 | 0.53 |
| 1:C:43:GLY:O | 1:C:47:ASP:CG | 2.47 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:194:LEU:HD12 | 2:D:428:LEU:HD21 | 1.91 | 0.53 |
| 2:D:206:ASN:ND2 | 5:D:503:GDP:N3 | 2.54 | 0.53 |
| 1:A:212:ILE:C | 1:A:214:ARG:H | 2.13 | 0.52 |
| 2:B:223:THR:C | 2:B:225:GLY:N | 2.61 | 0.52 |
| 2:B:381:SER:C | 2:B:383:ALA:H | 2.11 | 0.52 |
| 2:B:51:VAL:CG2 | 2:B:53:TYR:HB2 | 2.39 | 0.52 |
| 2:B:88:ARG:HH11 | 2:B:88:ARG:HA | 1.73 | 0.52 |
| 1:C:15:GLN:HE22 | 1:C:224:TYR:HD1 | 1.56 | 0.52 |
| 1:C:40:LYS:HD2 | 1:C:41:THR:H | 1.73 | 0.52 |
| 2:D:2:ARG:CG | 2:D:133:GLN:NE2 | 2.61 | 0.52 |
| 3:E:30:UNK:O | 3:E:33:UNK:N | 2.42 | 0.52 |
| 1:A:256:GLN:O | 1:A:258:ASN:N | 2.43 | 0.52 |
| 1:C:401:LYS:O | 1:C:402:ARG:CD | 2.57 | 0.52 |
| 2:D:154:ILE:O | 2:D:156:LYS:N | 2.42 | 0.52 |
| 2:D:25:SER:HB3 | 2:D:369:ARG:HH22 | 1.74 | 0.52 |
| 2:D:371:LEU:C | 2:D:373:MET:H | 2.10 | 0.52 |
| 2:D:413:MET:SD | 2:D:417:GLU:HG2 | 2.49 | 0.52 |
| 2:D:437:ASP:OD2 | 2:D:437:ASP:N | 2.43 | 0.52 |
| 1:A:101:ASN:C | 1:A:185:TYR:OH | 2.46 | 0.52 |
| 1:A:110:ILE:O | 1:A:111:GLY:C | 2.46 | 0.52 |
| 1:A:289:ALA:HA | 1:A:292:THR:HG22 | 1.89 | 0.52 |
| 1:A:333:ALA:O | 1:A:334:THR:C | 2.48 | 0.52 |
| 1:C:107:HIS:CE1 | 1:C:151:SER:HB2 | 2.43 | 0.52 |
| 1:C:276:ILE:CG1 | 1:C:282:TYR:CD2 | 2.92 | 0.52 |
| 1:C:276:ILE:HD12 | 1:C:277:SER:N | 2.25 | 0.52 |
| 1:C:322:ASP:OD1 | 1:C:357:TYR:O | 2.27 | 0.52 |
| 2:D:16:ILE:HG12 | 2:D:17:GLY:N | 2.24 | 0.52 |
| 2:D:223:THR:C | 2:D:225:GLY:N | 2.60 | 0.52 |
| 2:D:305:CYS:O | 2:D:306:ASP:C | 2.47 | 0.52 |
| 2:D:428:LEU:H | 2:D:428:LEU:CD1 | 2.23 | 0.52 |
| 2:D:264:ARG:NH2 | 2:D:431:GLU:HG3 | 2.24 | 0.52 |
| 3:E:73:UNK:C | 3:E:75:UNK:N | 2.66 | 0.52 |
| 1:A:213:CYS:SG | 1:A:230:LEU:HD23 | 2.50 | 0.52 |
| 1:A:314:ALA:O | 1:A:315:CYS:CB | 2.57 | 0.52 |
| 1:A:416:GLY:C | 1:A:418:PHE:N | 2.62 | 0.52 |
| 2:B:306:ASP:HB3 | 2:B:309:HIS:NE2 | 2.24 | 0.52 |
| 1:C:101:ASN:HD22 | 1:C:101:ASN:C | 2.13 | 0.52 |
| 1:C:321:GLY:HA2 | 1:C:358:GLU:O | 2.09 | 0.52 |
| 1:C:181:VAL:HG13 | 1:C:408:TYR:OH | 2.09 | 0.52 |
| 2:D:143:GLY:O | 5:D:503:GDP:O3B | 2.28 | 0.52 |
| 1:A:243:ARG:HA | 1:A:243:ARG:NE | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:298:PRO:O | 1:A:300:ASN:N | 2.42 | 0.52 |
| 2:B:70:LEU:HD11 | 2:B:110:GLU:O | 2.09 | 0.52 |
| 2:B:114:LEU:O | 2:B:115:VAL:C | 2.46 | 0.52 |
| 2:B:16:ILE:HD12 | 2:B:231:VAL:CG1 | 2.38 | 0.52 |
| 2:B:265:LEU:O | 2:B:266:HIS:CG | 2.63 | 0.52 |
| 2:B:276:THR:HG21 | 2:B:281:GLN:HB3 | 1.92 | 0.52 |
| 2:B:308:ARG:HH21 | 2:B:342:TYR:HD1 | 1.50 | 0.52 |
| 2:B:409:THR:HA | 2:B:412:GLY:O | 2.10 | 0.52 |
| 1:C:137:VAL:O | 1:C:168:GLU:HA | 2.10 | 0.52 |
| 1:C:103:TYR:HB2 | 1:C:185:TYR:HD1 | 1.74 | 0.52 |
| 1:C:293:ASN:C | 1:C:296:PHE:H | 2.13 | 0.52 |
| 2:D:179:ASP:HB3 | 2:D:181:VAL:CG1 | 2.37 | 0.52 |
| 2:D:182:VAL:CG1 | 2:D:182:VAL:O | 2.57 | 0.52 |
| 1:A:7:ILE:HG13 | 1:A:137:VAL:HG22 | 1.91 | 0.52 |
| 1:A:252:LEU:HD22 | 1:A:255:PHE:HD2 | 1.74 | 0.52 |
| 2:B:183:GLU:HB3 | 2:B:184:PRO:HD3 | 1.91 | 0.52 |
| 2:B:322:ARG:HG2 | 2:B:357:ASP:CA | 2.30 | 0.52 |
| 1:C:102:ASN:O | 1:C:105:ARG:N | 2.38 | 0.52 |
| 1:C:172:TYR:HB3 | 1:C:205:ASP:H | 1.74 | 0.52 |
| 1:C:294:ALA:HA | 1:C:297:GLU:OE1 | 2.09 | 0.52 |
| 1:C:311:LYS:CG | 1:C:344:VAL:HG22 | 2.40 | 0.52 |
| 1:C:35:GLN:HE22 | 1:C:88:HIS:CD2 | 2.28 | 0.52 |
| 2:D:260:VAL:HG12 | 2:D:260:VAL:O | 2.09 | 0.52 |
| 2:D:415:GLU:O | 2:D:416:MET:O | 2.27 | 0.52 |
| 1:A:142:GLY:O | 1:A:182:VAL:CG2 | 2.57 | 0.52 |
| 1:A:30:ILE:CG1 | 1:A:31:GLN:N | 2.70 | 0.52 |
| 2:B:129:CYS:O | 2:B:130:ASP:O | 2.27 | 0.52 |
| 2:B:287:THR:C | 2:B:289:PRO:HD2 | 2.29 | 0.52 |
| 1:C:152:LEU:O | 1:C:156:ARG:HG2 | 2.09 | 0.52 |
| 1:C:234:ILE:CD1 | 1:C:302:MET:SD | 2.97 | 0.52 |
| 1:C:402:ARG:CG | 1:C:403:ALA:N | 2.69 | 0.52 |
| 1:C:68:VAL:HG21 | 1:C:118:VAL:HG21 | 1.91 | 0.52 |
| 2:D:127:GLU:O | 2:D:128:SER:O | 2.28 | 0.52 |
| 2:D:132:LEU:HB3 | 2:D:164:ARG:CZ | 2.38 | 0.52 |
| 2:D:140:SER:HA | 2:D:171:VAL:H | 1.74 | 0.52 |
| 2:D:59:ASN:ND2 | 2:D:60:LYS:H | 2.07 | 0.52 |
| 1:A:134:GLY:H | 1:A:164:LYS:HG3 | 1.73 | 0.52 |
| 1:A:172:TYR:HB3 | 1:A:205:ASP:H | 1.75 | 0.52 |
| 1:A:286:LEU:HD12 | 1:A:291:ILE:HG12 | 1.90 | 0.52 |
| 2:B:103:TRP:O | 2:B:104:ALA:C | 2.48 | 0.52 |
| 2:B:179:ASP:HB3 | 2:B:181:VAL:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:325:MET:HG2 | 2:B:355:VAL:HG11 | 1.91 | 0.52 |
| 2:B:312:TYR:O | 2:B:344:VAL:HG13 | 2.09 | 0.52 |
| 2:B:69:ASP:CB | 2:B:74:THR:HG23 | 2.39 | 0.52 |
| 1:C:341:ILE:HG22 | 1:C:342:GLN:N | 2.25 | 0.52 |
| 1:C:307:PRO:HA | 1:C:383:ALA:HB3 | 1.92 | 0.52 |
| 1:C:388:TRP:HZ3 | 1:C:428:LEU:HD22 | 1.71 | 0.52 |
| 1:C:71:GLU:OE2 | 4:C:502:GTP:O1B | 2.28 | 0.52 |
| 2:D:239:THR:O | 2:D:241:CYS:N | 2.43 | 0.52 |
| 1:A:139:HIS:CG | 1:A:140:SER:N | 2.77 | 0.52 |
| 1:A:401:LYS:O | 1:A:402:ARG:CD | 2.58 | 0.52 |
| 1:A:414:GLU:N | 1:A:414:GLU:CD | 2.64 | 0.52 |
| 2:B:132:LEU:HD11 | 2:B:135:PHE:CE2 | 2.45 | 0.52 |
| 2:B:51:VAL:HG22 | 2:B:245:PRO:HG2 | 1.90 | 0.52 |
| 2:B:399:PHE:HE2 | 2:B:404:PHE:HB3 | 1.74 | 0.52 |
| 1:C:101:ASN:C | 1:C:185:TYR:OH | 2.47 | 0.52 |
| 1:C:139:HIS:O | 1:C:140:SER:CB | 2.58 | 0.52 |
| 1:C:190:THR:CG2 | 1:C:425:MET:HG2 | 2.40 | 0.52 |
| 1:C:213:CYS:O | 1:C:219:ILE:HB | 2.10 | 0.52 |
| 1:C:398:MET:C | 1:C:400:ALA:H | 2.13 | 0.52 |
| 2:D:142:GLY:HA2 | 2:D:185:TYR:CB | 2.35 | 0.52 |
| 2:D:265:LEU:O | 2:D:266:HIS:CG | 2.63 | 0.52 |
| 2:D:93:VAL:HG23 | 2:D:95:GLY:N | 2.25 | 0.52 |
| 1:A:212:ILE:HD11 | 1:A:230:LEU:HD21 | 1.91 | 0.52 |
| 1:A:2:ARG:NH2 | 1:A:133:GLN:NE2 | 2.53 | 0.52 |
| 1:A:414:GLU:CA | 1:A:417:GLU:HB2 | 2.39 | 0.52 |
| 2:B:158:ARG:HG3 | 2:B:159:GLU:HG3 | 1.92 | 0.52 |
| 2:B:391:ILE:O | 2:B:391:ILE:HG22 | 2.09 | 0.52 |
| 2:B:400:ARG:C | 2:B:402:LYS:H | 2.13 | 0.52 |
| 2:B:405:LEU:C | 2:B:405:LEU:HD22 | 2.30 | 0.52 |
| 1:C:292:THR:O | 1:C:292:THR:OG1 | 2.22 | 0.52 |
| 1:C:389:ALA:CB | 1:C:429:GLU:OE2 | 2.58 | 0.52 |
| 1:C:44:GLY:C | 1:C:46:ASP:N | 2.61 | 0.52 |
| 2:D:197:ASN:O | 2:D:198:THR:HB | 2.08 | 0.52 |
| 2:D:2:ARG:HE | 2:D:243:ARG:HD2 | 1.75 | 0.52 |
| 1:A:115:ILE:O | 1:A:119:LEU:HB2 | 2.09 | 0.51 |
| 1:A:221:ARG:CD | 1:A:221:ARG:H | 2.23 | 0.51 |
| 1:A:387:ALA:HB1 | 1:A:390:ARG:CZ | 2.40 | 0.51 |
| 2:B:264:ARG:NH1 | 2:B:264:ARG:HG3 | 2.25 | 0.51 |
| 2:B:339:ASN:C | 2:B:341:SER:N | 2.60 | 0.51 |
| 2:B:396:THR:HA | 2:B:400:ARG:HB3 | 1.92 | 0.51 |
| 2:B:58:GLY:O | 2:B:64:ARG:CZ | 2.59 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:298:PRO:O | 1:C:300:ASN:N | 2.43 | 0.51 |
| 1:C:344:VAL:HG11 | 1:C:346:TRP:CE2 | 2.45 | 0.51 |
| 1:C:44:GLY:HA3 | 1:C:47:ASP:HA | 1.91 | 0.51 |
| 1:C:88:HIS:CB | 1:C:91:GLN:HE22 | 2.18 | 0.51 |
| 2:D:320:ARG:HB2 | 2:D:374:SER:OG | 2.10 | 0.51 |
| 2:D:397:ALA:O | 2:D:398:MET:HB2 | 2.10 | 0.51 |
| 1:A:20:CYS:C | 1:A:22:GLU:N | 2.63 | 0.51 |
| 1:A:285:GLN:C | 1:A:286:LEU:HD23 | 2.31 | 0.51 |
| 1:A:264:ARG:HH22 | 1:A:427:ALA:HB3 | 1.75 | 0.51 |
| 2:B:179:ASP:CB | 2:B:182:VAL:HG23 | 2.37 | 0.51 |
| 2:B:198:THR:C | 2:B:200:GLU:N | 2.62 | 0.51 |
| 2:B:249:ASN:CG | 2:B:250:ALA:N | 2.62 | 0.51 |
| 2:D:75:MET:O | 2:D:76:ASP:O | 2.27 | 0.51 |
| 2:B:247:GLN:OE1 | 2:B:355:VAL:O | 2.28 | 0.51 |
| 2:B:273:ALA:O | 2:B:275:LEU:N | 2.40 | 0.51 |
| 2:B:333:LEU:O | 2:B:337:ASN:N | 2.43 | 0.51 |
| 2:B:357:ASP:CB | 2:B:358:ILE:HD12 | 2.41 | 0.51 |
| 2:B:104:ALA:HB1 | 2:B:411:GLU:HB2 | 1.93 | 0.51 |
| 2:B:415:GLU:O | 2:B:416:MET:O | 2.28 | 0.51 |
| 1:C:322:ASP:HA | 1:C:357:TYR:CD1 | 2.37 | 0.51 |
| 1:C:388:TRP:CZ3 | 1:C:428:LEU:HD13 | 2.45 | 0.51 |
| 2:D:18:ALA:C | 2:D:20:PHE:N | 2.60 | 0.51 |
| 2:D:223:THR:HG23 | 2:D:225:GLY:N | 2.25 | 0.51 |
| 2:D:415:GLU:HG2 | 2:D:416:MET:H | 1.75 | 0.51 |
| 1:A:202:PHE:CE1 | 1:A:378:LEU:HD22 | 2.42 | 0.51 |
| 2:B:123:ARG:NH2 | 2:B:160:GLU:OE2 | 2.44 | 0.51 |
| 2:B:234:THR:O | 2:B:238:VAL:HG23 | 2.11 | 0.51 |
| 2:B:241:CYS:O | 2:B:242:LEU:C | 2.49 | 0.51 |
| 2:B:371:LEU:C | 2:B:373:MET:H | 2.14 | 0.51 |
| 2:B:5:VAL:HG22 | 2:B:64:ARG:HD3 | 1.92 | 0.51 |
| 1:C:168:GLU:HG3 | 1:C:201:ALA:CB | 2.39 | 0.51 |
| 1:C:216:ASN:HB3 | 1:C:275:VAL:CG1 | 2.40 | 0.51 |
| 2:D:87:PHE:O | 2:D:89:PRO:N | 2.43 | 0.51 |
| 1:A:37:PRO:HA | 1:A:45:GLY:O | 2.10 | 0.51 |
| 1:A:5:ILE:O | 1:A:135:PHE:HA | 2.10 | 0.51 |
| 2:B:7:ILE:HB | 2:B:137:LEU:HA | 1.91 | 0.51 |
| 2:B:24:ILE:HG22 | 2:B:24:ILE:O | 2.10 | 0.51 |
| 2:B:401:ARG:O | 2:B:402:LYS:HG3 | 2.10 | 0.51 |
| 1:C:277:SER:O | 1:C:278:ALA:HB2 | 2.10 | 0.51 |
| 1:C:365:GLY:O | 1:C:368:LEU:CD1 | 2.59 | 0.51 |
| 2:D:154:ILE:HD11 | 2:D:168:THR:HG21 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:212:ILE:C | 2:D:214:PHE:H | 2.13 | 0.51 |
| 2:D:318:VAL:HG12 | 2:D:318:VAL:O | 2.11 | 0.51 |
| 2:D:51:VAL:CG2 | 2:D:53:TYR:HB2 | 2.40 | 0.51 |
| 2:D:60:LYS:HD2 | 2:D:60:LYS:H | 1.74 | 0.51 |
| 1:A:160:ASP:O | 1:A:161:TYR:CG | 2.64 | 0.51 |
| 1:A:184:PRO:HA | 1:A:395:PHE:HD2 | 1.76 | 0.51 |
| 1:A:288:VAL:HA | 1:A:373:ARG:HD3 | 1.92 | 0.51 |
| 1:A:320:ARG:CB | 1:A:374:ALA:HB3 | 2.37 | 0.51 |
| 1:A:41:THR:O | 1:A:42:ILE:HB | 2.09 | 0.51 |
| 2:B:166:MET:HG3 | 2:B:167:ASN:N | 2.24 | 0.51 |
| 2:B:179:ASP:OD1 | 1:C:352:LYS:NZ | 2.43 | 0.51 |
| 1:C:413:MET:HE2 | 1:C:413:MET:H | 1.75 | 0.51 |
| 1:C:78:VAL:HG11 | 1:C:92:LEU:CD2 | 2.39 | 0.51 |
| 2:D:179:ASP:HB2 | 2:D:182:VAL:N | 2.25 | 0.51 |
| 2:D:400:ARG:C | 2:D:402:LYS:N | 2.63 | 0.51 |
| 2:D:59:ASN:CA | 2:D:64:ARG:HH21 | 2.19 | 0.51 |
| 1:A:15:GLN:HE22 | 1:A:224:TYR:HD1 | 1.58 | 0.51 |
| 1:A:293:ASN:C | 1:A:296:PHE:H | 2.14 | 0.51 |
| 1:A:72:PRO:HG3 | 1:A:96:LYS:HA | 1.91 | 0.51 |
| 2:B:253:ARG:HG3 | 2:B:253:ARG:HH11 | 1.75 | 0.51 |
| 2:B:2:ARG:O | 2:B:57:ALA:HB1 | 2.11 | 0.51 |
| 1:C:171:ILE:HA | 1:C:204:VAL:HB | 1.92 | 0.51 |
| 1:C:69:ASP:OD2 | 1:C:74:VAL:HG12 | 2.11 | 0.51 |
| 2:D:103:TRP:O | 2:D:105:LYS:O | 2.28 | 0.51 |
| 2:D:11:GLN:HG3 | 2:D:15:GLN:NE2 | 2.26 | 0.51 |
| 2:D:6:HIS:ND1 | 2:D:21:TRP:HZ2 | 2.09 | 0.51 |
| 2:D:253:ARG:C | 2:D:255:LEU:N | 2.62 | 0.51 |
| 2:D:297:ASP:OD1 | 2:D:299:LYS:N | 2.32 | 0.51 |
| 2:D:51:VAL:C | 2:D:53:TYR:N | 2.64 | 0.51 |
| 3:E:90:UNK:O | 3:E:91:UNK:O | 2.29 | 0.51 |
| 1:A:101:ASN:C | 1:A:101:ASN:HD22 | 2.14 | 0.51 |
| 1:A:16:ILE:O | 1:A:17:GLY:C | 2.49 | 0.51 |
| 2:B:212:ILE:C | 2:B:214:PHE:H | 2.13 | 0.51 |
| 2:B:372:LYS:O | 2:B:373:MET:HG3 | 2.11 | 0.51 |
| 2:D:242:LEU:O | 2:D:243:ARG:NE | 2.44 | 0.51 |
| 2:D:297:ASP:O | 2:D:301:MET:HG2 | 2.11 | 0.51 |
| 2:D:424:ASN:O | 2:D:427:ASP:N | 2.44 | 0.51 |
| 2:D:59:ASN:HB2 | 2:D:64:ARG:HE | 1.74 | 0.51 |
| 1:A:238:ILE:O | 1:A:239:THR:C | 2.48 | 0.51 |
| 1:A:423:GLU:O | 1:A:426:ALA:HB3 | 2.11 | 0.51 |
| 2:B:162:PRO:O | 2:B:163:ASP:C | 2.47 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:391:ILE:CD1 | 2:B:391:ILE:N | 2.74 | 0.51 |
| 2:B:90:ASP:OD1 | 2:B:91:ASN:ND2 | 2.44 | 0.51 |
| 1:C:220:GLU:HB3 | 1:C:221:ARG:CZ | 2.40 | 0.51 |
| 1:C:215:ARG:NH2 | 1:C:300:ASN:HD21 | 2.07 | 0.51 |
| 1:C:38:SER:O | 1:C:39:ASP:HB3 | 2.11 | 0.51 |
| 1:C:405:VAL:O | 1:C:409:VAL:HG23 | 2.11 | 0.51 |
| 2:D:158:ARG:O | 2:D:159:GLU:C | 2.49 | 0.51 |
| 2:D:179:ASP:HB3 | 2:D:182:VAL:H | 1.73 | 0.51 |
| 2:D:241:CYS:O | 2:D:242:LEU:C | 2.50 | 0.51 |
| 2:D:264:ARG:O | 2:D:265:LEU:O | 2.29 | 0.51 |
| 2:D:283:TYR:CG | 2:D:283:TYR:O | 2.64 | 0.51 |
| 2:D:59:ASN:CA | 2:D:60:LYS:HZ3 | 2.24 | 0.51 |
| 2:D:86:ILE:H | 2:D:88:ARG:CZ | 2.24 | 0.51 |
| 1:A:247:ALA:O | 1:A:249:ASN:CG | 2.49 | 0.51 |
| 1:A:21:TRP:HA | 1:A:24:TYR:HB2 | 1.93 | 0.51 |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:HG13 | 1.93 | 0.51 |
| 2:B:79:ARG:HG3 | 2:B:88:ARG:HE | 1.75 | 0.51 |
| 1:C:247:ALA:O | 1:C:249:ASN:CG | 2.48 | 0.51 |
| 1:C:186:ASN:HD21 | 1:C:391:LEU:HD11 | 1.75 | 0.51 |
| 2:D:313:LEU:HD21 | 2:D:435:TYR:HD2 | 1.76 | 0.51 |
| 2:D:159:GLU:CD | 3:E:82:UNK:CB | 2.80 | 0.51 |
| 1:A:177:VAL:HG11 | 2:B:349:ASN:HB3 | 1.93 | 0.50 |
| 1:A:180:ALA:O | 1:A:182:VAL:N | 2.44 | 0.50 |
| 1:A:143:GLY:O | 4:A:500:GTP:O3G | 2.29 | 0.50 |
| 1:A:8:HIS:HE2 | 1:A:21:TRP:HE1 | 1.59 | 0.50 |
| 2:B:203:CYS:SG | 2:B:384:ILE:HD11 | 2.52 | 0.50 |
| 1:C:239:THR:OG1 | 1:C:240:ALA:N | 2.41 | 0.50 |
| 1:C:273:ALA:HB2 | 1:C:295:CYS:CA | 2.41 | 0.50 |
| 2:B:402:LYS:HE3 | 1:C:440:VAL:CG1 | 2.41 | 0.50 |
| 1:C:5:ILE:CD1 | 1:C:125:LEU:HD22 | 2.41 | 0.50 |
| 2:D:186:ASN:HA | 2:D:189:LEU:HD12 | 1.93 | 0.50 |
| 2:D:19:LYS:HZ2 | 2:D:82:PRO:HG3 | 1.76 | 0.50 |
| 3:E:4:UNK:C | 3:E:6:UNK:N | 2.74 | 0.50 |
| 1:A:101:ASN:ND2 | 1:A:185:TYR:OH | 2.44 | 0.50 |
| 1:A:294:ALA:HA | 1:A:297:GLU:OE1 | 2.11 | 0.50 |
| 1:A:368:LEU:N | 1:A:368:LEU:HD12 | 2.26 | 0.50 |
| 2:B:277:SER:O | 2:B:278:ARG:O | 2.29 | 0.50 |
| 2:B:395:PHE:CE2 | 2:B:418:PHE:O | 2.64 | 0.50 |
| 1:C:75:ILE:CG1 | 1:C:75:ILE:O | 2.58 | 0.50 |
| 2:D:205:ASP:HB3 | 2:D:303:ALA:HA | 1.93 | 0.50 |
| 2:D:218:LYS:NZ | 2:D:277:SER:HB3 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:4:UNK:O | 3:E:5:UNK:C | 2.59 | 0.50 |
| 1:A:333:ALA:O | 1:A:336:LYS:N | 2.43 | 0.50 |
| 2:B:154:ILE:C | 2:B:156:LYS:N | 2.64 | 0.50 |
| 2:B:205:ASP:HB3 | 2:B:303:ALA:HA | 1.93 | 0.50 |
| 2:B:6:HIS:CE1 | 2:B:21:TRP:HE1 | 2.30 | 0.50 |
| 2:B:93:VAL:HG23 | 2:B:94:PHE:N | 2.25 | 0.50 |
| 1:C:181:VAL:HG13 | 1:C:181:VAL:O | 2.11 | 0.50 |
| 1:C:260:VAL:O | 1:C:260:VAL:HG12 | 2.10 | 0.50 |
| 1:C:208:ALA:HB2 | 1:C:302:MET:O | 2.11 | 0.50 |
| 1:C:341:ILE:N | 1:C:341:ILE:HD12 | 2.26 | 0.50 |
| 1:C:311:LYS:HB2 | 1:C:344:VAL:HG22 | 1.92 | 0.50 |
| 1:C:381:THR:C | 1:C:383:ALA:H | 2.14 | 0.50 |
| 1:C:414:GLU:CG | 1:C:415:GLU:N | 2.69 | 0.50 |
| 2:D:123:ARG:NH2 | 2:D:160:GLU:OE2 | 2.44 | 0.50 |
| 2:D:308:ARG:HH21 | 2:D:342:TYR:HD1 | 1.48 | 0.50 |
| 2:D:398:MET:C | 2:D:400:ARG:N | 2.65 | 0.50 |
| 1:A:363:VAL:HG22 | 1:A:367:ASP:OD2 | 2.10 | 0.50 |
| 1:A:38:SER:O | 1:A:39:ASP:CB | 2.59 | 0.50 |
| 1:A:82:THR:HG22 | 1:A:83:TYR:H | 1.76 | 0.50 |
| 2:B:403:ALA:HB3 | 1:C:262:TYR:HE2 | 1.76 | 0.50 |
| 1:C:25:CYS:O | 1:C:25:CYS:SG | 2.69 | 0.50 |
| 1:C:350:GLY:O | 1:C:351:PHE:HD1 | 1.93 | 0.50 |
| 1:C:317:LEU:HD23 | 1:C:377:MET:HB3 | 1.92 | 0.50 |
| 2:D:10:GLY:CA | 2:D:146:GLY:HA3 | 2.41 | 0.50 |
| 2:D:191:VAL:HG22 | 2:D:421:ALA:O | 2.11 | 0.50 |
| 2:D:289:PRO:O | 2:D:292:THR:OG1 | 2.25 | 0.50 |
| 2:D:4:ILE:CD1 | 2:D:252:LEU:HD13 | 2.42 | 0.50 |
| 1:A:152:LEU:O | 1:A:156:ARG:HG2 | 2.10 | 0.50 |
| 2:B:133:GLN:OE1 | 2:B:133:GLN:HA | 2.11 | 0.50 |
| 2:B:179:ASP:HB3 | 2:B:182:VAL:H | 1.73 | 0.50 |
| 2:B:228:ASN:O | 2:B:231:VAL:HB | 2.11 | 0.50 |
| 2:B:51:VAL:N | 2:B:245:PRO:HG2 | 2.27 | 0.50 |
| 2:B:343:PHE:HB3 | 2:B:350:ASN:OD1 | 2.11 | 0.50 |
| 2:B:71:GLU:CB | 2:B:72:PRO:CD | 2.90 | 0.50 |
| 2:D:111:GLY:O | 2:D:114:LEU:N | 2.44 | 0.50 |
| 2:D:212:ILE:O | 2:D:217:LEU:HB3 | 2.10 | 0.50 |
| 2:D:326:LYS:O | 2:D:330:GLU:HG3 | 2.11 | 0.50 |
| 1:A:101:ASN:O | 1:A:101:ASN:ND2 | 2.39 | 0.50 |
| 1:A:206:ASN:O | 1:A:210:TYR:HD2 | 1.95 | 0.50 |
| 2:B:127:GLU:O | 2:B:128:SER:C | 2.50 | 0.50 |
| 2:B:140:SER:HA | 2:B:171:VAL:H | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:158:ARG:CZ | 2:B:197:ASN:HA | 2.41 | 0.50 |
| 1:C:155:GLU:O | 1:C:159:VAL:HG23 | 2.12 | 0.50 |
| 1:C:174:ALA:HB2 | 1:C:206:ASN:HB2 | 1.94 | 0.50 |
| 1:C:66:VAL:HG21 | 1:C:122:ILE:HG12 | 1.93 | 0.50 |
| 2:D:295:MET:O | 2:D:297:ASP:N | 2.43 | 0.50 |
| 1:A:181:VAL:HG23 | 1:A:404:PHE:HB2 | 1.93 | 0.50 |
| 1:A:258:ASN:H | 1:A:258:ASN:HD22 | 1.52 | 0.50 |
| 1:A:344:VAL:CG1 | 1:A:346:TRP:NE1 | 2.73 | 0.50 |
| 1:A:332:ILE:HG23 | 1:A:351:PHE:CE2 | 2.46 | 0.50 |
| 1:A:40:LYS:HD2 | 1:A:41:THR:H | 1.76 | 0.50 |
| 1:A:413:MET:C | 1:A:414:GLU:OE1 | 2.49 | 0.50 |
| 1:A:74:VAL:HG13 | 1:A:75:ILE:N | 2.27 | 0.50 |
| 1:A:9:VAL:HA | 1:A:68:VAL:O | 2.12 | 0.50 |
| 2:B:115:VAL:HG23 | 2:B:149:MET:HE1 | 1.94 | 0.50 |
| 2:B:211:ASP:O | 2:B:215:ARG:N | 2.44 | 0.50 |
| 2:B:311:ARG:NH1 | 2:B:344:VAL:HA | 2.26 | 0.50 |
| 2:B:400:ARG:C | 2:B:402:LYS:N | 2.62 | 0.50 |
| 2:B:266:HIS:ND1 | 2:B:432:TYR:CE1 | 2.79 | 0.50 |
| 1:C:190:THR:CA | 1:C:193:THR:HG22 | 2.36 | 0.50 |
| 1:C:266:HIS:H | 1:C:266:HIS:HD1 | 1.60 | 0.50 |
| 1:C:203:MET:HE1 | 1:C:388:TRP:HD1 | 1.76 | 0.50 |
| 1:C:417:GLU:HB3 | 1:C:418:PHE:HE2 | 1.74 | 0.50 |
| 2:D:284:ARG:HG3 | 2:D:284:ARG:HH11 | 1.77 | 0.50 |
| 2:D:2:ARG:NE | 2:D:243:ARG:CD | 2.72 | 0.50 |
| 1:A:208:ALA:O | 1:A:212:ILE:HG23 | 2.12 | 0.50 |
| 1:A:244:PHE:HE1 | 1:A:358:GLU:OE2 | 1.95 | 0.50 |
| 1:A:184:PRO:CG | 1:A:399:TYR:CZ | 2.93 | 0.50 |
| 1:A:401:LYS:O | 1:A:402:ARG:NE | 2.45 | 0.50 |
| 2:B:107:HIS:ND1 | 2:B:107:HIS:O | 2.44 | 0.50 |
| 2:B:115:VAL:CG1 | 2:B:156:LYS:NZ | 2.73 | 0.50 |
| 2:B:313:LEU:HD21 | 2:B:435:TYR:HD2 | 1.76 | 0.50 |
| 1:C:103:TYR:O | 1:C:104:ALA:C | 2.47 | 0.50 |
| 1:C:181:VAL:O | 1:C:184:PRO:HG2 | 2.11 | 0.50 |
| 1:C:184:PRO:O | 1:C:188:ILE:HG13 | 2.11 | 0.50 |
| 1:C:39:ASP:CG | 1:C:40:LYS:N | 2.62 | 0.50 |
| 1:C:77:GLU:C | 1:C:83:TYR:HB2 | 2.32 | 0.50 |
| 2:D:272:PHE:HD1 | 2:D:275:LEU:HD23 | 1.77 | 0.50 |
| 2:D:306:ASP:HB3 | 2:D:309:HIS:NE2 | 2.26 | 0.50 |
| 2:D:311:ARG:HH11 | 2:D:344:VAL:HA | 1.77 | 0.50 |
| 1:C:183:GLU:OE2 | 2:D:348:PRO:HB2 | 2.12 | 0.50 |
| 3:E:50:UNK:O | 3:E:53:UNK:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:144:GLY:CA | 1:A:147:SER:HB3 | 2.42 | 0.50 |
| 1:A:171:ILE:CD1 | 1:A:171:ILE:H | 2.25 | 0.50 |
| 1:A:187:SER:C | 1:A:189:LEU:H | 2.15 | 0.50 |
| 1:A:194:THR:O | 1:A:195:LEU:C | 2.49 | 0.50 |
| 1:A:194:THR:O | 1:A:196:GLU:N | 2.45 | 0.50 |
| 1:A:215:ARG:NH1 | 1:A:299:ALA:HB1 | 2.26 | 0.50 |
| 1:A:311:LYS:HD3 | 1:A:344:VAL:CG2 | 2.42 | 0.50 |
| 1:A:346:TRP:HZ2 | 1:A:435:VAL:HB | 1.76 | 0.50 |
| 1:A:9:VAL:HG21 | 1:A:150:THR:CG2 | 2.42 | 0.50 |
| 2:B:84:GLY:HA2 | 2:B:88:ARG:HH21 | 1.77 | 0.50 |
| 2:B:96:GLN:OE1 | 1:C:130:THR:HB | 2.12 | 0.50 |
| 1:C:177:VAL:HG11 | 2:D:349:ASN:CB | 2.42 | 0.50 |
| 1:C:194:THR:O | 1:C:195:LEU:C | 2.50 | 0.50 |
| 1:C:210:TYR:CE2 | 1:C:227:LEU:CD2 | 2.95 | 0.50 |
| 1:C:269:LEU:HD21 | 1:C:301:GLN:NE2 | 2.27 | 0.50 |
| 2:D:241:CYS:SG | 2:D:320:ARG:NH1 | 2.85 | 0.50 |
| 3:E:71:UNK:O | 3:E:72:UNK:C | 2.60 | 0.50 |
| 1:A:71:GLU:O | 1:A:73:THR:N | 2.44 | 0.49 |
| 2:B:280:SER:O | 2:B:282:GLN:N | 2.45 | 0.49 |
| 2:B:315:VAL:HG23 | 2:B:351:VAL:HG22 | 1.94 | 0.49 |
| 1:C:242:LEU:O | 1:C:243:ARG:HG2 | 2.12 | 0.49 |
| 1:C:283:HIS:O | 1:C:284:GLU:HB3 | 2.12 | 0.49 |
| 2:D:100:GLY:C | 2:D:101:ASN:HD22 | 2.15 | 0.49 |
| 2:D:11:GLN:C | 2:D:13:GLY:H | 2.15 | 0.49 |
| 2:D:218:LYS:O | 2:D:219:LEU:CB | 2.60 | 0.49 |
| 2:D:6:HIS:O | 2:D:66:ILE:HG22 | 2.12 | 0.49 |
| 1:A:102:ASN:O | 1:A:105:ARG:N | 2.34 | 0.49 |
| 1:A:100:ALA:CA | 1:A:105:ARG:HD2 | 2.41 | 0.49 |
| 1:A:174:ALA:CB | 1:A:176:GLN:HG2 | 2.42 | 0.49 |
| 1:A:331:ALA:C | 1:A:333:ALA:H | 2.16 | 0.49 |
| 2:B:154:ILE:C | 2:B:156:LYS:H | 2.15 | 0.49 |
| 2:B:158:ARG:C | 2:B:160:GLU:N | 2.64 | 0.49 |
| 2:B:282:GLN:O | 2:B:284:ARG:N | 2.45 | 0.49 |
| 2:B:427:ASP:O | 2:B:430:SER:N | 2.45 | 0.49 |
| 2:B:51:VAL:N | 2:B:245:PRO:HB2 | 2.26 | 0.49 |
| 1:C:393:HIS:C | 1:C:395:PHE:N | 2.65 | 0.49 |
| 1:C:402:ARG:HD2 | 2:D:346:TRP:CE3 | 2.47 | 0.49 |
| 1:C:41:THR:O | 1:C:42:ILE:HB | 2.11 | 0.49 |
| 2:D:204:ILE:HG21 | 2:D:209:LEU:HD11 | 1.93 | 0.49 |
| 2:D:390:ARG:HB2 | 2:D:391:ILE:HD12 | 1.94 | 0.49 |
| 2:D:87:PHE:O | 2:D:89:PRO:HD2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:154:MET:HE3 | 1:A:197:HIS:NE2 | 2.27 | 0.49 |
| 1:A:381:THR:C | 1:A:383:ALA:H | 2.15 | 0.49 |
| 1:A:386:GLU:C | 1:A:388:TRP:N | 2.66 | 0.49 |
| 2:B:344:VAL:O | 2:B:345:GLU:HB3 | 2.13 | 0.49 |
| 2:B:428:LEU:H | 2:B:428:LEU:HD12 | 1.76 | 0.49 |
| 2:B:4:ILE:CD1 | 2:B:252:LEU:HD13 | 2.42 | 0.49 |
| 2:B:59:ASN:HB3 | 2:B:64:ARG:HB2 | 1.93 | 0.49 |
| 1:C:213:CYS:SG | 1:C:217:LEU:CD2 | 2.99 | 0.49 |
| 1:C:350:GLY:C | 1:C:351:PHE:CD1 | 2.80 | 0.49 |
| 2:D:107:HIS:ND1 | 2:D:107:HIS:O | 2.46 | 0.49 |
| 2:D:114:LEU:O | 2:D:115:VAL:C | 2.49 | 0.49 |
| 2:D:2:ARG:CG | 2:D:133:GLN:HE21 | 2.23 | 0.49 |
| 1:A:190:THR:CA | 1:A:193:THR:HG22 | 2.37 | 0.49 |
| 1:A:306:ASP:OD1 | 1:A:306:ASP:O | 2.30 | 0.49 |
| 1:A:343:PHE:CD2 | 1:A:349:THR:HB | 2.47 | 0.49 |
| 1:A:307:PRO:HA | 1:A:383:ALA:CB | 2.41 | 0.49 |
| 2:B:271:GLY:O | 2:B:272:PHE:O | 2.30 | 0.49 |
| 2:B:398:MET:O | 2:B:401:ARG:N | 2.45 | 0.49 |
| 2:B:5:VAL:HA | 2:B:64:ARG:HD2 | 1.93 | 0.49 |
| 1:C:414:GLU:CG | 1:C:415:GLU:H | 2.17 | 0.49 |
| 2:D:184:PRO:CB | 2:D:399:PHE:CZ | 2.95 | 0.49 |
| 2:D:382:THR:HB | 2:D:436:GLN:HG2 | 1.95 | 0.49 |
| 2:D:424:ASN:O | 2:D:427:ASP:HB2 | 2.12 | 0.49 |
| 2:D:79:ARG:O | 2:D:79:ARG:HG2 | 2.13 | 0.49 |
| 1:A:181:VAL:HG22 | 1:A:408:TYR:OH | 2.12 | 0.49 |
| 2:B:295:MET:O | 2:B:297:ASP:N | 2.44 | 0.49 |
| 1:C:194:THR:O | 1:C:196:GLU:N | 2.45 | 0.49 |
| 1:C:202:PHE:CE1 | 1:C:378:LEU:HD22 | 2.43 | 0.49 |
| 1:C:264:ARG:HH22 | 1:C:427:ALA:HB3 | 1.78 | 0.49 |
| 1:C:93:ILE:HD13 | 1:C:118:VAL:HA | 1.95 | 0.49 |
| 2:D:158:ARG:HB2 | 2:D:197:ASN:CB | 2.31 | 0.49 |
| 2:D:71:GLU:CB | 2:D:72:PRO:CD | 2.90 | 0.49 |
| 1:A:123:ARG:O | 1:A:127:ASP:HB2 | 2.12 | 0.49 |
| 1:A:142:GLY:O | 1:A:182:VAL:HG23 | 2.13 | 0.49 |
| 1:A:20:CYS:C | 1:A:22:GLU:H | 2.16 | 0.49 |
| 1:A:213:CYS:SG | 1:A:230:LEU:CD2 | 3.01 | 0.49 |
| 1:A:238:ILE:O | 1:A:242:LEU:HD12 | 2.12 | 0.49 |
| 2:B:189:LEU:O | 2:B:192:HIS:ND1 | 2.38 | 0.49 |
| 1:C:171:ILE:N | 1:C:171:ILE:CD1 | 2.76 | 0.49 |
| 1:C:37:PRO:HA | 1:C:45:GLY:O | 2.13 | 0.49 |
| 2:D:242:LEU:O | 2:D:243:ARG:CD | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:259:MET:CE | 2:D:316:ALA:HB2 | 2.42 | 0.49 |
| 3:E:25:UNK:O | 3:E:27:UNK:N | 2.44 | 0.49 |
| 1:A:93:ILE:CD1 | 1:A:118:VAL:HA | 2.42 | 0.49 |
| 1:A:217:LEU:HG | 1:A:217:LEU:O | 2.12 | 0.49 |
| 2:B:132:LEU:CB | 2:B:164:ARG:HH21 | 2.15 | 0.49 |
| 2:B:395:PHE:CD2 | 2:B:422:GLU:OE1 | 2.66 | 0.49 |
| 2:B:59:ASN:CB | 2:B:64:ARG:HE | 2.25 | 0.49 |
| 1:C:255:PHE:CD1 | 1:C:259:LEU:HD12 | 2.48 | 0.49 |
| 1:C:393:HIS:O | 1:C:397:LEU:HB2 | 2.13 | 0.49 |
| 1:C:7:ILE:HG21 | 1:C:122:ILE:CD1 | 2.42 | 0.49 |
| 2:D:174:SER:C | 2:D:176:LYS:N | 2.66 | 0.49 |
| 2:D:289:PRO:CB | 2:D:331:GLN:HE21 | 2.25 | 0.49 |
| 2:D:2:ARG:NH2 | 2:D:243:ARG:HA | 2.28 | 0.49 |
| 2:D:325:MET:HG2 | 2:D:355:VAL:HG11 | 1.95 | 0.49 |
| 1:A:2:ARG:HH22 | 1:A:133:GLN:HE22 | 1.57 | 0.49 |
| 1:A:168:GLU:HG3 | 1:A:201:ALA:CB | 2.42 | 0.49 |
| 1:A:241:SER:CB | 1:A:242:LEU:HD12 | 2.43 | 0.49 |
| 1:A:68:VAL:O | 1:A:68:VAL:HG13 | 2.13 | 0.49 |
| 2:B:102:ASN:HD22 | 2:B:105:LYS:CB | 2.26 | 0.49 |
| 2:B:188:THR:HA | 2:B:191:VAL:HG21 | 1.95 | 0.49 |
| 2:B:381:SER:O | 2:B:383:ALA:N | 2.46 | 0.49 |
| 1:C:183:GLU:N | 1:C:184:PRO:CD | 2.75 | 0.49 |
| 1:C:283:HIS:C | 1:C:285:GLN:H | 2.16 | 0.49 |
| 1:C:420:GLU:O | 1:C:420:GLU:OE1 | 2.30 | 0.49 |
| 2:D:144:GLY:HA3 | 2:D:185:TYR:OH | 2.13 | 0.49 |
| 2:D:403:ALA:O | 2:D:404:PHE:HB2 | 2.12 | 0.49 |
| 1:A:311:LYS:HB2 | 1:A:344:VAL:CG2 | 2.43 | 0.49 |
| 1:A:186:ASN:HD21 | 1:A:391:LEU:HD11 | 1.70 | 0.49 |
| 1:A:427:ALA:HA | 1:A:430:LYS:CB | 2.43 | 0.49 |
| 2:B:388:PHE:C | 2:B:390:ARG:H | 2.14 | 0.49 |
| 1:C:102:ASN:HB2 | 1:C:105:ARG:HB3 | 1.91 | 0.49 |
| 1:C:176:GLN:OE1 | 1:C:210:TYR:CE1 | 2.66 | 0.49 |
| 1:C:291:ILE:HG22 | 1:C:292:THR:N | 2.28 | 0.49 |
| 1:C:68:VAL:HG21 | 1:C:149:PHE:HE1 | 1.77 | 0.49 |
| 1:C:9:VAL:HG21 | 1:C:150:THR:HB | 1.93 | 0.49 |
| 2:D:6:HIS:CE1 | 2:D:21:TRP:HE1 | 2.31 | 0.49 |
| 3:E:58:UNK:O | 3:E:59:UNK:C | 2.58 | 0.49 |
| 1:A:26:LEU:HG | 1:A:361:THR:HB | 1.95 | 0.49 |
| 1:A:317:LEU:HD13 | 1:A:319:TYR:CE1 | 2.48 | 0.49 |
| 1:A:395:PHE:C | 1:A:397:LEU:N | 2.63 | 0.49 |
| 2:B:133:GLN:NE2 | 2:B:252:LEU:CB | 2.65 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:115:VAL:HG21 | 2:B:152:LEU:HD21 | 1.93 | 0.49 |
| 2:B:149:MET:CE | 2:B:152:LEU:HD23 | 2.43 | 0.49 |
| 2:B:158:ARG:O | 2:B:159:GLU:C | 2.51 | 0.49 |
| 2:B:242:LEU:O | 2:B:243:ARG:HD3 | 2.12 | 0.49 |
| 1:C:350:GLY:O | 1:C:351:PHE:CD1 | 2.66 | 0.49 |
| 2:D:181:VAL:O | 2:D:183:GLU:N | 2.42 | 0.49 |
| 2:D:188:THR:HA | 2:D:191:VAL:HG21 | 1.95 | 0.49 |
| 2:D:395:PHE:CE2 | 2:D:418:PHE:O | 2.66 | 0.49 |
| 2:D:60:LYS:NZ | 2:D:60:LYS:H | 2.11 | 0.49 |
| 1:A:126:ALA:HB1 | 1:A:132:LEU:HD11 | 1.93 | 0.48 |
| 1:A:174:ALA:C | 1:A:176:GLN:N | 2.65 | 0.48 |
| 1:A:256:GLN:HA | 1:A:260:VAL:CG2 | 2.43 | 0.48 |
| 1:A:398:MET:C | 1:A:400:ALA:H | 2.14 | 0.48 |
| 2:B:119:LEU:HD13 | 2:B:123:ARG:NH2 | 2.28 | 0.48 |
| 2:B:238:VAL:HG22 | 2:B:376:THR:HG21 | 1.95 | 0.48 |
| 1:C:185:TYR:O | 1:C:186:ASN:C | 2.51 | 0.48 |
| 2:D:106:GLY:O | 2:D:149:MET:HA | 2.13 | 0.48 |
| 2:D:154:ILE:C | 2:D:156:LYS:N | 2.65 | 0.48 |
| 2:D:204:ILE:HD13 | 2:D:231:VAL:HG13 | 1.94 | 0.48 |
| 2:D:344:VAL:CG2 | 2:D:345:GLU:N | 2.76 | 0.48 |
| 2:D:8:GLN:O | 2:D:67:LEU:HA | 2.13 | 0.48 |
| 2:D:87:PHE:O | 2:D:89:PRO:CD | 2.61 | 0.48 |
| 1:A:102:ASN:HB2 | 1:A:105:ARG:HB3 | 1.88 | 0.48 |
| 1:A:294:ALA:HA | 1:A:297:GLU:HB2 | 1.95 | 0.48 |
| 1:A:307:PRO:HA | 1:A:383:ALA:HB3 | 1.95 | 0.48 |
| 1:A:428:LEU:C | 1:A:430:LYS:N | 2.66 | 0.48 |
| 2:B:102:ASN:HB3 | 2:B:105:LYS:CD | 2.43 | 0.48 |
| 2:B:18:ALA:C | 2:B:20:PHE:N | 2.66 | 0.48 |
| 2:B:20:PHE:HZ | 2:B:239:THR:HG21 | 1.78 | 0.48 |
| 2:B:262:PHE:O | 2:B:265:LEU:CA | 2.57 | 0.48 |
| 2:B:265:LEU:O | 2:B:266:HIS:ND1 | 2.46 | 0.48 |
| 2:B:283:TYR:C | 2:B:285:ALA:H | 2.16 | 0.48 |
| 1:C:31:GLN:HB3 | 1:C:32:PRO:CD | 2.37 | 0.48 |
| 1:C:303:VAL:HG21 | 1:C:384:ILE:HD11 | 1.94 | 0.48 |
| 2:D:283:TYR:C | 2:D:285:ALA:H | 2.15 | 0.48 |
| 2:D:291:LEU:CD2 | 2:D:291:LEU:H | 2.26 | 0.48 |
| 2:D:313:LEU:O | 2:D:314:THR:CG2 | 2.61 | 0.48 |
| 2:D:394:GLN:O | 2:D:398:MET:CB | 2.59 | 0.48 |
| 3:E:34:UNK:O | 3:E:38:UNK:N | 2.47 | 0.48 |
| 1:A:284:GLU:OE2 | 1:A:285:GLN:NE2 | 2.46 | 0.48 |
| 2:B:154:ILE:O | 2:B:156:LYS:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:239:THR:O | 2:B:241:CYS:N | 2.46 | 0.48 |
| 2:B:25:SER:HB3 | 2:B:369:ARG:HH22 | 1.79 | 0.48 |
| 2:B:289:PRO:CB | 2:B:331:GLN:HE21 | 2.26 | 0.48 |
| 2:B:269:MET:SD | 2:B:381:SER:HB3 | 2.54 | 0.48 |
| 1:C:174:ALA:CB | 1:C:176:GLN:HG2 | 2.43 | 0.48 |
| 1:C:344:VAL:HG12 | 1:C:345:ASP:OD2 | 2.13 | 0.48 |
| 2:D:311:ARG:HG3 | 2:D:311:ARG:NH1 | 2.29 | 0.48 |
| 3:E:35:UNK:O | 3:E:37:UNK:C | 2.61 | 0.48 |
| 1:A:179:THR:HB | 1:A:182:VAL:HB | 1.94 | 0.48 |
| 1:A:96:LYS:O | 1:A:98:ASP:N | 2.46 | 0.48 |
| 2:B:4:ILE:HG12 | 2:B:133:GLN:HG2 | 1.95 | 0.48 |
| 1:C:139:HIS:CG | 1:C:140:SER:N | 2.80 | 0.48 |
| 2:B:407:TRP:HE1 | 1:C:257:THR:HA | 1.79 | 0.48 |
| 1:C:393:HIS:O | 1:C:395:PHE:N | 2.38 | 0.48 |
| 1:C:427:ALA:HA | 1:C:430:LYS:CB | 2.43 | 0.48 |
| 1:C:77:GLU:OE2 | 1:C:83:TYR:CG | 2.66 | 0.48 |
| 2:D:163:ASP:OD1 | 2:D:164:ARG:HG2 | 2.13 | 0.48 |
| 2:D:320:ARG:HB3 | 2:D:320:ARG:CZ | 2.42 | 0.48 |
| 2:D:286:LEU:CD1 | 2:D:371:LEU:O | 2.61 | 0.48 |
| 2:D:79:ARG:HA | 2:D:84:GLY:CA | 2.44 | 0.48 |
| 1:A:283:HIS:C | 1:A:285:GLN:H | 2.16 | 0.48 |
| 2:B:386:GLU:C | 2:B:388:PHE:N | 2.66 | 0.48 |
| 1:C:244:PHE:HE1 | 1:C:358:GLU:OE2 | 1.97 | 0.48 |
| 1:C:274:PRO:HG3 | 1:C:373:ARG:O | 2.13 | 0.48 |
| 1:C:181:VAL:HG23 | 1:C:404:PHE:HB2 | 1.96 | 0.48 |
| 1:C:414:GLU:CA | 1:C:417:GLU:HB2 | 2.44 | 0.48 |
| 2:D:179:ASP:CB | 2:D:182:VAL:HG23 | 2.41 | 0.48 |
| 2:D:51:VAL:HG22 | 2:D:245:PRO:HG2 | 1.96 | 0.48 |
| 1:C:101:ASN:CB | 2:D:254:LYS:HD3 | 2.42 | 0.48 |
| 2:D:279:GLY:O | 2:D:281:GLN:N | 2.47 | 0.48 |
| 2:D:90:ASP:OD1 | 2:D:91:ASN:ND2 | 2.47 | 0.48 |
| 1:A:408:TYR:HB2 | 1:A:418:PHE:HZ | 1.79 | 0.48 |
| 2:B:137:LEU:CD2 | 2:B:154:ILE:HG13 | 2.43 | 0.48 |
| 2:B:181:VAL:C | 2:B:184:PRO:HD2 | 2.34 | 0.48 |
| 1:C:229:ARG:HB3 | 1:C:366:GLY:O | 2.14 | 0.48 |
| 2:B:402:LYS:CE | 1:C:440:VAL:C | 2.82 | 0.48 |
| 2:D:103:TRP:O | 2:D:104:ALA:C | 2.52 | 0.48 |
| 2:D:132:LEU:HD22 | 2:D:164:ARG:NE | 2.29 | 0.48 |
| 2:D:132:LEU:CB | 2:D:164:ARG:HH21 | 2.21 | 0.48 |
| 3:E:48:UNK:C | 3:E:50:UNK:N | 2.75 | 0.48 |
| 1:A:139:HIS:CD2 | 1:A:146:GLY:O | 2.66 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:GLN:OE1 | 1:A:210:TYR:CE1 | 2.67 | 0.48 |
| 1:A:213:CYS:O | 1:A:219:ILE:HB | 2.14 | 0.48 |
| 1:A:26:LEU:CG | 1:A:361:THR:OG1 | 2.62 | 0.48 |
| 2:B:189:LEU:HA | 2:B:192:HIS:CE1 | 2.48 | 0.48 |
| 2:B:284:ARG:HB3 | 2:B:287:THR:OG1 | 2.14 | 0.48 |
| 2:B:397:ALA:O | 2:B:398:MET:HB2 | 2.13 | 0.48 |
| 2:B:62:VAL:O | 2:B:63:PRO:C | 2.51 | 0.48 |
| 2:B:93:VAL:HG23 | 2:B:95:GLY:N | 2.28 | 0.48 |
| 1:C:343:PHE:CD1 | 1:C:349:THR:HA | 2.49 | 0.48 |
| 1:C:398:MET:HB2 | 1:C:403:ALA:HB2 | 1.96 | 0.48 |
| 2:D:158:ARG:HD3 | 2:D:197:ASN:HD22 | 1.67 | 0.48 |
| 2:D:174:SER:C | 2:D:176:LYS:H | 2.16 | 0.48 |
| 2:D:284:ARG:HB2 | 2:D:290:GLU:OE1 | 2.14 | 0.48 |
| 2:D:400:ARG:C | 2:D:402:LYS:H | 2.17 | 0.48 |
| 1:A:104:ALA:CA | 1:A:108:TYR:HD2 | 2.23 | 0.48 |
| 1:A:209:ILE:CG2 | 1:A:227:LEU:HG | 2.44 | 0.48 |
| 1:A:220:GLU:HB3 | 1:A:221:ARG:CZ | 2.43 | 0.48 |
| 1:A:239:THR:OG1 | 1:A:240:ALA:N | 2.45 | 0.48 |
| 1:A:23:LEU:C | 1:A:25:CYS:N | 2.67 | 0.48 |
| 1:A:286:LEU:O | 1:A:287:SER:C | 2.50 | 0.48 |
| 1:A:322:ASP:HA | 1:A:357:TYR:CD1 | 2.42 | 0.48 |
| 1:A:321:GLY:HA2 | 1:A:358:GLU:O | 2.14 | 0.48 |
| 2:B:102:ASN:ND2 | 2:B:104:ALA:HB3 | 2.27 | 0.48 |
| 2:B:139:HIS:C | 2:B:139:HIS:HD2 | 2.17 | 0.48 |
| 2:B:182:VAL:CG1 | 2:B:182:VAL:O | 2.53 | 0.48 |
| 2:B:212:ILE:HG21 | 2:B:230:LEU:HD21 | 1.96 | 0.48 |
| 1:C:103:TYR:CG | 1:C:188:ILE:HD13 | 2.48 | 0.48 |
| 1:C:108:TYR:O | 1:C:109:THR:C | 2.52 | 0.48 |
| 2:D:350:ASN:C | 2:D:350:ASN:HD22 | 2.17 | 0.48 |
| 2:D:383:ALA:C | 2:D:385:GLN:N | 2.67 | 0.48 |
| 2:D:84:GLY:HA2 | 2:D:88:ARG:HH21 | 1.78 | 0.48 |
| 1:A:174:ALA:HB2 | 1:A:206:ASN:HB2 | 1.94 | 0.48 |
| 1:A:417:GLU:HB3 | 1:A:418:PHE:HE2 | 1.74 | 0.48 |
| 1:A:426:ALA:C | 1:A:428:LEU:H | 2.17 | 0.48 |
| 2:B:148:GLY:HA2 | 2:B:151:THR:HG22 | 1.95 | 0.48 |
| 2:B:293:GLN:C | 2:B:295:MET:N | 2.67 | 0.48 |
| 2:B:424:ASN:O | 2:B:427:ASP:N | 2.46 | 0.48 |
| 2:B:59:ASN:CA | 2:B:64:ARG:HH21 | 2.23 | 0.48 |
| 1:C:218:ASP:CG | 1:C:219:ILE:H | 2.16 | 0.48 |
| 1:C:221:ARG:H | 1:C:221:ARG:NE | 2.11 | 0.48 |
| 1:C:256:GLN:HA | 1:C:260:VAL:CG2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:289:ALA:HA | 1:C:292:THR:HG23 | 1.95 | 0.48 |
| 1:C:69:ASP:OD1 | 1:C:71:GLU:HG3 | 2.14 | 0.48 |
| 2:D:253:ARG:HG3 | 2:D:253:ARG:NH1 | 2.27 | 0.48 |
| 2:D:287:THR:C | 2:D:289:PRO:HD2 | 2.34 | 0.48 |
| 2:D:62:VAL:CG2 | 2:D:62:VAL:O | 2.62 | 0.48 |
| 1:A:182:VAL:HG12 | 1:A:183:GLU:H | 1.79 | 0.48 |
| 1:A:242:LEU:HB3 | 1:A:250:VAL:CG1 | 2.44 | 0.48 |
| 1:A:326:LYS:HG2 | 1:A:326:LYS:O | 2.13 | 0.48 |
| 1:A:39:ASP:CG | 1:A:40:LYS:N | 2.60 | 0.48 |
| 1:A:77:GLU:C | 1:A:83:TYR:HB2 | 2.35 | 0.48 |
| 2:B:106:GLY:O | 2:B:149:MET:HA | 2.14 | 0.48 |
| 2:B:22:GLU:HG3 | 2:B:83:PHE:CE1 | 2.49 | 0.48 |
| 1:A:101:ASN:CG | 2:B:254:LYS:HD3 | 2.34 | 0.48 |
| 2:B:297:ASP:OD1 | 2:B:299:LYS:N | 2.36 | 0.48 |
| 2:B:2:ARG:NH2 | 2:B:243:ARG:CA | 2.76 | 0.48 |
| 1:C:180:ALA:O | 1:C:182:VAL:N | 2.47 | 0.48 |
| 1:C:212:ILE:C | 1:C:214:ARG:H | 2.17 | 0.48 |
| 1:C:296:PHE:HZ | 1:C:317:LEU:HD21 | 1.79 | 0.48 |
| 2:D:262:PHE:HB3 | 2:D:263:PRO:CD | 2.36 | 0.48 |
| 1:A:164:LYS:CB | 1:A:164:LYS:NZ | 2.77 | 0.47 |
| 1:A:311:LYS:CB | 1:A:344:VAL:HG22 | 2.43 | 0.47 |
| 1:A:398:MET:CE | 1:A:399:TYR:HE1 | 2.27 | 0.47 |
| 2:B:121:VAL:O | 2:B:121:VAL:CG1 | 2.61 | 0.47 |
| 2:B:224:TYR:O | 2:B:228:ASN:HB2 | 2.14 | 0.47 |
| 2:B:297:ASP:O | 2:B:301:MET:HG2 | 2.13 | 0.47 |
| 2:B:320:ARG:HG2 | 2:B:320:ARG:NH1 | 2.29 | 0.47 |
| 1:C:346:TRP:HZ2 | 1:C:435:VAL:HB | 1.79 | 0.47 |
| 2:D:18:ALA:O | 2:D:22:GLU:OE2 | 2.32 | 0.47 |
| 2:D:381:SER:C | 2:D:383:ALA:H | 2.16 | 0.47 |
| 1:A:115:ILE:HG12 | 1:A:149:PHE:HE2 | 1.80 | 0.47 |
| 1:A:7:ILE:HG21 | 1:A:122:ILE:CD1 | 2.40 | 0.47 |
| 1:A:294:ALA:C | 1:A:296:PHE:N | 2.67 | 0.47 |
| 1:A:355:ILE:N | 1:A:355:ILE:CD1 | 2.76 | 0.47 |
| 1:A:407:TRP:C | 1:A:409:VAL:N | 2.67 | 0.47 |
| 1:A:46:ASP:O | 1:A:47:ASP:C | 2.52 | 0.47 |
| 2:B:429:VAL:O | 2:B:433:GLN:HG2 | 2.13 | 0.47 |
| 1:C:16:ILE:O | 1:C:17:GLY:C | 2.52 | 0.47 |
| 1:C:103:TYR:N | 1:C:185:TYR:CE1 | 2.82 | 0.47 |
| 1:C:20:CYS:C | 1:C:22:GLU:N | 2.66 | 0.47 |
| 1:C:255:PHE:HD1 | 1:C:259:LEU:HD12 | 1.79 | 0.47 |
| 1:C:284:GLU:OE2 | 1:C:285:GLN:NE2 | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:296:PHE:CZ | 1:C:317:LEU:HD21 | 2.48 | 0.47 |
| 1:C:417:GLU:C | 1:C:418:PHE:HD2 | 2.15 | 0.47 |
| 2:D:118:VAL:C | 2:D:120:ASP:N | 2.66 | 0.47 |
| 2:D:130:ASP:OD2 | 2:D:130:ASP:C | 2.52 | 0.47 |
| 2:D:3:GLU:O | 2:D:133:GLN:N | 2.38 | 0.47 |
| 2:D:60:LYS:N | 2:D:60:LYS:HZ3 | 2.12 | 0.47 |
| 1:A:174:ALA:C | 1:A:176:GLN:H | 2.18 | 0.47 |
| 1:A:209:ILE:H | 1:A:209:ILE:CD1 | 2.28 | 0.47 |
| 1:A:426:ALA:C | 1:A:428:LEU:N | 2.67 | 0.47 |
| 2:B:14:ASN:O | 2:B:18:ALA:N | 2.47 | 0.47 |
| 2:B:200:GLU:CD | 2:B:268:PHE:HE2 | 2.17 | 0.47 |
| 2:B:79:ARG:HG2 | 2:B:79:ARG:O | 2.13 | 0.47 |
| 1:C:128:GLN:HA | 1:C:128:GLN:OE1 | 2.14 | 0.47 |
| 1:C:243:ARG:NE | 1:C:243:ARG:HA | 2.29 | 0.47 |
| 2:D:161:TYR:O | 2:D:162:PRO:C | 2.52 | 0.47 |
| 2:D:389:LYS:HA | 2:D:392:SER:OG | 2.14 | 0.47 |
| 1:A:217:LEU:HD23 | 1:A:219:ILE:CD1 | 2.44 | 0.47 |
| 2:B:427:ASP:O | 2:B:428:LEU:C | 2.53 | 0.47 |
| 1:C:307:PRO:HA | 1:C:383:ALA:CB | 2.45 | 0.47 |
| 1:C:428:LEU:C | 1:C:430:LYS:N | 2.68 | 0.47 |
| 2:D:142:GLY:HA3 | 2:D:186:ASN:OD1 | 2.15 | 0.47 |
| 2:D:212:ILE:HG21 | 2:D:230:LEU:HD21 | 1.95 | 0.47 |
| 2:D:283:TYR:HD1 | 2:D:284:ARG:HH21 | 1.62 | 0.47 |
| 2:D:303:ALA:HB1 | 2:D:387:LEU:HD12 | 1.95 | 0.47 |
| 2:D:387:LEU:O | 2:D:387:LEU:CD2 | 2.57 | 0.47 |
| 2:D:405:LEU:C | 2:D:407:TRP:H | 2.17 | 0.47 |
| 1:A:343:PHE:CG | 1:A:349:THR:HB | 2.49 | 0.47 |
| 2:B:144:GLY:HA3 | 2:B:185:TYR:OH | 2.14 | 0.47 |
| 2:B:154:ILE:HD11 | 2:B:168:THR:HG21 | 1.96 | 0.47 |
| 2:B:223:THR:HG23 | 2:B:225:GLY:H | 1.79 | 0.47 |
| 2:B:206:ASN:ND2 | 2:B:227:LEU:CD2 | 2.71 | 0.47 |
| 2:B:235:MET:O | 2:B:239:THR:OG1 | 2.31 | 0.47 |
| 2:B:242:LEU:O | 2:B:243:ARG:NE | 2.46 | 0.47 |
| 2:B:51:VAL:HG23 | 2:B:53:TYR:HB2 | 1.95 | 0.47 |
| 1:C:241:SER:HA | 1:C:320:ARG:CZ | 2.43 | 0.47 |
| 1:C:311:LYS:HD3 | 1:C:344:VAL:CG1 | 2.39 | 0.47 |
| 1:C:327:ASP:O | 1:C:330:ALA:HB3 | 2.14 | 0.47 |
| 1:C:408:TYR:HB2 | 1:C:418:PHE:HZ | 1.79 | 0.47 |
| 1:C:426:ALA:C | 1:C:428:LEU:N | 2.67 | 0.47 |
| 2:D:137:LEU:O | 2:D:137:LEU:HG | 2.15 | 0.47 |
| 2:D:255:LEU:HD21 | 2:D:259:MET:HG3 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:315:VAL:HA | 2:D:379:GLY:HA2 | 1.97 | 0.47 |
| 3:E:57:UNK:O | 3:E:60:UNK:N | 2.48 | 0.47 |
| 1:A:189:LEU:HD13 | 1:A:193:THR:CG2 | 2.44 | 0.47 |
| 1:A:217:LEU:HD23 | 1:A:219:ILE:HD12 | 1.95 | 0.47 |
| 2:B:100:GLY:C | 2:B:101:ASN:HD22 | 2.18 | 0.47 |
| 2:B:119:LEU:CD1 | 2:B:123:ARG:NH2 | 2.78 | 0.47 |
| 2:B:174:SER:O | 2:B:176:LYS:N | 2.47 | 0.47 |
| 2:B:179:ASP:HB2 | 2:B:182:VAL:N | 2.29 | 0.47 |
| 2:B:178:SER:O | 2:B:179:ASP:O | 2.32 | 0.47 |
| 2:B:133:GLN:NE2 | 2:B:252:LEU:N | 2.59 | 0.47 |
| 1:C:137:VAL:HG21 | 1:C:154:MET:CE | 2.45 | 0.47 |
| 1:C:286:LEU:HB3 | 1:C:290:GLU:HB3 | 1.97 | 0.47 |
| 1:C:295:CYS:SG | 1:C:295:CYS:O | 2.73 | 0.47 |
| 1:C:426:ALA:C | 1:C:428:LEU:H | 2.17 | 0.47 |
| 1:C:73:THR:HG23 | 1:C:74:VAL:H | 1.79 | 0.47 |
| 2:D:115:VAL:HG21 | 2:D:152:LEU:HD21 | 1.95 | 0.47 |
| 2:D:139:HIS:HD2 | 2:D:139:HIS:O | 1.98 | 0.47 |
| 2:D:158:ARG:HG3 | 2:D:159:GLU:HG3 | 1.97 | 0.47 |
| 2:D:202:TYR:HE1 | 2:D:378:ILE:HD12 | 1.76 | 0.47 |
| 2:B:286:LEU:CD1 | 2:B:371:LEU:O | 2.63 | 0.47 |
| 1:C:179:THR:HG22 | 1:C:180:ALA:O | 2.15 | 0.47 |
| 1:C:286:LEU:O | 1:C:287:SER:C | 2.51 | 0.47 |
| 1:C:35:GLN:HE22 | 1:C:88:HIS:CG | 2.32 | 0.47 |
| 2:D:19:LYS:HA | 2:D:22:GLU:CG | 2.45 | 0.47 |
| 2:D:295:MET:HG2 | 2:D:377:PHE:HD2 | 1.79 | 0.47 |
| 2:D:386:GLU:C | 2:D:388:PHE:N | 2.66 | 0.47 |
| 2:D:1:MET:C | 2:D:3:GLU:N | 2.68 | 0.47 |
| 1:A:242:LEU:HD11 | 1:A:318:LEU:HG | 1.97 | 0.47 |
| 1:A:172:TYR:CE2 | 1:A:391:LEU:HD22 | 2.49 | 0.47 |
| 2:B:154:ILE:HG23 | 2:B:197:ASN:HB3 | 1.97 | 0.47 |
| 2:B:282:GLN:C | 2:B:285:ALA:H | 2.17 | 0.47 |
| 1:C:294:ALA:C | 1:C:296:PHE:N | 2.67 | 0.47 |
| 1:C:294:ALA:HA | 1:C:297:GLU:HB2 | 1.96 | 0.47 |
| 1:C:312:TYR:O | 1:C:344:VAL:HG23 | 2.14 | 0.47 |
| 1:C:368:LEU:HD12 | 1:C:368:LEU:N | 2.29 | 0.47 |
| 1:C:385:ALA:HB1 | 1:C:429:GLU:HG3 | 1.97 | 0.47 |
| 1:C:190:THR:HG21 | 1:C:425:MET:SD | 2.55 | 0.47 |
| 2:D:124:LYS:HG3 | 2:D:124:LYS:O | 2.15 | 0.47 |
| 2:D:271:GLY:O | 2:D:272:PHE:O | 2.33 | 0.47 |
| 2:D:307:PRO:C | 2:D:309:HIS:N | 2.68 | 0.47 |
| 2:D:81:GLY:N | 2:D:82:PRO:HD2 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:93:VAL:CG2 | 2:D:94:PHE:N | 2.78 | 0.47 |
| 1:A:152:LEU:O | 1:A:153:LEU:C | 2.52 | 0.47 |
| 1:A:184:PRO:O | 1:A:188:ILE:HG13 | 2.14 | 0.47 |
| 1:A:314:ALA:O | 1:A:315:CYS:HB3 | 2.15 | 0.47 |
| 1:A:311:LYS:CD | 1:A:344:VAL:HG13 | 2.31 | 0.47 |
| 1:A:77:GLU:OE2 | 1:A:83:TYR:CG | 2.68 | 0.47 |
| 1:A:86:LEU:HD13 | 1:A:89:PRO:HD3 | 1.97 | 0.47 |
| 2:B:129:CYS:O | 2:B:130:ASP:C | 2.52 | 0.47 |
| 2:B:253:ARG:C | 2:B:255:LEU:N | 2.68 | 0.47 |
| 2:B:293:GLN:C | 2:B:295:MET:H | 2.17 | 0.47 |
| 1:C:23:LEU:O | 1:C:26:LEU:CD1 | 2.63 | 0.47 |
| 1:C:401:LYS:O | 1:C:402:ARG:NE | 2.47 | 0.47 |
| 1:C:407:TRP:C | 1:C:409:VAL:N | 2.65 | 0.47 |
| 2:D:209:LEU:CB | 2:D:227:LEU:HG | 2.45 | 0.47 |
| 2:D:312:TYR:CE2 | 2:D:377:PHE:HZ | 2.32 | 0.47 |
| 1:A:274:PRO:HG3 | 1:A:373:ARG:O | 2.14 | 0.47 |
| 1:A:306:ASP:HB3 | 1:A:386:GLU:OE1 | 2.15 | 0.47 |
| 2:B:174:SER:C | 2:B:176:LYS:N | 2.68 | 0.47 |
| 2:B:243:ARG:HD3 | 2:B:243:ARG:HA | 1.47 | 0.47 |
| 2:B:218:LYS:NZ | 2:B:277:SER:HB3 | 2.29 | 0.47 |
| 1:C:16:ILE:CG2 | 1:C:17:GLY:N | 2.67 | 0.47 |
| 1:C:20:CYS:O | 1:C:24:TYR:N | 2.34 | 0.47 |
| 1:C:243:ARG:NH1 | 1:C:250:VAL:HG13 | 2.19 | 0.47 |
| 1:C:256:GLN:HB3 | 1:C:260:VAL:CB | 2.41 | 0.47 |
| 1:C:311:LYS:CD | 1:C:344:VAL:HG22 | 2.44 | 0.47 |
| 1:C:419:SER:O | 1:C:422:ARG:HG2 | 2.14 | 0.47 |
| 1:C:9:VAL:HG21 | 1:C:150:THR:HG22 | 1.96 | 0.47 |
| 2:D:16:ILE:HD12 | 2:D:231:VAL:CG1 | 2.42 | 0.47 |
| 2:D:22:GLU:HG3 | 2:D:83:PHE:CE1 | 2.50 | 0.47 |
| 2:D:283:TYR:C | 2:D:285:ALA:N | 2.67 | 0.47 |
| 1:A:144:GLY:H | 1:A:147:SER:HB3 | 1.76 | 0.47 |
| 1:A:177:VAL:HG11 | 2:B:349:ASN:CB | 2.45 | 0.47 |
| 1:A:206:ASN:O | 1:A:207:GLU:C | 2.53 | 0.47 |
| 1:A:209:ILE:HG22 | 1:A:227:LEU:HG | 1.97 | 0.47 |
| 2:B:118:VAL:C | 2:B:120:ASP:N | 2.65 | 0.47 |
| 2:B:11:GLN:C | 2:B:13:GLY:H | 2.18 | 0.47 |
| 2:B:220:THR:HB | 1:C:326:LYS:CE | 2.45 | 0.47 |
| 2:B:284:ARG:HG3 | 2:B:284:ARG:HH11 | 1.79 | 0.47 |
| 2:B:298:ALA:HB2 | 2:B:307:PRO:CD | 2.45 | 0.47 |
| 1:C:416:GLY:O | 1:C:420:GLU:HB3 | 2.14 | 0.47 |
| 1:C:73:THR:HA | 1:C:76:ASP:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:141:LEU:HG | 2:D:170:SER:HB3 | 1.97 | 0.47 |
| 2:D:186:ASN:O | 2:D:189:LEU:HB2 | 2.15 | 0.47 |
| 2:D:249:ASN:CG | 2:D:250:ALA:N | 2.68 | 0.47 |
| 2:D:320:ARG:CG | 2:D:320:ARG:HH11 | 2.25 | 0.47 |
| 2:D:357:ASP:CB | 2:D:358:ILE:HD12 | 2.45 | 0.47 |
| 2:D:203:CYS:SG | 2:D:384:ILE:CD1 | 3.02 | 0.47 |
| 2:D:4:ILE:HG12 | 2:D:133:GLN:HG2 | 1.97 | 0.47 |
| 2:D:58:GLY:O | 2:D:64:ARG:CZ | 2.63 | 0.47 |
| 3:E:42:UNK:O | 3:E:45:UNK:N | 2.48 | 0.47 |
| 1:A:123:ARG:HA | 1:A:161:TYR:OH | 2.15 | 0.46 |
| 1:A:185:TYR:CE1 | 1:A:408:TYR:HE1 | 2.33 | 0.46 |
| 1:A:185:TYR:O | 1:A:188:ILE:HD12 | 2.15 | 0.46 |
| 1:A:264:ARG:O | 1:A:266:HIS:ND1 | 2.48 | 0.46 |
| 1:A:265:ALA:O | 1:A:266:HIS:O | 2.33 | 0.46 |
| 1:A:295:CYS:SG | 1:A:377:MET:HE1 | 2.55 | 0.46 |
| 1:A:362:VAL:O | 1:A:370:LYS:NZ | 2.48 | 0.46 |
| 2:B:191:VAL:CG1 | 2:B:191:VAL:O | 2.58 | 0.46 |
| 2:B:402:LYS:HE3 | 1:C:440:VAL:C | 2.35 | 0.46 |
| 1:C:273:ALA:HB2 | 1:C:295:CYS:HA | 1.97 | 0.46 |
| 1:C:343:PHE:CG | 1:C:349:THR:HB | 2.50 | 0.46 |
| 1:C:385:ALA:HB2 | 1:C:432:TYR:CD2 | 2.47 | 0.46 |
| 2:D:238:VAL:HG22 | 2:D:376:THR:HG21 | 1.96 | 0.46 |
| 3:E:61:UNK:C | 3:E:63:UNK:N | 2.78 | 0.46 |
| 1:A:102:ASN:O | 1:A:103:TYR:C | 2.54 | 0.46 |
| 2:B:320:ARG:HH11 | 2:B:320:ARG:CG | 2.25 | 0.46 |
| 1:C:172:TYR:CG | 1:C:173:PRO:HD2 | 2.50 | 0.46 |
| 1:C:26:LEU:HG | 1:C:361:THR:HB | 1.97 | 0.46 |
| 2:D:3:GLU:HG2 | 2:D:58:GLY:O | 2.15 | 0.46 |
| 2:D:401:ARG:O | 2:D:402:LYS:HG3 | 2.15 | 0.46 |
| 2:D:63:PRO:C | 2:D:65:ALA:N | 2.67 | 0.46 |
| 1:A:132:LEU:O | 1:A:133:GLN:CB | 2.61 | 0.46 |
| 1:A:317:LEU:HD23 | 1:A:377:MET:HB2 | 1.96 | 0.46 |
| 1:A:393:HIS:C | 1:A:395:PHE:N | 2.68 | 0.46 |
| 1:A:402:ARG:NH1 | 2:B:346:TRP:CD2 | 2.83 | 0.46 |
| 2:B:114:LEU:HD12 | 2:B:114:LEU:HA | 1.78 | 0.46 |
| 2:B:142:GLY:HA2 | 2:B:185:TYR:CB | 2.39 | 0.46 |
| 2:B:305:CYS:O | 2:B:306:ASP:C | 2.53 | 0.46 |
| 2:B:75:MET:SD | 2:B:79:ARG:CZ | 3.02 | 0.46 |
| 1:C:68:VAL:O | 1:C:68:VAL:HG13 | 2.14 | 0.46 |
| 1:C:9:VAL:CG2 | 1:C:9:VAL:O | 2.63 | 0.46 |
| 2:D:243:ARG:HD3 | 2:D:243:ARG:HA | 1.52 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:313:LEU:O | 2:D:314:THR:HG23 | 2.15 | 0.46 |
| 2:D:60:LYS:CD | 2:D:60:LYS:H | 2.28 | 0.46 |
| 1:A:181:VAL:O | 1:A:185:TYR:CD2 | 2.69 | 0.46 |
| 1:A:243:ARG:NH1 | 1:A:250:VAL:CG1 | 2.72 | 0.46 |
| 1:A:275:VAL:CG1 | 1:A:275:VAL:O | 2.63 | 0.46 |
| 2:B:103:TRP:N | 2:B:185:TYR:OH | 2.48 | 0.46 |
| 2:B:313:LEU:O | 2:B:314:THR:CG2 | 2.64 | 0.46 |
| 2:B:389:LYS:HA | 2:B:392:SER:OG | 2.14 | 0.46 |
| 1:C:101:ASN:OD1 | 2:D:254:LYS:CD | 2.59 | 0.46 |
| 1:C:24:TYR:HA | 1:C:26:LEU:CD1 | 2.46 | 0.46 |
| 1:C:273:ALA:HB2 | 1:C:295:CYS:CB | 2.42 | 0.46 |
| 2:D:3:GLU:OE2 | 2:D:128:SER:O | 2.33 | 0.46 |
| 2:D:137:LEU:CD2 | 2:D:154:ILE:HG13 | 2.46 | 0.46 |
| 2:D:132:LEU:H | 2:D:164:ARG:HH21 | 1.62 | 0.46 |
| 2:D:350:ASN:ND2 | 2:D:350:ASN:N | 2.62 | 0.46 |
| 1:A:122:ILE:HG22 | 1:A:123:ARG:N | 2.30 | 0.46 |
| 1:A:209:ILE:H | 1:A:209:ILE:HD12 | 1.79 | 0.46 |
| 1:A:388:TRP:CZ3 | 1:A:428:LEU:HD13 | 2.50 | 0.46 |
| 2:B:124:LYS:O | 2:B:124:LYS:HG3 | 2.15 | 0.46 |
| 2:B:405:LEU:C | 2:B:407:TRP:H | 2.18 | 0.46 |
| 1:C:344:VAL:CG1 | 1:C:345:ASP:N | 2.75 | 0.46 |
| 1:C:386:GLU:C | 1:C:388:TRP:N | 2.68 | 0.46 |
| 1:C:398:MET:CE | 1:C:399:TYR:HE1 | 2.29 | 0.46 |
| 2:D:322:ARG:NE | 2:D:357:ASP:CB | 2.74 | 0.46 |
| 2:D:350:ASN:ND2 | 2:D:350:ASN:H | 2.13 | 0.46 |
| 1:A:172:TYR:CG | 1:A:173:PRO:HD2 | 2.51 | 0.46 |
| 1:A:287:SER:O | 1:A:289:ALA:N | 2.49 | 0.46 |
| 2:B:320:ARG:HB3 | 2:B:320:ARG:CZ | 2.45 | 0.46 |
| 2:B:60:LYS:HD2 | 2:B:60:LYS:H | 1.79 | 0.46 |
| 2:B:73:GLY:O | 2:B:78:VAL:HG21 | 2.16 | 0.46 |
| 1:C:122:ILE:O | 1:C:125:LEU:N | 2.48 | 0.46 |
| 1:C:265:ALA:O | 1:C:266:HIS:O | 2.33 | 0.46 |
| 1:C:344:VAL:HG12 | 1:C:345:ASP:CG | 2.36 | 0.46 |
| 2:D:148:GLY:CA | 2:D:151:THR:HG22 | 2.46 | 0.46 |
| 2:D:239:THR:HB | 2:D:240:THR:H | 1.42 | 0.46 |
| 1:A:112:LYS:HZ1 | 3:E:12:UNK:CB | 2.29 | 0.46 |
| 1:A:218:ASP:CG | 1:A:219:ILE:N | 2.69 | 0.46 |
| 1:A:23:LEU:O | 1:A:26:LEU:CD1 | 2.63 | 0.46 |
| 1:A:341:ILE:HD12 | 1:A:341:ILE:N | 2.30 | 0.46 |
| 1:A:416:GLY:O | 1:A:420:GLU:HB3 | 2.16 | 0.46 |
| 2:B:137:LEU:HD23 | 2:B:154:ILE:CD1 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:149:PHE:CD2 | 1:C:149:PHE:O | 2.69 | 0.46 |
| 1:C:154:MET:CE | 1:C:197:HIS:NE2 | 2.79 | 0.46 |
| 1:C:245:ASP:O | 1:C:249:ASN:OD1 | 2.33 | 0.46 |
| 2:D:18:ALA:O | 2:D:21:TRP:N | 2.46 | 0.46 |
| 2:D:378:ILE:O | 2:D:378:ILE:HG22 | 2.16 | 0.46 |
| 1:C:159:VAL:HG21 | 3:E:56:UNK:HA | 1.98 | 0.46 |
| 1:A:398:MET:HB2 | 1:A:403:ALA:HB2 | 1.96 | 0.46 |
| 1:A:84:ARG:C | 1:A:85:GLN:HG2 | 2.36 | 0.46 |
| 2:B:194:LEU:HD12 | 2:B:428:LEU:HD21 | 1.97 | 0.46 |
| 2:B:283:TYR:C | 2:B:285:ALA:N | 2.68 | 0.46 |
| 2:B:308:ARG:HG3 | 2:B:342:TYR:CZ | 2.51 | 0.46 |
| 2:B:315:VAL:HA | 2:B:379:GLY:HA2 | 1.98 | 0.46 |
| 2:B:383:ALA:C | 2:B:385:GLN:N | 2.68 | 0.46 |
| 1:C:166:LYS:HD2 | 1:C:197:HIS:HD2 | 1.81 | 0.46 |
| 1:C:171:ILE:CG2 | 4:C:502:GTP:HN22 | 2.29 | 0.46 |
| 1:C:182:VAL:HG12 | 1:C:183:GLU:N | 2.31 | 0.46 |
| 1:C:20:CYS:C | 1:C:22:GLU:H | 2.19 | 0.46 |
| 1:C:251:ASP:O | 1:C:254:GLU:N | 2.49 | 0.46 |
| 1:C:274:PRO:HB3 | 1:C:291:ILE:CD1 | 2.45 | 0.46 |
| 2:D:174:SER:O | 2:D:176:LYS:N | 2.49 | 0.46 |
| 2:D:20:PHE:O | 2:D:23:VAL:N | 2.48 | 0.46 |
| 2:D:291:LEU:HD22 | 2:D:291:LEU:N | 2.30 | 0.46 |
| 2:D:331:GLN:OE1 | 2:D:331:GLN:HA | 2.15 | 0.46 |
| 1:C:159:VAL:CG2 | 3:E:56:UNK:HA | 2.46 | 0.46 |
| 1:A:103:TYR:CD1 | 1:A:188:ILE:HD13 | 2.51 | 0.46 |
| 1:A:149:PHE:O | 1:A:149:PHE:CD2 | 2.69 | 0.46 |
| 1:A:206:ASN:O | 1:A:210:TYR:CD2 | 2.69 | 0.46 |
| 1:A:225:THR:HA | 1:A:228:ASN:HB2 | 1.98 | 0.46 |
| 1:A:265:ALA:O | 1:A:266:HIS:C | 2.54 | 0.46 |
| 1:A:44:GLY:C | 1:A:46:ASP:N | 2.69 | 0.46 |
| 2:B:279:GLY:O | 2:B:281:GLN:N | 2.49 | 0.46 |
| 2:B:398:MET:HG3 | 1:C:346:TRP:O | 2.16 | 0.46 |
| 2:B:428:LEU:HD12 | 2:B:428:LEU:N | 2.31 | 0.46 |
| 2:B:430:SER:O | 2:B:431:GLU:C | 2.54 | 0.46 |
| 1:C:175:PRO:HB2 | 1:C:207:GLU:OE2 | 2.16 | 0.46 |
| 2:D:169:PHE:CG | 2:D:235:MET:SD | 3.09 | 0.46 |
| 2:D:215:ARG:NE | 2:D:215:ARG:CA | 2.78 | 0.46 |
| 2:D:238:VAL:HG21 | 2:D:378:ILE:HD11 | 1.98 | 0.46 |
| 1:A:306:ASP:OD1 | 1:A:309:HIS:NE2 | 2.49 | 0.46 |
| 1:A:371:VAL:CG1 | 1:A:372:GLN:N | 2.78 | 0.46 |
| 1:A:371:VAL:HG11 | 1:A:373:ARG:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:11:GLN:OE1 | 2:B:73:GLY:HA3 | 2.15 | 0.46 |
| 2:B:119:LEU:HD13 | 2:B:123:ARG:CZ | 2.46 | 0.46 |
| 2:B:6:HIS:ND1 | 2:B:21:TRP:HZ2 | 2.14 | 0.46 |
| 2:B:238:VAL:HG21 | 2:B:378:ILE:HD11 | 1.98 | 0.46 |
| 2:B:283:TYR:HD1 | 2:B:284:ARG:HH21 | 1.64 | 0.46 |
| 1:C:184:PRO:CG | 1:C:399:TYR:CZ | 2.98 | 0.46 |
| 1:C:331:ALA:O | 1:C:335:ILE:HG23 | 2.15 | 0.46 |
| 1:C:42:ILE:HD12 | 1:C:43:GLY:H | 1.81 | 0.46 |
| 2:D:122:VAL:CG1 | 2:D:123:ARG:N | 2.78 | 0.46 |
| 2:D:259:MET:HE1 | 2:D:316:ALA:HB2 | 1.98 | 0.46 |
| 2:D:416:MET:HA | 2:D:419:THR:OG1 | 2.16 | 0.46 |
| 1:A:21:TRP:N | 1:A:21:TRP:CD1 | 2.84 | 0.45 |
| 1:A:210:TYR:CE2 | 1:A:227:LEU:CD2 | 2.98 | 0.45 |
| 1:A:242:LEU:O | 1:A:250:VAL:HG12 | 2.16 | 0.45 |
| 1:A:276:ILE:CG1 | 1:A:282:TYR:CD2 | 2.98 | 0.45 |
| 1:A:262:TYR:HE1 | 1:A:346:TRP:CH2 | 2.35 | 0.45 |
| 1:A:36:MET:HE2 | 1:A:37:PRO:HD2 | 1.98 | 0.45 |
| 2:B:287:THR:CB | 2:B:289:PRO:HD2 | 2.41 | 0.45 |
| 1:C:104:ALA:CA | 1:C:108:TYR:HD2 | 2.23 | 0.45 |
| 1:C:316:CYS:HB2 | 1:C:352:LYS:CB | 2.24 | 0.45 |
| 1:C:419:SER:O | 1:C:420:GLU:C | 2.55 | 0.45 |
| 2:D:20:PHE:HZ | 2:D:239:THR:HG21 | 1.81 | 0.45 |
| 2:D:290:GLU:HG2 | 2:D:294:GLN:HB2 | 1.97 | 0.45 |
| 2:D:351:VAL:HG12 | 2:D:352:LYS:N | 2.32 | 0.45 |
| 2:D:351:VAL:O | 2:D:352:LYS:HG3 | 2.17 | 0.45 |
| 1:A:10:GLY:O | 1:A:11:GLN:C | 2.54 | 0.45 |
| 1:A:244:PHE:HD2 | 1:A:244:PHE:H | 1.63 | 0.45 |
| 1:A:280:LYS:O | 1:A:282:TYR:CD2 | 2.69 | 0.45 |
| 2:B:174:SER:C | 2:B:176:LYS:H | 2.19 | 0.45 |
| 2:B:158:ARG:HB2 | 2:B:197:ASN:HD22 | 1.81 | 0.45 |
| 2:B:208:ALA:HB2 | 2:B:304:ALA:CB | 2.47 | 0.45 |
| 2:B:211:ASP:O | 2:B:215:ARG:HB2 | 2.16 | 0.45 |
| 2:B:247:GLN:OE1 | 2:B:356:CYS:HA | 2.16 | 0.45 |
| 2:B:73:GLY:C | 2:B:75:MET:H | 2.20 | 0.45 |
| 2:B:81:GLY:N | 2:B:82:PRO:HD2 | 2.32 | 0.45 |
| 1:C:102:ASN:O | 1:C:103:TYR:C | 2.53 | 0.45 |
| 1:C:206:ASN:O | 1:C:210:TYR:CD2 | 2.69 | 0.45 |
| 1:C:398:MET:HE3 | 1:C:399:TYR:HE1 | 1.80 | 0.45 |
| 2:D:119:LEU:HD13 | 2:D:123:ARG:NH2 | 2.30 | 0.45 |
| 2:D:298:ALA:HB2 | 2:D:307:PRO:CD | 2.46 | 0.45 |
| 2:D:58:GLY:O | 2:D:64:ARG:NH2 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:242:LEU:O | 1:A:250:VAL:CG1 | 2.64 | 0.45 |
| 1:A:255:PHE:HD1 | 1:A:259:LEU:HD12 | 1.81 | 0.45 |
| 1:A:74:VAL:CG1 | 1:A:75:ILE:N | 2.78 | 0.45 |
| 2:B:313:LEU:O | 2:B:314:THR:HG23 | 2.16 | 0.45 |
| 2:B:5:VAL:HG12 | 2:B:5:VAL:O | 2.17 | 0.45 |
| 1:C:139:HIS:CD2 | 1:C:146:GLY:O | 2.69 | 0.45 |
| 1:C:197:HIS:CG | 1:C:198:SER:N | 2.83 | 0.45 |
| 1:C:209:ILE:O | 1:C:211:ASP:N | 2.49 | 0.45 |
| 2:D:14:ASN:O | 2:D:18:ALA:N | 2.46 | 0.45 |
| 2:D:235:MET:O | 2:D:239:THR:OG1 | 2.35 | 0.45 |
| 2:D:247:GLN:OE1 | 2:D:356:CYS:HA | 2.16 | 0.45 |
| 2:D:276:THR:HG21 | 2:D:281:GLN:CG | 2.47 | 0.45 |
| 1:A:221:ARG:HA | 1:A:222:PRO:HD2 | 1.71 | 0.45 |
| 1:A:238:ILE:O | 1:A:239:THR:O | 2.35 | 0.45 |
| 1:A:414:GLU:HA | 1:A:417:GLU:HB2 | 1.98 | 0.45 |
| 1:C:189:LEU:HD13 | 1:C:193:THR:CG2 | 2.45 | 0.45 |
| 1:C:5:ILE:O | 1:C:136:SER:N | 2.48 | 0.45 |
| 1:C:99:ALA:O | 1:C:100:ALA:HB2 | 2.17 | 0.45 |
| 2:D:276:THR:HG21 | 2:D:281:GLN:CB | 2.47 | 0.45 |
| 2:D:399:PHE:HE2 | 2:D:404:PHE:HB3 | 1.80 | 0.45 |
| 3:E:10:UNK:C | 3:E:12:UNK:N | 2.71 | 0.45 |
| 1:A:143:GLY:O | 1:A:144:GLY:C | 2.55 | 0.45 |
| 1:A:179:THR:HB | 1:A:182:VAL:CG2 | 2.47 | 0.45 |
| 1:A:277:SER:O | 1:A:278:ALA:CB | 2.62 | 0.45 |
| 1:A:5:ILE:HG22 | 1:A:6:SER:N | 2.31 | 0.45 |
| 2:B:51:VAL:HG13 | 2:B:245:PRO:HB2 | 1.99 | 0.45 |
| 2:B:403:ALA:O | 2:B:404:PHE:HB2 | 2.16 | 0.45 |
| 2:B:424:ASN:O | 2:B:427:ASP:HB2 | 2.17 | 0.45 |
| 2:B:60:LYS:CD | 2:B:60:LYS:H | 2.29 | 0.45 |
| 2:B:87:PHE:O | 2:B:89:PRO:N | 2.49 | 0.45 |
| 1:C:119:LEU:HD22 | 1:C:156:ARG:HE | 1.81 | 0.45 |
| 1:C:197:HIS:CE1 | 1:C:198:SER:HB3 | 2.52 | 0.45 |
| 1:C:365:GLY:O | 1:C:368:LEU:HD11 | 2.17 | 0.45 |
| 1:C:380:ASN:O | 1:C:380:ASN:CG | 2.53 | 0.45 |
| 1:C:67:PHE:O | 1:C:92:LEU:HA | 2.16 | 0.45 |
| 2:D:284:ARG:O | 2:D:285:ALA:C | 2.54 | 0.45 |
| 2:D:2:ARG:O | 2:D:2:ARG:HG2 | 2.17 | 0.45 |
| 1:A:108:TYR:O | 1:A:109:THR:C | 2.55 | 0.45 |
| 1:A:363:VAL:HG22 | 1:A:367:ASP:CG | 2.36 | 0.45 |
| 1:A:364:PRO:C | 1:A:366:GLY:H | 2.20 | 0.45 |
| 1:A:398:MET:HE3 | 1:A:399:TYR:HE1 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:176:LYS:HD2 | 2:B:210:TYR:CE1 | 2.52 | 0.45 |
| 2:B:272:PHE:CE1 | 2:B:274:PRO:HG2 | 2.51 | 0.45 |
| 1:C:115:ILE:HG12 | 1:C:149:PHE:HE2 | 1.80 | 0.45 |
| 1:C:164:LYS:HB2 | 1:C:164:LYS:NZ | 2.29 | 0.45 |
| 1:C:206:ASN:O | 1:C:207:GLU:C | 2.55 | 0.45 |
| 1:C:287:SER:O | 1:C:289:ALA:N | 2.50 | 0.45 |
| 1:C:332:ILE:HG23 | 1:C:351:PHE:CE2 | 2.52 | 0.45 |
| 2:D:140:SER:O | 2:D:147:SER:OG | 2.33 | 0.45 |
| 2:D:211:ASP:O | 2:D:215:ARG:N | 2.50 | 0.45 |
| 2:D:234:THR:O | 2:D:238:VAL:HG23 | 2.17 | 0.45 |
| 2:D:405:LEU:HD22 | 2:D:405:LEU:O | 2.16 | 0.45 |
| 2:D:311:ARG:NE | 2:D:436:GLN:O | 2.50 | 0.45 |
| 2:D:59:ASN:HA | 2:D:60:LYS:NZ | 2.32 | 0.45 |
| 1:A:327:ASP:O | 1:A:330:ALA:HB3 | 2.16 | 0.45 |
| 2:B:133:GLN:CG | 2:B:252:LEU:HD22 | 2.47 | 0.45 |
| 1:C:16:ILE:HG22 | 1:C:17:GLY:H | 1.79 | 0.45 |
| 1:C:371:VAL:HG12 | 1:C:372:GLN:H | 1.81 | 0.45 |
| 1:C:408:TYR:O | 1:C:414:GLU:HG3 | 2.17 | 0.45 |
| 2:D:206:ASN:ND2 | 5:D:503:GDP:N2 | 2.64 | 0.45 |
| 2:D:334:ASN:O | 2:D:338:LYS:N | 2.50 | 0.45 |
| 1:A:206:ASN:CB | 1:A:210:TYR:HE2 | 2.28 | 0.45 |
| 1:A:344:VAL:CG1 | 1:A:345:ASP:N | 2.76 | 0.45 |
| 1:A:417:GLU:C | 1:A:418:PHE:HD2 | 2.17 | 0.45 |
| 1:A:171:ILE:HG21 | 4:A:500:GTP:HN22 | 1.81 | 0.45 |
| 2:B:102:ASN:HB3 | 2:B:105:LYS:CG | 2.47 | 0.45 |
| 1:C:172:TYR:H | 1:C:205:ASP:H | 1.65 | 0.45 |
| 1:C:344:VAL:HG12 | 1:C:345:ASP:H | 1.81 | 0.45 |
| 1:C:355:ILE:N | 1:C:355:ILE:CD1 | 2.79 | 0.45 |
| 2:D:209:LEU:HD21 | 2:D:302:MET:HG3 | 1.98 | 0.45 |
| 2:D:436:GLN:HE21 | 2:D:436:GLN:C | 2.20 | 0.45 |
| 1:A:155:GLU:OE2 | 1:A:196:GLU:HB3 | 2.17 | 0.45 |
| 2:B:298:ALA:HA | 2:B:301:MET:CG | 2.47 | 0.45 |
| 1:C:223:THR:O | 1:C:226:ASN:N | 2.50 | 0.45 |
| 1:C:31:GLN:CB | 1:C:32:PRO:CD | 2.94 | 0.45 |
| 1:C:326:LYS:O | 1:C:326:LYS:HG2 | 2.16 | 0.45 |
| 1:C:343:PHE:CD2 | 1:C:349:THR:HB | 2.52 | 0.45 |
| 1:C:396:ASP:O | 1:C:400:ALA:HB3 | 2.17 | 0.45 |
| 1:C:171:ILE:HG21 | 4:C:502:GTP:N3 | 2.32 | 0.45 |
| 2:D:158:ARG:HB2 | 2:D:197:ASN:ND2 | 2.30 | 0.45 |
| 2:D:403:ALA:HB1 | 2:D:405:LEU:HD12 | 1.99 | 0.45 |
| 2:D:85:GLN:HA | 2:D:88:ARG:HG2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:ILE:N | 1:A:171:ILE:CD1 | 2.78 | 0.45 |
| 1:A:255:PHE:CD1 | 1:A:259:LEU:HD12 | 2.52 | 0.45 |
| 1:A:346:TRP:N | 1:A:346:TRP:CD1 | 2.74 | 0.45 |
| 1:A:351:PHE:HB3 | 1:A:352:LYS:H | 1.63 | 0.45 |
| 1:A:83:TYR:O | 1:A:84:ARG:HB2 | 2.17 | 0.45 |
| 2:B:126:SER:O | 2:B:127:GLU:C | 2.54 | 0.45 |
| 2:B:115:VAL:HG21 | 2:B:152:LEU:CD2 | 2.47 | 0.45 |
| 2:B:217:LEU:CG | 2:B:218:LYS:N | 2.75 | 0.45 |
| 2:B:226:ASP:C | 2:B:228:ASN:N | 2.70 | 0.45 |
| 2:B:290:GLU:O | 2:B:291:LEU:C | 2.55 | 0.45 |
| 2:B:351:VAL:HG12 | 2:B:352:LYS:N | 2.32 | 0.45 |
| 2:B:428:LEU:O | 2:B:429:VAL:C | 2.54 | 0.45 |
| 1:C:101:ASN:ND2 | 1:C:101:ASN:O | 2.44 | 0.45 |
| 1:C:101:ASN:ND2 | 1:C:185:TYR:OH | 2.50 | 0.45 |
| 1:C:197:HIS:CD2 | 1:C:198:SER:HB3 | 2.52 | 0.45 |
| 1:C:402:ARG:O | 1:C:405:VAL:HG12 | 2.17 | 0.45 |
| 1:C:433:GLU:C | 1:C:435:VAL:N | 2.69 | 0.45 |
| 3:E:3:UNK:C | 3:E:5:UNK:N | 2.80 | 0.45 |
| 1:A:284:GLU:O | 1:A:285:GLN:CG | 2.65 | 0.44 |
| 2:B:115:VAL:CG1 | 2:B:156:LYS:HZ3 | 2.30 | 0.44 |
| 2:B:307:PRO:C | 2:B:309:HIS:N | 2.69 | 0.44 |
| 2:B:59:ASN:CA | 2:B:60:LYS:HZ3 | 2.29 | 0.44 |
| 1:C:185:TYR:HA | 1:C:188:ILE:CD1 | 2.33 | 0.44 |
| 1:C:256:GLN:C | 1:C:258:ASN:H | 2.19 | 0.44 |
| 2:D:115:VAL:CG1 | 2:D:156:LYS:HZ3 | 2.30 | 0.44 |
| 2:D:178:SER:O | 2:D:179:ASP:O | 2.35 | 0.44 |
| 1:A:88:HIS:HA | 1:A:89:PRO:HD2 | 1.87 | 0.44 |
| 2:B:242:LEU:O | 2:B:243:ARG:CD | 2.64 | 0.44 |
| 2:B:51:VAL:O | 2:B:53:TYR:N | 2.50 | 0.44 |
| 1:C:163:LYS:C | 1:C:164:LYS:HZ1 | 2.20 | 0.44 |
| 1:C:86:LEU:HD13 | 1:C:89:PRO:HD3 | 1.99 | 0.44 |
| 2:D:102:ASN:HA | 2:D:408:TYR:HE1 | 1.82 | 0.44 |
| 2:D:185:TYR:O | 2:D:188:THR:HG22 | 2.16 | 0.44 |
| 2:D:155:SER:HB2 | 2:D:196:GLU:HG2 | 1.98 | 0.44 |
| 2:D:287:THR:CB | 2:D:289:PRO:HD2 | 2.39 | 0.44 |
| 1:A:100:ALA:CB | 1:A:105:ARG:HD2 | 2.47 | 0.44 |
| 1:A:137:VAL:HG21 | 1:A:154:MET:SD | 2.57 | 0.44 |
| 1:A:169:PHE:HE1 | 1:A:238:ILE:CD1 | 2.30 | 0.44 |
| 1:A:24:TYR:HA | 1:A:26:LEU:HD12 | 1.99 | 0.44 |
| 1:A:276:ILE:HD12 | 1:A:277:SER:H | 1.79 | 0.44 |
| 1:A:9:VAL:O | 1:A:9:VAL:CG2 | 2.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:2:ARG:CZ | 2:B:243:ARG:HD3 | 2.47 | 0.44 |
| 2:B:286:LEU:HA | 2:B:290:GLU:CD | 2.37 | 0.44 |
| 2:B:184:PRO:CB | 2:B:399:PHE:CZ | 3.00 | 0.44 |
| 1:C:331:ALA:O | 1:C:333:ALA:N | 2.51 | 0.44 |
| 2:D:25:SER:HB3 | 2:D:369:ARG:NH2 | 2.31 | 0.44 |
| 2:D:280:SER:O | 2:D:282:GLN:N | 2.50 | 0.44 |
| 2:D:284:ARG:O | 2:D:287:THR:N | 2.51 | 0.44 |
| 2:D:88:ARG:CB | 2:D:89:PRO:HD3 | 2.34 | 0.44 |
| 1:A:164:LYS:NZ | 1:A:164:LYS:N | 2.60 | 0.44 |
| 1:A:420:GLU:C | 1:A:420:GLU:OE1 | 2.54 | 0.44 |
| 2:B:138:THR:HG22 | 2:B:139:HIS:N | 2.32 | 0.44 |
| 2:B:298:ALA:HB2 | 2:B:307:PRO:HD2 | 2.00 | 0.44 |
| 2:B:308:ARG:NH2 | 2:B:342:TYR:CG | 2.83 | 0.44 |
| 1:C:16:ILE:O | 1:C:19:ALA:N | 2.41 | 0.44 |
| 1:C:273:ALA:CB | 1:C:295:CYS:HB2 | 2.45 | 0.44 |
| 1:C:363:VAL:HG22 | 1:C:367:ASP:OD2 | 2.18 | 0.44 |
| 1:C:380:ASN:O | 1:C:380:ASN:OD1 | 2.35 | 0.44 |
| 1:C:413:MET:C | 1:C:414:GLU:CD | 2.76 | 0.44 |
| 1:C:11:GLN:OE1 | 4:C:502:GTP:O1B | 2.35 | 0.44 |
| 2:D:139:HIS:O | 2:D:170:SER:HA | 2.17 | 0.44 |
| 2:D:151:THR:HG21 | 2:D:189:LEU:HD21 | 1.99 | 0.44 |
| 1:A:139:HIS:NE2 | 1:A:150:THR:CG2 | 2.79 | 0.44 |
| 1:A:214:ARG:CA | 1:A:218:ASP:O | 2.61 | 0.44 |
| 1:A:256:GLN:C | 1:A:258:ASN:H | 2.20 | 0.44 |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:OD2 | 2.17 | 0.44 |
| 2:B:338:LYS:O | 2:B:340:SER:N | 2.43 | 0.44 |
| 2:B:407:TRP:HE1 | 1:C:257:THR:CA | 2.31 | 0.44 |
| 2:B:4:ILE:N | 2:B:58:GLY:HA2 | 2.33 | 0.44 |
| 1:C:188:ILE:H | 1:C:188:ILE:HG13 | 1.62 | 0.44 |
| 1:C:344:VAL:CG1 | 1:C:345:ASP:H | 2.30 | 0.44 |
| 1:C:347:CYS:O | 1:C:349:THR:N | 2.50 | 0.44 |
| 1:C:428:LEU:C | 1:C:430:LYS:H | 2.21 | 0.44 |
| 1:C:67:PHE:O | 1:C:75:ILE:HD11 | 2.17 | 0.44 |
| 1:C:7:ILE:O | 1:C:7:ILE:HG13 | 2.18 | 0.44 |
| 1:C:96:LYS:HE3 | 1:C:96:LYS:HB2 | 1.77 | 0.44 |
| 2:D:97:SER:HG | 2:D:110:GLU:CG | 2.30 | 0.44 |
| 2:D:187:ALA:HB2 | 2:D:391:ILE:CG2 | 2.48 | 0.44 |
| 2:D:344:VAL:O | 2:D:346:TRP:CD1 | 2.70 | 0.44 |
| 2:D:95:GLY:O | 2:D:96:GLN:HB3 | 2.18 | 0.44 |
| 1:A:111:GLY:C | 1:A:113:GLU:N | 2.71 | 0.44 |
| 1:A:306:ASP:C | 1:A:308:ARG:N | 2.68 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:414:GLU:CG | 1:A:415:GLU:H | 2.13 | 0.44 |
| 2:B:2:ARG:CZ | 2:B:243:ARG:CD | 2.96 | 0.44 |
| 2:B:271:GLY:O | 2:B:377:PHE:HB2 | 2.18 | 0.44 |
| 2:B:273:ALA:HB3 | 2:B:274:PRO:CD | 2.48 | 0.44 |
| 2:B:334:ASN:O | 2:B:338:LYS:N | 2.51 | 0.44 |
| 2:B:12:CYS:HB2 | 5:B:501:GDP:PA | 2.58 | 0.44 |
| 2:B:59:ASN:ND2 | 2:B:60:LYS:H | 2.16 | 0.44 |
| 2:B:58:GLY:O | 2:B:64:ARG:NH2 | 2.50 | 0.44 |
| 1:C:10:GLY:O | 1:C:11:GLN:C | 2.56 | 0.44 |
| 2:B:407:TRP:HE1 | 1:C:257:THR:N | 2.15 | 0.44 |
| 1:C:340:THR:O | 1:C:342:GLN:HG2 | 2.17 | 0.44 |
| 1:C:46:ASP:O | 1:C:47:ASP:C | 2.56 | 0.44 |
| 2:D:179:ASP:HB2 | 2:D:182:VAL:CB | 2.47 | 0.44 |
| 3:E:13:UNK:C | 3:E:15:UNK:N | 2.77 | 0.44 |
| 1:A:142:GLY:HA2 | 1:A:185:TYR:HB2 | 1.98 | 0.44 |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:CG | 2.38 | 0.44 |
| 2:B:103:TRP:O | 2:B:105:LYS:N | 2.50 | 0.44 |
| 2:B:283:TYR:O | 2:B:290:GLU:OE1 | 2.36 | 0.44 |
| 2:B:303:ALA:HB1 | 2:B:387:LEU:HD13 | 1.99 | 0.44 |
| 2:B:182:VAL:HG11 | 5:B:501:GDP:O3' | 2.17 | 0.44 |
| 1:C:177:VAL:HG21 | 2:D:349:ASN:HB2 | 1.99 | 0.44 |
| 1:C:227:LEU:N | 1:C:227:LEU:CD1 | 2.81 | 0.44 |
| 1:C:259:LEU:HD21 | 1:C:378:LEU:CB | 2.45 | 0.44 |
| 1:C:312:TYR:H | 1:C:312:TYR:HD1 | 1.65 | 0.44 |
| 2:D:223:THR:C | 2:D:225:GLY:H | 2.20 | 0.44 |
| 2:D:358:ILE:HD12 | 2:D:358:ILE:N | 2.21 | 0.44 |
| 3:E:71:UNK:O | 3:E:74:UNK:N | 2.51 | 0.44 |
| 1:A:289:ALA:HA | 1:A:292:THR:HG23 | 1.96 | 0.44 |
| 1:A:305:CYS:C | 1:A:386:GLU:OE1 | 2.56 | 0.44 |
| 2:B:121:VAL:O | 2:B:121:VAL:HG12 | 2.16 | 0.44 |
| 2:B:165:ILE:HG13 | 2:B:253:ARG:CG | 2.48 | 0.44 |
| 2:B:274:PRO:HB2 | 2:B:371:LEU:HD11 | 1.99 | 0.44 |
| 2:B:320:ARG:NH1 | 2:B:320:ARG:CG | 2.79 | 0.44 |
| 1:C:277:SER:O | 1:C:368:LEU:HB3 | 2.17 | 0.44 |
| 1:C:306:ASP:C | 1:C:308:ARG:N | 2.69 | 0.44 |
| 1:C:288:VAL:HA | 1:C:373:ARG:CD | 2.47 | 0.44 |
| 2:D:273:ALA:H | 2:D:274:PRO:HD2 | 1.83 | 0.44 |
| 2:D:430:SER:O | 2:D:431:GLU:C | 2.56 | 0.44 |
| 2:D:51:VAL:HG23 | 2:D:53:TYR:HB2 | 1.99 | 0.44 |
| 1:A:126:ALA:O | 1:A:132:LEU:HD12 | 2.17 | 0.44 |
| 1:A:181:VAL:HG13 | 1:A:181:VAL:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:PRO:HB2 | 1:A:399:TYR:CE2 | 2.53 | 0.44 |
| 2:B:179:ASP:HB2 | 2:B:182:VAL:CB | 2.48 | 0.44 |
| 2:B:223:THR:C | 2:B:225:GLY:H | 2.20 | 0.44 |
| 2:B:324:SER:HB3 | 2:B:327:GLU:OE1 | 2.18 | 0.44 |
| 2:B:428:LEU:O | 2:B:432:TYR:HB2 | 2.18 | 0.44 |
| 1:C:152:LEU:O | 1:C:153:LEU:C | 2.55 | 0.44 |
| 1:C:206:ASN:CB | 1:C:210:TYR:HE2 | 2.28 | 0.44 |
| 1:C:244:PHE:CZ | 1:C:358:GLU:OE1 | 2.71 | 0.44 |
| 1:C:265:ALA:O | 1:C:266:HIS:C | 2.55 | 0.44 |
| 1:C:284:GLU:O | 1:C:285:GLN:CG | 2.65 | 0.44 |
| 1:C:349:THR:OG1 | 1:C:349:THR:O | 2.29 | 0.44 |
| 1:C:402:ARG:HG2 | 1:C:403:ALA:N | 2.24 | 0.44 |
| 2:D:106:GLY:HA2 | 2:D:111:GLY:HA3 | 1.99 | 0.44 |
| 2:D:381:SER:O | 2:D:383:ALA:N | 2.51 | 0.44 |
| 2:D:427:ASP:O | 2:D:430:SER:N | 2.51 | 0.44 |
| 2:D:75:MET:SD | 2:D:79:ARG:CZ | 3.06 | 0.44 |
| 1:A:411:GLU:O | 1:A:411:GLU:OE2 | 2.36 | 0.43 |
| 1:A:67:PHE:O | 1:A:92:LEU:HA | 2.18 | 0.43 |
| 2:B:223:THR:HG23 | 2:B:225:GLY:C | 2.38 | 0.43 |
| 2:B:322:ARG:NE | 2:B:357:ASP:CB | 2.81 | 0.43 |
| 1:C:320:ARG:CB | 1:C:374:ALA:HB3 | 2.40 | 0.43 |
| 1:C:395:PHE:C | 1:C:395:PHE:HD1 | 2.21 | 0.43 |
| 1:C:398:MET:O | 1:C:401:LYS:N | 2.42 | 0.43 |
| 2:D:185:TYR:HB3 | 2:D:186:ASN:H | 1.56 | 0.43 |
| 2:D:431:GLU:HA | 2:D:434:GLN:HE21 | 1.83 | 0.43 |
| 1:A:306:ASP:O | 1:A:308:ARG:N | 2.51 | 0.43 |
| 1:A:307:PRO:CB | 1:A:381:THR:HG21 | 2.48 | 0.43 |
| 2:B:137:LEU:O | 2:B:168:THR:HA | 2.18 | 0.43 |
| 2:B:272:PHE:HD1 | 2:B:275:LEU:CD2 | 2.31 | 0.43 |
| 2:B:333:LEU:O | 2:B:336:GLN:HB3 | 2.18 | 0.43 |
| 2:B:3:GLU:HG2 | 2:B:58:GLY:O | 2.18 | 0.43 |
| 1:C:132:LEU:HB3 | 1:C:133:GLN:H | 1.63 | 0.43 |
| 1:C:103:TYR:CD2 | 1:C:148:GLY:HA2 | 2.53 | 0.43 |
| 1:C:174:ALA:C | 1:C:176:GLN:N | 2.71 | 0.43 |
| 1:C:256:GLN:O | 1:C:257:THR:C | 2.57 | 0.43 |
| 1:C:3:GLU:HG3 | 1:C:3:GLU:O | 2.18 | 0.43 |
| 1:C:171:ILE:HG21 | 4:C:502:GTP:HN22 | 1.82 | 0.43 |
| 1:C:91:GLN:HG2 | 1:C:92:LEU:CD1 | 2.47 | 0.43 |
| 2:D:133:GLN:NE2 | 2:D:252:LEU:CB | 2.75 | 0.43 |
| 2:D:308:ARG:NH2 | 2:D:342:TYR:CB | 2.81 | 0.43 |
| 2:D:383:ALA:C | 2:D:385:GLN:H | 2.20 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:305:CYS:O | 2:D:383:ALA:HB1 | 2.18 | 0.43 |
| 2:D:427:ASP:C | 2:D:429:VAL:N | 2.72 | 0.43 |
| 2:D:51:VAL:N | 2:D:245:PRO:CB | 2.81 | 0.43 |
| 2:D:88:ARG:HA | 2:D:91:ASN:ND2 | 2.33 | 0.43 |
| 1:A:303:VAL:O | 1:A:305:CYS:N | 2.51 | 0.43 |
| 1:A:402:ARG:HG2 | 1:A:403:ALA:N | 2.22 | 0.43 |
| 2:B:139:HIS:O | 2:B:170:SER:HA | 2.17 | 0.43 |
| 2:B:19:LYS:HA | 2:B:22:GLU:OE2 | 2.18 | 0.43 |
| 2:B:284:ARG:HB2 | 2:B:290:GLU:OE1 | 2.17 | 0.43 |
| 1:C:229:ARG:HD2 | 1:C:366:GLY:HA3 | 1.99 | 0.43 |
| 1:C:328:VAL:O | 1:C:330:ALA:N | 2.52 | 0.43 |
| 1:C:33:ASP:O | 1:C:34:GLY:C | 2.57 | 0.43 |
| 2:D:198:THR:C | 2:D:200:GLU:H | 2.21 | 0.43 |
| 2:D:320:ARG:CG | 2:D:320:ARG:NH1 | 2.80 | 0.43 |
| 1:A:174:ALA:HB1 | 1:A:176:GLN:HG2 | 2.01 | 0.43 |
| 1:A:203:MET:HE1 | 1:A:388:TRP:HD1 | 1.83 | 0.43 |
| 1:A:209:ILE:N | 1:A:209:ILE:CD1 | 2.81 | 0.43 |
| 1:A:371:VAL:CG1 | 1:A:372:GLN:H | 2.32 | 0.43 |
| 1:A:88:HIS:O | 1:A:90:GLU:N | 2.51 | 0.43 |
| 2:B:107:HIS:HB2 | 2:B:148:GLY:O | 2.17 | 0.43 |
| 2:B:154:ILE:O | 2:B:157:ILE:N | 2.50 | 0.43 |
| 2:B:3:GLU:O | 2:B:133:GLN:N | 2.40 | 0.43 |
| 1:C:93:ILE:CD1 | 1:C:118:VAL:HA | 2.48 | 0.43 |
| 1:C:143:GLY:O | 1:C:144:GLY:C | 2.56 | 0.43 |
| 1:C:217:LEU:HD23 | 1:C:219:ILE:HD11 | 1.99 | 0.43 |
| 1:C:371:VAL:HG11 | 1:C:373:ARG:O | 2.18 | 0.43 |
| 2:D:137:LEU:HD23 | 2:D:154:ILE:CD1 | 2.47 | 0.43 |
| 2:D:174:SER:OG | 2:D:207:GLU:HA | 2.18 | 0.43 |
| 2:D:291:LEU:CD2 | 2:D:291:LEU:N | 2.81 | 0.43 |
| 2:B:159:GLU:OE2 | 3:E:30:UNK:HA | 2.17 | 0.43 |
| 1:A:9:VAL:HG21 | 1:A:150:THR:CB | 2.46 | 0.43 |
| 1:A:178:SER:O | 1:A:179:THR:CB | 2.66 | 0.43 |
| 1:A:205:ASP:OD2 | 1:A:205:ASP:C | 2.56 | 0.43 |
| 1:A:344:VAL:HG11 | 1:A:346:TRP:CE2 | 2.52 | 0.43 |
| 2:B:209:LEU:CB | 2:B:227:LEU:HG | 2.48 | 0.43 |
| 2:B:327:GLU:O | 2:B:331:GLN:HB2 | 2.19 | 0.43 |
| 1:C:187:SER:C | 1:C:189:LEU:H | 2.21 | 0.43 |
| 1:C:242:LEU:HD11 | 1:C:318:LEU:HG | 2.00 | 0.43 |
| 1:C:276:ILE:HG12 | 1:C:282:TYR:HD2 | 1.79 | 0.43 |
| 1:C:27:GLU:CG | 1:C:28:HIS:N | 2.81 | 0.43 |
| 2:D:158:ARG:C | 2:D:160:GLU:N | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:238:VAL:CG2 | 2:D:376:THR:HG21 | 2.49 | 0.43 |
| 2:D:287:THR:O | 2:D:291:LEU:HD23 | 2.18 | 0.43 |
| 2:D:91:ASN:ND2 | 2:D:91:ASN:N | 2.50 | 0.43 |
| 1:A:15:GLN:O | 1:A:16:ILE:O | 2.36 | 0.43 |
| 1:A:278:ALA:HA | 1:A:282:TYR:OH | 2.19 | 0.43 |
| 1:A:368:LEU:O | 1:A:369:ALA:HB3 | 2.19 | 0.43 |
| 1:A:36:MET:CE | 1:A:37:PRO:HD2 | 2.48 | 0.43 |
| 2:B:151:THR:HG21 | 2:B:189:LEU:HD21 | 1.99 | 0.43 |
| 2:B:18:ALA:O | 2:B:21:TRP:N | 2.51 | 0.43 |
| 1:C:403:ALA:C | 1:C:405:VAL:H | 2.22 | 0.43 |
| 2:D:193:GLN:HE21 | 2:D:193:GLN:HB3 | 1.66 | 0.43 |
| 2:D:63:PRO:C | 2:D:65:ALA:H | 2.20 | 0.43 |
| 1:A:179:THR:HG22 | 1:A:180:ALA:O | 2.18 | 0.43 |
| 1:A:23:LEU:O | 1:A:25:CYS:N | 2.42 | 0.43 |
| 2:B:132:LEU:H | 2:B:164:ARG:HH21 | 1.66 | 0.43 |
| 2:B:346:TRP:HZ2 | 2:B:435:TYR:HB3 | 1.82 | 0.43 |
| 2:B:59:ASN:CG | 2:B:60:LYS:HD2 | 2.39 | 0.43 |
| 1:C:179:THR:HB | 1:C:182:VAL:HB | 2.01 | 0.43 |
| 1:C:333:ALA:O | 1:C:336:LYS:N | 2.52 | 0.43 |
| 1:C:71:GLU:CD | 4:C:502:GTP:O3G | 2.57 | 0.43 |
| 2:D:343:PHE:HB3 | 2:D:350:ASN:OD1 | 2.17 | 0.43 |
| 2:D:353:THR:HG23 | 2:D:354:ALA:H | 1.83 | 0.43 |
| 2:D:180:THR:CB | 2:D:404:PHE:CE1 | 2.97 | 0.43 |
| 2:D:51:VAL:N | 2:D:245:PRO:CG | 2.81 | 0.43 |
| 1:A:197:HIS:CG | 1:A:198:SER:N | 2.85 | 0.43 |
| 1:A:256:GLN:HB3 | 1:A:260:VAL:CB | 2.46 | 0.43 |
| 1:A:43:GLY:O | 1:A:47:ASP:OD2 | 2.37 | 0.43 |
| 2:B:200:GLU:HG2 | 2:B:268:PHE:CE2 | 2.53 | 0.43 |
| 2:B:269:MET:HB3 | 2:B:269:MET:HE2 | 1.86 | 0.43 |
| 2:B:272:PHE:HB3 | 2:B:275:LEU:HD21 | 2.00 | 0.43 |
| 2:B:419:THR:O | 2:B:423:SER:N | 2.51 | 0.43 |
| 1:C:122:ILE:HG22 | 1:C:123:ARG:N | 2.34 | 0.43 |
| 1:C:78:VAL:O | 1:C:82:THR:CG2 | 2.63 | 0.43 |
| 2:D:208:ALA:O | 2:D:212:ILE:HG13 | 2.19 | 0.43 |
| 1:A:100:ALA:HA | 1:A:105:ARG:CD | 2.49 | 0.43 |
| 1:A:163:LYS:HB2 | 1:A:163:LYS:NZ | 2.34 | 0.43 |
| 1:A:171:ILE:HA | 1:A:204:VAL:HB | 2.01 | 0.43 |
| 1:A:229:ARG:NH1 | 1:A:229:ARG:HG3 | 2.34 | 0.43 |
| 1:A:292:THR:O | 1:A:292:THR:OG1 | 2.33 | 0.43 |
| 1:A:328:VAL:HG11 | 1:A:353:VAL:HG11 | 2.00 | 0.43 |
| 1:A:26:LEU:HD23 | 1:A:361:THR:OG1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:PHE:C | 1:A:397:LEU:H | 2.20 | 0.43 |
| 1:A:409:VAL:HA | 1:A:414:GLU:CD | 2.32 | 0.43 |
| 1:A:428:LEU:C | 1:A:430:LYS:H | 2.22 | 0.43 |
| 1:A:77:GLU:HB3 | 1:A:83:TYR:HD2 | 1.76 | 0.43 |
| 2:B:276:THR:HG21 | 2:B:281:GLN:CG | 2.49 | 0.43 |
| 2:B:59:ASN:CA | 2:B:64:ARG:HE | 2.32 | 0.43 |
| 1:C:294:ALA:C | 1:C:296:PHE:H | 2.22 | 0.43 |
| 1:C:346:TRP:CE3 | 1:C:347:CYS:SG | 3.12 | 0.43 |
| 1:C:409:VAL:C | 1:C:411:GLU:N | 2.71 | 0.43 |
| 2:D:10:GLY:HA3 | 2:D:146:GLY:HA3 | 1.99 | 0.43 |
| 2:D:348:PRO:O | 2:D:349:ASN:CB | 2.66 | 0.43 |
| 2:D:428:LEU:HD12 | 2:D:428:LEU:N | 2.33 | 0.43 |
| 2:D:92:PHE:CZ | 2:D:117:SER:O | 2.71 | 0.43 |
| 3:E:68:UNK:O | 3:E:72:UNK:CB | 2.66 | 0.43 |
| 3:E:83:UNK:O | 3:E:85:UNK:N | 2.51 | 0.43 |
| 1:A:100:ALA:HB1 | 1:A:105:ARG:HD2 | 2.00 | 0.43 |
| 1:A:185:TYR:O | 1:A:186:ASN:C | 2.56 | 0.43 |
| 1:A:242:LEU:CG | 1:A:318:LEU:HD11 | 2.47 | 0.43 |
| 2:B:132:LEU:O | 2:B:164:ARG:NE | 2.41 | 0.43 |
| 2:B:402:LYS:HE3 | 1:C:440:VAL:HG12 | 1.99 | 0.43 |
| 2:B:59:ASN:HA | 2:B:60:LYS:NZ | 2.33 | 0.43 |
| 1:C:270:ALA:HB3 | 1:C:302:MET:HG2 | 2.00 | 0.43 |
| 2:D:121:VAL:CG1 | 2:D:121:VAL:O | 2.66 | 0.43 |
| 2:D:183:GLU:HB3 | 2:D:184:PRO:HD3 | 2.01 | 0.43 |
| 2:D:60:LYS:HZ2 | 2:D:60:LYS:N | 2.15 | 0.43 |
| 1:A:181:VAL:HG13 | 1:A:185:TYR:CE2 | 2.53 | 0.42 |
| 1:A:189:LEU:C | 1:A:189:LEU:HD13 | 2.40 | 0.42 |
| 1:A:39:ASP:OD2 | 1:A:40:LYS:HB2 | 2.19 | 0.42 |
| 2:B:111:GLY:O | 2:B:113:GLU:N | 2.52 | 0.42 |
| 2:B:189:LEU:HA | 2:B:192:HIS:HE1 | 1.82 | 0.42 |
| 2:B:211:ASP:N | 2:B:211:ASP:OD1 | 2.52 | 0.42 |
| 2:B:273:ALA:HB3 | 2:B:274:PRO:HD3 | 2.01 | 0.42 |
| 2:B:286:LEU:CG | 2:B:373:MET:HE3 | 2.44 | 0.42 |
| 2:B:88:ARG:O | 2:B:91:ASN:ND2 | 2.52 | 0.42 |
| 1:C:217:LEU:CD2 | 1:C:219:ILE:HD11 | 2.49 | 0.42 |
| 2:D:211:ASP:O | 2:D:215:ARG:HB2 | 2.19 | 0.42 |
| 2:D:273:ALA:HB3 | 2:D:274:PRO:HD3 | 2.00 | 0.42 |
| 2:D:283:TYR:HE2 | 2:D:294:GLN:NE2 | 2.17 | 0.42 |
| 2:D:311:ARG:HD3 | 2:D:311:ARG:H | 1.84 | 0.42 |
| 2:D:312:TYR:CE2 | 2:D:377:PHE:CZ | 3.06 | 0.42 |
| 2:D:389:LYS:C | 2:D:392:SER:HG | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:86:ILE:H | 2:D:88:ARG:NH2 | 2.17 | 0.42 |
| 3:E:14:UNK:C | 3:E:16:UNK:N | 2.81 | 0.42 |
| 1:A:306:ASP:N | 1:A:307:PRO:HD3 | 2.33 | 0.42 |
| 1:A:46:ASP:O | 1:A:47:ASP:O | 2.37 | 0.42 |
| 2:B:283:TYR:CG | 2:B:283:TYR:O | 2.72 | 0.42 |
| 2:B:287:THR:OG1 | 2:B:290:GLU:CB | 2.67 | 0.42 |
| 2:B:335:VAL:C | 2:B:338:LYS:H | 2.22 | 0.42 |
| 2:B:344:VAL:O | 2:B:346:TRP:CD1 | 2.72 | 0.42 |
| 1:C:209:ILE:HG12 | 1:C:231:ILE:HD11 | 2.00 | 0.42 |
| 1:C:284:GLU:CG | 1:C:285:GLN:HE21 | 2.22 | 0.42 |
| 1:C:273:ALA:HB3 | 1:C:291:ILE:HG23 | 2.01 | 0.42 |
| 1:C:312:TYR:N | 1:C:312:TYR:CD1 | 2.87 | 0.42 |
| 1:C:305:CYS:C | 1:C:386:GLU:OE1 | 2.57 | 0.42 |
| 1:C:306:ASP:HB3 | 1:C:386:GLU:OE1 | 2.18 | 0.42 |
| 2:D:200:GLU:CD | 2:D:268:PHE:HE2 | 2.21 | 0.42 |
| 2:D:226:ASP:O | 2:D:228:ASN:N | 2.44 | 0.42 |
| 2:D:327:GLU:O | 2:D:331:GLN:HB2 | 2.19 | 0.42 |
| 2:D:311:ARG:NH1 | 2:D:344:VAL:HA | 2.35 | 0.42 |
| 2:D:52:TYR:CG | 2:D:52:TYR:O | 2.72 | 0.42 |
| 3:E:75:UNK:C | 3:E:77:UNK:N | 2.78 | 0.42 |
| 1:A:154:MET:C | 1:A:156:ARG:N | 2.70 | 0.42 |
| 1:A:284:GLU:CG | 1:A:285:GLN:HE21 | 2.24 | 0.42 |
| 1:A:242:LEU:CD2 | 1:A:318:LEU:HD21 | 2.33 | 0.42 |
| 2:B:10:GLY:HA3 | 2:B:146:GLY:HA3 | 2.01 | 0.42 |
| 2:B:212:ILE:O | 2:B:217:LEU:HB3 | 2.19 | 0.42 |
| 2:B:2:ARG:HH21 | 2:B:243:ARG:HB3 | 1.84 | 0.42 |
| 2:B:322:ARG:CG | 2:B:357:ASP:HA | 2.33 | 0.42 |
| 1:C:119:LEU:HD22 | 1:C:156:ARG:CZ | 2.49 | 0.42 |
| 1:C:264:ARG:HD3 | 1:C:264:ARG:HA | 1.97 | 0.42 |
| 1:C:31:GLN:OE1 | 1:C:32:PRO:HD3 | 2.19 | 0.42 |
| 2:D:181:VAL:C | 2:D:184:PRO:HD2 | 2.40 | 0.42 |
| 2:D:176:LYS:NZ | 2:D:210:TYR:CG | 2.84 | 0.42 |
| 2:D:312:TYR:HE2 | 2:D:377:PHE:CZ | 2.37 | 0.42 |
| 2:D:395:PHE:CD2 | 2:D:422:GLU:OE1 | 2.71 | 0.42 |
| 1:A:411:GLU:CA | 1:A:411:GLU:OE2 | 2.68 | 0.42 |
| 2:B:97:SER:HG | 2:B:110:GLU:CG | 2.32 | 0.42 |
| 2:B:22:GLU:HG3 | 2:B:83:PHE:CD1 | 2.55 | 0.42 |
| 2:B:256:ALA:O | 2:B:260:VAL:HB | 2.19 | 0.42 |
| 2:B:312:TYR:CE2 | 2:B:377:PHE:HZ | 2.38 | 0.42 |
| 2:B:327:GLU:O | 2:B:331:GLN:N | 2.53 | 0.42 |
| 2:B:93:VAL:CG2 | 2:B:94:PHE:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:95:GLY:O | 2:B:96:GLN:O | 2.37 | 0.42 |
| 1:C:158:SER:HB3 | 1:C:166:LYS:HZ1 | 1.83 | 0.42 |
| 1:C:20:CYS:SG | 1:C:232:GLY:HA2 | 2.59 | 0.42 |
| 1:C:241:SER:CB | 1:C:242:LEU:HD12 | 2.48 | 0.42 |
| 1:C:321:GLY:N | 1:C:356:ASN:O | 2.52 | 0.42 |
| 2:D:322:ARG:CG | 2:D:357:ASP:HA | 2.34 | 0.42 |
| 2:D:4:ILE:HD11 | 2:D:252:LEU:HD13 | 2.00 | 0.42 |
| 2:D:84:GLY:C | 2:D:85:GLN:HG2 | 2.39 | 0.42 |
| 1:A:339:ARG:C | 1:A:339:ARG:CD | 2.75 | 0.42 |
| 1:A:340:THR:C | 1:A:341:ILE:HD12 | 2.40 | 0.42 |
| 1:A:311:LYS:CE | 1:A:344:VAL:HA | 2.50 | 0.42 |
| 1:A:349:THR:OG1 | 1:A:349:THR:O | 2.31 | 0.42 |
| 1:A:291:ILE:CG2 | 1:A:375:VAL:HG21 | 2.44 | 0.42 |
| 1:A:412:GLY:HA2 | 1:A:413:MET:HE1 | 2.02 | 0.42 |
| 2:B:3:GLU:HB3 | 2:B:132:LEU:HA | 2.01 | 0.42 |
| 2:B:174:SER:HB2 | 2:B:206:ASN:C | 2.39 | 0.42 |
| 2:B:383:ALA:C | 2:B:385:GLN:H | 2.23 | 0.42 |
| 1:C:123:ARG:O | 1:C:127:ASP:HB2 | 2.19 | 0.42 |
| 1:C:190:THR:O | 1:C:193:THR:N | 2.52 | 0.42 |
| 1:C:286:LEU:HD12 | 1:C:291:ILE:CG1 | 2.48 | 0.42 |
| 1:C:332:ILE:HG23 | 1:C:351:PHE:CZ | 2.55 | 0.42 |
| 1:C:44:GLY:O | 1:C:46:ASP:N | 2.52 | 0.42 |
| 1:C:5:ILE:HG22 | 1:C:6:SER:N | 2.34 | 0.42 |
| 1:C:83:TYR:O | 1:C:84:ARG:HB2 | 2.20 | 0.42 |
| 2:D:165:ILE:HD13 | 2:D:199:ASP:OD1 | 2.18 | 0.42 |
| 3:E:30:UNK:O | 3:E:31:UNK:C | 2.67 | 0.42 |
| 1:A:126:ALA:O | 1:A:132:LEU:CD1 | 2.67 | 0.42 |
| 1:A:216:ASN:HB3 | 1:A:275:VAL:HG11 | 2.01 | 0.42 |
| 1:A:305:CYS:O | 1:A:306:ASP:HB2 | 2.19 | 0.42 |
| 1:A:73:THR:O | 1:A:76:ASP:N | 2.48 | 0.42 |
| 1:A:97:GLU:CD | 1:A:97:GLU:H | 2.23 | 0.42 |
| 2:B:230:LEU:H | 2:B:230:LEU:CD1 | 2.25 | 0.42 |
| 2:B:88:ARG:HA | 2:B:91:ASN:ND2 | 2.35 | 0.42 |
| 1:C:111:GLY:C | 1:C:113:GLU:N | 2.73 | 0.42 |
| 1:C:190:THR:HA | 1:C:193:THR:CG2 | 2.39 | 0.42 |
| 1:C:21:TRP:CD1 | 1:C:21:TRP:N | 2.87 | 0.42 |
| 1:C:335:ILE:O | 1:C:338:LYS:HG2 | 2.19 | 0.42 |
| 1:C:398:MET:CG | 1:C:399:TYR:H | 2.33 | 0.42 |
| 1:C:88:HIS:O | 1:C:90:GLU:N | 2.52 | 0.42 |
| 2:D:126:SER:O | 2:D:127:GLU:C | 2.57 | 0.42 |
| 2:D:415:GLU:HG2 | 2:D:416:MET:SD | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:346:TRP:HZ2 | 2:D:435:TYR:HB3 | 1.85 | 0.42 |
| 2:D:22:GLU:HG3 | 2:D:83:PHE:CD1 | 2.55 | 0.42 |
| 2:D:95:GLY:O | 2:D:96:GLN:O | 2.38 | 0.42 |
| 1:A:119:LEU:HD22 | 1:A:156:ARG:NE | 2.34 | 0.42 |
| 1:A:190:THR:O | 1:A:193:THR:N | 2.50 | 0.42 |
| 1:A:286:LEU:HD12 | 1:A:291:ILE:CG1 | 2.49 | 0.42 |
| 2:B:350:ASN:HD22 | 2:B:350:ASN:C | 2.21 | 0.42 |
| 2:B:415:GLU:HG2 | 2:B:416:MET:H | 1.85 | 0.42 |
| 1:C:185:TYR:CE1 | 1:C:408:TYR:CE1 | 3.06 | 0.42 |
| 1:C:209:ILE:CG2 | 1:C:213:CYS:HB2 | 2.43 | 0.42 |
| 1:C:239:THR:O | 1:C:243:ARG:HB2 | 2.19 | 0.42 |
| 1:C:91:GLN:HE21 | 1:C:91:GLN:HB3 | 1.58 | 0.42 |
| 2:D:311:ARG:HB3 | 2:D:343:PHE:N | 2.35 | 0.42 |
| 1:A:209:ILE:CG2 | 1:A:213:CYS:HB2 | 2.47 | 0.42 |
| 1:A:294:ALA:C | 1:A:296:PHE:H | 2.23 | 0.42 |
| 2:B:123:ARG:C | 2:B:125:GLU:N | 2.72 | 0.42 |
| 2:B:178:SER:C | 2:B:182:VAL:HB | 2.35 | 0.42 |
| 2:B:350:ASN:ND2 | 2:B:350:ASN:N | 2.67 | 0.42 |
| 1:C:320:ARG:HH21 | 1:C:356:ASN:ND2 | 2.18 | 0.42 |
| 1:C:405:VAL:O | 1:C:405:VAL:CG2 | 2.68 | 0.42 |
| 1:C:413:MET:O | 1:C:414:GLU:CB | 2.66 | 0.42 |
| 1:C:431:ASP:C | 1:C:433:GLU:H | 2.23 | 0.42 |
| 2:D:224:TYR:O | 2:D:228:ASN:HB2 | 2.20 | 0.42 |
| 2:D:269:MET:HG2 | 2:D:384:ILE:HB | 2.01 | 0.42 |
| 2:D:320:ARG:HG2 | 2:D:320:ARG:NH1 | 2.32 | 0.42 |
| 2:D:88:ARG:HA | 2:D:91:ASN:HD21 | 1.85 | 0.42 |
| 1:A:312:TYR:HD1 | 1:A:312:TYR:H | 1.67 | 0.42 |
| 2:B:333:LEU:HG | 2:B:337:ASN:HD21 | 1.82 | 0.42 |
| 2:B:405:LEU:HD13 | 2:B:406:HIS:H | 1.79 | 0.42 |
| 2:B:346:TRP:CZ2 | 2:B:435:TYR:HB3 | 2.54 | 0.42 |
| 2:B:6:HIS:HD2 | 2:B:136:GLN:OE1 | 2.03 | 0.42 |
| 1:C:192:HIS:C | 1:C:194:THR:H | 2.23 | 0.42 |
| 1:C:229:ARG:NH1 | 1:C:229:ARG:HG3 | 2.33 | 0.42 |
| 1:C:88:HIS:HA | 1:C:89:PRO:HD2 | 1.84 | 0.42 |
| 2:D:102:ASN:HD22 | 2:D:105:LYS:H | 1.62 | 0.42 |
| 1:A:208:ALA:HB2 | 1:A:302:MET:O | 2.20 | 0.42 |
| 2:B:224:TYR:C | 2:B:226:ASP:H | 2.22 | 0.42 |
| 2:B:273:ALA:H | 2:B:274:PRO:HD2 | 1.84 | 0.42 |
| 2:B:1:MET:C | 2:B:3:GLU:N | 2.73 | 0.42 |
| 1:C:174:ALA:HB1 | 1:C:176:GLN:HG2 | 2.02 | 0.42 |
| 1:C:208:ALA:O | 1:C:212:ILE:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:269:LEU:C | 1:C:269:LEU:CD1 | 2.84 | 0.42 |
| 1:C:275:VAL:HG12 | 1:C:275:VAL:O | 2.18 | 0.42 |
| 1:C:277:SER:HA | 1:C:368:LEU:HB3 | 2.02 | 0.42 |
| 1:C:321:GLY:CA | 1:C:358:GLU:O | 2.68 | 0.42 |
| 1:C:8:HIS:HE2 | 1:C:21:TRP:HE1 | 1.66 | 0.42 |
| 2:D:104:ALA:HB1 | 2:D:411:GLU:HB2 | 2.02 | 0.42 |
| 2:D:69:ASP:HB3 | 2:D:74:THR:HG23 | 2.02 | 0.42 |
| 1:A:115:ILE:HG12 | 1:A:149:PHE:CE2 | 2.54 | 0.41 |
| 1:A:197:HIS:CD2 | 1:A:198:SER:HB3 | 2.55 | 0.41 |
| 2:B:122:VAL:CG1 | 2:B:123:ARG:N | 2.82 | 0.41 |
| 2:B:1:MET:C | 2:B:3:GLU:H | 2.20 | 0.41 |
| 1:C:209:ILE:HA | 1:C:212:ILE:HG12 | 2.01 | 0.41 |
| 1:C:181:VAL:HG22 | 1:C:399:TYR:OH | 2.18 | 0.41 |
| 2:D:179:ASP:OD2 | 2:D:181:VAL:HG12 | 2.20 | 0.41 |
| 2:D:60:LYS:H | 2:D:60:LYS:HZ3 | 1.68 | 0.41 |
| 1:A:181:VAL:O | 1:A:184:PRO:HG2 | 2.20 | 0.41 |
| 1:A:182:VAL:HA | 1:A:185:TYR:HD2 | 1.86 | 0.41 |
| 1:A:245:ASP:O | 1:A:249:ASN:OD1 | 2.37 | 0.41 |
| 1:A:33:ASP:O | 1:A:34:GLY:C | 2.59 | 0.41 |
| 1:A:403:ALA:C | 1:A:405:VAL:H | 2.23 | 0.41 |
| 1:A:420:GLU:OE1 | 1:A:420:GLU:O | 2.38 | 0.41 |
| 2:B:86:ILE:H | 2:B:88:ARG:CZ | 2.33 | 0.41 |
| 1:C:161:TYR:O | 1:C:162:GLY:C | 2.59 | 0.41 |
| 1:C:168:GLU:O | 1:C:168:GLU:HG3 | 2.20 | 0.41 |
| 1:C:215:ARG:HG2 | 1:C:216:ASN:N | 2.36 | 0.41 |
| 1:C:242:LEU:CG | 1:C:318:LEU:HD11 | 2.50 | 0.41 |
| 2:D:273:ALA:HB3 | 2:D:274:PRO:CD | 2.49 | 0.41 |
| 3:E:16:UNK:O | 3:E:20:UNK:N | 2.53 | 0.41 |
| 1:A:117:LEU:O | 1:A:121:ARG:HB2 | 2.21 | 0.41 |
| 1:A:214:ARG:HG3 | 1:A:214:ARG:O | 2.20 | 0.41 |
| 1:A:237:SER:C | 1:A:241:SER:CB | 2.88 | 0.41 |
| 1:A:312:TYR:HD2 | 1:A:315:CYS:HB2 | 1.84 | 0.41 |
| 1:A:5:ILE:O | 1:A:136:SER:N | 2.47 | 0.41 |
| 2:B:165:ILE:HG13 | 2:B:253:ARG:HG2 | 2.02 | 0.41 |
| 2:B:291:LEU:H | 2:B:291:LEU:CD2 | 2.32 | 0.41 |
| 1:C:163:LYS:NZ | 1:C:163:LYS:HB2 | 2.34 | 0.41 |
| 1:C:312:TYR:N | 1:C:312:TYR:HD1 | 2.17 | 0.41 |
| 1:C:38:SER:O | 1:C:39:ASP:CB | 2.68 | 0.41 |
| 1:C:42:ILE:HA | 1:C:42:ILE:HD12 | 1.87 | 0.41 |
| 2:D:121:VAL:O | 2:D:121:VAL:HG12 | 2.20 | 0.41 |
| 2:D:214:PHE:CE2 | 2:D:215:ARG:NE | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:286:LEU:HA | 2:D:290:GLU:CD | 2.40 | 0.41 |
| 2:D:73:GLY:O | 2:D:78:VAL:HG21 | 2.20 | 0.41 |
| 1:A:229:ARG:HB3 | 1:A:366:GLY:O | 2.20 | 0.41 |
| 1:A:30:ILE:HG13 | 1:A:31:GLN:H | 1.81 | 0.41 |
| 1:A:387:ALA:CB | 1:A:390:ARG:NH1 | 2.83 | 0.41 |
| 1:A:3:GLU:O | 1:A:3:GLU:HG3 | 2.19 | 0.41 |
| 1:A:414:GLU:HB2 | 1:A:417:GLU:CB | 2.46 | 0.41 |
| 1:A:35:GLN:HE22 | 1:A:88:HIS:CD2 | 2.38 | 0.41 |
| 2:B:103:TRP:HE1 | 2:B:151:THR:HG21 | 1.85 | 0.41 |
| 2:B:215:ARG:NE | 2:B:215:ARG:CA | 2.80 | 0.41 |
| 2:B:395:PHE:CE1 | 2:B:399:PHE:CD1 | 3.08 | 0.41 |
| 2:B:404:PHE:CD2 | 2:B:404:PHE:O | 2.69 | 0.41 |
| 1:C:10:GLY:O | 1:C:12:ALA:N | 2.54 | 0.41 |
| 1:C:253:THR:OG1 | 1:C:254:GLU:N | 2.53 | 0.41 |
| 1:C:363:VAL:HG22 | 1:C:367:ASP:CG | 2.41 | 0.41 |
| 1:C:317:LEU:HD23 | 1:C:377:MET:HB2 | 2.00 | 0.41 |
| 1:C:69:ASP:CG | 1:C:71:GLU:H | 2.23 | 0.41 |
| 2:D:132:LEU:HD22 | 2:D:164:ARG:CG | 2.48 | 0.41 |
| 2:D:218:LYS:NZ | 2:D:278:ARG:CB | 2.80 | 0.41 |
| 2:D:283:TYR:O | 2:D:284:ARG:HB2 | 2.20 | 0.41 |
| 2:D:208:ALA:HB2 | 2:D:304:ALA:CB | 2.51 | 0.41 |
| 2:D:3:GLU:OE2 | 2:D:130:ASP:CB | 2.60 | 0.41 |
| 1:A:27:GLU:OE1 | 1:A:28:HIS:CE1 | 2.73 | 0.41 |
| 1:A:203:MET:SD | 1:A:388:TRP:CD1 | 3.13 | 0.41 |
| 2:B:191:VAL:HG21 | 2:B:421:ALA:CB | 2.28 | 0.41 |
| 2:B:313:LEU:C | 2:B:314:THR:HG23 | 2.41 | 0.41 |
| 1:A:177:VAL:HG21 | 2:B:349:ASN:HB2 | 2.03 | 0.41 |
| 2:B:407:TRP:NE1 | 1:C:257:THR:HA | 2.34 | 0.41 |
| 2:B:190:SER:O | 2:B:425:MET:HB2 | 2.21 | 0.41 |
| 1:C:107:HIS:HB2 | 1:C:148:GLY:O | 2.21 | 0.41 |
| 1:C:115:ILE:HG23 | 1:C:116:ASP:OD1 | 2.20 | 0.41 |
| 1:C:121:ARG:O | 1:C:122:ILE:C | 2.57 | 0.41 |
| 1:C:139:HIS:HB3 | 1:C:170:SER:CA | 2.44 | 0.41 |
| 2:D:176:LYS:HD2 | 2:D:210:TYR:CE1 | 2.55 | 0.41 |
| 2:D:223:THR:HG23 | 2:D:225:GLY:C | 2.41 | 0.41 |
| 2:D:265:LEU:HB2 | 2:D:266:HIS:H | 1.58 | 0.41 |
| 2:D:335:VAL:C | 2:D:338:LYS:H | 2.23 | 0.41 |
| 1:A:105:ARG:HG3 | 1:A:411:GLU:HG3 | 2.03 | 0.41 |
| 1:A:180:ALA:HB3 | 2:B:258:ASN:ND2 | 2.36 | 0.41 |
| 1:A:238:ILE:N | 1:A:241:SER:CB | 2.84 | 0.41 |
| 1:A:167:LEU:HD13 | 1:A:252:LEU:HD11 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:VAL:C | 1:A:411:GLU:N | 2.73 | 0.41 |
| 1:A:419:SER:O | 1:A:420:GLU:C | 2.59 | 0.41 |
| 2:B:158:ARG:HD3 | 2:B:197:ASN:HD22 | 1.73 | 0.41 |
| 2:B:351:VAL:O | 2:B:352:LYS:HG3 | 2.21 | 0.41 |
| 2:B:427:ASP:C | 2:B:429:VAL:N | 2.73 | 0.41 |
| 1:C:144:GLY:O | 1:C:145:THR:C | 2.59 | 0.41 |
| 1:C:174:ALA:HB2 | 1:C:206:ASN:CB | 2.50 | 0.41 |
| 1:C:395:PHE:C | 1:C:397:LEU:H | 2.23 | 0.41 |
| 1:C:416:GLY:C | 1:C:418:PHE:H | 2.19 | 0.41 |
| 1:C:228:ASN:ND2 | 4:C:502:GTP:O6 | 2.53 | 0.41 |
| 1:C:84:ARG:C | 1:C:85:GLN:HG2 | 2.41 | 0.41 |
| 2:D:115:VAL:HG11 | 2:D:156:LYS:HZ3 | 1.80 | 0.41 |
| 2:D:115:VAL:HG23 | 2:D:149:MET:HE1 | 2.02 | 0.41 |
| 2:D:154:ILE:HG23 | 2:D:166:MET:HE3 | 2.03 | 0.41 |
| 2:D:320:ARG:HE | 2:D:360:PRO:HG3 | 1.85 | 0.41 |
| 2:D:333:LEU:O | 2:D:336:GLN:HB3 | 2.20 | 0.41 |
| 2:D:372:LYS:HA | 2:D:372:LYS:HE2 | 2.02 | 0.41 |
| 2:D:97:SER:HG | 2:D:110:GLU:CD | 2.23 | 0.41 |
| 1:A:139:HIS:O | 1:A:140:SER:CB | 2.68 | 0.41 |
| 1:A:242:LEU:HD21 | 1:A:318:LEU:CD2 | 2.32 | 0.41 |
| 1:A:239:THR:O | 1:A:243:ARG:HB2 | 2.19 | 0.41 |
| 1:A:24:TYR:HA | 1:A:26:LEU:CD1 | 2.50 | 0.41 |
| 1:A:251:ASP:OD2 | 1:A:252:LEU:N | 2.54 | 0.41 |
| 1:A:317:LEU:HA | 1:A:377:MET:HB2 | 2.02 | 0.41 |
| 1:A:409:VAL:HG22 | 1:A:414:GLU:CD | 2.40 | 0.41 |
| 2:B:103:TRP:HB2 | 2:B:185:TYR:CE2 | 2.56 | 0.41 |
| 2:B:103:TRP:H | 2:B:408:TYR:HE1 | 1.69 | 0.41 |
| 2:B:236:SER:C | 2:B:238:VAL:H | 2.24 | 0.41 |
| 2:B:4:ILE:HD13 | 2:B:252:LEU:HD13 | 2.03 | 0.41 |
| 2:B:262:PHE:CE1 | 2:B:435:TYR:CE2 | 3.08 | 0.41 |
| 2:B:304:ALA:O | 2:B:305:CYS:SG | 2.77 | 0.41 |
| 2:B:310:GLY:HA3 | 2:B:436:GLN:HG2 | 2.03 | 0.41 |
| 2:B:313:LEU:HD21 | 2:B:435:TYR:CD2 | 2.54 | 0.41 |
| 2:D:102:ASN:N | 2:D:185:TYR:OH | 2.53 | 0.41 |
| 2:D:103:TRP:HE1 | 2:D:151:THR:HG21 | 1.85 | 0.41 |
| 2:D:289:PRO:HA | 2:D:292:THR:OG1 | 2.21 | 0.41 |
| 2:D:73:GLY:C | 2:D:75:MET:H | 2.24 | 0.41 |
| 1:A:197:HIS:O | 1:A:198:SER:OG | 2.35 | 0.41 |
| 1:A:30:ILE:HD12 | 1:A:30:ILE:C | 2.40 | 0.41 |
| 1:A:335:ILE:O | 1:A:336:LYS:C | 2.59 | 0.41 |
| 1:A:335:ILE:CG1 | 1:A:336:LYS:N | 2.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:343:PHE:CD1 | 1:A:349:THR:HA | 2.55 | 0.41 |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:H | 1.83 | 0.41 |
| 2:B:102:ASN:HD22 | 2:B:105:LYS:H | 1.58 | 0.41 |
| 2:B:271:GLY:C | 2:B:272:PHE:O | 2.58 | 0.41 |
| 2:B:95:GLY:O | 2:B:96:GLN:HB3 | 2.21 | 0.41 |
| 1:C:142:GLY:HA2 | 1:C:185:TYR:HB2 | 2.03 | 0.41 |
| 1:C:255:PHE:O | 1:C:259:LEU:HB2 | 2.21 | 0.41 |
| 2:D:176:LYS:O | 2:D:177:VAL:HB | 2.21 | 0.41 |
| 2:D:267:PHE:N | 2:D:267:PHE:CD2 | 2.89 | 0.41 |
| 2:D:59:ASN:CG | 2:D:60:LYS:HD2 | 2.41 | 0.41 |
| 1:A:115:ILE:HG13 | 1:A:152:LEU:CG | 2.50 | 0.41 |
| 1:A:178:SER:O | 1:A:182:VAL:HG21 | 2.21 | 0.41 |
| 1:A:339:ARG:O | 1:A:339:ARG:HD2 | 2.21 | 0.41 |
| 1:A:388:TRP:HZ3 | 1:A:428:LEU:HD22 | 1.82 | 0.41 |
| 2:B:232:SER:C | 2:B:234:THR:H | 2.22 | 0.41 |
| 2:B:247:GLN:HG2 | 2:B:355:VAL:HB | 2.03 | 0.41 |
| 2:B:76:ASP:HB2 | 2:B:77:SER:H | 1.46 | 0.41 |
| 1:C:306:ASP:N | 1:C:307:PRO:HD3 | 2.35 | 0.41 |
| 1:C:311:LYS:HB2 | 1:C:344:VAL:CG2 | 2.50 | 0.41 |
| 1:C:371:VAL:CG1 | 1:C:372:GLN:N | 2.82 | 0.41 |
| 1:C:9:VAL:HG21 | 1:C:150:THR:CB | 2.51 | 0.41 |
| 2:D:16:ILE:CD1 | 2:D:231:VAL:CG1 | 2.99 | 0.41 |
| 2:D:158:ARG:NH1 | 2:D:197:ASN:OD1 | 2.54 | 0.41 |
| 2:D:226:ASP:C | 2:D:228:ASN:N | 2.74 | 0.41 |
| 2:D:88:ARG:O | 2:D:91:ASN:ND2 | 2.54 | 0.41 |
| 1:A:273:ALA:HB2 | 1:A:295:CYS:CB | 2.51 | 0.41 |
| 1:A:311:LYS:HD3 | 1:A:344:VAL:CB | 2.51 | 0.41 |
| 1:A:365:GLY:O | 1:A:368:LEU:HD12 | 2.20 | 0.41 |
| 1:A:184:PRO:CB | 1:A:399:TYR:CE2 | 3.04 | 0.41 |
| 1:A:398:MET:CG | 1:A:399:TYR:H | 2.34 | 0.41 |
| 1:A:413:MET:C | 1:A:414:GLU:CD | 2.80 | 0.41 |
| 2:B:136:GLN:O | 2:B:136:GLN:HG3 | 2.21 | 0.41 |
| 2:B:204:ILE:CG2 | 2:B:209:LEU:HD11 | 2.51 | 0.41 |
| 2:B:384:ILE:O | 2:B:384:ILE:HG12 | 2.20 | 0.41 |
| 2:B:51:VAL:HG22 | 2:B:245:PRO:CB | 2.51 | 0.41 |
| 2:B:52:TYR:CG | 2:B:52:TYR:O | 2.74 | 0.41 |
| 2:B:63:PRO:C | 2:B:65:ALA:N | 2.74 | 0.41 |
| 2:B:404:PHE:HZ | 1:C:257:THR:O | 2.04 | 0.41 |
| 2:D:103:TRP:H | 2:D:408:TYR:HE1 | 1.68 | 0.41 |
| 2:D:51:VAL:HG22 | 2:D:245:PRO:CB | 2.51 | 0.41 |
| 2:D:8:GLN:O | 2:D:68:VAL:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:128:GLN:HA | 1:A:128:GLN:OE1 | 2.21 | 0.41 |
| 1:A:158:SER:HB3 | 1:A:166:LYS:HZ1 | 1.86 | 0.41 |
| 1:A:174:ALA:HB2 | 1:A:206:ASN:CB | 2.51 | 0.41 |
| 1:A:204:VAL:O | 1:A:205:ASP:HB3 | 2.21 | 0.41 |
| 1:A:398:MET:HE2 | 1:A:399:TYR:CE1 | 2.56 | 0.41 |
| 2:B:103:TRP:C | 2:B:105:LYS:N | 2.74 | 0.41 |
| 2:B:148:GLY:CA | 2:B:151:THR:HG22 | 2.51 | 0.41 |
| 2:B:179:ASP:CB | 2:B:181:VAL:HG12 | 2.46 | 0.41 |
| 2:B:19:LYS:HA | 2:B:22:GLU:CG | 2.51 | 0.41 |
| 2:B:25:SER:HB3 | 2:B:369:ARG:NH2 | 2.34 | 0.41 |
| 2:B:325:MET:CG | 2:B:355:VAL:HG11 | 2.51 | 0.41 |
| 1:C:238:ILE:O | 1:C:239:THR:O | 2.38 | 0.41 |
| 1:C:244:PHE:H | 1:C:244:PHE:HD2 | 1.67 | 0.41 |
| 1:C:244:PHE:N | 1:C:244:PHE:CD2 | 2.89 | 0.41 |
| 2:B:407:TRP:CZ2 | 1:C:256:GLN:CB | 2.91 | 0.41 |
| 1:C:108:TYR:HB3 | 1:C:413:MET:HE3 | 2.03 | 0.41 |
| 1:C:414:GLU:HA | 1:C:417:GLU:HB2 | 2.02 | 0.41 |
| 2:D:182:VAL:O | 2:D:183:GLU:HB2 | 2.21 | 0.41 |
| 1:A:183:GLU:N | 1:A:184:PRO:CD | 2.83 | 0.40 |
| 1:A:269:LEU:HD11 | 1:A:301:GLN:HB3 | 2.03 | 0.40 |
| 1:A:295:CYS:O | 1:A:295:CYS:SG | 2.78 | 0.40 |
| 1:A:244:PHE:CE1 | 1:A:358:GLU:OE2 | 2.74 | 0.40 |
| 1:A:431:ASP:C | 1:A:433:GLU:H | 2.22 | 0.40 |
| 2:B:162:PRO:HG2 | 2:B:163:ASP:H | 1.86 | 0.40 |
| 2:B:269:MET:HG2 | 2:B:384:ILE:HB | 2.03 | 0.40 |
| 1:C:107:HIS:HA | 1:C:148:GLY:O | 2.21 | 0.40 |
| 1:C:164:LYS:N | 1:C:164:LYS:NZ | 2.69 | 0.40 |
| 1:C:320:ARG:N | 1:C:374:ALA:O | 2.49 | 0.40 |
| 2:D:114:LEU:HD12 | 2:D:114:LEU:HA | 1.78 | 0.40 |
| 2:D:115:VAL:HG21 | 2:D:152:LEU:CD2 | 2.51 | 0.40 |
| 2:D:253:ARG:C | 2:D:255:LEU:H | 2.22 | 0.40 |
| 2:D:350:ASN:C | 2:D:351:VAL:CG2 | 2.89 | 0.40 |
| 3:E:83:UNK:O | 3:E:84:UNK:C | 2.67 | 0.40 |
| 1:A:101:ASN:OD1 | 2:B:254:LYS:NZ | 2.39 | 0.40 |
| 1:A:346:TRP:CZ2 | 1:A:435:VAL:HB | 2.56 | 0.40 |
| 1:A:72:PRO:HB3 | 1:A:94:THR:HG1 | 1.86 | 0.40 |
| 2:B:7:ILE:HG21 | 2:B:137:LEU:HD13 | 2.03 | 0.40 |
| 2:B:174:SER:CB | 2:B:207:GLU:N | 2.82 | 0.40 |
| 2:B:264:ARG:O | 2:B:265:LEU:O | 2.38 | 0.40 |
| 2:B:408:TYR:CD2 | 2:B:418:PHE:CZ | 3.09 | 0.40 |
| 1:C:109:THR:OG1 | 1:C:110:ILE:N | 2.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:214:ARG:NH1 | 1:C:214:ARG:HG3 | 2.35 | 0.40 |
| 1:C:362:VAL:HG12 | 1:C:363:VAL:N | 2.36 | 0.40 |
| 1:C:405:VAL:O | 1:C:405:VAL:HG22 | 2.20 | 0.40 |
| 2:D:123:ARG:C | 2:D:125:GLU:N | 2.74 | 0.40 |
| 2:D:154:ILE:O | 2:D:157:ILE:N | 2.46 | 0.40 |
| 2:D:180:THR:HB | 2:D:404:PHE:CZ | 2.55 | 0.40 |
| 2:D:346:TRP:CZ2 | 2:D:435:TYR:HB3 | 2.57 | 0.40 |
| 1:A:132:LEU:HB3 | 1:A:133:GLN:H | 1.66 | 0.40 |
| 1:A:175:PRO:HB2 | 1:A:207:GLU:OE2 | 2.22 | 0.40 |
| 1:A:322:ASP:OD1 | 1:A:357:TYR:O | 2.39 | 0.40 |
| 1:A:380:ASN:CG | 1:A:380:ASN:O | 2.60 | 0.40 |
| 1:A:409:VAL:HA | 1:A:412:GLY:O | 2.22 | 0.40 |
| 2:B:132:LEU:CD2 | 2:B:164:ARG:NE | 2.83 | 0.40 |
| 2:B:172:VAL:CG1 | 2:B:173:PRO:HD2 | 2.42 | 0.40 |
| 1:C:139:HIS:NE2 | 1:C:150:THR:CG2 | 2.84 | 0.40 |
| 1:C:225:THR:HA | 1:C:228:ASN:HB2 | 2.04 | 0.40 |
| 1:C:305:CYS:O | 1:C:306:ASP:HB2 | 2.22 | 0.40 |
| 1:C:411:GLU:O | 1:C:411:GLU:OE2 | 2.39 | 0.40 |
| 2:D:144:GLY:N | 2:D:185:TYR:CZ | 2.89 | 0.40 |
| 2:D:179:ASP:CB | 2:D:181:VAL:HG12 | 2.42 | 0.40 |
| 2:D:427:ASP:O | 2:D:428:LEU:C | 2.59 | 0.40 |
| 2:D:429:VAL:O | 2:D:433:GLN:HG2 | 2.22 | 0.40 |
| 1:A:142:GLY:O | 1:A:182:VAL:HG22 | 2.20 | 0.40 |
| 1:A:181:VAL:HG13 | 1:A:408:TYR:HH | 1.86 | 0.40 |
| 1:A:187:SER:C | 1:A:189:LEU:N | 2.74 | 0.40 |
| 1:A:145:THR:CB | 4:A:500:GTP:PG | 3.10 | 0.40 |
| 1:A:79:ARG:HD3 | 1:A:86:LEU:HD11 | 2.04 | 0.40 |
| 2:B:109:THR:O | 2:B:112:ALA:N | 2.49 | 0.40 |
| 2:B:147:SER:O | 2:B:189:LEU:HD11 | 2.22 | 0.40 |
| 2:B:192:HIS:CA | 2:B:195:VAL:HG22 | 2.26 | 0.40 |
| 2:B:267:PHE:CD2 | 2:B:267:PHE:N | 2.89 | 0.40 |
| 2:B:403:ALA:HB1 | 2:B:405:LEU:CD1 | 2.51 | 0.40 |
| 2:B:436:GLN:HE21 | 2:B:436:GLN:C | 2.23 | 0.40 |
| 1:C:107:HIS:CB | 1:C:148:GLY:O | 2.69 | 0.40 |
| 1:C:174:ALA:C | 1:C:176:GLN:H | 2.25 | 0.40 |
| 1:C:328:VAL:HG11 | 1:C:353:VAL:HG11 | 2.04 | 0.40 |
| 1:C:184:PRO:HB2 | 1:C:399:TYR:CE2 | 2.56 | 0.40 |
| 2:D:12:CYS:HB3 | 5:D:503:GDP:H8 | 1.79 | 0.40 |
| 2:D:223:THR:HG23 | 2:D:225:GLY:H | 1.85 | 0.40 |
| 2:D:308:ARG:NH2 | 2:D:339:ASN:CB | 2.85 | 0.40 |
| 2:D:350:ASN:O | 2:D:351:VAL:HG22 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:62:VAL:O | 2:D:63:PRO:C | 2.59 | 0.40 |
| 3:E:21:UNK:O | 3:E:24:UNK:CA | 2.69 | 0.40 |
| 1:A:221:ARG:NE | 1:A:221:ARG:H | 2.20 | 0.40 |
| 1:A:31:GLN:HB3 | 1:A:32:PRO:CD | 2.39 | 0.40 |
| 1:A:313:MET:HE2 | 1:A:346:TRP:HH2 | 1.87 | 0.40 |
| 1:A:317:LEU:CD2 | 1:A:377:MET:HB3 | 2.50 | 0.40 |
| 1:A:402:ARG:O | 1:A:405:VAL:HG12 | 2.21 | 0.40 |
| 2:B:117:SER:O | 2:B:120:ASP:HB2 | 2.21 | 0.40 |
| 2:B:151:THR:HG21 | 2:B:189:LEU:HD22 | 2.03 | 0.40 |
| 2:B:153:LEU:O | 2:B:156:LYS:HB3 | 2.21 | 0.40 |
| 2:B:168:THR:OG1 | 2:B:201:THR:CB | 2.64 | 0.40 |
| 2:B:144:GLY:N | 2:B:185:TYR:CZ | 2.90 | 0.40 |
| 2:B:258:ASN:OD1 | 2:B:352:LYS:HD2 | 2.21 | 0.40 |
| 2:B:88:ARG:HA | 2:B:91:ASN:HD21 | 1.87 | 0.40 |
| 1:C:115:ILE:CD1 | 1:C:156:ARG:HG3 | 2.34 | 0.40 |
| 2:D:290:GLU:O | 2:D:291:LEU:C | 2.59 | 0.40 |
| 2:D:333:LEU:HA | 2:D:336:GLN:HB3 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|---|
| 1 | A | 419/451 (93%) | 221 (53%) | 111 (26%) | 87 (21%) | 0 | 2 |
| 1 | C | 419/451 (93%) | 219 (52%) | 114 (27%) | 86 (20%) | 0 | 2 |
| 2 | B | 406/445 (91%) | 184 (45%) | 133 (33%) | 89 (22%) | 0 | 1 |
| 2 | D | 406/445 (91%) | 186 (46%) | 130 (32%) | 90 (22%) | 0 | 1 |
| All | All | 1650/1792 (92%) | 810 (49%) | 488 (30%) | 352 (21%) | 0 | 1 |

All (352) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | ILE |
| 1 | A | 32 | PRO |
| 1 | A | 46 | ASP |
| 1 | A | 83 | TYR |
| 1 | A | 90 | GLU |
| 1 | A | 97 | GLU |
| 1 | A | 98 | ASP |
| 1 | A | 100 | ALA |
| 1 | A | 103 | TYR |
| 1 | A | 109 | THR |
| 1 | A | 140 | SER |
| 1 | A | 177 | VAL |
| 1 | A | 181 | VAL |
| 1 | A | 191 | THR |
| 1 | A | 197 | HIS |
| 1 | A | 222 | PRO |
| 1 | A | 238 | ILE |
| 1 | A | 239 | THR |
| 1 | A | 265 | ALA |
| 1 | A | 266 | HIS |
| 1 | A | 278 | ALA |
| 1 | A | 322 | ASP |
| 1 | A | 346 | TRP |
| 1 | A | 349 | THR |
| 1 | A | 352 | LYS |
| 1 | A | 399 | TYR |
| 1 | A | 402 | ARG |
| 1 | A | 403 | ALA |
| 1 | A | 414 | GLU |
| 2 | B | 19 | LYS |
| 2 | B | 76 | ASP |
| 2 | B | 82 | PRO |
| 2 | B | 88 | ARG |
| 2 | B | 110 | GLU |
| 2 | B | 127 | GLU |
| 2 | B | 129 | CYS |
| 2 | B | 130 | ASP |
| 2 | B | 144 | GLY |
| 2 | B | 159 | GLU |
| 2 | B | 179 | ASP |
| 2 | B | 183 | GLU |
| 2 | B | 198 | THR |
| 2 | B | 240 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 245 | PRO |
| 2 | B | 265 | LEU |
| 2 | B | 272 | PHE |
| 2 | B | 278 | ARG |
| 2 | B | 281 | GLN |
| 2 | B | 296 | PHE |
| 2 | B | 308 | ARG |
| 2 | B | 324 | SER |
| 2 | B | 344 | VAL |
| 2 | B | 360 | PRO |
| 2 | B | 378 | ILE |
| 2 | B | 391 | ILE |
| 2 | B | 398 | MET |
| 2 | B | 399 | PHE |
| 2 | B | 402 | LYS |
| 2 | B | 404 | PHE |
| 2 | B | 416 | MET |
| 2 | B | 428 | LEU |
| 1 | C | 11 | GLN |
| 1 | C | 32 | PRO |
| 1 | C | 83 | TYR |
| 1 | C | 90 | GLU |
| 1 | C | 97 | GLU |
| 1 | C | 98 | ASP |
| 1 | C | 99 | ALA |
| 1 | C | 100 | ALA |
| 1 | C | 103 | TYR |
| 1 | C | 109 | THR |
| 1 | C | 140 | SER |
| 1 | C | 144 | GLY |
| 1 | C | 177 | VAL |
| 1 | C | 181 | VAL |
| 1 | C | 191 | THR |
| 1 | C | 197 | HIS |
| 1 | C | 222 | PRO |
| 1 | C | 238 | ILE |
| 1 | C | 259 | LEU |
| 1 | C | 265 | ALA |
| 1 | C | 266 | HIS |
| 1 | C | 277 | SER |
| 1 | C | 278 | ALA |
| 1 | C | 299 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 322 | ASP |
| 1 | C | 340 | THR |
| 1 | C | 346 | TRP |
| 1 | C | 349 | THR |
| 1 | C | 352 | LYS |
| 1 | C | 399 | TYR |
| 1 | C | 402 | ARG |
| 1 | C | 403 | ALA |
| 1 | C | 414 | GLU |
| 2 | D | 19 | LYS |
| 2 | D | 27 | GLU |
| 2 | D | 61 | TYR |
| 2 | D | 71 | GLU |
| 2 | D | 76 | ASP |
| 2 | D | 82 | PRO |
| 2 | D | 88 | ARG |
| 2 | D | 110 | GLU |
| 2 | D | 127 | GLU |
| 2 | D | 129 | CYS |
| 2 | D | 130 | ASP |
| 2 | D | 144 | GLY |
| 2 | D | 159 | GLU |
| 2 | D | 179 | ASP |
| 2 | D | 183 | GLU |
| 2 | D | 198 | THR |
| 2 | D | 240 | THR |
| 2 | D | 245 | PRO |
| 2 | D | 265 | LEU |
| 2 | D | 272 | PHE |
| 2 | D | 278 | ARG |
| 2 | D | 281 | GLN |
| 2 | D | 296 | PHE |
| 2 | D | 308 | ARG |
| 2 | D | 324 | SER |
| 2 | D | 344 | VAL |
| 2 | D | 360 | PRO |
| 2 | D | 378 | ILE |
| 2 | D | 391 | ILE |
| 2 | D | 398 | MET |
| 2 | D | 402 | LYS |
| 2 | D | 404 | PHE |
| 2 | D | 416 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 428 | LEU |
| 1 | A | 11 | GLN |
| 1 | A | 39 | ASP |
| 1 | A | 73 | THR |
| 1 | A | 99 | ALA |
| 1 | A | 112 | LYS |
| 1 | A | 144 | GLY |
| 1 | A | 195 | LEU |
| 1 | A | 237 | SER |
| 1 | A | 245 | ASP |
| 1 | A | 259 | LEU |
| 1 | A | 277 | SER |
| 1 | A | 299 | ALA |
| 1 | A | 340 | THR |
| 1 | A | 341 | ILE |
| 1 | A | 344 | VAL |
| 1 | A | 353 | VAL |
| 1 | A | 419 | SER |
| 2 | B | 26 | ASP |
| 2 | B | 27 | GLU |
| 2 | B | 56 | ALA |
| 2 | B | 60 | LYS |
| 2 | B | 61 | TYR |
| 2 | B | 71 | GLU |
| 2 | B | 96 | GLN |
| 2 | B | 115 | VAL |
| 2 | B | 119 | LEU |
| 2 | B | 128 | SER |
| 2 | B | 139 | HIS |
| 2 | B | 185 | TYR |
| 2 | B | 199 | ASP |
| 2 | B | 219 | LEU |
| 2 | B | 239 | THR |
| 2 | B | 264 | ARG |
| 2 | B | 293 | GLN |
| 2 | B | 304 | ALA |
| 2 | B | 340 | SER |
| 2 | B | 349 | ASN |
| 2 | B | 382 | THR |
| 2 | B | 387 | LEU |
| 1 | C | 16 | ILE |
| 1 | C | 38 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 39 | ASP |
| 1 | C | 46 | ASP |
| 1 | C | 73 | THR |
| 1 | C | 112 | LYS |
| 1 | C | 195 | LEU |
| 1 | C | 237 | SER |
| 1 | C | 239 | THR |
| 1 | C | 245 | ASP |
| 1 | C | 257 | THR |
| 1 | C | 264 | ARG |
| 1 | C | 315 | CYS |
| 1 | C | 341 | ILE |
| 1 | C | 344 | VAL |
| 1 | C | 353 | VAL |
| 1 | C | 404 | PHE |
| 1 | C | 419 | SER |
| 2 | D | 2 | ARG |
| 2 | D | 26 | ASP |
| 2 | D | 56 | ALA |
| 2 | D | 96 | GLN |
| 2 | D | 115 | VAL |
| 2 | D | 119 | LEU |
| 2 | D | 128 | SER |
| 2 | D | 139 | HIS |
| 2 | D | 185 | TYR |
| 2 | D | 186 | ASN |
| 2 | D | 199 | ASP |
| 2 | D | 219 | LEU |
| 2 | D | 239 | THR |
| 2 | D | 293 | GLN |
| 2 | D | 340 | SER |
| 2 | D | 382 | THR |
| 2 | D | 387 | LEU |
| 2 | D | 399 | PHE |
| 1 | A | 28 | HIS |
| 1 | A | 29 | GLY |
| 1 | A | 38 | SER |
| 1 | A | 89 | PRO |
| 1 | A | 101 | ASN |
| 1 | A | 115 | ILE |
| 1 | A | 129 | CYS |
| 1 | A | 175 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 198 | SER |
| 1 | A | 210 | TYR |
| 1 | A | 219 | ILE |
| 1 | A | 257 | THR |
| 1 | A | 261 | PRO |
| 1 | A | 264 | ARG |
| 1 | A | 306 | ASP |
| 1 | A | 315 | CYS |
| 1 | A | 404 | PHE |
| 2 | B | 2 | ARG |
| 2 | B | 91 | ASN |
| 2 | B | 94 | PHE |
| 2 | B | 97 | SER |
| 2 | B | 186 | ASN |
| 2 | B | 190 | SER |
| 2 | B | 192 | HIS |
| 2 | B | 194 | LEU |
| 2 | B | 211 | ASP |
| 2 | B | 227 | LEU |
| 2 | B | 273 | ALA |
| 2 | B | 277 | SER |
| 2 | B | 348 | PRO |
| 2 | B | 370 | GLY |
| 1 | C | 29 | GLY |
| 1 | C | 72 | PRO |
| 1 | C | 89 | PRO |
| 1 | C | 101 | ASN |
| 1 | C | 129 | CYS |
| 1 | C | 130 | THR |
| 1 | C | 161 | TYR |
| 1 | C | 198 | SER |
| 1 | C | 208 | ALA |
| 1 | C | 219 | ILE |
| 1 | C | 261 | PRO |
| 1 | C | 329 | ASN |
| 1 | C | 364 | PRO |
| 1 | C | 432 | TYR |
| 2 | D | 78 | VAL |
| 2 | D | 81 | GLY |
| 2 | D | 91 | ASN |
| 2 | D | 94 | PHE |
| 2 | D | 97 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 155 | SER |
| 2 | D | 190 | SER |
| 2 | D | 192 | HIS |
| 2 | D | 194 | LEU |
| 2 | D | 264 | ARG |
| 2 | D | 273 | ALA |
| 2 | D | 277 | SER |
| 2 | D | 283 | TYR |
| 2 | D | 304 | ALA |
| 2 | D | 339 | ASN |
| 2 | D | 348 | PRO |
| 2 | D | 370 | GLY |
| 1 | A | 72 | PRO |
| 1 | A | 125 | LEU |
| 1 | A | 130 | THR |
| 1 | A | 131 | GLY |
| 1 | A | 145 | THR |
| 1 | A | 314 | ALA |
| 1 | A | 326 | LYS |
| 1 | A | 436 | GLY |
| 2 | B | 30 | ILE |
| 2 | B | 52 | TYR |
| 2 | B | 63 | PRO |
| 2 | B | 78 | VAL |
| 2 | B | 177 | VAL |
| 2 | B | 424 | ASN |
| 1 | C | 28 | HIS |
| 1 | C | 132 | LEU |
| 1 | C | 145 | THR |
| 1 | C | 292 | THR |
| 1 | C | 306 | ASP |
| 1 | C | 314 | ALA |
| 1 | C | 326 | LYS |
| 1 | C | 348 | PRO |
| 1 | C | 382 | THR |
| 1 | C | 408 | TYR |
| 1 | C | 436 | GLY |
| 2 | D | 63 | PRO |
| 2 | D | 154 | ILE |
| 2 | D | 177 | VAL |
| 2 | D | 211 | ASP |
| 2 | D | 227 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 318 | VAL |
| 2 | D | 349 | ASN |
| 2 | D | 424 | ASN |
| 2 | D | 431 | GLU |
| 1 | A | 161 | TYR |
| 1 | A | 329 | ASN |
| 1 | A | 342 | GLN |
| 1 | A | 348 | PRO |
| 1 | A | 364 | PRO |
| 1 | A | 369 | ALA |
| 1 | A | 382 | THR |
| 1 | A | 432 | TYR |
| 2 | B | 3 | GLU |
| 2 | B | 162 | PRO |
| 2 | B | 193 | GLN |
| 2 | B | 339 | ASN |
| 1 | C | 125 | LEU |
| 1 | C | 175 | PRO |
| 1 | C | 369 | ALA |
| 2 | D | 148 | GLY |
| 2 | D | 160 | GLU |
| 2 | D | 193 | GLN |
| 1 | A | 17 | GLY |
| 1 | A | 307 | PRO |
| 2 | B | 81 | GLY |
| 2 | B | 154 | ILE |
| 2 | B | 163 | ASP |
| 2 | B | 182 | VAL |
| 2 | B | 431 | GLU |
| 1 | C | 115 | ILE |
| 1 | C | 298 | PRO |
| 1 | C | 342 | GLN |
| 2 | D | 30 | ILE |
| 2 | D | 107 | HIS |
| 2 | D | 111 | GLY |
| 2 | D | 162 | PRO |
| 2 | D | 182 | VAL |
| 1 | A | 298 | PRO |
| 2 | B | 93 | VAL |
| 2 | B | 222 | PRO |
| 2 | B | 318 | VAL |
| 1 | C | 78 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 131 | GLY |
| 2 | D | 93 | VAL |
| 2 | D | 222 | PRO |
| 1 | A | 288 | VAL |
| 2 | B | 86 | ILE |
| 1 | A | 30 | ILE |
| 2 | B | 111 | GLY |
| 1 | C | 307 | PRO |
| 2 | D | 184 | PRO |
| 1 | A | 78 | VAL |
| 2 | B | 279 | GLY |
| 1 | C | 273 | ALA |
| 1 | A | 273 | ALA |
| 1 | A | 435 | VAL |
| 2 | D | 271 | GLY |

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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1 | A | 354/377 (94%) | 278 (78%) | 76 (22%) | 1 | 6 |
| 1 | C | 354/377 (94%) | 279 (79%) | 75 (21%) | 1 | 6 |
| 2 | B | 347/381 (91%) | 274 (79%) | 73 (21%) | 1 | 6 |
| 2 | D | 347/381 (91%) | 270 (78%) | 77 (22%) | 1 | 6 |
| All | All | 1402/1516 (92%) | 1101 (78%) | 301 (22%) | 1 | 6 |

All (301) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | HIS |
| 1 | A | 16 | ILE |
| 1 | A | 23 | LEU |
| 1 | A | 25 | CYS |
| 1 | A | 30 | ILE |
| 1 | A | 32 | PRO |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 40 | LYS |
| 1 | A | 46 | ASP |
| 1 | A | 47 | ASP |
| 1 | A | 71 | GLU |
| 1 | A | 73 | THR |
| 1 | A | 77 | GLU |
| 1 | A | 83 | TYR |
| 1 | A | 86 | LEU |
| 1 | A | 87 | PHE |
| 1 | A | 91 | GLN |
| 1 | A | 92 | LEU |
| 1 | A | 101 | ASN |
| 1 | A | 105 | ARG |
| 1 | A | 115 | ILE |
| 1 | A | 125 | LEU |
| 1 | A | 130 | THR |
| 1 | A | 141 | PHE |
| 1 | A | 150 | THR |
| 1 | A | 164 | LYS |
| 1 | A | 179 | THR |
| 1 | A | 181 | VAL |
| 1 | A | 182 | VAL |
| 1 | A | 196 | GLU |
| 1 | A | 197 | HIS |
| 1 | A | 199 | ASP |
| 1 | A | 210 | TYR |
| 1 | A | 212 | ILE |
| 1 | A | 213 | CYS |
| 1 | A | 214 | ARG |
| 1 | A | 216 | ASN |
| 1 | A | 221 | ARG |
| 1 | A | 244 | PHE |
| 1 | A | 250 | VAL |
| 1 | A | 252 | LEU |
| 1 | A | 255 | PHE |
| 1 | A | 258 | ASN |
| 1 | A | 267 | PHE |
| 1 | A | 269 | LEU |
| 1 | A | 275 | VAL |
| 1 | A | 276 | ILE |
| 1 | A | 279 | GLU |
| 1 | A | 282 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 285 | GLN |
| 1 | A | 292 | THR |
| 1 | A | 295 | CYS |
| 1 | A | 297 | GLU |
| 1 | A | 302 | MET |
| 1 | A | 309 | HIS |
| 1 | A | 316 | CYS |
| 1 | A | 318 | LEU |
| 1 | A | 322 | ASP |
| 1 | A | 335 | ILE |
| 1 | A | 336 | LYS |
| 1 | A | 345 | ASP |
| 1 | A | 346 | TRP |
| 1 | A | 349 | THR |
| 1 | A | 356 | ASN |
| 1 | A | 373 | ARG |
| 1 | A | 376 | CYS |
| 1 | A | 402 | ARG |
| 1 | A | 404 | PHE |
| 1 | A | 411 | GLU |
| 1 | A | 413 | MET |
| 1 | A | 414 | GLU |
| 1 | A | 418 | PHE |
| 1 | A | 420 | GLU |
| 1 | A | 425 | MET |
| 1 | A | 428 | LEU |
| 1 | A | 431 | ASP |
| 1 | A | 439 | SER |
| 2 | B | 16 | ILE |
| 2 | B | 25 | SER |
| 2 | B | 53 | TYR |
| 2 | B | 55 | GLU |
| 2 | B | 60 | LYS |
| 2 | B | 70 | LEU |
| 2 | B | 76 | ASP |
| 2 | B | 88 | ARG |
| 2 | B | 91 | ASN |
| 2 | B | 113 | GLU |
| 2 | B | 119 | LEU |
| 2 | B | 128 | SER |
| 2 | B | 136 | GLN |
| 2 | B | 139 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 149 | MET |
| 2 | B | 157 | ILE |
| 2 | B | 158 | ARG |
| 2 | B | 160 | GLU |
| 2 | B | 163 | ASP |
| 2 | B | 167 | ASN |
| 2 | B | 168 | THR |
| 2 | B | 180 | THR |
| 2 | B | 185 | TYR |
| 2 | B | 186 | ASN |
| 2 | B | 192 | HIS |
| 2 | B | 193 | GLN |
| 2 | B | 194 | LEU |
| 2 | B | 201 | THR |
| 2 | B | 203 | CYS |
| 2 | B | 211 | ASP |
| 2 | B | 218 | LYS |
| 2 | B | 228 | ASN |
| 2 | B | 239 | THR |
| 2 | B | 244 | PHE |
| 2 | B | 245 | PRO |
| 2 | B | 249 | ASN |
| 2 | B | 251 | ASP |
| 2 | B | 252 | LEU |
| 2 | B | 253 | ARG |
| 2 | B | 254 | LYS |
| 2 | B | 255 | LEU |
| 2 | B | 265 | LEU |
| 2 | B | 278 | ARG |
| 2 | B | 283 | TYR |
| 2 | B | 284 | ARG |
| 2 | B | 286 | LEU |
| 2 | B | 292 | THR |
| 2 | B | 302 | MET |
| 2 | B | 308 | ARG |
| 2 | B | 311 | ARG |
| 2 | B | 315 | VAL |
| 2 | B | 323 | MET |
| 2 | B | 341 | SER |
| 2 | B | 345 | GLU |
| 2 | B | 346 | TRP |
| 2 | B | 350 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 352 | LYS |
| 2 | B | 377 | PHE |
| 2 | B | 380 | ASN |
| 2 | B | 388 | PHE |
| 2 | B | 395 | PHE |
| 2 | B | 401 | ARG |
| 2 | B | 404 | PHE |
| 2 | B | 405 | LEU |
| 2 | B | 407 | TRP |
| 2 | B | 409 | THR |
| 2 | B | 414 | ASP |
| 2 | B | 416 | MET |
| 2 | B | 419 | THR |
| 2 | B | 424 | ASN |
| 2 | B | 426 | ASN |
| 2 | B | 436 | GLN |
| 2 | B | 437 | ASP |
| 1 | C | 8 | HIS |
| 1 | C | 16 | ILE |
| 1 | C | 23 | LEU |
| 1 | C | 25 | CYS |
| 1 | C | 30 | ILE |
| 1 | C | 32 | PRO |
| 1 | C | 40 | LYS |
| 1 | C | 42 | ILE |
| 1 | C | 46 | ASP |
| 1 | C | 47 | ASP |
| 1 | C | 71 | GLU |
| 1 | C | 73 | THR |
| 1 | C | 77 | GLU |
| 1 | C | 83 | TYR |
| 1 | C | 86 | LEU |
| 1 | C | 87 | PHE |
| 1 | C | 91 | GLN |
| 1 | C | 101 | ASN |
| 1 | C | 105 | ARG |
| 1 | C | 115 | ILE |
| 1 | C | 125 | LEU |
| 1 | C | 130 | THR |
| 1 | C | 141 | PHE |
| 1 | C | 150 | THR |
| 1 | C | 164 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 175 | PRO |
| 1 | C | 179 | THR |
| 1 | C | 181 | VAL |
| 1 | C | 182 | VAL |
| 1 | C | 196 | GLU |
| 1 | C | 197 | HIS |
| 1 | C | 199 | ASP |
| 1 | C | 212 | ILE |
| 1 | C | 213 | CYS |
| 1 | C | 214 | ARG |
| 1 | C | 216 | ASN |
| 1 | C | 221 | ARG |
| 1 | C | 244 | PHE |
| 1 | C | 252 | LEU |
| 1 | C | 255 | PHE |
| 1 | C | 258 | ASN |
| 1 | C | 267 | PHE |
| 1 | C | 269 | LEU |
| 1 | C | 275 | VAL |
| 1 | C | 279 | GLU |
| 1 | C | 282 | TYR |
| 1 | C | 285 | GLN |
| 1 | C | 292 | THR |
| 1 | C | 297 | GLU |
| 1 | C | 302 | MET |
| 1 | C | 309 | HIS |
| 1 | C | 316 | CYS |
| 1 | C | 318 | LEU |
| 1 | C | 322 | ASP |
| 1 | C | 336 | LYS |
| 1 | C | 345 | ASP |
| 1 | C | 346 | TRP |
| 1 | C | 349 | THR |
| 1 | C | 356 | ASN |
| 1 | C | 373 | ARG |
| 1 | C | 376 | CYS |
| 1 | C | 395 | PHE |
| 1 | C | 398 | MET |
| 1 | C | 402 | ARG |
| 1 | C | 404 | PHE |
| 1 | C | 411 | GLU |
| 1 | C | 413 | MET |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 414 | GLU |
| 1 | C | 418 | PHE |
| 1 | C | 420 | GLU |
| 1 | C | 425 | MET |
| 1 | C | 428 | LEU |
| 1 | C | 431 | ASP |
| 1 | C | 433 | GLU |
| 1 | C | 439 | SER |
| 2 | D | 16 | ILE |
| 2 | D | 25 | SER |
| 2 | D | 53 | TYR |
| 2 | D | 55 | GLU |
| 2 | D | 60 | LYS |
| 2 | D | 70 | LEU |
| 2 | D | 76 | ASP |
| 2 | D | 88 | ARG |
| 2 | D | 91 | ASN |
| 2 | D | 94 | PHE |
| 2 | D | 113 | GLU |
| 2 | D | 119 | LEU |
| 2 | D | 128 | SER |
| 2 | D | 136 | GLN |
| 2 | D | 139 | HIS |
| 2 | D | 149 | MET |
| 2 | D | 157 | ILE |
| 2 | D | 158 | ARG |
| 2 | D | 160 | GLU |
| 2 | D | 163 | ASP |
| 2 | D | 167 | ASN |
| 2 | D | 180 | THR |
| 2 | D | 185 | TYR |
| 2 | D | 186 | ASN |
| 2 | D | 192 | HIS |
| 2 | D | 193 | GLN |
| 2 | D | 194 | LEU |
| 2 | D | 201 | THR |
| 2 | D | 203 | CYS |
| 2 | D | 218 | LYS |
| 2 | D | 228 | ASN |
| 2 | D | 239 | THR |
| 2 | D | 244 | PHE |
| 2 | D | 245 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 249 | ASN |
| 2 | D | 251 | ASP |
| 2 | D | 252 | LEU |
| 2 | D | 253 | ARG |
| 2 | D | 254 | LYS |
| 2 | D | 255 | LEU |
| 2 | D | 265 | LEU |
| 2 | D | 278 | ARG |
| 2 | D | 283 | TYR |
| 2 | D | 284 | ARG |
| 2 | D | 286 | LEU |
| 2 | D | 292 | THR |
| 2 | D | 302 | MET |
| 2 | D | 308 | ARG |
| 2 | D | 311 | ARG |
| 2 | D | 312 | TYR |
| 2 | D | 315 | VAL |
| 2 | D | 323 | MET |
| 2 | D | 341 | SER |
| 2 | D | 345 | GLU |
| 2 | D | 346 | TRP |
| 2 | D | 350 | ASN |
| 2 | D | 352 | LYS |
| 2 | D | 377 | PHE |
| 2 | D | 380 | ASN |
| 2 | D | 381 | SER |
| 2 | D | 382 | THR |
| 2 | D | 388 | PHE |
| 2 | D | 395 | PHE |
| 2 | D | 398 | MET |
| 2 | D | 401 | ARG |
| 2 | D | 404 | PHE |
| 2 | D | 405 | LEU |
| 2 | D | 407 | TRP |
| 2 | D | 409 | THR |
| 2 | D | 414 | ASP |
| 2 | D | 416 | MET |
| 2 | D | 419 | THR |
| 2 | D | 424 | ASN |
| 2 | D | 425 | MET |
| 2 | D | 426 | ASN |
| 2 | D | 436 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 437 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 35 | GLN |
| 1 | A | 102 | ASN |
| 1 | A | 133 | GLN |
| 1 | A | 176 | GLN |
| 1 | A | 186 | ASN |
| 1 | A | 258 | ASN |
| 1 | A | 285 | GLN |
| 1 | A | 300 | ASN |
| 1 | A | 301 | GLN |
| 1 | A | 356 | ASN |
| 1 | A | 380 | ASN |
| 2 | B | 6 | HIS |
| 2 | B | 8 | GLN |
| 2 | B | 14 | ASN |
| 2 | B | 15 | GLN |
| 2 | B | 85 | GLN |
| 2 | B | 91 | ASN |
| 2 | B | 101 | ASN |
| 2 | B | 102 | ASN |
| 2 | B | 133 | GLN |
| 2 | B | 139 | HIS |
| 2 | B | 193 | GLN |
| 2 | B | 197 | ASN |
| 2 | B | 206 | ASN |
| 2 | B | 228 | ASN |
| 2 | B | 282 | GLN |
| 2 | B | 294 | GLN |
| 2 | B | 337 | ASN |
| 2 | B | 350 | ASN |
| 2 | B | 380 | ASN |
| 2 | B | 426 | ASN |
| 2 | B | 433 | GLN |
| 2 | B | 434 | GLN |
| 1 | C | 15 | GLN |
| 1 | C | 35 | GLN |
| 1 | C | 102 | ASN |
| 1 | C | 133 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 176 | GLN |
| 1 | C | 186 | ASN |
| 1 | C | 256 | GLN |
| 1 | C | 258 | ASN |
| 1 | C | 285 | GLN |
| 1 | C | 300 | ASN |
| 1 | C | 301 | GLN |
| 1 | C | 356 | ASN |
| 2 | D | 6 | HIS |
| 2 | D | 8 | GLN |
| 2 | D | 14 | ASN |
| 2 | D | 15 | GLN |
| 2 | D | 85 | GLN |
| 2 | D | 91 | ASN |
| 2 | D | 101 | ASN |
| 2 | D | 102 | ASN |
| 2 | D | 133 | GLN |
| 2 | D | 193 | GLN |
| 2 | D | 197 | ASN |
| 2 | D | 206 | ASN |
| 2 | D | 228 | ASN |
| 2 | D | 282 | GLN |
| 2 | D | 294 | GLN |
| 2 | D | 349 | ASN |
| 2 | D | 350 | ASN |
| 2 | D | 380 | ASN |
| 2 | D | 426 | ASN |
| 2 | D | 433 | GLN |
| 2 | D | 434 | 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 ⓘ

4 ligands are modelled in this entry.

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 |
| 4 | GTP | C | 502 | - | 26,34,34 | 1.58 | 2 (7%) | 33,54,54 | 2.13 | 6 (18%) |
| 5 | GDP | D | 503 | - | 24,30,30 | 1.69 | 4 (16%) | 31,47,47 | 2.13 | 6 (19%) |
| 4 | GTP | A | 500 | - | 26,34,34 | 1.52 | 5 (19%) | 33,54,54 | 2.08 | 4 (12%) |
| 5 | GDP | B | 501 | - | 24,30,30 | 1.85 | 5 (20%) | 31,47,47 | 2.22 | 4 (12%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | GTP | C | 502 | - | - | 3/18/38/38 | 0/3/3/3 |
| 5 | GDP | D | 503 | - | - | 6/12/32/32 | 0/3/3/3 |
| 4 | GTP | A | 500 | - | - | 5/18/38/38 | 0/3/3/3 |
| 5 | GDP | B | 501 | - | - | 4/12/32/32 | 0/3/3/3 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | B | 501 | GDP | C6-N1 | 6.02 | 1.43 | 1.33 |
| 5 | D | 503 | GDP | C6-N1 | 5.72 | 1.43 | 1.33 |
| 4 | C | 502 | GTP | C6-N1 | 5.34 | 1.42 | 1.33 |
| 4 | A | 500 | GTP | C6-N1 | 4.87 | 1.41 | 1.33 |
| 5 | B | 501 | GDP | C2'-C1' | -3.28 | 1.48 | 1.53 |
| 4 | C | 502 | GTP | C2-N1 | 3.20 | 1.41 | 1.35 |
| 5 | B | 501 | GDP | C2-N1 | 3.08 | 1.40 | 1.35 |
| 5 | D | 503 | GDP | C2'-C1' | -2.77 | 1.49 | 1.53 |
| 5 | B | 501 | GDP | O4'-C1' | -2.74 | 1.37 | 1.41 |
| 4 | A | 500 | GTP | C2-N1 | 2.48 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | A | 500 | GTP | O5'-C5' | -2.23 | 1.36 | 1.44 |
| 5 | D | 503 | GDP | C2-N1 | 2.15 | 1.39 | 1.35 |
| 4 | A | 500 | GTP | C8-N7 | -2.12 | 1.30 | 1.34 |
| 5 | D | 503 | GDP | PA-O2A | -2.10 | 1.45 | 1.55 |
| 4 | A | 500 | GTP | PA-O2A | -2.08 | 1.45 | 1.55 |
| 5 | B | 501 | GDP | PA-O2A | -2.03 | 1.45 | 1.55 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5 | B | 501 | GDP | C5-C6-N1 | -8.30 | 112.08 | 123.43 |
| 5 | D | 503 | GDP | C5-C6-N1 | -7.87 | 112.67 | 123.43 |
| 4 | C | 502 | GTP | C5-C6-N1 | -7.80 | 112.76 | 123.43 |
| 4 | A | 500 | GTP | C5-C6-N1 | -7.64 | 112.99 | 123.43 |
| 5 | B | 501 | GDP | C6-N1-C2 | 6.00 | 125.46 | 115.93 |
| 4 | C | 502 | GTP | C6-N1-C2 | 5.70 | 124.98 | 115.93 |
| 4 | A | 500 | GTP | C6-N1-C2 | 5.69 | 124.97 | 115.93 |
| 5 | D | 503 | GDP | C6-N1-C2 | 5.65 | 124.91 | 115.93 |
| 4 | A | 500 | GTP | N3-C2-N1 | -3.54 | 122.50 | 127.22 |
| 5 | B | 501 | GDP | N3-C2-N1 | -3.41 | 122.68 | 127.22 |
| 4 | C | 502 | GTP | N3-C2-N1 | -3.40 | 122.68 | 127.22 |
| 5 | B | 501 | GDP | C6-C5-C4 | -3.25 | 117.69 | 120.80 |
| 4 | A | 500 | GTP | C6-C5-C4 | -3.24 | 117.71 | 120.80 |
| 5 | D | 503 | GDP | C6-C5-C4 | -3.14 | 117.80 | 120.80 |
| 4 | C | 502 | GTP | C6-C5-C4 | -3.11 | 117.83 | 120.80 |
| 5 | D | 503 | GDP | N3-C2-N1 | -2.90 | 123.35 | 127.22 |
| 4 | C | 502 | GTP | PA-O3A-PB | 2.75 | 142.26 | 132.83 |
| 4 | C | 502 | GTP | O2G-PG-O3B | 2.65 | 113.51 | 104.64 |
| 5 | D | 503 | GDP | O2B-PB-O3A | 2.31 | 112.38 | 104.64 |
| 5 | D | 503 | GDP | O3B-PB-O3A | 2.10 | 111.68 | 104.64 |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | D | 503 | GDP | C5'-O5'-PA-O1A |
| 5 | D | 503 | GDP | C5'-O5'-PA-O2A |
| 5 | D | 503 | GDP | C4'-C5'-O5'-PA |
| 5 | D | 503 | GDP | C3'-C4'-C5'-O5' |
| 4 | A | 500 | GTP | C3'-C4'-C5'-O5' |
| 5 | B | 501 | GDP | C5'-O5'-PA-O1A |
| 5 | B | 501 | GDP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | B | 501 | GDP | C4'-C5'-O5'-PA |
| 5 | D | 503 | GDP | O4'-C4'-C5'-O5' |
| 4 | A | 500 | GTP | O4'-C4'-C5'-O5' |
| 4 | A | 500 | GTP | PG-O3B-PB-O1B |
| 4 | C | 502 | GTP | C3'-C4'-C5'-O5' |
| 4 | A | 500 | GTP | PA-O3A-PB-O1B |
| 4 | C | 502 | GTP | O4'-C4'-C5'-O5' |
| 5 | D | 503 | GDP | C5'-O5'-PA-O3A |
| 5 | B | 501 | GDP | C5'-O5'-PA-O3A |
| 4 | C | 502 | GTP | C5'-O5'-PA-O1A |
| 4 | A | 500 | GTP | C5'-O5'-PA-O1A |

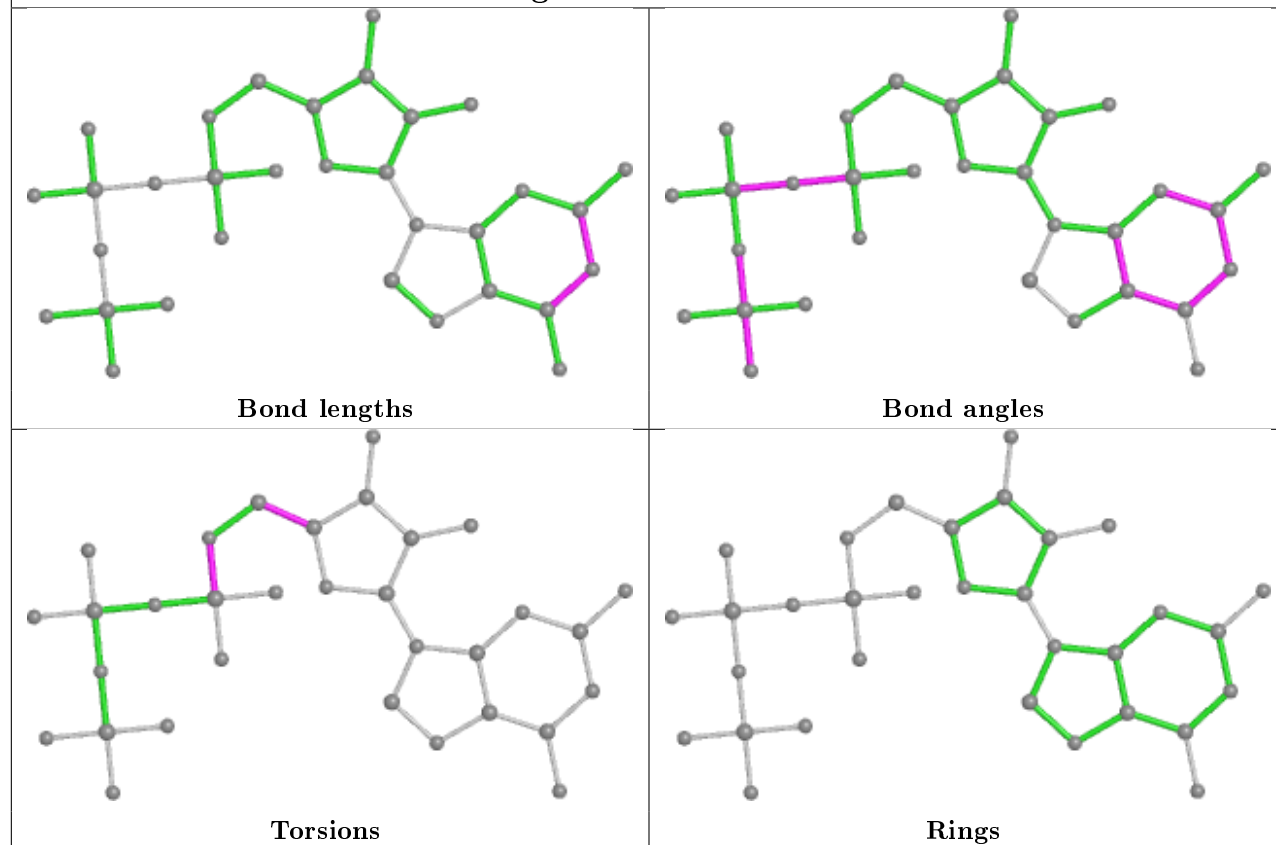
There are no ring outliers.

4 monomers are involved in 26 short contacts:

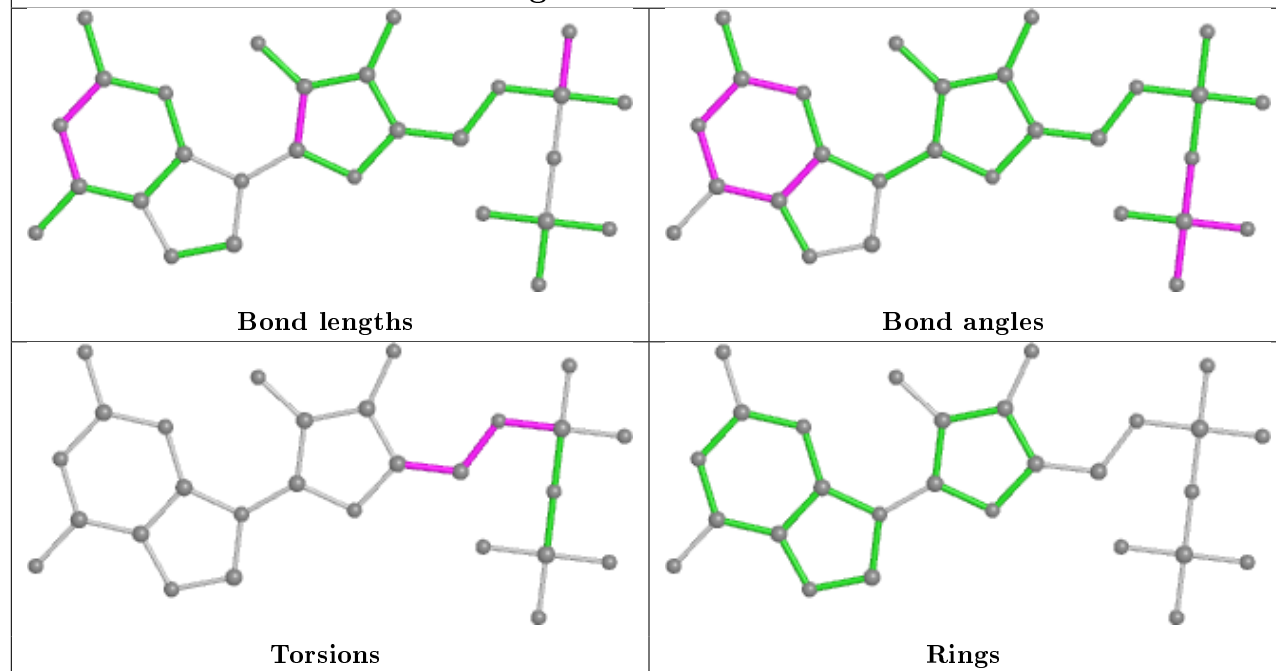
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | C | 502 | GTP | 8 | 0 |
| 5 | D | 503 | GDP | 9 | 0 |
| 4 | A | 500 | GTP | 4 | 0 |
| 5 | B | 501 | GDP | 5 | 0 |

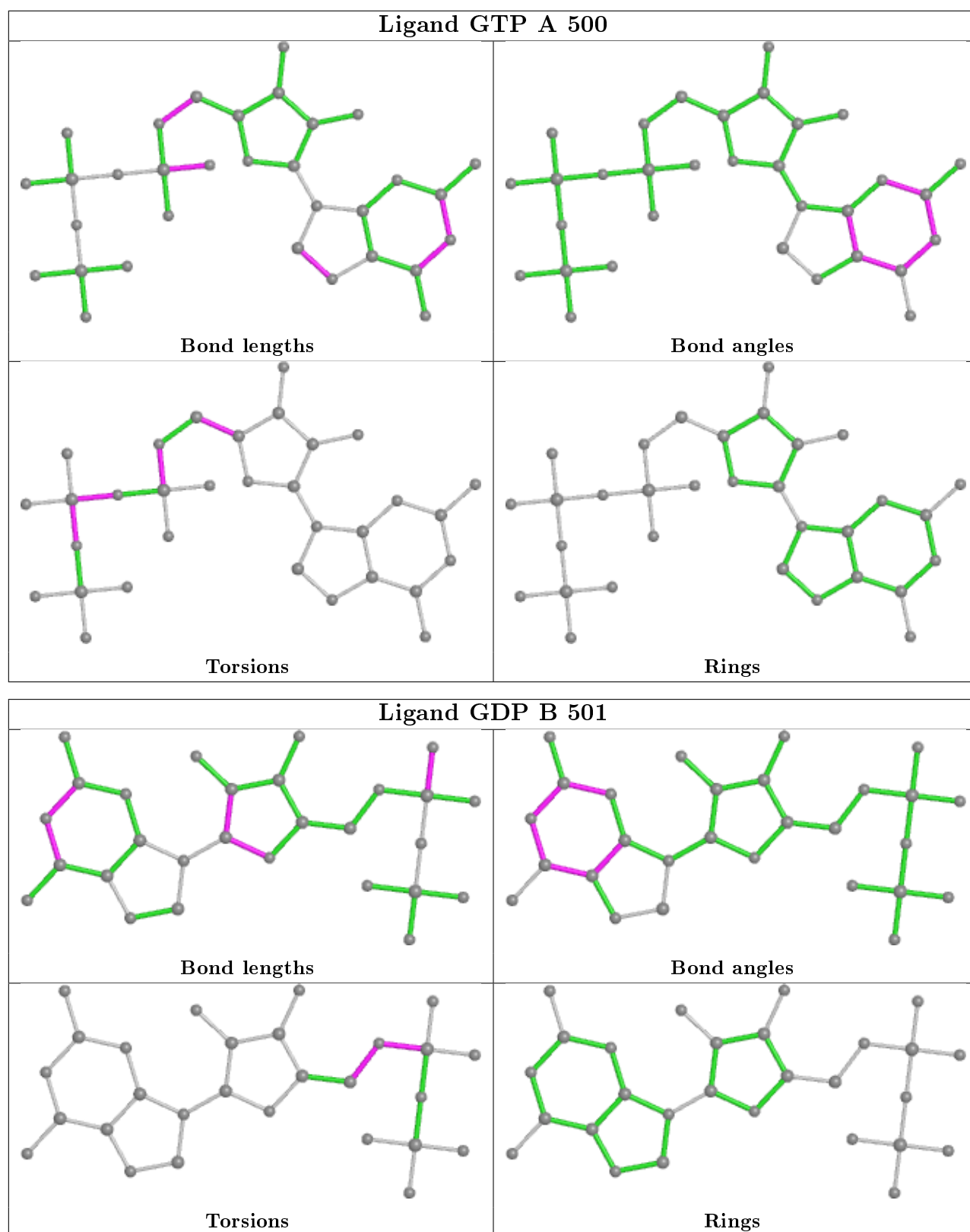
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP C 502



Ligand GDP D 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.