# Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Nov 3, 2016 – 05:34 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 3DCO |
| EMDB ID: | : | EMD-5038 |
| Title | : | Drosophila NOD (3DC4) and Bovine Tubulin (1JFF) Docked into the 11-Angstrom Cryo-EM Map of Nucleotide-Free NOD Complexed to the Microtubule |
| Authors | : | Sindelar, C.V.; Cochran, J.C.; Kull, F.J. |
| Deposited on | : | 2008-06-04 |
| Resolution | : | 11.00 Å(reported) |
| Based on PDB ID | : | 3DC4, 1JFF |

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

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

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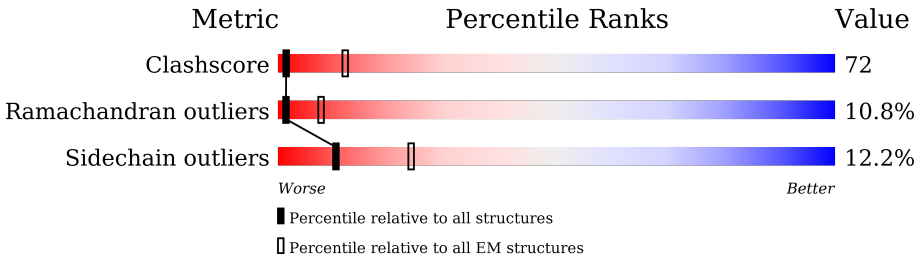
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| EM map analysis | : | NOT EXECUTED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20028320 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.00 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | N | 344 | 55% 26% • • 15% |
| 2 | A | 451 | 16% 57% 17% • 9% |
| 3 | B | 445 | 20% 56% 18% • • |

## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Kinesin-like protein Nod.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | N | 291 | Total | C | N | O | S | 0 | 0 |
| | | | 2247 | 1420 | 397 | 416 | 14 | | |

There are 26 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| N | -14 | MET | - | EXPRESSION TAG | UNP P18105 |
| N | -13 | ALA | - | EXPRESSION TAG | UNP P18105 |
| N | -12 | SER | - | EXPRESSION TAG | UNP P18105 |
| N | -11 | ASP | - | EXPRESSION TAG | UNP P18105 |
| N | -10 | TYR | - | EXPRESSION TAG | UNP P18105 |
| N | -9 | LYS | - | EXPRESSION TAG | UNP P18105 |
| N | -8 | ASP | - | EXPRESSION TAG | UNP P18105 |
| N | -7 | ASP | - | EXPRESSION TAG | UNP P18105 |
| N | -6 | ASP | - | EXPRESSION TAG | UNP P18105 |
| N | -5 | ASP | - | EXPRESSION TAG | UNP P18105 |
| N | -4 | LYS | - | EXPRESSION TAG | UNP P18105 |
| N | -3 | ARG | - | EXPRESSION TAG | UNP P18105 |
| N | -2 | ARG | - | EXPRESSION TAG | UNP P18105 |
| N | -1 | ARG | - | EXPRESSION TAG | UNP P18105 |
| N | 0 | GLY | - | EXPRESSION TAG | UNP P18105 |
| N | 319 | ALA | - | EXPRESSION TAG | UNP P18105 |
| N | 320 | ALA | - | EXPRESSION TAG | UNP P18105 |
| N | 321 | ALA | - | EXPRESSION TAG | UNP P18105 |
| N | 322 | LEU | - | EXPRESSION TAG | UNP P18105 |
| N | 323 | GLU | - | EXPRESSION TAG | UNP P18105 |
| N | 324 | HIS | - | EXPRESSION TAG | UNP P18105 |
| N | 325 | HIS | - | EXPRESSION TAG | UNP P18105 |
| N | 326 | HIS | - | EXPRESSION TAG | UNP P18105 |
| N | 327 | HIS | - | EXPRESSION TAG | UNP P18105 |
| N | 328 | HIS | - | EXPRESSION TAG | UNP P18105 |
| N | 329 | HIS | - | EXPRESSION TAG | UNP P18105 |

- Molecule 2 is a protein called Bovine Alpha Tubulin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 412 | Total | C | N | O | S | 0 | 0 |
| | | | 3227 | 2043 | 551 | 613 | 20 | | |

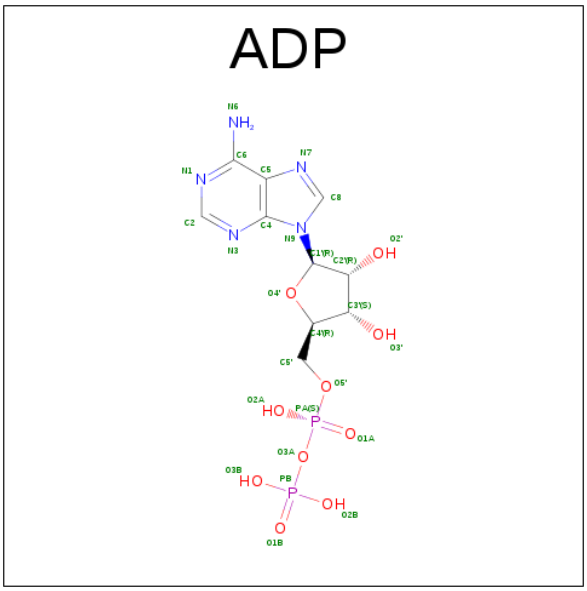
- Molecule 3 is a protein called Bovine Beta Tubulin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | B | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2105 | 575 | 646 | 25 | | |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 4 | A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 4 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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

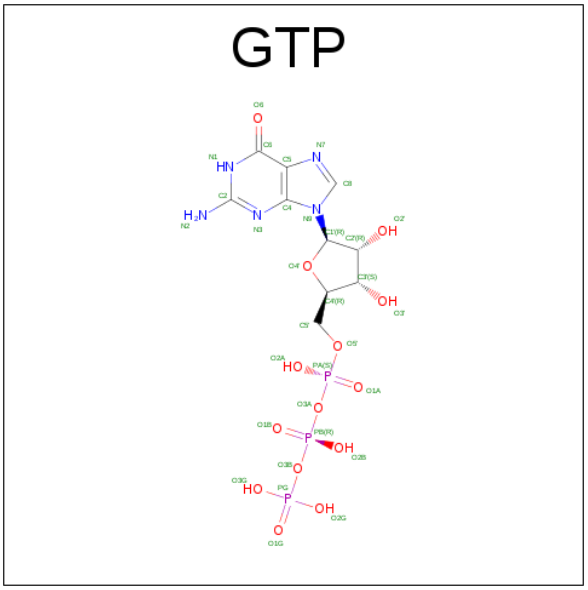



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | N | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

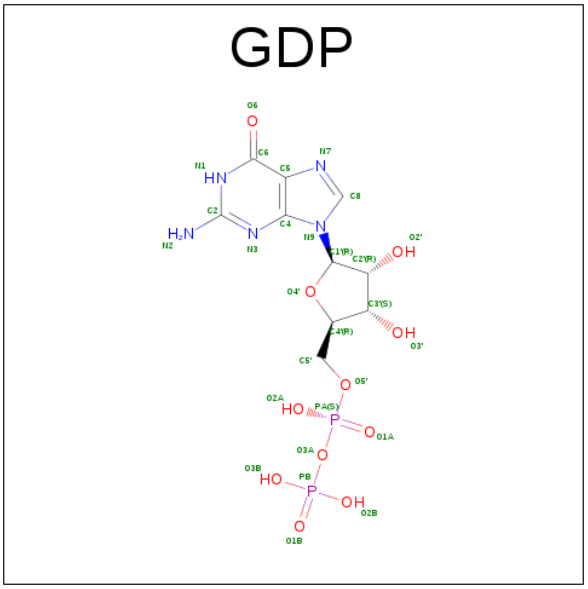
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 6 | A | 1 | 1 | 1 | 0 |

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



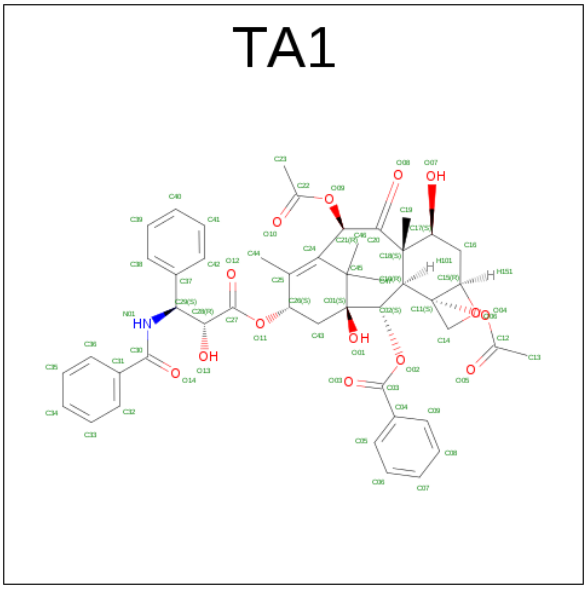

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 7 | B | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 8 | B | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



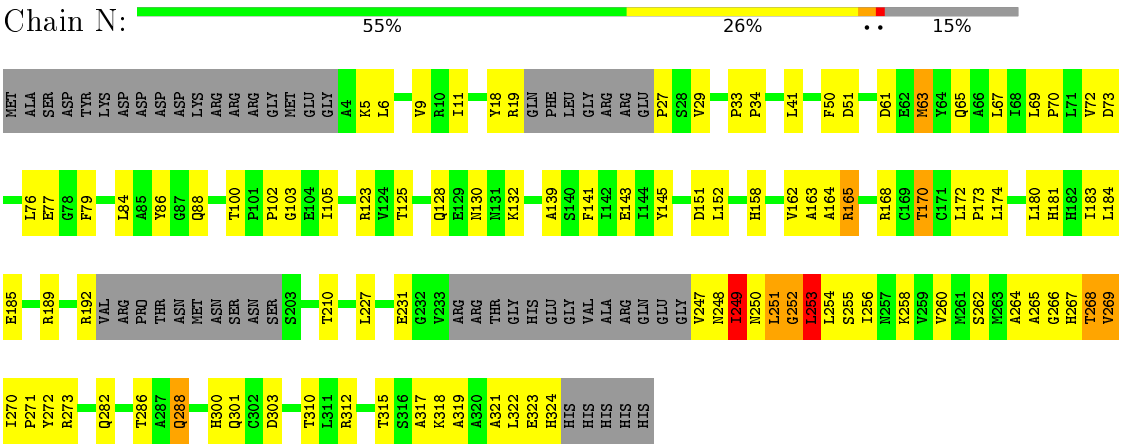

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 9 | B | 1 | Total | C | N | O | 0 |
| | | | 62 | 47 | 1 | 14 | |

# 3 Residue-property plots (i)

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

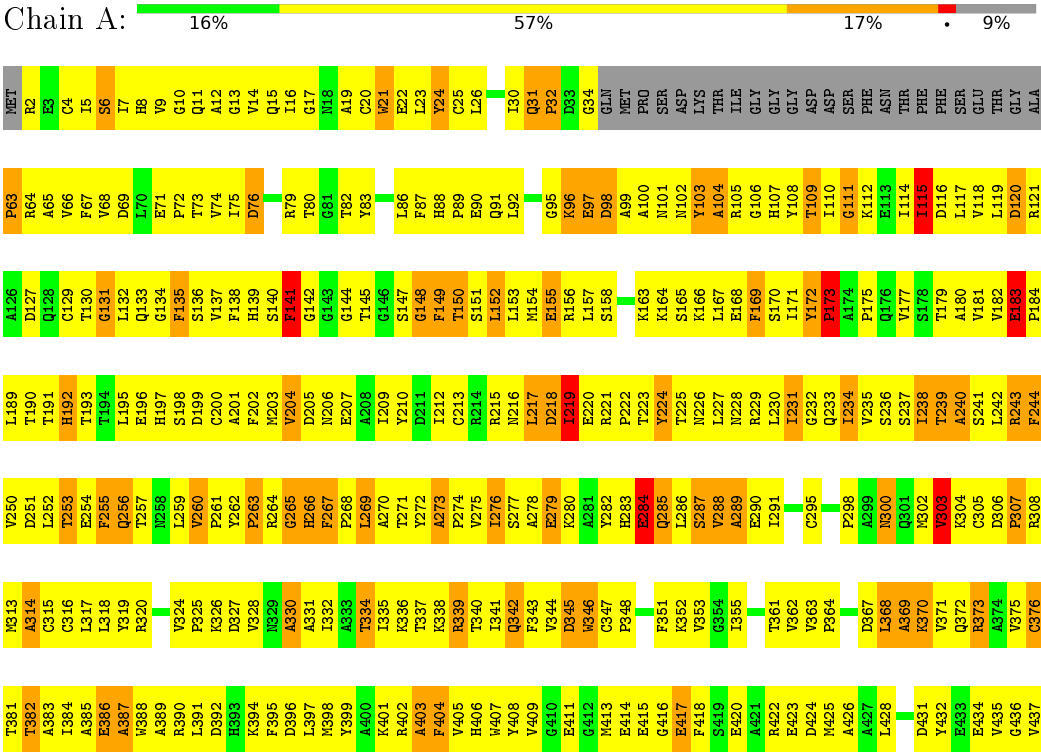
- Molecule 1: Kinesin-like protein Nod

Chain N:



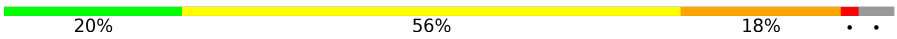

- Molecule 2: Bovine Alpha Tubulin

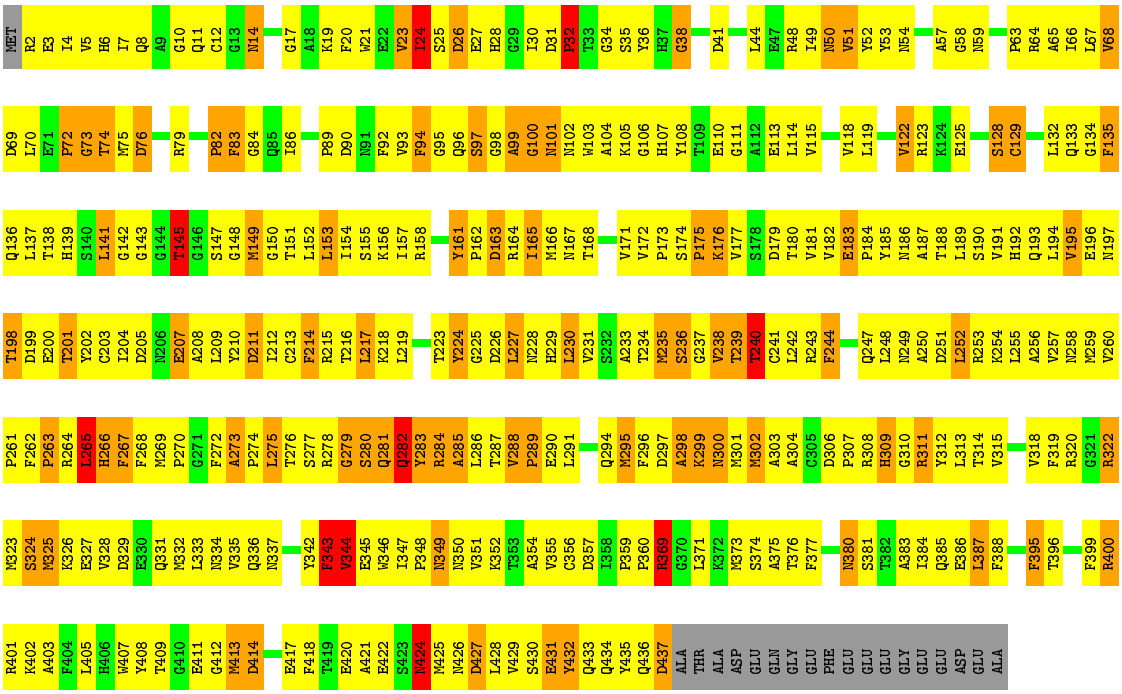
Chain A:




- Molecule 3: Bovine Beta Tubulin

Chain B:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | Integrated with fourier inversion (similar to FREALIGN) | Depositor |
| Microscope | JEOL 4000EX | Depositor |
| Voltage (kV) | 400 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 700 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | 60000 | Depositor |
| Image detector | Not provided | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, TA1, ADP, ZN, 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 | $\#\|Z\| > 2$ | RMSZ | $\#\|Z\| > 2$ |
| 1 | N | 0.31 | 0/2293 | 0.60 | 3/3110 (0.1%) |
| 2 | A | 0.50 | 0/3300 | 0.73 | 0/4482 |
| 3 | B | 0.51 | 0/3426 | 0.76 | 2/4642 (0.0%) |
| All | All | 0.46 | 0/9019 | 0.71 | 5/12234 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 268 | THR | CB-CA-C | -9.04 | 87.20 | 111.60 |
| 1 | N | 288 | GLN | CB-CA-C | -6.56 | 97.29 | 110.40 |
| 3 | B | 235 | MET | CG-SD-CE | 6.09 | 109.95 | 100.20 |
| 1 | N | 130 | ASN | N-CA-C | -5.55 | 96.02 | 111.00 |
| 3 | B | 217 | LEU | N-CA-C | -5.37 | 96.51 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | N | 2247 | 0 | 2247 | 212 | 0 |
| 2 | A | 3227 | 0 | 3143 | 580 | 0 |
| 3 | B | 3351 | 0 | 3227 | 619 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | N | 1 | 0 | 0 | 0 | 0 |
| 5 | N | 27 | 0 | 12 | 0 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 7 | B | 32 | 0 | 12 | 4 | 0 |
| 8 | B | 28 | 0 | 12 | 1 | 0 |
| 9 | B | 62 | 0 | 51 | 6 | 0 |
| All | All | 8977 | 0 | 8704 | 1270 | 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 72.

All (1270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:254:LEU:CD2 | 2:A:409:VAL:CG1 | 1.78 | 1.58 |
| 1:N:271:PRO:HB3 | 3:B:263:PRO:CG | 1.22 | 1.57 |
| 1:N:271:PRO:CB | 3:B:263:PRO:CG | 1.92 | 1.47 |
| 1:N:254:LEU:HD22 | 2:A:409:VAL:CG1 | 1.01 | 1.46 |
| 1:N:271:PRO:CB | 3:B:263:PRO:HG2 | 1.48 | 1.36 |
| 1:N:266:GLY:O | 3:B:434:GLN:CB | 1.72 | 1.34 |
| 1:N:268:THR:HG23 | 3:B:430:SER:O | 1.26 | 1.28 |
| 1:N:248:ASN:O | 1:N:249:ILE:CG2 | 1.81 | 1.27 |
| 1:N:248:ASN:O | 1:N:249:ILE:HG23 | 1.29 | 1.24 |
| 1:N:227:LEU:CD1 | 1:N:253:LEU:HD21 | 1.67 | 1.23 |
| 1:N:254:LEU:CD1 | 2:A:409:VAL:HG12 | 1.70 | 1.21 |
| 1:N:268:THR:HG23 | 3:B:430:SER:C | 1.40 | 1.17 |
| 3:B:234:THR:HG21 | 3:B:270:PRO:HB2 | 1.23 | 1.16 |
| 1:N:266:GLY:C | 3:B:434:GLN:CB | 2.14 | 1.16 |
| 2:A:243:ARG:NH2 | 2:A:252:LEU:H | 1.45 | 1.13 |
| 1:N:266:GLY:O | 3:B:434:GLN:HB2 | 1.36 | 1.13 |
| 1:N:254:LEU:HD13 | 2:A:409:VAL:HG12 | 1.20 | 1.12 |
| 1:N:271:PRO:HB3 | 3:B:263:PRO:CB | 1.79 | 1.12 |
| 1:N:312:ARG:HH22 | 2:A:417:GLU:HA | 1.05 | 1.11 |
| 1:N:266:GLY:C | 3:B:434:GLN:HB3 | 1.69 | 1.11 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:CA | 2.15 | 1.10 |
| 1:N:227:LEU:HD12 | 1:N:253:LEU:HD21 | 1.18 | 1.09 |
| 1:N:268:THR:O | 1:N:268:THR:HG22 | 1.50 | 1.09 |
| 3:B:93:VAL:HG11 | 3:B:118:VAL:HG22 | 1.30 | 1.09 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:HA | 1.68 | 1.07 |
| 1:N:254:LEU:CD2 | 2:A:409:VAL:HG13 | 1.58 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:268:THR:OG1 | 3:B:433:GLN:N | 1.89 | 1.05 |
| 2:A:109:THR:HG22 | 2:A:110:ILE:N | 1.70 | 1.04 |
| 1:N:271:PRO:CB | 3:B:263:PRO:HG3 | 1.87 | 1.03 |
| 2:A:243:ARG:HH21 | 2:A:252:LEU:N | 1.57 | 1.03 |
| 1:N:254:LEU:HD21 | 2:A:409:VAL:HG13 | 1.40 | 1.02 |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:HD21 | 1.37 | 1.02 |
| 1:N:268:THR:OG1 | 3:B:434:GLN:N | 1.91 | 1.01 |
| 2:A:11:GLN:HG3 | 2:A:74:VAL:HG11 | 1.43 | 1.01 |
| 1:N:254:LEU:CD2 | 2:A:409:VAL:HG11 | 1.62 | 1.01 |
| 3:B:236:SER:O | 3:B:240:THR:HG23 | 1.61 | 1.01 |
| 1:N:268:THR:O | 3:B:432:TYR:N | 1.72 | 1.01 |
| 1:N:273:ARG:HH11 | 3:B:196:GLU:CB | 1.73 | 1.00 |
| 3:B:299:LYS:H | 3:B:299:LYS:HD3 | 1.24 | 1.00 |
| 1:N:266:GLY:CA | 3:B:434:GLN:HB3 | 1.89 | 1.00 |
| 1:N:268:THR:CG2 | 3:B:430:SER:C | 2.28 | 1.00 |
| 1:N:268:THR:HB | 3:B:431:GLU:OE1 | 1.60 | 1.00 |
| 1:N:254:LEU:HD22 | 2:A:409:VAL:HG13 | 1.19 | 0.97 |
| 2:A:98:ASP:HB2 | 2:A:105:ARG:HH21 | 1.31 | 0.96 |
| 1:N:266:GLY:O | 3:B:434:GLN:C | 2.03 | 0.95 |
| 1:N:266:GLY:C | 3:B:434:GLN:HB2 | 1.80 | 0.95 |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:HD13 | 1.47 | 0.94 |
| 3:B:273:ALA:HB3 | 3:B:274:PRO:HD3 | 1.48 | 0.94 |
| 3:B:281:GLN:O | 3:B:283:TYR:N | 2.00 | 0.94 |
| 1:N:265:ALA:HB2 | 2:A:401:LYS:HG2 | 1.49 | 0.94 |
| 2:A:251:ASP:N | 2:A:254:GLU:HG3 | 1.82 | 0.94 |
| 1:N:268:THR:OG1 | 3:B:432:TYR:C | 2.04 | 0.94 |
| 2:A:237:SER:HB2 | 2:A:376:CYS:SG | 2.08 | 0.94 |
| 3:B:132:LEU:HD23 | 3:B:164:ARG:HG3 | 1.50 | 0.93 |
| 2:A:31:GLN:HB3 | 2:A:32:PRO:HD2 | 1.51 | 0.93 |
| 2:A:316:CYS:HB3 | 2:A:378:LEU:HD11 | 1.48 | 0.93 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:HG2 | 1.83 | 0.92 |
| 3:B:264:ARG:O | 3:B:265:LEU:HB3 | 1.69 | 0.92 |
| 2:A:251:ASP:H | 2:A:254:GLU:HG3 | 1.33 | 0.92 |
| 1:N:265:ALA:HB1 | 2:A:401:LYS:HD3 | 1.50 | 0.92 |
| 1:N:271:PRO:CG | 3:B:263:PRO:HG2 | 2.00 | 0.92 |
| 1:N:271:PRO:CG | 3:B:263:PRO:CG | 2.47 | 0.92 |
| 1:N:268:THR:H | 3:B:434:GLN:HG3 | 1.35 | 0.91 |
| 1:N:248:ASN:C | 1:N:249:ILE:HG22 | 1.88 | 0.91 |
| 3:B:70:LEU:H | 3:B:145:THR:HG21 | 1.33 | 0.91 |
| 2:A:151:SER:HB3 | 2:A:193:THR:HG21 | 1.51 | 0.90 |
| 1:N:248:ASN:O | 1:N:249:ILE:HG22 | 1.71 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:147:SER:O | 3:B:151:THR:HB | 1.71 | 0.89 |
| 3:B:8:GLN:OE1 | 3:B:67:LEU:HD22 | 1.72 | 0.89 |
| 3:B:93:VAL:HG11 | 3:B:118:VAL:CG2 | 2.03 | 0.89 |
| 3:B:102:ASN:HD21 | 3:B:408:TYR:HA | 1.38 | 0.88 |
| 2:A:343:PHE:CZ | 2:A:351:PHE:CE1 | 2.61 | 0.88 |
| 3:B:101:ASN:HD21 | 3:B:143:GLY:HA2 | 1.38 | 0.88 |
| 1:N:227:LEU:CD1 | 1:N:253:LEU:CD2 | 2.51 | 0.88 |
| 2:A:119:LEU:HD23 | 2:A:122:ILE:HD11 | 1.53 | 0.88 |
| 3:B:264:ARG:HB2 | 3:B:266:HIS:CD2 | 2.08 | 0.88 |
| 3:B:311:ARG:HD3 | 3:B:342:TYR:HA | 1.56 | 0.88 |
| 1:N:268:THR:HA | 3:B:434:GLN:CG | 2.03 | 0.88 |
| 2:A:147:SER:HB2 | 2:A:190:THR:OG1 | 1.73 | 0.88 |
| 1:N:268:THR:CG2 | 3:B:430:SER:O | 2.18 | 0.88 |
| 2:A:109:THR:HG22 | 2:A:110:ILE:H | 1.33 | 0.88 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:CG | 2.36 | 0.87 |
| 3:B:276:THR:HB | 3:B:281:GLN:HG3 | 1.56 | 0.87 |
| 2:A:407:TRP:HE1 | 3:B:260:VAL:HG23 | 1.38 | 0.87 |
| 2:A:110:ILE:HG23 | 2:A:111:GLY:H | 1.38 | 0.87 |
| 2:A:122:ILE:HD12 | 2:A:157:LEU:HD21 | 1.54 | 0.87 |
| 3:B:6:HIS:CE1 | 3:B:8:GLN:HG2 | 2.10 | 0.86 |
| 3:B:153:LEU:O | 3:B:157:ILE:HG12 | 1.75 | 0.86 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:N | 2.23 | 0.86 |
| 1:N:248:ASN:C | 1:N:249:ILE:CG2 | 2.36 | 0.86 |
| 1:N:268:THR:CG2 | 3:B:433:GLN:H | 1.85 | 0.86 |
| 1:N:254:LEU:CG | 2:A:409:VAL:CG1 | 2.53 | 0.86 |
| 3:B:195:VAL:HG13 | 3:B:196:GLU:HG2 | 1.57 | 0.86 |
| 3:B:360:PRO:HG2 | 3:B:371:LEU:HB3 | 1.56 | 0.86 |
| 3:B:10:GLY:HA2 | 3:B:145:THR:HB | 1.55 | 0.86 |
| 2:A:264:ARG:O | 2:A:266:HIS:N | 2.09 | 0.85 |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:H | 1.41 | 0.85 |
| 1:N:266:GLY:O | 3:B:434:GLN:HB3 | 1.63 | 0.85 |
| 2:A:234:ILE:HG13 | 2:A:270:ALA:HB1 | 1.59 | 0.84 |
| 3:B:234:THR:HG21 | 3:B:270:PRO:CB | 2.06 | 0.84 |
| 1:N:84:LEU:HD21 | 1:N:253:LEU:CD2 | 2.06 | 0.84 |
| 2:A:204:VAL:HG11 | 2:A:231:ILE:HD12 | 1.59 | 0.84 |
| 1:N:312:ARG:HH22 | 2:A:417:GLU:CA | 1.81 | 0.84 |
| 3:B:20:PHE:CD2 | 3:B:235:MET:SD | 2.71 | 0.84 |
| 3:B:4:ILE:HD13 | 3:B:136:GLN:HE21 | 1.42 | 0.84 |
| 3:B:19:LYS:HG3 | 3:B:228:ASN:HB3 | 1.57 | 0.84 |
| 3:B:324:SER:HB3 | 3:B:327:GLU:HG2 | 1.60 | 0.84 |
| 2:A:264:ARG:HB2 | 2:A:266:HIS:CD2 | 2.13 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:273:ARG:HH11 | 3:B:196:GLU:HB3 | 1.42 | 0.83 |
| 2:A:316:CYS:HB3 | 2:A:378:LEU:CD1 | 2.08 | 0.83 |
| 3:B:3:GLU:O | 3:B:133:GLN:HB3 | 1.78 | 0.83 |
| 3:B:101:ASN:ND2 | 3:B:143:GLY:HA2 | 1.94 | 0.83 |
| 3:B:209:LEU:HB3 | 3:B:227:LEU:HD22 | 1.59 | 0.83 |
| 3:B:148:GLY:O | 3:B:151:THR:HG22 | 1.79 | 0.83 |
| 3:B:156:LYS:HE2 | 3:B:156:LYS:HA | 1.61 | 0.83 |
| 2:A:184:PRO:HG2 | 2:A:398:MET:HE1 | 1.60 | 0.82 |
| 1:N:254:LEU:CG | 2:A:409:VAL:HG12 | 2.08 | 0.82 |
| 1:N:227:LEU:HD11 | 1:N:253:LEU:HD21 | 1.62 | 0.82 |
| 2:A:106:GLY:O | 2:A:111:GLY:HA3 | 1.78 | 0.82 |
| 1:N:268:THR:CA | 3:B:434:GLN:CG | 2.58 | 0.82 |
| 2:A:23:LEU:HD23 | 2:A:236:SER:HB2 | 1.61 | 0.82 |
| 3:B:147:SER:HB2 | 3:B:190:SER:HB3 | 1.60 | 0.81 |
| 3:B:287:THR:O | 3:B:288:VAL:HG23 | 1.78 | 0.81 |
| 1:N:268:THR:H | 3:B:434:GLN:CG | 1.92 | 0.81 |
| 2:A:151:SER:CB | 2:A:193:THR:HG21 | 2.09 | 0.81 |
| 3:B:110:GLU:O | 3:B:113:GLU:HG2 | 1.79 | 0.81 |
| 1:N:103:GLY:H | 1:N:181:HIS:HD2 | 1.29 | 0.81 |
| 3:B:150:GLY:HA2 | 3:B:153:LEU:HD22 | 1.59 | 0.81 |
| 1:N:267:HIS:C | 3:B:431:GLU:HG2 | 1.83 | 0.81 |
| 2:A:248:LEU:HD23 | 2:A:353:VAL:O | 1.80 | 0.81 |
| 3:B:264:ARG:HB2 | 3:B:266:HIS:HD2 | 1.45 | 0.81 |
| 2:A:267:PHE:CD1 | 2:A:267:PHE:N | 2.49 | 0.81 |
| 1:N:268:THR:N | 3:B:434:GLN:HB2 | 1.96 | 0.81 |
| 3:B:54:ASN:HD21 | 3:B:64:ARG:HD3 | 1.46 | 0.81 |
| 3:B:20:PHE:CZ | 3:B:24:ILE:HD12 | 2.15 | 0.80 |
| 3:B:236:SER:O | 3:B:240:THR:CG2 | 2.29 | 0.80 |
| 2:A:234:ILE:HD13 | 2:A:234:ILE:O | 1.81 | 0.80 |
| 3:B:191:VAL:HG11 | 3:B:425:MET:HG3 | 1.60 | 0.80 |
| 1:N:268:THR:N | 3:B:434:GLN:HG3 | 1.95 | 0.80 |
| 2:A:220:GLU:C | 2:A:222:PRO:HD3 | 2.02 | 0.80 |
| 2:A:6:SER:HB3 | 2:A:136:SER:OG | 1.81 | 0.80 |
| 1:N:273:ARG:NH1 | 3:B:196:GLU:CB | 2.45 | 0.80 |
| 1:N:312:ARG:HH21 | 2:A:417:GLU:HG2 | 1.44 | 0.80 |
| 3:B:68:VAL:HG12 | 3:B:149:MET:SD | 2.22 | 0.80 |
| 1:N:268:THR:N | 3:B:434:GLN:CG | 2.45 | 0.80 |
| 2:A:313:MET:HB3 | 2:A:344:VAL:HG21 | 1.63 | 0.79 |
| 2:A:7:ILE:HG22 | 2:A:66:VAL:HG22 | 1.63 | 0.79 |
| 2:A:132:LEU:HD23 | 2:A:132:LEU:H | 1.46 | 0.79 |
| 3:B:265:LEU:HD12 | 3:B:265:LEU:O | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:271:PRO:CG | 3:B:263:PRO:HG3 | 2.10 | 0.79 |
| 3:B:413:MET:HG3 | 3:B:414:ASP:H | 1.47 | 0.79 |
| 2:A:241:SER:O | 2:A:244:PHE:HB3 | 1.82 | 0.79 |
| 2:A:204:VAL:HG13 | 2:A:209:ILE:HD11 | 1.65 | 0.79 |
| 3:B:259:MET:HA | 3:B:314:THR:HG21 | 1.65 | 0.79 |
| 2:A:69:ASP:HA | 2:A:145:THR:HG21 | 1.66 | 0.78 |
| 2:A:11:GLN:HG3 | 2:A:74:VAL:CG1 | 2.13 | 0.78 |
| 1:N:253:LEU:O | 1:N:256:ILE:HB | 1.83 | 0.78 |
| 2:A:199:ASP:HB3 | 2:A:256:GLN:NE2 | 1.98 | 0.78 |
| 2:A:109:THR:CG2 | 2:A:110:ILE:N | 2.44 | 0.78 |
| 2:A:172:TYR:HD1 | 2:A:172:TYR:C | 1.87 | 0.78 |
| 1:N:265:ALA:HB2 | 2:A:401:LYS:CG | 2.13 | 0.78 |
| 2:A:155:GLU:HA | 2:A:197:HIS:ND1 | 1.99 | 0.78 |
| 3:B:234:THR:CG2 | 3:B:270:PRO:HB2 | 2.11 | 0.78 |
| 1:N:273:ARG:HH11 | 3:B:196:GLU:HB2 | 1.46 | 0.78 |
| 2:A:243:ARG:HH21 | 2:A:252:LEU:H | 0.79 | 0.77 |
| 3:B:396:THR:HG23 | 3:B:422:GLU:OE2 | 1.83 | 0.77 |
| 3:B:205:ASP:OD1 | 3:B:304:ALA:HB2 | 1.84 | 0.77 |
| 3:B:192:HIS:ND1 | 3:B:424:ASN:OD1 | 2.18 | 0.77 |
| 2:A:223:THR:HB | 2:A:225:THR:HG22 | 1.67 | 0.77 |
| 2:A:425:MET:HE2 | 2:A:428:LEU:HD23 | 1.64 | 0.77 |
| 3:B:259:MET:HG2 | 3:B:314:THR:HG21 | 1.67 | 0.77 |
| 2:A:110:ILE:HG23 | 2:A:111:GLY:N | 1.99 | 0.77 |
| 1:N:268:THR:CG2 | 3:B:433:GLN:N | 2.45 | 0.77 |
| 1:N:268:THR:HA | 3:B:434:GLN:HG3 | 1.64 | 0.77 |
| 1:N:266:GLY:O | 3:B:434:GLN:CA | 2.33 | 0.76 |
| 2:A:231:ILE:HA | 2:A:234:ILE:HG22 | 1.66 | 0.76 |
| 3:B:35:SER:HB3 | 3:B:59:ASN:HA | 1.65 | 0.76 |
| 1:N:271:PRO:HB3 | 3:B:263:PRO:HG2 | 0.77 | 0.76 |
| 2:A:221:ARG:HD3 | 2:A:221:ARG:O | 1.85 | 0.76 |
| 3:B:176:LYS:HE3 | 3:B:207:GLU:HG3 | 1.68 | 0.76 |
| 3:B:250:ALA:HA | 3:B:254:LYS:HE2 | 1.68 | 0.76 |
| 1:N:253:LEU:HA | 1:N:256:ILE:HD12 | 1.65 | 0.76 |
| 2:A:7:ILE:HD12 | 2:A:153:LEU:HD21 | 1.68 | 0.76 |
| 3:B:198:THR:O | 3:B:265:LEU:HD22 | 1.85 | 0.75 |
| 1:N:273:ARG:NH1 | 3:B:196:GLU:HB2 | 2.01 | 0.75 |
| 2:A:167:LEU:HG | 2:A:200:CYS:HB3 | 1.69 | 0.75 |
| 2:A:225:THR:O | 2:A:229:ARG:HG3 | 1.85 | 0.75 |
| 2:A:101:ASN:ND2 | 3:B:254:LYS:HD2 | 2.02 | 0.75 |
| 2:A:344:VAL:HG11 | 2:A:346:TRP:CE2 | 2.21 | 0.75 |
| 2:A:163:LYS:O | 2:A:164:LYS:HG2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:205:ASP:CB | 2:A:303:VAL:HA | 2.17 | 0.75 |
| 1:N:268:THR:HA | 3:B:434:GLN:HG2 | 1.67 | 0.75 |
| 1:N:19:ARG:H | 1:N:300:HIS:HE1 | 1.32 | 0.75 |
| 3:B:19:LYS:HG3 | 3:B:228:ASN:CB | 2.17 | 0.75 |
| 3:B:209:LEU:HG | 3:B:230:LEU:HD22 | 1.69 | 0.75 |
| 2:A:4:CYS:SG | 2:A:252:LEU:HD11 | 2.27 | 0.75 |
| 1:N:271:PRO:CB | 3:B:263:PRO:CB | 2.53 | 0.75 |
| 3:B:103:TRP:CZ3 | 3:B:108:TYR:HE1 | 2.05 | 0.74 |
| 2:A:331:ALA:O | 2:A:335:ILE:HG12 | 1.86 | 0.74 |
| 1:N:269:VAL:C | 3:B:264:ARG:HD3 | 2.08 | 0.74 |
| 2:A:172:TYR:OH | 2:A:387:ALA:HB1 | 1.87 | 0.74 |
| 1:N:164:ALA:HB1 | 1:N:168:ARG:HB3 | 1.69 | 0.74 |
| 2:A:362:VAL:HG13 | 2:A:368:LEU:HD12 | 1.68 | 0.74 |
| 1:N:266:GLY:HA3 | 3:B:434:GLN:HB3 | 1.69 | 0.74 |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:CB | 2.16 | 0.74 |
| 2:A:264:ARG:C | 2:A:266:HIS:H | 1.91 | 0.74 |
| 3:B:242:LEU:HD13 | 3:B:250:ALA:C | 2.08 | 0.74 |
| 2:A:317:LEU:HB3 | 2:A:319:TYR:HE1 | 1.52 | 0.74 |
| 3:B:168:THR:HB | 3:B:201:THR:HG23 | 1.68 | 0.74 |
| 2:A:104:ALA:HB2 | 2:A:413:MET:HG3 | 1.71 | 0.73 |
| 2:A:63:PRO:O | 2:A:64:ARG:HG2 | 1.88 | 0.73 |
| 3:B:8:GLN:CD | 3:B:67:LEU:HD22 | 2.08 | 0.73 |
| 2:A:112:LYS:O | 2:A:115:ILE:HG22 | 1.89 | 0.73 |
| 2:A:104:ALA:CB | 2:A:413:MET:HG3 | 2.18 | 0.73 |
| 3:B:217:LEU:O | 3:B:219:LEU:N | 2.22 | 0.73 |
| 3:B:76:ASP:HA | 3:B:79:ARG:HG2 | 1.71 | 0.73 |
| 2:A:7:ILE:HD11 | 2:A:137:VAL:HG22 | 1.71 | 0.73 |
| 3:B:217:LEU:C | 3:B:219:LEU:H | 1.91 | 0.73 |
| 3:B:191:VAL:CG1 | 3:B:425:MET:HG3 | 2.19 | 0.73 |
| 2:A:105:ARG:O | 2:A:110:ILE:HG22 | 1.89 | 0.72 |
| 2:A:31:GLN:HB3 | 2:A:32:PRO:CD | 2.18 | 0.72 |
| 3:B:274:PRO:HG2 | 3:B:371:LEU:HD21 | 1.70 | 0.72 |
| 2:A:25:CYS:HB2 | 2:A:30:ILE:O | 1.89 | 0.72 |
| 1:N:270:ILE:N | 3:B:264:ARG:HD3 | 2.04 | 0.72 |
| 2:A:103:TYR:CD2 | 2:A:189:LEU:HD13 | 2.24 | 0.72 |
| 1:N:271:PRO:HG3 | 3:B:263:PRO:HG3 | 1.70 | 0.72 |
| 3:B:356:CYS:SG | 3:B:357:ASP:N | 2.62 | 0.72 |
| 1:N:227:LEU:HD11 | 1:N:253:LEU:CD2 | 2.18 | 0.72 |
| 1:N:265:ALA:HB1 | 2:A:401:LYS:CD | 2.20 | 0.72 |
| 2:A:242:LEU:HG | 2:A:250:VAL:O | 1.88 | 0.72 |
| 2:A:7:ILE:CG1 | 2:A:137:VAL:HG22 | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:268:THR:CA | 3:B:434:GLN:HG2 | 2.19 | 0.72 |
| 2:A:306:ASP:O | 2:A:308:ARG:N | 2.20 | 0.72 |
| 3:B:6:HIS:HE1 | 3:B:8:GLN:HG2 | 1.52 | 0.72 |
| 1:N:265:ALA:CB | 2:A:401:LYS:HG2 | 2.20 | 0.72 |
| 2:A:172:TYR:C | 2:A:172:TYR:CD1 | 2.61 | 0.72 |
| 3:B:70:LEU:HG | 3:B:145:THR:CG2 | 2.20 | 0.72 |
| 3:B:48:ARG:HG2 | 3:B:243:ARG:O | 1.90 | 0.71 |
| 3:B:237:GLY:O | 3:B:241:CYS:HB3 | 1.90 | 0.71 |
| 3:B:243:ARG:NH2 | 3:B:252:LEU:HG | 2.05 | 0.71 |
| 3:B:201:THR:OG1 | 3:B:265:LEU:HD11 | 1.90 | 0.71 |
| 1:N:268:THR:O | 1:N:269:VAL:HG23 | 1.88 | 0.71 |
| 3:B:111:GLY:O | 3:B:115:VAL:HG23 | 1.89 | 0.71 |
| 3:B:431:GLU:OE1 | 3:B:432:TYR:HA | 1.91 | 0.71 |
| 3:B:255:LEU:O | 3:B:259:MET:HG3 | 1.91 | 0.71 |
| 2:A:12:ALA:HB3 | 2:A:140:SER:OG | 1.91 | 0.71 |
| 2:A:317:LEU:HD12 | 2:A:351:PHE:HD2 | 1.56 | 0.71 |
| 2:A:166:LYS:HE3 | 2:A:199:ASP:OD1 | 1.90 | 0.70 |
| 3:B:10:GLY:O | 3:B:14:ASN:HB2 | 1.90 | 0.70 |
| 3:B:299:LYS:N | 3:B:299:LYS:HD3 | 2.04 | 0.70 |
| 3:B:8:GLN:NE2 | 3:B:17:GLY:HA3 | 2.06 | 0.70 |
| 1:N:268:THR:HG21 | 3:B:433:GLN:N | 1.99 | 0.70 |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:CD1 | 2.20 | 0.70 |
| 3:B:175:PRO:HD2 | 3:B:207:GLU:OE2 | 1.91 | 0.70 |
| 3:B:70:LEU:HG | 3:B:145:THR:HG23 | 1.74 | 0.70 |
| 2:A:148:GLY:O | 2:A:151:SER:HB2 | 1.91 | 0.70 |
| 2:A:312:TYR:O | 2:A:344:VAL:HG23 | 1.90 | 0.70 |
| 3:B:291:LEU:O | 3:B:295:MET:HG3 | 1.91 | 0.70 |
| 2:A:5:ILE:HG22 | 2:A:6:SER:N | 2.07 | 0.70 |
| 1:N:271:PRO:HG3 | 3:B:263:PRO:CG | 2.21 | 0.70 |
| 1:N:254:LEU:HD22 | 2:A:409:VAL:HG11 | 0.70 | 0.70 |
| 2:A:343:PHE:CZ | 2:A:351:PHE:HE1 | 2.08 | 0.70 |
| 2:A:88:HIS:C | 2:A:90:GLU:H | 1.95 | 0.70 |
| 1:N:268:THR:CA | 3:B:434:GLN:HG3 | 2.20 | 0.70 |
| 2:A:242:LEU:HD21 | 2:A:250:VAL:HB | 1.71 | 0.69 |
| 2:A:205:ASP:HB3 | 2:A:303:VAL:HA | 1.73 | 0.69 |
| 3:B:24:ILE:HD11 | 3:B:52:TYR:CE1 | 2.28 | 0.69 |
| 2:A:234:ILE:HG21 | 2:A:302:MET:HE3 | 1.72 | 0.69 |
| 2:A:237:SER:CB | 2:A:376:CYS:SG | 2.80 | 0.69 |
| 3:B:234:THR:O | 3:B:238:VAL:HG23 | 1.92 | 0.69 |
| 2:A:63:PRO:C | 2:A:64:ARG:HG2 | 2.12 | 0.69 |
| 3:B:180:THR:HG22 | 3:B:181:VAL:N | 2.07 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:244:PHE:HD2 | 2:A:245:ASP:N | 1.89 | 0.69 |
| 2:A:381:THR:C | 2:A:383:ALA:H | 1.95 | 0.69 |
| 3:B:209:LEU:HD23 | 3:B:227:LEU:HB3 | 1.75 | 0.69 |
| 1:N:312:ARG:NH2 | 2:A:417:GLU:CB | 2.56 | 0.69 |
| 2:A:394:LYS:HG2 | 3:B:348:PRO:HG3 | 1.75 | 0.69 |
| 2:A:222:PRO:HD2 | 3:B:326:LYS:HB3 | 1.74 | 0.69 |
| 3:B:359:PRO:HB2 | 3:B:360:PRO:HD2 | 1.74 | 0.69 |
| 2:A:133:GLN:HG2 | 2:A:243:ARG:HH22 | 1.57 | 0.68 |
| 1:N:268:THR:O | 1:N:269:VAL:CG2 | 2.41 | 0.68 |
| 1:N:88:GLN:HE22 | 1:N:303:ASP:HB3 | 1.58 | 0.68 |
| 2:A:141:PHE:O | 2:A:147:SER:HB3 | 1.94 | 0.68 |
| 2:A:199:ASP:HB3 | 2:A:256:GLN:HE21 | 1.57 | 0.68 |
| 1:N:271:PRO:HB3 | 3:B:263:PRO:HB2 | 1.73 | 0.68 |
| 2:A:407:TRP:HE1 | 3:B:260:VAL:CG2 | 2.07 | 0.68 |
| 2:A:217:LEU:HD12 | 2:A:277:SER:HB3 | 1.75 | 0.68 |
| 2:A:371:VAL:HG12 | 2:A:372:GLN:H | 1.57 | 0.68 |
| 2:A:71:GLU:HG3 | 3:B:2:ARG:HH21 | 1.58 | 0.68 |
| 1:N:268:THR:H | 3:B:434:GLN:CB | 2.06 | 0.68 |
| 2:A:221:ARG:N | 2:A:222:PRO:HD3 | 2.09 | 0.68 |
| 3:B:204:ILE:HD13 | 3:B:231:VAL:HG22 | 1.76 | 0.68 |
| 2:A:95:GLY:O | 2:A:97:GLU:N | 2.27 | 0.68 |
| 2:A:115:ILE:CD1 | 2:A:119:LEU:HG | 2.23 | 0.68 |
| 2:A:152:LEU:HA | 2:A:155:GLU:HB2 | 1.76 | 0.68 |
| 2:A:7:ILE:HD12 | 2:A:153:LEU:CD2 | 2.24 | 0.68 |
| 2:A:298:PRO:HB3 | 2:A:307:PRO:HD2 | 1.74 | 0.67 |
| 3:B:251:ASP:O | 3:B:253:ARG:N | 2.26 | 0.67 |
| 3:B:257:VAL:O | 3:B:257:VAL:HG12 | 1.93 | 0.67 |
| 3:B:328:VAL:O | 3:B:332:MET:HG2 | 1.94 | 0.67 |
| 3:B:325:MET:CE | 3:B:355:VAL:HG21 | 2.24 | 0.67 |
| 2:A:343:PHE:HZ | 2:A:351:PHE:CE1 | 2.10 | 0.67 |
| 3:B:107:HIS:CD2 | 3:B:151:THR:CG2 | 2.78 | 0.67 |
| 3:B:242:LEU:CD2 | 3:B:250:ALA:H | 2.06 | 0.67 |
| 2:A:102:ASN:HB2 | 2:A:408:TYR:CE2 | 2.29 | 0.67 |
| 3:B:230:LEU:HD23 | 3:B:231:VAL:N | 2.10 | 0.67 |
| 3:B:250:ALA:HB1 | 3:B:254:LYS:HB2 | 1.75 | 0.67 |
| 3:B:256:ALA:O | 3:B:260:VAL:HG22 | 1.94 | 0.67 |
| 1:N:271:PRO:HB2 | 3:B:263:PRO:CG | 2.20 | 0.67 |
| 3:B:276:THR:HB | 3:B:281:GLN:CG | 2.25 | 0.67 |
| 3:B:310:GLY:HA3 | 3:B:436:GLN:HE21 | 1.59 | 0.67 |
| 2:A:251:ASP:O | 2:A:254:GLU:HB2 | 1.94 | 0.67 |
| 2:A:175:PRO:HG3 | 2:A:304:LYS:HG2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:265:ALA:CB | 2:A:401:LYS:CG | 2.72 | 0.67 |
| 1:N:315:THR:HG21 | 2:A:420:GLU:OE2 | 1.94 | 0.67 |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:CD2 | 2.22 | 0.67 |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:HD21 | 1.60 | 0.67 |
| 3:B:66:ILE:C | 3:B:67:LEU:HD23 | 2.15 | 0.67 |
| 1:N:162:VAL:HA | 1:N:165:ARG:NH1 | 2.09 | 0.67 |
| 2:A:276:ILE:O | 2:A:369:ALA:HB2 | 1.95 | 0.66 |
| 3:B:108:TYR:CD1 | 3:B:413:MET:HE1 | 2.30 | 0.66 |
| 1:N:185:GLU:HG2 | 1:N:189:ARG:NH1 | 2.10 | 0.66 |
| 3:B:44:LEU:HD12 | 3:B:49:ILE:HD13 | 1.76 | 0.66 |
| 3:B:243:ARG:HH22 | 3:B:252:LEU:HG | 1.59 | 0.66 |
| 1:N:50:PHE:HA | 1:N:318:LYS:HE3 | 1.76 | 0.66 |
| 2:A:172:TYR:HD1 | 2:A:173:PRO:N | 1.93 | 0.66 |
| 3:B:325:MET:HE2 | 3:B:355:VAL:HG21 | 1.78 | 0.66 |
| 2:A:100:ALA:CB | 2:A:105:ARG:HD3 | 2.26 | 0.66 |
| 1:N:268:THR:N | 3:B:434:GLN:CB | 2.58 | 0.66 |
| 3:B:4:ILE:HG21 | 3:B:136:GLN:HG2 | 1.76 | 0.66 |
| 2:A:68:VAL:HG11 | 2:A:149:PHE:CZ | 2.30 | 0.66 |
| 3:B:281:GLN:O | 3:B:283:TYR:HB2 | 1.96 | 0.66 |
| 1:N:266:GLY:O | 3:B:434:GLN:O | 2.13 | 0.66 |
| 2:A:206:ASN:OD1 | 2:A:227:LEU:HD13 | 1.96 | 0.65 |
| 3:B:265:LEU:HD12 | 3:B:265:LEU:C | 2.16 | 0.65 |
| 2:A:243:ARG:NH2 | 2:A:252:LEU:N | 2.28 | 0.65 |
| 2:A:341:ILE:HG12 | 2:A:341:ILE:O | 1.95 | 0.65 |
| 1:N:151:ASP:OD2 | 1:N:170:THR:HG22 | 1.96 | 0.65 |
| 2:A:217:LEU:HD11 | 2:A:367:ASP:O | 1.96 | 0.65 |
| 3:B:325:MET:HE3 | 3:B:325:MET:HA | 1.77 | 0.65 |
| 1:N:312:ARG:HH21 | 2:A:417:GLU:CB | 2.09 | 0.65 |
| 3:B:158:ARG:NE | 3:B:197:ASN:O | 2.30 | 0.65 |
| 3:B:66:ILE:CD1 | 3:B:122:VAL:HG12 | 2.26 | 0.65 |
| 3:B:267:PHE:CD1 | 3:B:267:PHE:N | 2.62 | 0.65 |
| 3:B:103:TRP:HZ3 | 3:B:108:TYR:HE1 | 1.42 | 0.65 |
| 1:N:139:ALA:HB2 | 1:N:174:LEU:HD11 | 1.78 | 0.65 |
| 1:N:312:ARG:HB3 | 2:A:416:GLY:HA3 | 1.78 | 0.65 |
| 3:B:242:LEU:CD1 | 3:B:255:LEU:HD11 | 2.25 | 0.65 |
| 2:A:344:VAL:HG12 | 2:A:345:ASP:N | 2.12 | 0.65 |
| 3:B:66:ILE:HD13 | 3:B:122:VAL:HG12 | 1.79 | 0.65 |
| 2:A:271:THR:HG23 | 2:A:300:ASN:O | 1.97 | 0.65 |
| 2:A:313:MET:HB3 | 2:A:344:VAL:CG2 | 2.26 | 0.65 |
| 3:B:422:GLU:O | 3:B:426:ASN:HB2 | 1.97 | 0.65 |
| 3:B:431:GLU:O | 3:B:434:GLN:HG2 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:372:GLN:O | 2:A:373:ARG:HB3 | 1.96 | 0.65 |
| 2:A:305:CYS:SG | 2:A:384:ILE:HD13 | 2.37 | 0.65 |
| 3:B:413:MET:HG2 | 3:B:418:PHE:HE1 | 1.61 | 0.65 |
| 2:A:115:ILE:HG23 | 2:A:116:ASP:N | 2.12 | 0.64 |
| 2:A:315:CYS:HB3 | 2:A:377:MET:HE2 | 1.78 | 0.64 |
| 2:A:402:ARG:O | 2:A:403:ALA:C | 2.36 | 0.64 |
| 2:A:224:TYR:CD1 | 3:B:325:MET:HG2 | 2.33 | 0.64 |
| 3:B:241:CYS:O | 3:B:244:PHE:HB2 | 1.97 | 0.64 |
| 3:B:35:SER:HB3 | 3:B:59:ASN:CA | 2.26 | 0.64 |
| 3:B:242:LEU:HD12 | 3:B:255:LEU:HD11 | 1.78 | 0.64 |
| 3:B:105:LYS:O | 3:B:110:GLU:HB2 | 1.98 | 0.64 |
| 3:B:192:HIS:O | 3:B:195:VAL:HG12 | 1.98 | 0.64 |
| 3:B:284:ARG:O | 3:B:286:LEU:N | 2.31 | 0.64 |
| 3:B:332:MET:HE3 | 3:B:351:VAL:HG11 | 1.78 | 0.64 |
| 3:B:427:ASP:O | 3:B:430:SER:HB3 | 1.97 | 0.64 |
| 2:A:209:ILE:HG23 | 2:A:230:LEU:HD23 | 1.79 | 0.64 |
| 2:A:317:LEU:HD12 | 2:A:351:PHE:CD2 | 2.32 | 0.64 |
| 3:B:243:ARG:HH21 | 3:B:252:LEU:H | 1.45 | 0.64 |
| 2:A:151:SER:O | 2:A:155:GLU:HB2 | 1.98 | 0.64 |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:HB2 | 1.80 | 0.63 |
| 1:N:312:ARG:HH21 | 2:A:417:GLU:CG | 2.02 | 0.63 |
| 3:B:133:GLN:HG3 | 3:B:165:ILE:HD11 | 1.80 | 0.63 |
| 3:B:172:VAL:CG1 | 3:B:387:LEU:HD21 | 2.24 | 0.63 |
| 2:A:175:PRO:HG2 | 2:A:207:GLU:OE1 | 1.98 | 0.63 |
| 3:B:180:THR:CG2 | 3:B:181:VAL:N | 2.61 | 0.63 |
| 1:N:271:PRO:CB | 3:B:263:PRO:HB2 | 2.26 | 0.63 |
| 2:A:273:ALA:HB3 | 2:A:274:PRO:HD3 | 1.81 | 0.63 |
| 2:A:386:GLU:O | 2:A:389:ALA:N | 2.31 | 0.63 |
| 9:B:601:TA1:H261 | 9:B:601:TA1:H463 | 1.80 | 0.63 |
| 2:A:7:ILE:HG22 | 2:A:66:VAL:CG2 | 2.28 | 0.63 |
| 3:B:114:LEU:O | 3:B:118:VAL:HG23 | 1.97 | 0.63 |
| 3:B:205:ASP:OD1 | 3:B:304:ALA:N | 2.32 | 0.63 |
| 3:B:282:GLN:O | 3:B:282:GLN:HG2 | 1.97 | 0.63 |
| 1:N:11:ILE:HB | 1:N:318:LYS:NZ | 2.13 | 0.63 |
| 2:A:269:LEU:O | 2:A:378:LEU:HA | 1.99 | 0.63 |
| 3:B:315:VAL:HG13 | 3:B:377:PHE:CE1 | 2.34 | 0.63 |
| 1:N:268:THR:HG21 | 3:B:433:GLN:H | 1.54 | 0.63 |
| 1:N:6:LEU:H | 1:N:324:HIS:HD2 | 1.46 | 0.63 |
| 3:B:318:VAL:HA | 3:B:354:ALA:HB3 | 1.81 | 0.63 |
| 2:A:234:ILE:HD13 | 2:A:234:ILE:C | 2.18 | 0.63 |
| 3:B:4:ILE:HA | 3:B:134:GLY:O | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:107:HIS:HD2 | 3:B:151:THR:CG2 | 2.12 | 0.63 |
| 2:A:315:CYS:HB3 | 2:A:377:MET:CE | 2.29 | 0.62 |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:CG2 | 2.28 | 0.62 |
| 3:B:299:LYS:O | 3:B:300:ASN:HB2 | 1.97 | 0.62 |
| 1:N:6:LEU:H | 1:N:324:HIS:CD2 | 2.17 | 0.62 |
| 1:N:84:LEU:HD21 | 1:N:253:LEU:HD21 | 1.80 | 0.62 |
| 2:A:7:ILE:CD1 | 2:A:137:VAL:HG22 | 2.29 | 0.62 |
| 2:A:288:VAL:O | 2:A:290:GLU:N | 2.33 | 0.62 |
| 2:A:317:LEU:HD11 | 2:A:351:PHE:HE2 | 1.63 | 0.62 |
| 2:A:236:SER:O | 2:A:240:ALA:HB3 | 1.99 | 0.62 |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:CD2 | 2.30 | 0.62 |
| 2:A:278:ALA:HA | 2:A:282:TYR:OH | 2.00 | 0.62 |
| 1:N:269:VAL:HG22 | 3:B:428:LEU:HD12 | 1.81 | 0.62 |
| 2:A:317:LEU:HB3 | 2:A:319:TYR:CE1 | 2.33 | 0.62 |
| 3:B:253:ARG:O | 3:B:256:ALA:N | 2.33 | 0.62 |
| 2:A:152:LEU:HD12 | 2:A:153:LEU:N | 2.14 | 0.62 |
| 2:A:267:PHE:H | 2:A:267:PHE:HD1 | 1.47 | 0.62 |
| 2:A:205:ASP:HB2 | 2:A:303:VAL:HA | 1.82 | 0.62 |
| 3:B:63:PRO:HD2 | 3:B:86:ILE:HG12 | 1.80 | 0.62 |
| 3:B:4:ILE:HG23 | 3:B:134:GLY:O | 2.00 | 0.61 |
| 3:B:230:LEU:O | 3:B:233:ALA:HB3 | 2.00 | 0.61 |
| 2:A:179:THR:HG22 | 3:B:352:LYS:NZ | 2.15 | 0.61 |
| 2:A:166:LYS:H | 2:A:199:ASP:CG | 2.03 | 0.61 |
| 3:B:70:LEU:CG | 3:B:145:THR:HG23 | 2.30 | 0.61 |
| 2:A:177:VAL:HG11 | 3:B:329:ASP:HB3 | 1.82 | 0.61 |
| 2:A:102:ASN:OD1 | 2:A:105:ARG:HB3 | 1.99 | 0.61 |
| 2:A:118:VAL:HG11 | 2:A:149:PHE:HZ | 1.65 | 0.61 |
| 3:B:273:ALA:HB3 | 3:B:274:PRO:CD | 2.29 | 0.61 |
| 3:B:54:ASN:ND2 | 3:B:64:ARG:HD3 | 2.15 | 0.61 |
| 2:A:23:LEU:HD22 | 2:A:232:GLY:O | 1.99 | 0.61 |
| 3:B:114:LEU:HD23 | 3:B:149:MET:CE | 2.30 | 0.61 |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD21 | 1.81 | 0.61 |
| 2:A:88:HIS:O | 2:A:90:GLU:N | 2.33 | 0.61 |
| 2:A:115:ILE:HG13 | 2:A:152:LEU:HD13 | 1.81 | 0.61 |
| 2:A:169:PHE:CE1 | 2:A:235:VAL:HG22 | 2.36 | 0.61 |
| 2:A:179:THR:HG21 | 3:B:248:LEU:CD2 | 2.30 | 0.61 |
| 2:A:362:VAL:HG13 | 2:A:368:LEU:HB2 | 1.83 | 0.61 |
| 2:A:168:GLU:OE1 | 2:A:198:SER:HB2 | 2.01 | 0.60 |
| 3:B:211:ASP:OD1 | 3:B:212:ILE:N | 2.33 | 0.60 |
| 3:B:204:ILE:CD1 | 3:B:231:VAL:HG13 | 2.30 | 0.60 |
| 2:A:181:VAL:HG21 | 3:B:258:ASN:O | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:167:LEU:HA | 2:A:200:CYS:O | 2.01 | 0.60 |
| 2:A:311:LYS:HE3 | 2:A:342:GLN:CD | 2.22 | 0.60 |
| 2:A:435:VAL:HG12 | 2:A:435:VAL:O | 2.02 | 0.60 |
| 2:A:407:TRP:NE1 | 3:B:260:VAL:HG23 | 2.14 | 0.60 |
| 1:N:268:THR:CB | 3:B:433:GLN:N | 2.59 | 0.60 |
| 3:B:205:ASP:OD1 | 3:B:304:ALA:CB | 2.50 | 0.60 |
| 3:B:19:LYS:CG | 3:B:228:ASN:HB3 | 2.31 | 0.60 |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:HG22 | 1.84 | 0.60 |
| 3:B:70:LEU:H | 3:B:145:THR:CG2 | 2.10 | 0.60 |
| 2:A:11:GLN:HE21 | 2:A:74:VAL:HG22 | 1.66 | 0.60 |
| 2:A:177:VAL:CG1 | 3:B:329:ASP:HB3 | 2.31 | 0.60 |
| 2:A:345:ASP:C | 2:A:347:CYS:H | 2.04 | 0.60 |
| 3:B:285:ALA:HB1 | 3:B:290:GLU:HG2 | 1.82 | 0.60 |
| 1:N:158:HIS:HA | 1:N:192:ARG:NH2 | 2.16 | 0.60 |
| 3:B:324:SER:C | 3:B:326:LYS:H | 2.03 | 0.60 |
| 3:B:324:SER:CB | 3:B:327:GLU:HG2 | 2.30 | 0.60 |
| 1:N:250:ASN:O | 1:N:251:LEU:CB | 2.49 | 0.60 |
| 3:B:279:GLY:O | 3:B:282:GLN:HB3 | 2.01 | 0.60 |
| 2:A:191:THR:HG21 | 2:A:425:MET:SD | 2.41 | 0.60 |
| 3:B:70:LEU:N | 3:B:145:THR:HG21 | 2.11 | 0.60 |
| 3:B:324:SER:O | 3:B:328:VAL:HG23 | 2.01 | 0.60 |
| 2:A:229:ARG:NH1 | 2:A:363:VAL:HG21 | 2.16 | 0.60 |
| 3:B:49:ILE:O | 3:B:51:VAL:N | 2.35 | 0.60 |
| 1:N:18:TYR:HH | 1:N:27:PRO:N | 1.99 | 0.60 |
| 2:A:119:LEU:O | 2:A:122:ILE:HG12 | 2.02 | 0.59 |
| 2:A:344:VAL:HG11 | 2:A:346:TRP:NE1 | 2.16 | 0.59 |
| 3:B:102:ASN:ND2 | 3:B:407:TRP:O | 2.35 | 0.59 |
| 1:N:273:ARG:CZ | 3:B:196:GLU:HG3 | 2.32 | 0.59 |
| 3:B:68:VAL:CG1 | 3:B:149:MET:SD | 2.90 | 0.59 |
| 1:N:163:ALA:H | 1:N:165:ARG:NH2 | 1.99 | 0.59 |
| 2:A:115:ILE:HD13 | 2:A:115:ILE:O | 2.02 | 0.59 |
| 2:A:278:ALA:HB2 | 2:A:369:ALA:HA | 1.85 | 0.59 |
| 3:B:161:TYR:C | 3:B:163:ASP:H | 2.05 | 0.59 |
| 3:B:30:ILE:HD13 | 3:B:53:TYR:CE2 | 2.38 | 0.59 |
| 2:A:371:VAL:HG12 | 2:A:372:GLN:N | 2.17 | 0.59 |
| 3:B:93:VAL:CG1 | 3:B:118:VAL:HG22 | 2.19 | 0.59 |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:HD23 | 1.84 | 0.59 |
| 3:B:89:PRO:HA | 3:B:92:PHE:CD1 | 2.38 | 0.59 |
| 2:A:119:LEU:CD2 | 2:A:122:ILE:HD11 | 2.28 | 0.59 |
| 2:A:284:GLU:O | 2:A:286:LEU:N | 2.35 | 0.59 |
| 3:B:128:SER:OG | 3:B:129:CYS:N | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:141:LEU:N | 3:B:141:LEU:CD1 | 2.65 | 0.59 |
| 3:B:332:MET:CE | 3:B:351:VAL:HG11 | 2.32 | 0.59 |
| 2:A:6:SER:HA | 2:A:136:SER:O | 2.02 | 0.58 |
| 3:B:408:TYR:CG | 3:B:418:PHE:HZ | 2.20 | 0.58 |
| 2:A:369:ALA:O | 2:A:370:LYS:HB3 | 2.03 | 0.58 |
| 2:A:110:ILE:CG2 | 2:A:111:GLY:H | 2.15 | 0.58 |
| 2:A:248:LEU:CD2 | 2:A:353:VAL:O | 2.49 | 0.58 |
| 2:A:413:MET:O | 2:A:414:GLU:HG3 | 2.03 | 0.58 |
| 2:A:317:LEU:HD11 | 2:A:351:PHE:CE2 | 2.38 | 0.58 |
| 2:A:88:HIS:C | 2:A:90:GLU:N | 2.57 | 0.58 |
| 3:B:307:PRO:HB3 | 3:B:312:TYR:OH | 2.04 | 0.58 |
| 2:A:166:LYS:HD2 | 2:A:197:HIS:O | 2.04 | 0.58 |
| 2:A:268:PRO:HA | 2:A:379:SER:O | 2.04 | 0.58 |
| 2:A:2:ARG:N | 2:A:131:GLY:O | 2.36 | 0.58 |
| 2:A:381:THR:C | 2:A:383:ALA:N | 2.56 | 0.58 |
| 3:B:198:THR:HG22 | 3:B:265:LEU:HD22 | 1.86 | 0.58 |
| 1:N:253:LEU:O | 1:N:256:ILE:N | 2.36 | 0.58 |
| 2:A:218:ASP:O | 2:A:219:ILE:HG23 | 2.04 | 0.58 |
| 3:B:180:THR:CG2 | 3:B:181:VAL:H | 2.17 | 0.58 |
| 3:B:299:LYS:O | 3:B:300:ASN:CB | 2.51 | 0.58 |
| 3:B:320:ARG:O | 3:B:359:PRO:HA | 2.04 | 0.58 |
| 2:A:407:TRP:O | 2:A:411:GLU:HG2 | 2.02 | 0.58 |
| 3:B:183:GLU:HB3 | 3:B:184:PRO:CD | 2.33 | 0.58 |
| 3:B:70:LEU:C | 3:B:99:ALA:HB2 | 2.24 | 0.57 |
| 2:A:362:VAL:HG11 | 2:A:368:LEU:O | 2.04 | 0.57 |
| 2:A:345:ASP:O | 2:A:347:CYS:N | 2.38 | 0.57 |
| 3:B:283:TYR:C | 3:B:284:ARG:HG2 | 2.25 | 0.57 |
| 3:B:319:PHE:CD2 | 3:B:375:ALA:HB2 | 2.40 | 0.57 |
| 1:N:252:GLY:O | 1:N:255:SER:N | 2.37 | 0.57 |
| 3:B:5:VAL:CG2 | 3:B:135:PHE:HD2 | 2.18 | 0.57 |
| 3:B:253:ARG:O | 3:B:254:LYS:C | 2.42 | 0.57 |
| 3:B:349:ASN:C | 3:B:349:ASN:HD22 | 2.06 | 0.57 |
| 3:B:270:PRO:HA | 3:B:377:PHE:O | 2.04 | 0.57 |
| 1:N:63:MET:HE2 | 1:N:67:LEU:HB3 | 1.85 | 0.57 |
| 2:A:152:LEU:HA | 2:A:155:GLU:CB | 2.35 | 0.57 |
| 2:A:362:VAL:CG1 | 2:A:368:LEU:HB2 | 2.35 | 0.57 |
| 2:A:202:PHE:CE2 | 2:A:378:LEU:HD22 | 2.38 | 0.57 |
| 3:B:151:THR:OG1 | 3:B:193:GLN:HB3 | 2.03 | 0.57 |
| 3:B:149:MET:O | 3:B:153:LEU:HD13 | 2.05 | 0.57 |
| 3:B:217:LEU:C | 3:B:219:LEU:N | 2.55 | 0.57 |
| 1:N:264:ALA:HB2 | 1:N:324:HIS:CE1 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:139:HIS:CE1 | 2:A:170:SER:HB3 | 2.40 | 0.57 |
| 2:A:165:SER:HA | 2:A:199:ASP:OD2 | 2.04 | 0.57 |
| 2:A:175:PRO:HG3 | 2:A:304:LYS:CG | 2.35 | 0.57 |
| 2:A:63:PRO:HD3 | 2:A:86:LEU:O | 2.04 | 0.57 |
| 2:A:117:LEU:HD11 | 2:A:121:ARG:HH22 | 1.69 | 0.57 |
| 3:B:273:ALA:CB | 3:B:274:PRO:HD3 | 2.30 | 0.57 |
| 3:B:30:ILE:HA | 3:B:35:SER:O | 2.04 | 0.57 |
| 2:A:286:LEU:HD12 | 2:A:290:GLU:HG2 | 1.87 | 0.57 |
| 3:B:132:LEU:CD2 | 3:B:164:ARG:HG3 | 2.32 | 0.57 |
| 3:B:259:MET:CA | 3:B:314:THR:HG21 | 2.35 | 0.57 |
| 3:B:6:HIS:HB3 | 3:B:65:ALA:HB2 | 1.87 | 0.57 |
| 3:B:14:ASN:OD1 | 3:B:75:MET:HG2 | 2.05 | 0.57 |
| 2:A:210:TYR:CE2 | 2:A:227:LEU:HD11 | 2.40 | 0.56 |
| 2:A:394:LYS:HG2 | 3:B:348:PRO:CG | 2.35 | 0.56 |
| 3:B:301:MET:CE | 3:B:377:PHE:HE2 | 2.18 | 0.56 |
| 1:N:63:MET:CE | 1:N:67:LEU:HB3 | 2.35 | 0.56 |
| 2:A:209:ILE:CG2 | 2:A:227:LEU:HD22 | 2.35 | 0.56 |
| 2:A:19:ALA:CB | 2:A:228:ASN:HB3 | 2.35 | 0.56 |
| 2:A:338:LYS:O | 2:A:340:THR:N | 2.34 | 0.56 |
| 3:B:216:THR:O | 3:B:217:LEU:HD12 | 2.05 | 0.56 |
| 2:A:11:GLN:HE22 | 3:B:249:ASN:ND2 | 2.03 | 0.56 |
| 2:A:436:GLY:C | 2:A:438:ASP:H | 2.08 | 0.56 |
| 2:A:71:GLU:HG3 | 3:B:2:ARG:NH2 | 2.19 | 0.56 |
| 3:B:31:ASP:O | 3:B:32:PRO:C | 2.44 | 0.56 |
| 3:B:319:PHE:HA | 3:B:375:ALA:HA | 1.86 | 0.56 |
| 2:A:409:VAL:C | 2:A:411:GLU:H | 2.09 | 0.56 |
| 3:B:50:ASN:O | 3:B:64:ARG:NH2 | 2.38 | 0.56 |
| 2:A:216:ASN:O | 2:A:217:LEU:HB2 | 2.05 | 0.56 |
| 2:A:264:ARG:HB2 | 2:A:266:HIS:HD2 | 1.67 | 0.56 |
| 2:A:331:ALA:O | 2:A:334:THR:HG22 | 2.05 | 0.56 |
| 3:B:274:PRO:CG | 3:B:371:LEU:HD21 | 2.34 | 0.56 |
| 2:A:209:ILE:HG22 | 2:A:227:LEU:HD22 | 1.88 | 0.56 |
| 1:N:268:THR:H | 3:B:434:GLN:HB2 | 1.63 | 0.56 |
| 3:B:312:TYR:O | 3:B:344:VAL:HB | 2.05 | 0.56 |
| 3:B:70:LEU:CD1 | 3:B:145:THR:HG23 | 2.35 | 0.56 |
| 1:N:312:ARG:HH21 | 2:A:417:GLU:CA | 2.11 | 0.56 |
| 3:B:139:HIS:HE1 | 3:B:168:THR:HG23 | 1.71 | 0.56 |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:CG2 | 2.36 | 0.56 |
| 3:B:422:GLU:O | 3:B:426:ASN:N | 2.37 | 0.56 |
| 3:B:4:ILE:HD13 | 3:B:136:GLN:NE2 | 2.18 | 0.56 |
| 2:A:242:LEU:C | 2:A:244:PHE:H | 2.09 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:324:SER:C | 3:B:326:LYS:N | 2.59 | 0.56 |
| 1:N:253:LEU:HA | 1:N:256:ILE:HB | 1.87 | 0.56 |
| 2:A:313:MET:O | 2:A:314:ALA:HB2 | 2.04 | 0.56 |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:ND2 | 2.20 | 0.56 |
| 3:B:151:THR:OG1 | 3:B:193:GLN:CB | 2.54 | 0.56 |
| 3:B:272:PHE:HB3 | 3:B:275:LEU:HD22 | 1.88 | 0.56 |
| 3:B:191:VAL:HA | 3:B:194:LEU:HD12 | 1.87 | 0.55 |
| 3:B:311:ARG:HD2 | 3:B:344:VAL:H | 1.71 | 0.55 |
| 2:A:388:TRP:HA | 2:A:388:TRP:CE3 | 2.41 | 0.55 |
| 3:B:165:ILE:HD13 | 3:B:165:ILE:H | 1.71 | 0.55 |
| 1:N:163:ALA:H | 1:N:165:ARG:CZ | 2.20 | 0.55 |
| 2:A:16:ILE:HD12 | 2:A:171:ILE:HD11 | 1.87 | 0.55 |
| 3:B:250:ALA:CA | 3:B:254:LYS:HE2 | 2.35 | 0.55 |
| 3:B:19:LYS:O | 3:B:23:VAL:HG23 | 2.06 | 0.55 |
| 1:N:158:HIS:HA | 1:N:192:ARG:HH21 | 1.71 | 0.55 |
| 3:B:190:SER:O | 3:B:194:LEU:HG | 2.06 | 0.55 |
| 3:B:311:ARG:HG2 | 3:B:311:ARG:HH11 | 1.71 | 0.55 |
| 2:A:253:THR:O | 2:A:256:GLN:HG2 | 2.06 | 0.55 |
| 3:B:223:THR:HG22 | 3:B:224:TYR:N | 2.21 | 0.55 |
| 2:A:382:THR:O | 2:A:382:THR:HG22 | 2.05 | 0.55 |
| 3:B:119:LEU:O | 3:B:123:ARG:HG3 | 2.06 | 0.55 |
| 3:B:147:SER:O | 3:B:151:THR:CB | 2.52 | 0.55 |
| 1:N:253:LEU:HA | 1:N:256:ILE:CD1 | 2.36 | 0.55 |
| 2:A:381:THR:OG1 | 2:A:383:ALA:HB3 | 2.07 | 0.55 |
| 2:A:231:ILE:HA | 2:A:234:ILE:CG2 | 2.36 | 0.55 |
| 2:A:6:SER:O | 2:A:65:ALA:HB1 | 2.07 | 0.55 |
| 3:B:166:MET:HB3 | 3:B:198:THR:OG1 | 2.06 | 0.55 |
| 1:N:29:VAL:HG11 | 1:N:301:GLN:HA | 1.88 | 0.55 |
| 3:B:5:VAL:HG22 | 3:B:135:PHE:CD2 | 2.42 | 0.55 |
| 3:B:253:ARG:O | 3:B:257:VAL:N | 2.33 | 0.55 |
| 3:B:310:GLY:CA | 3:B:436:GLN:HE21 | 2.19 | 0.55 |
| 2:A:408:TYR:CD1 | 2:A:418:PHE:HZ | 2.24 | 0.54 |
| 3:B:210:TYR:HD2 | 3:B:227:LEU:HD21 | 1.71 | 0.54 |
| 2:A:101:ASN:CG | 3:B:254:LYS:HD2 | 2.28 | 0.54 |
| 3:B:20:PHE:CE2 | 3:B:24:ILE:HD12 | 2.43 | 0.54 |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:CZ | 2.42 | 0.54 |
| 3:B:239:THR:O | 3:B:241:CYS:N | 2.41 | 0.54 |
| 2:A:98:ASP:CB | 2:A:105:ARG:HH21 | 2.14 | 0.54 |
| 2:A:9:VAL:CG1 | 2:A:139:HIS:HB3 | 2.38 | 0.54 |
| 3:B:44:LEU:O | 3:B:49:ILE:HG12 | 2.07 | 0.54 |
| 2:A:150:THR:O | 2:A:153:LEU:N | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:194:LEU:C | 3:B:196:GLU:H | 2.11 | 0.54 |
| 2:A:115:ILE:C | 2:A:115:ILE:HD13 | 2.28 | 0.54 |
| 2:A:17:GLY:O | 2:A:21:TRP:HB2 | 2.08 | 0.54 |
| 3:B:297:ASP:OD1 | 3:B:298:ALA:N | 2.39 | 0.54 |
| 3:B:325:MET:CE | 3:B:355:VAL:HG11 | 2.38 | 0.54 |
| 3:B:325:MET:O | 3:B:329:ASP:HB2 | 2.07 | 0.54 |
| 3:B:331:GLN:O | 3:B:335:VAL:HG23 | 2.08 | 0.54 |
| 2:A:5:ILE:CG2 | 2:A:6:SER:N | 2.70 | 0.54 |
| 3:B:204:ILE:HD13 | 3:B:231:VAL:HG13 | 1.89 | 0.54 |
| 3:B:239:THR:HG22 | 3:B:240:THR:N | 2.22 | 0.54 |
| 3:B:27:GLU:HG2 | 3:B:27:GLU:O | 2.08 | 0.54 |
| 1:N:84:LEU:HD21 | 1:N:253:LEU:HD23 | 1.88 | 0.54 |
| 2:A:173:PRO:HB2 | 2:A:391:LEU:CD1 | 2.38 | 0.54 |
| 3:B:322:ARG:HH11 | 3:B:322:ARG:HG3 | 1.73 | 0.54 |
| 3:B:323:MET:HG3 | 3:B:328:VAL:HG21 | 1.90 | 0.54 |
| 3:B:31:ASP:HB3 | 3:B:32:PRO:HD2 | 1.89 | 0.54 |
| 3:B:424:ASN:C | 3:B:424:ASN:ND2 | 2.62 | 0.53 |
| 1:N:264:ALA:HB2 | 1:N:324:HIS:HE1 | 1.73 | 0.53 |
| 2:A:150:THR:O | 2:A:151:SER:C | 2.47 | 0.53 |
| 2:A:163:LYS:O | 2:A:163:LYS:HG2 | 2.08 | 0.53 |
| 2:A:339:ARG:C | 2:A:341:ILE:H | 2.11 | 0.53 |
| 2:A:5:ILE:O | 2:A:135:PHE:HA | 2.09 | 0.53 |
| 3:B:259:MET:HG2 | 3:B:314:THR:CG2 | 2.38 | 0.53 |
| 3:B:259:MET:CG | 3:B:314:THR:HG21 | 2.36 | 0.53 |
| 3:B:427:ASP:OD1 | 3:B:428:LEU:N | 2.41 | 0.53 |
| 3:B:431:GLU:O | 3:B:434:GLN:CG | 2.56 | 0.53 |
| 3:B:67:LEU:HD23 | 3:B:67:LEU:N | 2.22 | 0.53 |
| 2:A:215:ARG:C | 2:A:216:ASN:HD22 | 2.12 | 0.53 |
| 3:B:36:TYR:CZ | 3:B:38:GLY:HA3 | 2.43 | 0.53 |
| 3:B:424:ASN:HD22 | 3:B:424:ASN:C | 2.09 | 0.53 |
| 3:B:21:TRP:CZ2 | 3:B:65:ALA:HB2 | 2.44 | 0.53 |
| 3:B:68:VAL:HG12 | 3:B:149:MET:CE | 2.38 | 0.53 |
| 3:B:229:HIS:ND1 | 3:B:229:HIS:C | 2.62 | 0.53 |
| 3:B:343:PHE:O | 3:B:344:VAL:O | 2.26 | 0.53 |
| 2:A:110:ILE:O | 2:A:112:LYS:N | 2.41 | 0.53 |
| 3:B:4:ILE:CG2 | 3:B:136:GLN:HG2 | 2.38 | 0.53 |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:N | 2.19 | 0.53 |
| 2:A:98:ASP:O | 2:A:110:ILE:HD13 | 2.08 | 0.53 |
| 2:A:248:LEU:HB3 | 2:A:355:ILE:H | 1.73 | 0.53 |
| 1:N:251:LEU:O | 1:N:255:SER:OG | 2.26 | 0.53 |
| 2:A:182:VAL:O | 2:A:184:PRO:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:243:ARG:CZ | 2:A:252:LEU:HG | 2.39 | 0.53 |
| 3:B:213:CYS:SG | 3:B:219:LEU:HD23 | 2.48 | 0.53 |
| 3:B:133:GLN:HE21 | 3:B:252:LEU:HB2 | 1.73 | 0.53 |
| 1:N:79:PHE:HD2 | 1:N:288:GLN:O | 1.92 | 0.53 |
| 2:A:121:ARG:O | 2:A:125:LEU:HB2 | 2.08 | 0.53 |
| 3:B:179:ASP:HB2 | 8:B:600:GDP:H3' | 1.90 | 0.53 |
| 3:B:226:ASP:O | 3:B:227:LEU:C | 2.46 | 0.53 |
| 2:A:324:VAL:O | 2:A:327:ASP:HB2 | 2.08 | 0.53 |
| 3:B:141:LEU:HA | 3:B:147:SER:HB3 | 1.91 | 0.53 |
| 3:B:345:GLU:C | 3:B:347:ILE:H | 2.12 | 0.53 |
| 2:A:196:GLU:C | 2:A:197:HIS:CD2 | 2.82 | 0.53 |
| 2:A:275:VAL:HG21 | 2:A:300:ASN:OD1 | 2.09 | 0.53 |
| 3:B:212:ILE:O | 3:B:216:THR:HB | 2.09 | 0.53 |
| 3:B:210:TYR:CD2 | 3:B:227:LEU:HD21 | 2.44 | 0.52 |
| 2:A:101:ASN:ND2 | 7:B:500:GTP:O3G | 2.42 | 0.52 |
| 2:A:264:ARG:C | 2:A:266:HIS:N | 2.60 | 0.52 |
| 1:N:265:ALA:HB2 | 2:A:401:LYS:CB | 2.39 | 0.52 |
| 2:A:173:PRO:HB2 | 2:A:391:LEU:HD11 | 1.91 | 0.52 |
| 1:N:319:ALA:CB | 2:A:402:ARG:HH22 | 2.22 | 0.52 |
| 3:B:198:THR:HG22 | 3:B:265:LEU:CD2 | 2.39 | 0.52 |
| 3:B:431:GLU:OE1 | 3:B:432:TYR:CA | 2.57 | 0.52 |
| 2:A:344:VAL:HG12 | 2:A:345:ASP:H | 1.74 | 0.52 |
| 2:A:408:TYR:O | 2:A:411:GLU:N | 2.39 | 0.52 |
| 3:B:5:VAL:O | 3:B:5:VAL:HG23 | 2.09 | 0.52 |
| 2:A:206:ASN:OD1 | 2:A:227:LEU:CD1 | 2.58 | 0.52 |
| 3:B:107:HIS:HD2 | 3:B:151:THR:HG22 | 1.72 | 0.52 |
| 3:B:70:LEU:HD12 | 3:B:145:THR:HG23 | 1.91 | 0.52 |
| 3:B:226:ASP:O | 3:B:229:HIS:N | 2.42 | 0.52 |
| 2:A:251:ASP:OD1 | 2:A:252:LEU:N | 2.43 | 0.52 |
| 2:A:362:VAL:HG13 | 2:A:368:LEU:CD1 | 2.38 | 0.52 |
| 3:B:264:ARG:HA | 3:B:264:ARG:HE | 1.75 | 0.52 |
| 3:B:200:GLU:N | 3:B:265:LEU:HD13 | 2.25 | 0.52 |
| 3:B:188:THR:HA | 3:B:425:MET:CE | 2.40 | 0.52 |
| 3:B:360:PRO:HB2 | 9:B:601:TA1:H281 | 1.91 | 0.52 |
| 2:A:231:ILE:CA | 2:A:234:ILE:HG22 | 2.38 | 0.52 |
| 3:B:107:HIS:CD2 | 3:B:151:THR:HG22 | 2.45 | 0.52 |
| 3:B:314:THR:CG2 | 3:B:315:VAL:N | 2.73 | 0.52 |
| 3:B:295:MET:SD | 3:B:375:ALA:O | 2.68 | 0.52 |
| 3:B:149:MET:HG2 | 3:B:149:MET:O | 2.10 | 0.52 |
| 3:B:149:MET:O | 3:B:153:LEU:HD22 | 2.10 | 0.52 |
| 3:B:8:GLN:OE1 | 3:B:14:ASN:ND2 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:23:LEU:HD23 | 2:A:236:SER:CB | 2.37 | 0.52 |
| 3:B:425:MET:O | 3:B:428:LEU:HB3 | 2.09 | 0.52 |
| 2:A:119:LEU:HD11 | 2:A:156:ARG:CD | 2.40 | 0.51 |
| 2:A:243:ARG:NH2 | 2:A:251:ASP:OD1 | 2.44 | 0.51 |
| 2:A:345:ASP:OD2 | 2:A:439:SER:HB3 | 2.10 | 0.51 |
| 3:B:251:ASP:O | 3:B:252:LEU:C | 2.49 | 0.51 |
| 1:N:262:SER:HG | 3:B:262:PHE:HD2 | 1.57 | 0.51 |
| 2:A:201:ALA:O | 2:A:267:PHE:HA | 2.10 | 0.51 |
| 2:A:234:ILE:HB | 2:A:302:MET:HE1 | 1.91 | 0.51 |
| 2:A:8:HIS:HB3 | 2:A:13:GLY:O | 2.09 | 0.51 |
| 1:N:84:LEU:CD2 | 1:N:253:LEU:CD2 | 2.83 | 0.51 |
| 2:A:4:CYS:HA | 2:A:134:GLY:O | 2.10 | 0.51 |
| 2:A:171:ILE:O | 2:A:171:ILE:HG22 | 2.10 | 0.51 |
| 2:A:191:THR:HG23 | 2:A:192:HIS:N | 2.25 | 0.51 |
| 2:A:9:VAL:HG21 | 2:A:149:PHE:CD1 | 2.46 | 0.51 |
| 1:N:143:GLU:HB3 | 1:N:152:LEU:HD11 | 1.92 | 0.51 |
| 2:A:231:ILE:HD13 | 2:A:231:ILE:N | 2.25 | 0.51 |
| 2:A:283:HIS:O | 2:A:284:GLU:C | 2.47 | 0.51 |
| 3:B:103:TRP:CE2 | 3:B:189:LEU:HB3 | 2.45 | 0.51 |
| 3:B:320:ARG:HA | 3:B:356:CYS:HB3 | 1.92 | 0.51 |
| 3:B:49:ILE:O | 3:B:50:ASN:C | 2.48 | 0.51 |
| 2:A:239:THR:O | 2:A:240:ALA:C | 2.48 | 0.51 |
| 1:N:252:GLY:O | 1:N:256:ILE:N | 2.42 | 0.51 |
| 2:A:172:TYR:OH | 2:A:387:ALA:O | 2.24 | 0.51 |
| 3:B:240:THR:HG23 | 3:B:241:CYS:H | 1.76 | 0.51 |
| 3:B:260:VAL:HG23 | 3:B:260:VAL:O | 2.10 | 0.51 |
| 2:A:244:PHE:C | 2:A:244:PHE:CD2 | 2.83 | 0.51 |
| 2:A:244:PHE:CD2 | 2:A:245:ASP:N | 2.76 | 0.51 |
| 2:A:24:TYR:CE2 | 2:A:240:ALA:HB2 | 2.45 | 0.51 |
| 3:B:277:SER:OG | 3:B:281:GLN:HB2 | 2.10 | 0.51 |
| 3:B:21:TRP:HZ2 | 3:B:65:ALA:HB2 | 1.76 | 0.51 |
| 1:N:86:TYR:CE2 | 1:N:310:THR:HG23 | 2.46 | 0.51 |
| 2:A:133:GLN:HB3 | 2:A:243:ARG:HH12 | 1.76 | 0.51 |
| 2:A:67:PHE:HE1 | 2:A:87:PHE:CE2 | 2.29 | 0.51 |
| 3:B:113:GLU:HG3 | 3:B:114:LEU:N | 2.26 | 0.51 |
| 1:N:247:VAL:O | 1:N:248:ASN:HB2 | 2.10 | 0.51 |
| 2:A:417:GLU:OE1 | 2:A:417:GLU:HA | 2.10 | 0.50 |
| 3:B:5:VAL:CG2 | 3:B:135:PHE:CD2 | 2.94 | 0.50 |
| 2:A:12:ALA:CB | 2:A:140:SER:OG | 2.59 | 0.50 |
| 2:A:119:LEU:HA | 2:A:122:ILE:HG12 | 1.93 | 0.50 |
| 2:A:261:PRO:HB2 | 2:A:262:TYR:CD1 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:413:MET:HG3 | 3:B:414:ASP:N | 2.22 | 0.50 |
| 2:A:310:GLY:HA3 | 2:A:383:ALA:N | 2.26 | 0.50 |
| 3:B:168:THR:O | 3:B:201:THR:HA | 2.12 | 0.50 |
| 3:B:323:MET:HG3 | 3:B:328:VAL:CG2 | 2.41 | 0.50 |
| 3:B:265:LEU:O | 3:B:266:HIS:O | 2.29 | 0.50 |
| 3:B:296:PHE:CZ | 3:B:315:VAL:HG11 | 2.46 | 0.50 |
| 3:B:3:GLU:HA | 3:B:51:VAL:HA | 1.93 | 0.50 |
| 2:A:16:ILE:HG23 | 2:A:17:GLY:N | 2.26 | 0.50 |
| 2:A:196:GLU:O | 2:A:197:HIS:CD2 | 2.65 | 0.50 |
| 3:B:156:LYS:CE | 3:B:156:LYS:HA | 2.38 | 0.50 |
| 2:A:132:LEU:CD2 | 2:A:164:LYS:HE3 | 2.42 | 0.50 |
| 2:A:140:SER:O | 2:A:142:GLY:N | 2.44 | 0.50 |
| 2:A:402:ARG:O | 2:A:403:ALA:O | 2.29 | 0.50 |
| 3:B:298:ALA:O | 3:B:299:LYS:C | 2.50 | 0.50 |
| 3:B:49:ILE:HG13 | 3:B:50:ASN:H | 1.76 | 0.50 |
| 2:A:147:SER:CB | 2:A:190:THR:OG1 | 2.52 | 0.50 |
| 2:A:5:ILE:O | 2:A:136:SER:N | 2.40 | 0.50 |
| 3:B:176:LYS:CE | 3:B:207:GLU:HG3 | 2.39 | 0.50 |
| 1:N:253:LEU:O | 1:N:256:ILE:CB | 2.59 | 0.50 |
| 2:A:115:ILE:HD11 | 2:A:119:LEU:HG | 1.92 | 0.49 |
| 2:A:115:ILE:CG2 | 2:A:116:ASP:N | 2.75 | 0.49 |
| 2:A:11:GLN:O | 2:A:14:VAL:HB | 2.12 | 0.49 |
| 2:A:238:ILE:O | 2:A:242:LEU:HB2 | 2.11 | 0.49 |
| 3:B:333:LEU:O | 3:B:336:GLN:N | 2.45 | 0.49 |
| 3:B:369:ARG:C | 3:B:369:ARG:HD2 | 2.32 | 0.49 |
| 1:N:272:TYR:CG | 1:N:282:GLN:HG3 | 2.47 | 0.49 |
| 1:N:72:VAL:O | 1:N:76:LEU:HD13 | 2.12 | 0.49 |
| 2:A:227:LEU:O | 2:A:231:ILE:HG12 | 2.12 | 0.49 |
| 3:B:24:ILE:HG22 | 3:B:25:SER:N | 2.27 | 0.49 |
| 3:B:262:PHE:O | 3:B:264:ARG:N | 2.45 | 0.49 |
| 3:B:336:GLN:HE22 | 3:B:349:ASN:ND2 | 2.10 | 0.49 |
| 1:N:9:VAL:HB | 1:N:321:ALA:HB1 | 1.94 | 0.49 |
| 2:A:305:CYS:O | 2:A:306:ASP:C | 2.49 | 0.49 |
| 3:B:8:GLN:HB3 | 3:B:14:ASN:HA | 1.94 | 0.49 |
| 3:B:387:LEU:HD23 | 3:B:388:PHE:CD2 | 2.47 | 0.49 |
| 3:B:69:ASP:HA | 3:B:145:THR:HG21 | 1.95 | 0.49 |
| 3:B:265:LEU:HD12 | 3:B:266:HIS:O | 2.12 | 0.49 |
| 1:N:84:LEU:CD2 | 1:N:253:LEU:HD23 | 2.42 | 0.49 |
| 2:A:133:GLN:CB | 2:A:243:ARG:HH12 | 2.24 | 0.49 |
| 3:B:209:LEU:O | 3:B:210:TYR:C | 2.48 | 0.49 |
| 3:B:4:ILE:HG22 | 3:B:5:VAL:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:414:GLU:OE1 | 2:A:414:GLU:N | 2.46 | 0.49 |
| 3:B:102:ASN:HB3 | 3:B:105:LYS:HB2 | 1.95 | 0.49 |
| 3:B:199:ASP:O | 3:B:200:GLU:HG3 | 2.13 | 0.49 |
| 3:B:345:GLU:O | 3:B:347:ILE:N | 2.45 | 0.49 |
| 3:B:383:ALA:C | 3:B:385:GLN:H | 2.15 | 0.49 |
| 1:N:19:ARG:HA | 1:N:19:ARG:NE | 2.27 | 0.49 |
| 1:N:5:LYS:HD2 | 1:N:264:ALA:HA | 1.93 | 0.49 |
| 2:A:149:PHE:HE1 | 2:A:153:LEU:HD22 | 1.77 | 0.49 |
| 2:A:234:ILE:CG1 | 2:A:270:ALA:HB1 | 2.38 | 0.49 |
| 3:B:4:ILE:HD12 | 3:B:239:THR:CG2 | 2.42 | 0.49 |
| 1:N:319:ALA:HB3 | 2:A:402:ARG:HH22 | 1.78 | 0.49 |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:CE2 | 2.48 | 0.49 |
| 2:A:163:LYS:C | 2:A:164:LYS:HG2 | 2.33 | 0.49 |
| 2:A:192:HIS:CD2 | 2:A:424:ASP:OD2 | 2.66 | 0.49 |
| 2:A:158:SER:OG | 2:A:197:HIS:HB3 | 2.13 | 0.49 |
| 2:A:392:ASP:O | 2:A:395:PHE:HB3 | 2.13 | 0.49 |
| 3:B:142:GLY:HA3 | 3:B:183:GLU:OE2 | 2.13 | 0.49 |
| 2:A:115:ILE:O | 2:A:116:ASP:C | 2.51 | 0.49 |
| 2:A:122:ILE:CD1 | 2:A:157:LEU:HD21 | 2.35 | 0.49 |
| 2:A:191:THR:CG2 | 2:A:192:HIS:N | 2.76 | 0.49 |
| 2:A:274:PRO:CB | 2:A:371:VAL:HG21 | 2.43 | 0.49 |
| 3:B:280:SER:O | 3:B:282:GLN:N | 2.45 | 0.49 |
| 3:B:296:PHE:HZ | 3:B:315:VAL:HG11 | 1.78 | 0.49 |
| 3:B:173:PRO:HB3 | 3:B:183:GLU:HG2 | 1.93 | 0.49 |
| 1:N:271:PRO:HB2 | 3:B:263:PRO:HG3 | 1.88 | 0.49 |
| 3:B:175:PRO:CD | 3:B:207:GLU:OE1 | 2.61 | 0.48 |
| 1:N:63:MET:HE3 | 1:N:67:LEU:HD23 | 1.94 | 0.48 |
| 2:A:99:ALA:O | 2:A:100:ALA:HB3 | 2.14 | 0.48 |
| 2:A:9:VAL:HG11 | 2:A:150:THR:OG1 | 2.13 | 0.48 |
| 2:A:155:GLU:OE1 | 2:A:197:HIS:HE1 | 1.96 | 0.48 |
| 3:B:133:GLN:NE2 | 3:B:252:LEU:HB2 | 2.27 | 0.48 |
| 3:B:211:ASP:OD1 | 3:B:212:ILE:HG13 | 2.13 | 0.48 |
| 3:B:2:ARG:NH1 | 3:B:251:ASP:OD2 | 2.46 | 0.48 |
| 3:B:431:GLU:OE1 | 3:B:432:TYR:N | 2.46 | 0.48 |
| 2:A:188:ILE:O | 2:A:191:THR:HG22 | 2.13 | 0.48 |
| 2:A:283:HIS:O | 2:A:285:GLN:N | 2.45 | 0.48 |
| 2:A:151:SER:OG | 2:A:193:THR:HG21 | 2.13 | 0.48 |
| 3:B:173:PRO:HB3 | 3:B:183:GLU:CG | 2.42 | 0.48 |
| 3:B:49:ILE:HG13 | 3:B:50:ASN:N | 2.28 | 0.48 |
| 2:A:104:ALA:CB | 2:A:408:TYR:HD2 | 2.26 | 0.48 |
| 2:A:231:ILE:O | 2:A:235:VAL:HG23 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:20:PHE:CG | 3:B:235:MET:SD | 3.07 | 0.48 |
| 3:B:399:PHE:O | 3:B:400:ARG:C | 2.52 | 0.48 |
| 1:N:231:GLU:O | 1:N:249:ILE:CD1 | 2.61 | 0.48 |
| 1:N:251:LEU:O | 1:N:255:SER:N | 2.30 | 0.48 |
| 2:A:105:ARG:HG3 | 2:A:105:ARG:HH11 | 1.78 | 0.48 |
| 2:A:242:LEU:C | 2:A:244:PHE:N | 2.66 | 0.48 |
| 2:A:369:ALA:O | 2:A:370:LYS:CB | 2.62 | 0.48 |
| 3:B:103:TRP:HZ3 | 3:B:108:TYR:CE1 | 2.27 | 0.48 |
| 3:B:209:LEU:CD2 | 3:B:227:LEU:HD13 | 2.44 | 0.48 |
| 3:B:307:PRO:HB3 | 3:B:312:TYR:CZ | 2.49 | 0.48 |
| 2:A:253:THR:O | 2:A:254:GLU:C | 2.52 | 0.48 |
| 2:A:97:GLU:HB2 | 2:A:110:ILE:HD11 | 1.96 | 0.48 |
| 2:A:151:SER:HB3 | 2:A:193:THR:CG2 | 2.34 | 0.48 |
| 2:A:204:VAL:CG1 | 2:A:209:ILE:HD11 | 2.42 | 0.48 |
| 1:N:265:ALA:CB | 2:A:401:LYS:CD | 2.91 | 0.48 |
| 2:A:5:ILE:HG22 | 2:A:6:SER:H | 1.78 | 0.48 |
| 3:B:154:ILE:HG22 | 3:B:166:MET:CE | 2.44 | 0.48 |
| 3:B:176:LYS:HG3 | 3:B:177:VAL:H | 1.78 | 0.48 |
| 3:B:237:GLY:O | 3:B:241:CYS:CB | 2.61 | 0.48 |
| 3:B:269:MET:HB3 | 3:B:303:ALA:HB2 | 1.94 | 0.48 |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:HG21 | 1.95 | 0.48 |
| 3:B:175:PRO:O | 3:B:176:LYS:C | 2.52 | 0.48 |
| 3:B:209:LEU:O | 3:B:213:CYS:N | 2.47 | 0.48 |
| 3:B:308:ARG:HG3 | 3:B:342:TYR:OH | 2.13 | 0.48 |
| 2:A:132:LEU:HD21 | 2:A:164:LYS:HE3 | 1.96 | 0.48 |
| 2:A:203:MET:SD | 2:A:267:PHE:HB3 | 2.53 | 0.48 |
| 2:A:339:ARG:C | 2:A:341:ILE:N | 2.68 | 0.48 |
| 1:N:251:LEU:O | 1:N:255:SER:CB | 2.61 | 0.48 |
| 2:A:110:ILE:CG2 | 2:A:111:GLY:N | 2.71 | 0.47 |
| 2:A:107:HIS:CE1 | 2:A:152:LEU:HB3 | 2.49 | 0.47 |
| 3:B:191:VAL:HG13 | 3:B:192:HIS:N | 2.28 | 0.47 |
| 3:B:297:ASP:OD2 | 3:B:299:LYS:HE2 | 2.14 | 0.47 |
| 2:A:286:LEU:CD1 | 2:A:290:GLU:HG2 | 2.44 | 0.47 |
| 2:A:335:ILE:O | 2:A:337:THR:N | 2.47 | 0.47 |
| 2:A:34:GLY:C | 2:A:61:HIS:N | 2.68 | 0.47 |
| 2:A:317:LEU:CD1 | 2:A:351:PHE:CD2 | 2.97 | 0.47 |
| 3:B:198:THR:HG23 | 3:B:200:GLU:H | 1.79 | 0.47 |
| 1:N:102:PRO:HD3 | 1:N:184:LEU:HD12 | 1.96 | 0.47 |
| 1:N:231:GLU:O | 1:N:249:ILE:HD13 | 2.14 | 0.47 |
| 2:A:210:TYR:CE2 | 2:A:227:LEU:HD21 | 2.49 | 0.47 |
| 1:N:11:ILE:HB | 1:N:318:LYS:HZ1 | 1.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:148:GLY:O | 2:A:151:SER:CB | 2.61 | 0.47 |
| 2:A:155:GLU:HG2 | 2:A:197:HIS:CE1 | 2.49 | 0.47 |
| 2:A:175:PRO:HD2 | 2:A:207:GLU:HB3 | 1.97 | 0.47 |
| 2:A:19:ALA:HB2 | 2:A:228:ASN:HB3 | 1.96 | 0.47 |
| 2:A:345:ASP:C | 2:A:347:CYS:N | 2.68 | 0.47 |
| 2:A:386:GLU:O | 2:A:388:TRP:N | 2.47 | 0.47 |
| 1:N:254:LEU:HD21 | 2:A:409:VAL:CG1 | 2.03 | 0.47 |
| 3:B:243:ARG:HD3 | 3:B:243:ARG:N | 2.26 | 0.47 |
| 3:B:384:ILE:HG23 | 3:B:384:ILE:O | 2.14 | 0.47 |
| 1:N:267:HIS:O | 3:B:435:TYR:CD1 | 2.46 | 0.47 |
| 1:N:76:LEU:HD21 | 1:N:123:ARG:HB2 | 1.96 | 0.47 |
| 2:A:115:ILE:HG23 | 2:A:116:ASP:H | 1.79 | 0.47 |
| 2:A:154:MET:HA | 2:A:157:LEU:HD12 | 1.96 | 0.47 |
| 2:A:6:SER:OG | 2:A:65:ALA:HB2 | 2.14 | 0.47 |
| 3:B:185:TYR:HD2 | 3:B:395:PHE:CE1 | 2.33 | 0.47 |
| 2:A:230:LEU:O | 2:A:233:GLN:N | 2.35 | 0.47 |
| 2:A:217:LEU:CD1 | 2:A:277:SER:HA | 2.44 | 0.47 |
| 2:A:396:ASP:O | 2:A:397:LEU:C | 2.53 | 0.47 |
| 3:B:168:THR:CB | 3:B:201:THR:HG23 | 2.38 | 0.47 |
| 3:B:242:LEU:CD1 | 3:B:250:ALA:HB3 | 2.45 | 0.47 |
| 3:B:24:ILE:CD1 | 3:B:52:TYR:CE1 | 2.97 | 0.47 |
| 2:A:226:ASN:O | 2:A:229:ARG:N | 2.48 | 0.47 |
| 2:A:25:CYS:SG | 2:A:83:TYR:HE2 | 2.38 | 0.47 |
| 2:A:384:ILE:HG22 | 2:A:388:TRP:CD1 | 2.49 | 0.47 |
| 3:B:101:ASN:O | 3:B:101:ASN:ND2 | 2.47 | 0.47 |
| 3:B:115:VAL:CG2 | 3:B:152:LEU:HD23 | 2.44 | 0.47 |
| 1:N:252:GLY:O | 1:N:253:LEU:C | 2.52 | 0.47 |
| 2:A:256:GLN:HA | 2:A:260:VAL:HG13 | 1.97 | 0.47 |
| 2:A:96:LYS:O | 2:A:97:GLU:O | 2.31 | 0.47 |
| 3:B:134:GLY:HA3 | 3:B:165:ILE:HG12 | 1.97 | 0.47 |
| 1:N:267:HIS:C | 3:B:431:GLU:CG | 2.62 | 0.47 |
| 2:A:120:ASP:O | 2:A:124:LYS:HB2 | 2.15 | 0.47 |
| 2:A:191:THR:O | 2:A:195:LEU:HB2 | 2.15 | 0.47 |
| 3:B:264:ARG:HA | 3:B:264:ARG:NE | 2.29 | 0.47 |
| 3:B:287:THR:N | 3:B:290:GLU:OE1 | 2.48 | 0.47 |
| 1:N:165:ARG:H | 1:N:165:ARG:HD2 | 1.79 | 0.47 |
| 2:A:278:ALA:O | 2:A:279:GLU:HG2 | 2.15 | 0.47 |
| 2:A:147:SER:O | 2:A:190:THR:HG23 | 2.14 | 0.47 |
| 2:A:4:CYS:SG | 2:A:252:LEU:CD1 | 3.02 | 0.47 |
| 2:A:384:ILE:HG22 | 2:A:384:ILE:O | 2.15 | 0.47 |
| 3:B:387:LEU:O | 3:B:387:LEU:HG | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:185:TYR:OH | 2:A:399:TYR:HA | 2.15 | 0.46 |
| 3:B:242:LEU:HD11 | 3:B:250:ALA:HB3 | 1.97 | 0.46 |
| 2:A:114:ILE:O | 2:A:118:VAL:HG23 | 2.16 | 0.46 |
| 2:A:22:GLU:O | 2:A:23:LEU:C | 2.54 | 0.46 |
| 2:A:392:ASP:OD2 | 2:A:422:ARG:NE | 2.48 | 0.46 |
| 3:B:133:GLN:O | 3:B:165:ILE:CD1 | 2.64 | 0.46 |
| 3:B:226:ASP:O | 3:B:229:HIS:HB3 | 2.14 | 0.46 |
| 3:B:263:PRO:O | 3:B:264:ARG:C | 2.52 | 0.46 |
| 3:B:272:PHE:CE1 | 9:B:601:TA1:H391 | 2.50 | 0.46 |
| 3:B:237:GLY:HA3 | 3:B:376:THR:OG1 | 2.15 | 0.46 |
| 3:B:70:LEU:O | 3:B:99:ALA:HB2 | 2.15 | 0.46 |
| 2:A:11:GLN:O | 2:A:15:GLN:HG3 | 2.15 | 0.46 |
| 2:A:210:TYR:CZ | 2:A:227:LEU:HD11 | 2.51 | 0.46 |
| 2:A:407:TRP:O | 2:A:411:GLU:CG | 2.63 | 0.46 |
| 3:B:175:PRO:HD2 | 3:B:207:GLU:CD | 2.35 | 0.46 |
| 3:B:20:PHE:O | 3:B:24:ILE:HB | 2.14 | 0.46 |
| 1:N:271:PRO:CD | 3:B:263:PRO:HG2 | 2.44 | 0.46 |
| 2:A:117:LEU:HD12 | 2:A:121:ARG:HH12 | 1.80 | 0.46 |
| 2:A:243:ARG:NH2 | 2:A:252:LEU:CB | 2.78 | 0.46 |
| 3:B:307:PRO:C | 3:B:309:HIS:H | 2.18 | 0.46 |
| 1:N:253:LEU:HA | 1:N:256:ILE:CG1 | 2.45 | 0.46 |
| 2:A:224:TYR:CG | 3:B:325:MET:HG2 | 2.50 | 0.46 |
| 2:A:224:TYR:HD1 | 3:B:247:GLN:HB3 | 1.80 | 0.46 |
| 2:A:196:GLU:C | 2:A:197:HIS:HD2 | 2.19 | 0.46 |
| 2:A:260:VAL:O | 2:A:260:VAL:CG2 | 2.63 | 0.46 |
| 2:A:241:SER:HB3 | 2:A:320:ARG:NH2 | 2.29 | 0.46 |
| 2:A:278:ALA:HB2 | 2:A:369:ALA:CA | 2.45 | 0.46 |
| 3:B:243:ARG:HH21 | 3:B:252:LEU:N | 2.12 | 0.46 |
| 3:B:324:SER:OG | 3:B:326:LYS:HB3 | 2.16 | 0.46 |
| 9:B:601:TA1:C26 | 9:B:601:TA1:H463 | 2.46 | 0.46 |
| 2:A:145:THR:O | 2:A:149:PHE:HB3 | 2.15 | 0.46 |
| 2:A:179:THR:HG22 | 3:B:352:LYS:HZ2 | 1.80 | 0.46 |
| 2:A:23:LEU:CD2 | 2:A:232:GLY:O | 2.64 | 0.46 |
| 2:A:241:SER:C | 2:A:244:PHE:HB3 | 2.36 | 0.46 |
| 2:A:286:LEU:O | 2:A:287:SER:O | 2.34 | 0.46 |
| 2:A:324:VAL:HG12 | 2:A:326:LYS:H | 1.81 | 0.46 |
| 3:B:208:ALA:O | 3:B:212:ILE:HG13 | 2.16 | 0.46 |
| 2:A:155:GLU:HA | 2:A:197:HIS:CE1 | 2.49 | 0.46 |
| 2:A:265:GLY:O | 2:A:266:HIS:O | 2.33 | 0.46 |
| 2:A:203:MET:SD | 2:A:267:PHE:CB | 3.04 | 0.46 |
| 2:A:328:VAL:C | 2:A:330:ALA:H | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:381:THR:O | 2:A:383:ALA:N | 2.49 | 0.46 |
| 2:A:436:GLY:O | 2:A:438:ASP:N | 2.48 | 0.46 |
| 3:B:102:ASN:ND2 | 3:B:104:ALA:HB3 | 2.31 | 0.46 |
| 3:B:360:PRO:O | 3:B:369:ARG:C | 2.54 | 0.46 |
| 3:B:408:TYR:O | 3:B:411:GLU:HB2 | 2.16 | 0.46 |
| 1:N:273:ARG:HD3 | 3:B:196:GLU:HB3 | 1.59 | 0.46 |
| 2:A:317:LEU:CD1 | 2:A:351:PHE:CE2 | 2.99 | 0.46 |
| 2:A:11:GLN:CG | 2:A:74:VAL:HG11 | 2.28 | 0.46 |
| 2:A:95:GLY:C | 2:A:97:GLU:N | 2.69 | 0.46 |
| 3:B:103:TRP:CE3 | 3:B:189:LEU:HD13 | 2.50 | 0.46 |
| 3:B:196:GLU:O | 3:B:197:ASN:OD1 | 2.34 | 0.46 |
| 3:B:274:PRO:HG2 | 3:B:371:LEU:CD2 | 2.43 | 0.46 |
| 1:N:51:ASP:OD1 | 1:N:318:LYS:NZ | 2.49 | 0.46 |
| 2:A:10:GLY:O | 2:A:11:GLN:C | 2.53 | 0.46 |
| 2:A:9:VAL:HG21 | 2:A:149:PHE:HD1 | 1.80 | 0.46 |
| 2:A:204:VAL:HG21 | 2:A:231:ILE:HG23 | 1.97 | 0.46 |
| 2:A:286:LEU:HG | 2:A:290:GLU:HB2 | 1.97 | 0.46 |
| 2:A:316:CYS:HB3 | 2:A:378:LEU:HD12 | 1.95 | 0.46 |
| 2:A:423:GLU:O | 2:A:426:ALA:HB3 | 2.16 | 0.46 |
| 1:N:65:GLN:NE2 | 1:N:69:LEU:HD22 | 2.31 | 0.46 |
| 2:A:308:ARG:O | 2:A:309:HIS:HB3 | 2.16 | 0.45 |
| 2:A:99:ALA:H | 3:B:2:ARG:HH22 | 1.63 | 0.45 |
| 3:B:154:ILE:HD12 | 3:B:155:SER:N | 2.31 | 0.45 |
| 3:B:209:LEU:HD23 | 3:B:227:LEU:HD13 | 1.98 | 0.45 |
| 3:B:194:LEU:O | 3:B:265:LEU:HD23 | 2.16 | 0.45 |
| 3:B:288:VAL:N | 3:B:289:PRO:CD | 2.80 | 0.45 |
| 3:B:325:MET:HE2 | 3:B:355:VAL:CG2 | 2.46 | 0.45 |
| 3:B:323:MET:CE | 3:B:328:VAL:HG22 | 2.46 | 0.45 |
| 2:A:119:LEU:HD11 | 2:A:156:ARG:HD2 | 1.97 | 0.45 |
| 2:A:255:PHE:O | 2:A:256:GLN:C | 2.53 | 0.45 |
| 2:A:288:VAL:HA | 2:A:291:ILE:HG12 | 1.97 | 0.45 |
| 2:A:5:ILE:CG2 | 2:A:6:SER:H | 2.29 | 0.45 |
| 2:A:117:LEU:HD11 | 2:A:121:ARG:NH2 | 2.30 | 0.45 |
| 2:A:7:ILE:HG13 | 2:A:137:VAL:HG22 | 1.98 | 0.45 |
| 2:A:243:ARG:NH2 | 2:A:252:LEU:HB2 | 2.31 | 0.45 |
| 2:A:346:TRP:HZ2 | 2:A:435:VAL:HG12 | 1.81 | 0.45 |
| 3:B:113:GLU:CG | 3:B:114:LEU:N | 2.79 | 0.45 |
| 3:B:11:GLN:O | 3:B:14:ASN:HB3 | 2.16 | 0.45 |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:HG23 | 1.98 | 0.45 |
| 3:B:242:LEU:C | 3:B:244:PHE:H | 2.20 | 0.45 |
| 3:B:313:LEU:O | 3:B:347:ILE:HD12 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:180:ALA:HA | 3:B:352:LYS:NZ | 2.31 | 0.45 |
| 2:A:256:GLN:O | 2:A:260:VAL:HG13 | 2.15 | 0.45 |
| 2:A:344:VAL:CG1 | 2:A:345:ASP:N | 2.78 | 0.45 |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:HD21 | 1.98 | 0.45 |
| 3:B:188:THR:HA | 3:B:425:MET:HE3 | 1.97 | 0.45 |
| 3:B:210:TYR:CE2 | 3:B:227:LEU:HD11 | 2.52 | 0.45 |
| 1:N:269:VAL:HG13 | 3:B:264:ARG:CZ | 2.45 | 0.45 |
| 2:A:204:VAL:O | 2:A:204:VAL:HG12 | 2.17 | 0.45 |
| 2:A:212:ILE:HD11 | 2:A:302:MET:H | 1.82 | 0.45 |
| 2:A:404:PHE:CD1 | 2:A:404:PHE:N | 2.83 | 0.45 |
| 2:A:104:ALA:HB1 | 2:A:413:MET:HG3 | 1.96 | 0.45 |
| 2:A:434:GLU:C | 2:A:436:GLY:H | 2.18 | 0.45 |
| 2:A:7:ILE:HD11 | 2:A:137:VAL:CG2 | 2.44 | 0.45 |
| 3:B:6:HIS:HB3 | 3:B:21:TRP:HZ2 | 1.81 | 0.45 |
| 2:A:166:LYS:CE | 2:A:199:ASP:OD1 | 2.62 | 0.45 |
| 3:B:250:ALA:HB1 | 3:B:254:LYS:CB | 2.44 | 0.45 |
| 3:B:273:ALA:CB | 3:B:274:PRO:CD | 2.93 | 0.45 |
| 2:A:303:VAL:CG1 | 2:A:303:VAL:O | 2.65 | 0.45 |
| 2:A:271:THR:O | 2:A:376:CYS:HA | 2.17 | 0.45 |
| 3:B:324:SER:O | 3:B:326:LYS:N | 2.50 | 0.45 |
| 1:N:100:THR:HG21 | 1:N:105:ILE:HD11 | 1.98 | 0.45 |
| 2:A:392:ASP:OD2 | 2:A:422:ARG:CZ | 2.65 | 0.45 |
| 2:A:408:TYR:CG | 2:A:418:PHE:HZ | 2.34 | 0.45 |
| 3:B:194:LEU:C | 3:B:196:GLU:N | 2.70 | 0.45 |
| 3:B:167:ASN:HA | 3:B:200:GLU:O | 2.17 | 0.45 |
| 2:A:103:TYR:CD1 | 2:A:148:GLY:HA2 | 2.52 | 0.45 |
| 2:A:11:GLN:HE21 | 2:A:74:VAL:CG2 | 2.29 | 0.45 |
| 2:A:132:LEU:CD2 | 2:A:132:LEU:H | 2.23 | 0.45 |
| 2:A:148:GLY:O | 2:A:149:PHE:C | 2.54 | 0.45 |
| 2:A:182:VAL:O | 2:A:184:PRO:CD | 2.65 | 0.45 |
| 2:A:291:ILE:HD12 | 2:A:375:VAL:HG23 | 1.99 | 0.45 |
| 2:A:11:GLN:NE2 | 2:A:74:VAL:HG22 | 2.30 | 0.45 |
| 3:B:23:VAL:O | 3:B:25:SER:N | 2.50 | 0.45 |
| 3:B:72:PRO:O | 3:B:74:THR:N | 2.50 | 0.45 |
| 2:A:210:TYR:CD2 | 2:A:227:LEU:HD21 | 2.51 | 0.45 |
| 3:B:135:PHE:CD1 | 3:B:135:PHE:N | 2.84 | 0.45 |
| 3:B:224:TYR:O | 3:B:225:GLY:C | 2.53 | 0.45 |
| 3:B:307:PRO:C | 3:B:309:HIS:N | 2.71 | 0.45 |
| 3:B:360:PRO:HG2 | 3:B:371:LEU:CB | 2.38 | 0.45 |
| 3:B:82:PRO:C | 3:B:84:GLY:H | 2.20 | 0.45 |
| 2:A:172:TYR:CD1 | 2:A:173:PRO:N | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:229:ARG:HG2 | 2:A:229:ARG:NH1 | 2.31 | 0.44 |
| 2:A:286:LEU:O | 2:A:287:SER:C | 2.55 | 0.44 |
| 2:A:288:VAL:C | 2:A:290:GLU:N | 2.71 | 0.44 |
| 3:B:67:LEU:HD12 | 3:B:92:PHE:CD2 | 2.51 | 0.44 |
| 1:N:256:ILE:O | 1:N:260:VAL:HG23 | 2.17 | 0.44 |
| 2:A:152:LEU:HD12 | 2:A:152:LEU:C | 2.38 | 0.44 |
| 2:A:276:ILE:HG12 | 2:A:277:SER:N | 2.32 | 0.44 |
| 2:A:274:PRO:HB2 | 2:A:371:VAL:HG21 | 1.98 | 0.44 |
| 3:B:141:LEU:N | 3:B:141:LEU:HD12 | 2.33 | 0.44 |
| 3:B:106:GLY:O | 3:B:149:MET:HB2 | 2.16 | 0.44 |
| 3:B:24:ILE:CG2 | 3:B:25:SER:N | 2.80 | 0.44 |
| 2:A:180:ALA:HA | 3:B:352:LYS:HZ3 | 1.82 | 0.44 |
| 3:B:67:LEU:HD12 | 3:B:92:PHE:CE2 | 2.52 | 0.44 |
| 1:N:69:LEU:HB3 | 1:N:70:PRO:HD3 | 1.99 | 0.44 |
| 2:A:209:ILE:CD1 | 2:A:231:ILE:HD11 | 2.47 | 0.44 |
| 2:A:334:THR:CG2 | 2:A:335:ILE:N | 2.79 | 0.44 |
| 2:A:343:PHE:CE1 | 2:A:351:PHE:HE1 | 2.36 | 0.44 |
| 3:B:102:ASN:OD1 | 3:B:408:TYR:CZ | 2.70 | 0.44 |
| 3:B:4:ILE:HD12 | 3:B:239:THR:HG21 | 1.98 | 0.44 |
| 3:B:288:VAL:N | 3:B:289:PRO:HD2 | 2.32 | 0.44 |
| 3:B:230:LEU:HD21 | 3:B:302:MET:HE2 | 1.98 | 0.44 |
| 3:B:312:TYR:HA | 3:B:381:SER:HA | 1.99 | 0.44 |
| 1:N:269:VAL:CG2 | 3:B:428:LEU:HD12 | 2.47 | 0.44 |
| 3:B:94:PHE:CD2 | 3:B:94:PHE:N | 2.84 | 0.44 |
| 2:A:12:ALA:HB2 | 7:B:500:GTP:C8 | 2.52 | 0.44 |
| 3:B:189:LEU:HD23 | 3:B:421:ALA:CB | 2.48 | 0.44 |
| 2:A:153:LEU:O | 2:A:157:LEU:HG | 2.18 | 0.44 |
| 2:A:362:VAL:HG13 | 2:A:368:LEU:CG | 2.48 | 0.44 |
| 2:A:295:CYS:HB3 | 2:A:377:MET:HG2 | 1.99 | 0.44 |
| 2:A:72:PRO:HG2 | 2:A:73:THR:H | 1.83 | 0.44 |
| 3:B:239:THR:O | 3:B:240:THR:C | 2.56 | 0.44 |
| 2:A:144:GLY:H | 7:B:500:GTP:PG | 2.41 | 0.44 |
| 2:A:413:MET:C | 2:A:414:GLU:HG3 | 2.36 | 0.44 |
| 3:B:175:PRO:HG2 | 3:B:207:GLU:OE1 | 2.16 | 0.44 |
| 3:B:287:THR:O | 3:B:288:VAL:CG2 | 2.58 | 0.44 |
| 3:B:409:THR:HA | 3:B:413:MET:HB3 | 1.99 | 0.44 |
| 3:B:8:GLN:CG | 3:B:67:LEU:HD22 | 2.47 | 0.44 |
| 1:N:249:ILE:CG1 | 1:N:250:ASN:N | 2.80 | 0.44 |
| 2:A:121:ARG:HG2 | 2:A:121:ARG:HH11 | 1.83 | 0.44 |
| 2:A:272:TYR:CE2 | 2:A:274:PRO:HD2 | 2.53 | 0.44 |
| 2:A:278:ALA:CA | 2:A:282:TYR:OH | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:114:LEU:HD23 | 3:B:149:MET:HE3 | 2.00 | 0.44 |
| 3:B:12:CYS:C | 3:B:14:ASN:N | 2.71 | 0.44 |
| 3:B:295:MET:SD | 3:B:375:ALA:HB3 | 2.57 | 0.44 |
| 1:N:251:LEU:CA | 1:N:254:LEU:HB2 | 2.48 | 0.44 |
| 2:A:218:ASP:C | 2:A:219:ILE:HG12 | 2.37 | 0.44 |
| 2:A:377:MET:O | 2:A:377:MET:HG3 | 2.18 | 0.44 |
| 2:A:388:TRP:HA | 2:A:388:TRP:HE3 | 1.79 | 0.44 |
| 3:B:7:ILE:N | 3:B:136:GLN:O | 2.51 | 0.44 |
| 3:B:168:THR:CG2 | 3:B:201:THR:HG23 | 2.48 | 0.44 |
| 3:B:14:ASN:O | 3:B:17:GLY:N | 2.50 | 0.44 |
| 3:B:182:VAL:O | 3:B:183:GLU:C | 2.56 | 0.44 |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:O | 2.17 | 0.44 |
| 2:A:121:ARG:NH1 | 2:A:121:ARG:HG2 | 2.33 | 0.44 |
| 2:A:132:LEU:N | 2:A:132:LEU:HD23 | 2.26 | 0.44 |
| 2:A:115:ILE:CG1 | 2:A:152:LEU:HD13 | 2.46 | 0.44 |
| 2:A:231:ILE:H | 2:A:231:ILE:HD13 | 1.82 | 0.44 |
| 2:A:23:LEU:O | 2:A:26:LEU:HB3 | 2.17 | 0.44 |
| 1:N:312:ARG:HH21 | 2:A:417:GLU:N | 2.10 | 0.44 |
| 3:B:161:TYR:N | 3:B:161:TYR:CD1 | 2.86 | 0.44 |
| 3:B:161:TYR:O | 3:B:163:ASP:N | 2.51 | 0.44 |
| 3:B:52:TYR:HE1 | 3:B:240:THR:HB | 1.82 | 0.44 |
| 3:B:72:PRO:HG2 | 3:B:73:GLY:H | 1.83 | 0.44 |
| 2:A:224:TYR:HD2 | 2:A:224:TYR:HA | 1.73 | 0.43 |
| 2:A:268:PRO:CA | 2:A:379:SER:O | 2.65 | 0.43 |
| 2:A:283:HIS:ND1 | 2:A:283:HIS:O | 2.49 | 0.43 |
| 2:A:287:SER:N | 2:A:290:GLU:OE1 | 2.51 | 0.43 |
| 2:A:63:PRO:HG2 | 2:A:91:GLN:OE1 | 2.17 | 0.43 |
| 3:B:26:ASP:C | 3:B:28:HIS:H | 2.21 | 0.43 |
| 2:A:262:TYR:HB3 | 2:A:263:PRO:HD2 | 2.00 | 0.43 |
| 3:B:167:ASN:HD21 | 3:B:252:LEU:HD22 | 1.82 | 0.43 |
| 1:N:125:THR:O | 1:N:128:GLN:HG2 | 2.17 | 0.43 |
| 2:A:252:LEU:O | 2:A:253:THR:C | 2.56 | 0.43 |
| 2:A:175:PRO:CG | 2:A:304:LYS:HG2 | 2.47 | 0.43 |
| 2:A:363:VAL:CG1 | 2:A:364:PRO:HD2 | 2.48 | 0.43 |
| 1:N:258:LYS:HD2 | 2:A:406:HIS:HA | 1.74 | 0.43 |
| 3:B:409:THR:C | 3:B:411:GLU:H | 2.22 | 0.43 |
| 1:N:139:ALA:HA | 1:N:210:THR:O | 2.18 | 0.43 |
| 1:N:250:ASN:O | 1:N:251:LEU:HB2 | 2.19 | 0.43 |
| 1:N:322:LEU:O | 1:N:323:GLU:HB2 | 2.19 | 0.43 |
| 2:A:184:PRO:HG2 | 2:A:398:MET:CE | 2.41 | 0.43 |
| 3:B:161:TYR:C | 3:B:163:ASP:N | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:103:TYR:O | 2:A:104:ALA:C | 2.57 | 0.43 |
| 2:A:172:TYR:HA | 2:A:173:PRO:HD3 | 1.92 | 0.43 |
| 2:A:179:THR:HG22 | 3:B:352:LYS:HZ1 | 1.80 | 0.43 |
| 2:A:310:GLY:HA3 | 2:A:383:ALA:CA | 2.49 | 0.43 |
| 3:B:212:ILE:O | 3:B:212:ILE:HG22 | 2.18 | 0.43 |
| 3:B:229:HIS:HE2 | 9:B:601:TA1:H361 | 1.83 | 0.43 |
| 2:A:21:TRP:HE1 | 2:A:63:PRO:HB3 | 1.83 | 0.43 |
| 2:A:63:PRO:C | 2:A:64:ARG:CG | 2.83 | 0.43 |
| 3:B:68:VAL:HG11 | 3:B:153:LEU:HD21 | 2.00 | 0.43 |
| 2:A:13:GLY:C | 2:A:16:ILE:HG22 | 2.38 | 0.43 |
| 2:A:207:GLU:O | 2:A:210:TYR:N | 2.51 | 0.43 |
| 3:B:301:MET:O | 3:B:303:ALA:N | 2.51 | 0.43 |
| 3:B:435:TYR:C | 3:B:437:ASP:N | 2.72 | 0.43 |
| 3:B:168:THR:N | 3:B:200:GLU:O | 2.43 | 0.43 |
| 3:B:359:PRO:CB | 3:B:360:PRO:HD2 | 2.45 | 0.43 |
| 3:B:383:ALA:C | 3:B:385:GLN:N | 2.72 | 0.43 |
| 3:B:105:LYS:HG2 | 3:B:110:GLU:CG | 2.48 | 0.43 |
| 3:B:118:VAL:O | 3:B:122:VAL:HG13 | 2.19 | 0.43 |
| 3:B:108:TYR:CE1 | 3:B:413:MET:HE1 | 2.53 | 0.43 |
| 2:A:147:SER:HB2 | 2:A:186:ASN:O | 2.19 | 0.43 |
| 2:A:154:MET:CE | 2:A:166:LYS:HB3 | 2.48 | 0.43 |
| 2:A:209:ILE:CD1 | 2:A:231:ILE:CD1 | 2.97 | 0.43 |
| 2:A:238:ILE:O | 2:A:242:LEU:CB | 2.67 | 0.43 |
| 2:A:238:ILE:HD11 | 2:A:378:LEU:HD23 | 2.01 | 0.43 |
| 1:N:172:LEU:HA | 1:N:173:PRO:HD3 | 1.92 | 0.43 |
| 2:A:343:PHE:HZ | 2:A:351:PHE:CZ | 2.36 | 0.42 |
| 3:B:103:TRP:HB2 | 3:B:186:ASN:HA | 2.01 | 0.42 |
| 3:B:210:TYR:O | 3:B:214:PHE:N | 2.52 | 0.42 |
| 3:B:72:PRO:O | 3:B:73:GLY:C | 2.58 | 0.42 |
| 2:A:8:HIS:HA | 2:A:138:PHE:HB2 | 2.00 | 0.42 |
| 2:A:409:VAL:C | 2:A:411:GLU:N | 2.71 | 0.42 |
| 3:B:192:HIS:NE2 | 3:B:420:GLU:HG2 | 2.34 | 0.42 |
| 3:B:240:THR:HG23 | 3:B:241:CYS:N | 2.33 | 0.42 |
| 3:B:70:LEU:HB2 | 3:B:99:ALA:CB | 2.48 | 0.42 |
| 2:A:16:ILE:CG2 | 2:A:17:GLY:N | 2.82 | 0.42 |
| 2:A:436:GLY:C | 2:A:438:ASP:N | 2.72 | 0.42 |
| 3:B:288:VAL:C | 3:B:290:GLU:N | 2.70 | 0.42 |
| 3:B:399:PHE:O | 3:B:402:LYS:N | 2.29 | 0.42 |
| 1:N:73:ASP:O | 1:N:77:GLU:HG3 | 2.19 | 0.42 |
| 2:A:231:ILE:C | 2:A:233:GLN:N | 2.73 | 0.42 |
| 2:A:76:ASP:O | 2:A:79:ARG:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:204:ILE:HD13 | 3:B:231:VAL:CG2 | 2.45 | 0.42 |
| 3:B:48:ARG:HG2 | 3:B:243:ARG:HB3 | 2.01 | 0.42 |
| 1:N:268:THR:HG23 | 3:B:433:GLN:H | 1.75 | 0.42 |
| 1:N:103:GLY:H | 1:N:181:HIS:CD2 | 2.21 | 0.42 |
| 1:N:33:PRO:HA | 1:N:34:PRO:HD3 | 1.91 | 0.42 |
| 2:A:304:LYS:HG3 | 2:A:304:LYS:O | 2.19 | 0.42 |
| 2:A:363:VAL:HG13 | 2:A:364:PRO:HD2 | 2.02 | 0.42 |
| 2:A:8:HIS:CD2 | 2:A:138:PHE:CD1 | 3.07 | 0.42 |
| 3:B:243:ARG:HD3 | 3:B:243:ARG:HA | 1.62 | 0.42 |
| 3:B:333:LEU:O | 3:B:334:ASN:C | 2.58 | 0.42 |
| 2:A:105:ARG:O | 2:A:110:ILE:CG2 | 2.64 | 0.42 |
| 2:A:378:LEU:O | 2:A:378:LEU:HD12 | 2.19 | 0.42 |
| 2:A:390:ARG:HG3 | 2:A:390:ARG:HH11 | 1.83 | 0.42 |
| 3:B:153:LEU:HD13 | 3:B:153:LEU:N | 2.34 | 0.42 |
| 3:B:242:LEU:HB3 | 3:B:250:ALA:O | 2.20 | 0.42 |
| 3:B:299:LYS:CD | 3:B:299:LYS:H | 2.07 | 0.42 |
| 2:A:210:TYR:OH | 3:B:325:MET:HB3 | 2.20 | 0.42 |
| 3:B:343:PHE:CD2 | 3:B:350:ASN:ND2 | 2.88 | 0.42 |
| 2:A:101:ASN:ND2 | 3:B:254:LYS:CD | 2.75 | 0.42 |
| 2:A:13:GLY:HA2 | 2:A:16:ILE:CG2 | 2.50 | 0.42 |
| 2:A:213:CYS:O | 2:A:219:ILE:HG13 | 2.20 | 0.42 |
| 2:A:25:CYS:SG | 2:A:26:LEU:N | 2.92 | 0.42 |
| 3:B:250:ALA:CB | 3:B:254:LYS:HE2 | 2.50 | 0.42 |
| 2:A:15:GLN:NE2 | 7:B:500:GTP:N7 | 2.67 | 0.42 |
| 2:A:119:LEU:HD11 | 2:A:156:ARG:HD3 | 2.01 | 0.42 |
| 2:A:95:GLY:C | 2:A:97:GLU:H | 2.23 | 0.42 |
| 3:B:106:GLY:O | 3:B:149:MET:CA | 2.68 | 0.42 |
| 3:B:2:ARG:NH1 | 3:B:251:ASP:CG | 2.73 | 0.42 |
| 1:N:321:ALA:O | 1:N:324:HIS:HB2 | 2.19 | 0.42 |
| 2:A:149:PHE:O | 2:A:150:THR:C | 2.56 | 0.42 |
| 2:A:175:PRO:HG3 | 2:A:304:LYS:CB | 2.50 | 0.42 |
| 2:A:328:VAL:C | 2:A:330:ALA:N | 2.73 | 0.42 |
| 3:B:138:THR:O | 3:B:139:HIS:HB3 | 2.19 | 0.42 |
| 3:B:171:VAL:O | 3:B:171:VAL:HG12 | 2.20 | 0.42 |
| 3:B:25:SER:O | 3:B:28:HIS:N | 2.53 | 0.42 |
| 3:B:6:HIS:HB3 | 3:B:65:ALA:CB | 2.48 | 0.42 |
| 2:A:242:LEU:HD11 | 2:A:250:VAL:HG23 | 2.02 | 0.42 |
| 2:A:305:CYS:SG | 2:A:383:ALA:HB1 | 2.60 | 0.42 |
| 2:A:402:ARG:O | 2:A:405:VAL:N | 2.49 | 0.42 |
| 3:B:187:ALA:O | 3:B:188:THR:C | 2.57 | 0.42 |
| 3:B:422:GLU:O | 3:B:426:ASN:CB | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:35:SER:CB | 3:B:59:ASN:HA | 2.42 | 0.42 |
| 1:N:6:LEU:HD23 | 1:N:286:THR:O | 2.20 | 0.42 |
| 2:A:255:PHE:O | 2:A:257:THR:N | 2.53 | 0.41 |
| 2:A:104:ALA:HB3 | 2:A:408:TYR:HD2 | 1.84 | 0.41 |
| 3:B:199:ASP:C | 3:B:265:LEU:HD13 | 2.40 | 0.41 |
| 3:B:202:TYR:CE2 | 3:B:268:PHE:HD1 | 2.38 | 0.41 |
| 3:B:210:TYR:O | 3:B:211:ASP:C | 2.57 | 0.41 |
| 3:B:301:MET:HE1 | 3:B:377:PHE:HE2 | 1.84 | 0.41 |
| 3:B:82:PRO:HB2 | 3:B:83:PHE:H | 1.56 | 0.41 |
| 1:N:269:VAL:HG13 | 3:B:264:ARG:NH1 | 2.35 | 0.41 |
| 2:A:115:ILE:C | 2:A:115:ILE:CD1 | 2.87 | 0.41 |
| 2:A:67:PHE:HB2 | 2:A:92:LEU:HD23 | 2.02 | 0.41 |
| 2:A:76:ASP:O | 2:A:80:THR:N | 2.53 | 0.41 |
| 3:B:276:THR:O | 9:B:601:TA1:H192 | 2.20 | 0.41 |
| 3:B:175:PRO:O | 3:B:177:VAL:N | 2.53 | 0.41 |
| 3:B:273:ALA:HB1 | 3:B:291:LEU:HG | 2.01 | 0.41 |
| 3:B:310:GLY:HA3 | 3:B:436:GLN:NE2 | 2.29 | 0.41 |
| 3:B:274:PRO:HD3 | 3:B:374:SER:HA | 2.03 | 0.41 |
| 3:B:399:PHE:O | 3:B:401:ARG:N | 2.53 | 0.41 |
| 1:N:61:ASP:O | 1:N:65:GLN:HG2 | 2.20 | 0.41 |
| 2:A:152:LEU:CD1 | 2:A:152:LEU:C | 2.89 | 0.41 |
| 2:A:23:LEU:HD11 | 2:A:361:THR:O | 2.21 | 0.41 |
| 3:B:261:PRO:HB2 | 3:B:262:PHE:CD1 | 2.54 | 0.41 |
| 3:B:333:LEU:HD11 | 3:B:337:ASN:HD21 | 1.85 | 0.41 |
| 1:N:180:LEU:O | 1:N:183:ILE:HG13 | 2.20 | 0.41 |
| 3:B:119:LEU:O | 3:B:122:VAL:HG22 | 2.21 | 0.41 |
| 3:B:135:PHE:CD1 | 3:B:166:MET:SD | 3.14 | 0.41 |
| 3:B:239:THR:CG2 | 3:B:240:THR:N | 2.80 | 0.41 |
| 3:B:380:ASN:C | 3:B:380:ASN:HD22 | 2.24 | 0.41 |
| 3:B:269:MET:HE1 | 3:B:381:SER:OG | 2.20 | 0.41 |
| 3:B:427:ASP:OD1 | 3:B:427:ASP:C | 2.58 | 0.41 |
| 1:N:268:THR:CG2 | 3:B:429:VAL:O | 2.68 | 0.41 |
| 1:N:103:GLY:N | 1:N:181:HIS:HD2 | 2.08 | 0.41 |
| 2:A:115:ILE:CG2 | 2:A:116:ASP:H | 2.32 | 0.41 |
| 2:A:243:ARG:NH2 | 2:A:252:LEU:HG | 2.35 | 0.41 |
| 2:A:255:PHE:O | 2:A:259:LEU:N | 2.50 | 0.41 |
| 2:A:67:PHE:CE1 | 2:A:87:PHE:CE2 | 3.08 | 0.41 |
| 3:B:168:THR:HB | 3:B:198:THR:HG21 | 2.03 | 0.41 |
| 2:A:166:LYS:HB2 | 2:A:199:ASP:OD1 | 2.20 | 0.41 |
| 2:A:282:TYR:HD2 | 2:A:284:GLU:HG3 | 1.86 | 0.41 |
| 3:B:182:VAL:O | 3:B:184:PRO:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:409:THR:C | 3:B:411:GLU:N | 2.73 | 0.41 |
| 1:N:165:ARG:HD2 | 1:N:165:ARG:N | 2.36 | 0.41 |
| 2:A:149:PHE:CD1 | 2:A:150:THR:N | 2.89 | 0.41 |
| 2:A:414:GLU:C | 2:A:416:GLY:N | 2.74 | 0.41 |
| 3:B:132:LEU:O | 3:B:164:ARG:HD2 | 2.21 | 0.41 |
| 2:A:101:ASN:HD21 | 3:B:254:LYS:NZ | 2.18 | 0.41 |
| 3:B:259:MET:HE3 | 3:B:268:PHE:CE1 | 2.56 | 0.41 |
| 3:B:417:GLU:O | 3:B:420:GLU:HB3 | 2.21 | 0.41 |
| 1:N:249:ILE:HG12 | 1:N:250:ASN:N | 2.36 | 0.41 |
| 2:A:226:ASN:O | 2:A:227:LEU:C | 2.59 | 0.41 |
| 2:A:288:VAL:O | 2:A:289:ALA:C | 2.59 | 0.41 |
| 3:B:98:GLY:C | 3:B:100:GLY:H | 2.25 | 0.41 |
| 3:B:147:SER:CB | 3:B:190:SER:HB3 | 2.42 | 0.41 |
| 1:N:145:TYR:CD2 | 1:N:192:ARG:HD2 | 2.56 | 0.41 |
| 2:A:100:ALA:O | 2:A:102:ASN:N | 2.49 | 0.41 |
| 2:A:272:TYR:O | 2:A:300:ASN:ND2 | 2.54 | 0.41 |
| 2:A:384:ILE:O | 2:A:385:ALA:C | 2.59 | 0.41 |
| 3:B:102:ASN:ND2 | 3:B:408:TYR:HA | 2.20 | 0.41 |
| 1:N:11:ILE:HD11 | 1:N:317:ALA:HB3 | 2.03 | 0.41 |
| 2:A:251:ASP:CA | 2:A:254:GLU:HG3 | 2.49 | 0.41 |
| 2:A:263:PRO:O | 2:A:264:ARG:C | 2.56 | 0.41 |
| 2:A:332:ILE:CD1 | 2:A:353:VAL:HG22 | 2.51 | 0.41 |
| 2:A:401:LYS:O | 2:A:402:ARG:HB2 | 2.21 | 0.41 |
| 2:A:413:MET:C | 2:A:414:GLU:CG | 2.90 | 0.41 |
| 3:B:242:LEU:HA | 3:B:242:LEU:HD23 | 1.76 | 0.41 |
| 3:B:307:PRO:O | 3:B:309:HIS:N | 2.53 | 0.41 |
| 3:B:311:ARG:NH1 | 3:B:311:ARG:HG2 | 2.34 | 0.41 |
| 1:N:265:ALA:CB | 2:A:401:LYS:HB3 | 2.51 | 0.41 |
| 2:A:384:ILE:C | 2:A:386:GLU:N | 2.72 | 0.40 |
| 3:B:11:GLN:HA | 3:B:74:THR:HG21 | 2.04 | 0.40 |
| 3:B:125:GLU:O | 3:B:128:SER:HB3 | 2.22 | 0.40 |
| 3:B:187:ALA:O | 3:B:190:SER:N | 2.54 | 0.40 |
| 3:B:23:VAL:O | 3:B:24:ILE:C | 2.60 | 0.40 |
| 3:B:409:THR:O | 3:B:412:GLY:N | 2.48 | 0.40 |
| 1:N:29:VAL:CG1 | 1:N:301:GLN:HA | 2.50 | 0.40 |
| 2:A:199:ASP:CB | 2:A:256:GLN:NE2 | 2.77 | 0.40 |
| 3:B:291:LEU:HD21 | 3:B:373:MET:HG2 | 2.03 | 0.40 |
| 1:N:84:LEU:HD23 | 1:N:84:LEU:C | 2.41 | 0.40 |
| 2:A:273:ALA:O | 2:A:275:VAL:N | 2.54 | 0.40 |
| 2:A:289:ALA:HB3 | 2:A:290:GLU:OE2 | 2.21 | 0.40 |
| 2:A:14:VAL:HG11 | 2:A:75:ILE:HD13 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:20:PHE:CD2 | 3:B:235:MET:CG | 3.04 | 0.40 |
| 3:B:405:LEU:O | 3:B:405:LEU:HD23 | 2.21 | 0.40 |
| 3:B:98:GLY:O | 3:B:100:GLY:N | 2.49 | 0.40 |
| 2:A:182:VAL:O | 2:A:183:GLU:C | 2.60 | 0.40 |
| 2:A:209:ILE:HD13 | 2:A:231:ILE:HD11 | 2.04 | 0.40 |
| 2:A:335:ILE:C | 2:A:337:THR:N | 2.73 | 0.40 |
| 3:B:133:GLN:CG | 3:B:165:ILE:HD11 | 2.49 | 0.40 |
| 3:B:315:VAL:CG1 | 3:B:377:PHE:CE1 | 3.05 | 0.40 |
| 3:B:70:LEU:HB2 | 3:B:99:ALA:HB2 | 2.03 | 0.40 |
| 1:N:249:ILE:HG23 | 1:N:250:ASN:H | 1.87 | 0.40 |
| 1:N:265:ALA:CB | 2:A:401:LYS:CB | 3.00 | 0.40 |
| 2:A:318:LEU:HB2 | 2:A:376:CYS:SG | 2.61 | 0.40 |
| 3:B:35:SER:HB3 | 3:B:59:ASN:OD1 | 2.22 | 0.40 |
| 3:B:95:GLY:C | 3:B:97:SER:H | 2.25 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | N | 283/344 (82%) | 265 (94%) | 13 (5%) | 5 (2%) | 11 53 |
| 2 | A | 408/451 (90%) | 266 (65%) | 83 (20%) | 59 (14%) | 0 6 |
| 3 | B | 424/445 (95%) | 274 (65%) | 94 (22%) | 56 (13%) | 0 7 |
| All | All | 1115/1240 (90%) | 805 (72%) | 190 (17%) | 120 (11%) | 1 11 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 96 | LYS |
| 2 | A | 97 | GLU |
| 2 | A | 108 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 109 | THR |
| 2 | A | 141 | PHE |
| 2 | A | 183 | GLU |
| 2 | A | 217 | LEU |
| 2 | A | 240 | ALA |
| 2 | A | 249 | ASN |
| 2 | A | 255 | PHE |
| 2 | A | 266 | HIS |
| 2 | A | 280 | LYS |
| 2 | A | 284 | GLU |
| 2 | A | 285 | GLN |
| 2 | A | 289 | ALA |
| 2 | A | 309 | HIS |
| 2 | A | 346 | TRP |
| 2 | A | 370 | LYS |
| 2 | A | 387 | ALA |
| 2 | A | 403 | ALA |
| 2 | A | 437 | VAL |
| 3 | B | 23 | VAL |
| 3 | B | 24 | ILE |
| 3 | B | 32 | PRO |
| 3 | B | 50 | ASN |
| 3 | B | 82 | PRO |
| 3 | B | 97 | SER |
| 3 | B | 128 | SER |
| 3 | B | 176 | LYS |
| 3 | B | 183 | GLU |
| 3 | B | 218 | LYS |
| 3 | B | 238 | VAL |
| 3 | B | 239 | THR |
| 3 | B | 240 | THR |
| 3 | B | 252 | LEU |
| 3 | B | 263 | PRO |
| 3 | B | 266 | HIS |
| 3 | B | 273 | ALA |
| 3 | B | 278 | ARG |
| 3 | B | 280 | SER |
| 3 | B | 281 | GLN |
| 3 | B | 282 | GLN |
| 3 | B | 288 | VAL |
| 3 | B | 294 | GLN |
| 3 | B | 295 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 343 | PHE |
| 3 | B | 344 | VAL |
| 3 | B | 346 | TRP |
| 3 | B | 369 | ARG |
| 3 | B | 403 | ALA |
| 1 | N | 251 | LEU |
| 1 | N | 252 | GLY |
| 2 | A | 24 | TYR |
| 2 | A | 63 | PRO |
| 2 | A | 103 | TYR |
| 2 | A | 111 | GLY |
| 2 | A | 131 | GLY |
| 2 | A | 218 | ASP |
| 2 | A | 219 | ILE |
| 2 | A | 238 | ILE |
| 2 | A | 265 | GLY |
| 2 | A | 287 | SER |
| 2 | A | 314 | ALA |
| 2 | A | 339 | ARG |
| 2 | A | 342 | GLN |
| 2 | A | 373 | ARG |
| 2 | A | 386 | GLU |
| 3 | B | 38 | GLY |
| 3 | B | 73 | GLY |
| 3 | B | 175 | PRO |
| 3 | B | 265 | LEU |
| 3 | B | 279 | GLY |
| 3 | B | 298 | ALA |
| 3 | B | 300 | ASN |
| 3 | B | 311 | ARG |
| 2 | A | 104 | ALA |
| 2 | A | 148 | GLY |
| 2 | A | 149 | PHE |
| 2 | A | 173 | PRO |
| 2 | A | 239 | THR |
| 2 | A | 245 | ASP |
| 2 | A | 263 | PRO |
| 2 | A | 279 | GLU |
| 2 | A | 288 | VAL |
| 2 | A | 330 | ALA |
| 2 | A | 336 | LYS |
| 2 | A | 369 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 34 | GLY |
| 3 | B | 83 | PHE |
| 3 | B | 99 | ALA |
| 3 | B | 100 | GLY |
| 3 | B | 302 | MET |
| 3 | B | 386 | GLU |
| 2 | A | 89 | PRO |
| 2 | A | 129 | CYS |
| 2 | A | 300 | ASN |
| 2 | A | 348 | PRO |
| 3 | B | 96 | GLN |
| 3 | B | 395 | PHE |
| 2 | A | 256 | GLN |
| 2 | A | 303 | VAL |
| 2 | A | 307 | PRO |
| 2 | A | 382 | THR |
| 3 | B | 57 | ALA |
| 3 | B | 74 | THR |
| 3 | B | 285 | ALA |
| 1 | N | 253 | LEU |
| 2 | A | 31 | GLN |
| 2 | A | 273 | ALA |
| 3 | B | 51 | VAL |
| 3 | B | 58 | GLY |
| 3 | B | 145 | THR |
| 3 | B | 162 | PRO |
| 3 | B | 400 | ARG |
| 3 | B | 424 | ASN |
| 3 | B | 195 | VAL |
| 1 | N | 269 | VAL |
| 2 | A | 115 | ILE |
| 3 | B | 72 | PRO |
| 1 | N | 249 | ILE |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | N | 248/293 (85%) | 240 (97%) | 8 (3%) | 46 76 |
| 2 | A | 347/377 (92%) | 298 (86%) | 49 (14%) | 4 26 |
| 3 | B | 367/381 (96%) | 307 (84%) | 60 (16%) | 3 20 |
| All | All | 962/1051 (92%) | 845 (88%) | 117 (12%) | 10 31 |

All (117) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 41 | LEU |
| 1 | N | 63 | MET |
| 1 | N | 132 | LYS |
| 1 | N | 141 | PHE |
| 1 | N | 165 | ARG |
| 1 | N | 170 | THR |
| 1 | N | 249 | ILE |
| 1 | N | 253 | LEU |
| 2 | A | 6 | SER |
| 2 | A | 20 | CYS |
| 2 | A | 21 | TRP |
| 2 | A | 32 | PRO |
| 2 | A | 76 | ASP |
| 2 | A | 82 | THR |
| 2 | A | 98 | ASP |
| 2 | A | 115 | ILE |
| 2 | A | 120 | ASP |
| 2 | A | 125 | LEU |
| 2 | A | 127 | ASP |
| 2 | A | 130 | THR |
| 2 | A | 135 | PHE |
| 2 | A | 141 | PHE |
| 2 | A | 150 | THR |
| 2 | A | 152 | LEU |
| 2 | A | 155 | GLU |
| 2 | A | 169 | PHE |
| 2 | A | 172 | TYR |
| 2 | A | 173 | PRO |
| 2 | A | 183 | GLU |
| 2 | A | 192 | HIS |
| 2 | A | 204 | VAL |
| 2 | A | 219 | ILE |
| 2 | A | 224 | TYR |
| 2 | A | 231 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 234 | ILE |
| 2 | A | 243 | ARG |
| 2 | A | 244 | PHE |
| 2 | A | 253 | THR |
| 2 | A | 260 | VAL |
| 2 | A | 267 | PHE |
| 2 | A | 269 | LEU |
| 2 | A | 276 | ILE |
| 2 | A | 284 | GLU |
| 2 | A | 303 | VAL |
| 2 | A | 325 | PRO |
| 2 | A | 334 | THR |
| 2 | A | 345 | ASP |
| 2 | A | 352 | LYS |
| 2 | A | 368 | LEU |
| 2 | A | 376 | CYS |
| 2 | A | 378 | LEU |
| 2 | A | 380 | ASN |
| 2 | A | 404 | PHE |
| 2 | A | 415 | GLU |
| 2 | A | 417 | GLU |
| 2 | A | 431 | ASP |
| 2 | A | 432 | TYR |
| 3 | B | 14 | ASN |
| 3 | B | 24 | ILE |
| 3 | B | 26 | ASP |
| 3 | B | 32 | PRO |
| 3 | B | 41 | ASP |
| 3 | B | 68 | VAL |
| 3 | B | 76 | ASP |
| 3 | B | 90 | ASP |
| 3 | B | 94 | PHE |
| 3 | B | 101 | ASN |
| 3 | B | 122 | VAL |
| 3 | B | 129 | CYS |
| 3 | B | 135 | PHE |
| 3 | B | 141 | LEU |
| 3 | B | 145 | THR |
| 3 | B | 149 | MET |
| 3 | B | 153 | LEU |
| 3 | B | 161 | TYR |
| 3 | B | 163 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 165 | ILE |
| 3 | B | 174 | SER |
| 3 | B | 198 | THR |
| 3 | B | 201 | THR |
| 3 | B | 203 | CYS |
| 3 | B | 207 | GLU |
| 3 | B | 211 | ASP |
| 3 | B | 214 | PHE |
| 3 | B | 215 | ARG |
| 3 | B | 224 | TYR |
| 3 | B | 227 | LEU |
| 3 | B | 230 | LEU |
| 3 | B | 236 | SER |
| 3 | B | 240 | THR |
| 3 | B | 244 | PHE |
| 3 | B | 265 | LEU |
| 3 | B | 267 | PHE |
| 3 | B | 275 | LEU |
| 3 | B | 282 | GLN |
| 3 | B | 283 | TYR |
| 3 | B | 284 | ARG |
| 3 | B | 289 | PRO |
| 3 | B | 299 | LYS |
| 3 | B | 306 | ASP |
| 3 | B | 309 | HIS |
| 3 | B | 322 | ARG |
| 3 | B | 324 | SER |
| 3 | B | 325 | MET |
| 3 | B | 343 | PHE |
| 3 | B | 344 | VAL |
| 3 | B | 349 | ASN |
| 3 | B | 369 | ARG |
| 3 | B | 380 | ASN |
| 3 | B | 387 | LEU |
| 3 | B | 413 | MET |
| 3 | B | 414 | ASP |
| 3 | B | 424 | ASN |
| 3 | B | 427 | ASP |
| 3 | B | 431 | GLU |
| 3 | B | 432 | TYR |
| 3 | B | 437 | ASP |

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

sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 49 | HIS |
| 1 | N | 65 | GLN |
| 1 | N | 88 | GLN |
| 1 | N | 181 | HIS |
| 1 | N | 300 | HIS |
| 1 | N | 324 | HIS |
| 2 | A | 11 | GLN |
| 2 | A | 15 | GLN |
| 2 | A | 28 | HIS |
| 2 | A | 128 | GLN |
| 2 | A | 133 | GLN |
| 2 | A | 139 | HIS |
| 2 | A | 197 | HIS |
| 2 | A | 216 | ASN |
| 2 | A | 226 | ASN |
| 2 | A | 256 | GLN |
| 2 | A | 309 | HIS |
| 2 | A | 380 | ASN |
| 3 | B | 14 | ASN |
| 3 | B | 91 | ASN |
| 3 | B | 101 | ASN |
| 3 | B | 102 | ASN |
| 3 | B | 107 | HIS |
| 3 | B | 136 | GLN |
| 3 | B | 139 | HIS |
| 3 | B | 197 | ASN |
| 3 | B | 282 | GLN |
| 3 | B | 331 | GLN |
| 3 | B | 334 | ASN |
| 3 | B | 337 | ASN |
| 3 | B | 349 | ASN |
| 3 | B | 380 | ASN |
| 3 | B | 406 | HIS |
| 3 | B | 436 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 7 | GTP | B | 500 | 4 | 26,34,34 | 1.35 | 1 (3%) | 29,54,54 | 2.29 | 4 (13%) |
| 8 | GDP | B | 600 | - | 24,30,30 | 2.66 | 8 (33%) | 26,47,47 | 3.29 | 8 (30%) |
| 9 | TA1 | B | 601 | - | 68,68,68 | 1.93 | 20 (29%) | 102,105,105 | 1.31 | 8 (7%) |
| 5 | ADP | N | 401 | 4 | 24,29,29 | 1.32 | 2 (8%) | 23,45,45 | 2.24 | 4 (17%) |

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 |
|---|---|---|---|---|---|---|---|
| 7 | GTP | B | 500 | 4 | - | 0/18/38/38 | 0/3/3/3 |
| 8 | GDP | B | 600 | - | - | 0/12/32/32 | 0/3/3/3 |
| 9 | TA1 | B | 601 | - | - | 0/41/127/127 | 0/5/7/7 |
| 5 | ADP | N | 401 | 4 | - | 0/12/32/32 | 0/3/3/3 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | B | 601 | TA1 | C08-C07 | -4.93 | 1.25 | 1.38 |
| 8 | B | 600 | GDP | PB-O2B | -4.21 | 1.40 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | B | 601 | TA1 | C04-C03 | -2.31 | 1.44 | 1.49 |
| 9 | B | 601 | TA1 | C10-C02 | 2.03 | 1.62 | 1.57 |
| 5 | N | 401 | ADP | C2'-C3' | 2.04 | 1.58 | 1.53 |
| 9 | B | 601 | TA1 | C41-C42 | 2.04 | 1.42 | 1.38 |
| 9 | B | 601 | TA1 | C18-C20 | 2.07 | 1.62 | 1.56 |
| 8 | B | 600 | GDP | O3'-C3' | 2.10 | 1.47 | 1.43 |
| 9 | B | 601 | TA1 | C01-C45 | 2.15 | 1.66 | 1.56 |
| 9 | B | 601 | TA1 | C11-C10 | 2.16 | 1.61 | 1.55 |
| 9 | B | 601 | TA1 | C37-C29 | 2.16 | 1.54 | 1.51 |
| 9 | B | 601 | TA1 | C16-C15 | 2.18 | 1.56 | 1.52 |
| 9 | B | 601 | TA1 | C26-C25 | 2.40 | 1.56 | 1.51 |
| 8 | B | 600 | GDP | C5-C4 | 2.42 | 1.46 | 1.40 |
| 9 | B | 601 | TA1 | C43-C26 | 2.43 | 1.58 | 1.52 |
| 8 | B | 600 | GDP | PB-O3B | 2.66 | 1.63 | 1.54 |
| 9 | B | 601 | TA1 | C43-C01 | 2.87 | 1.60 | 1.54 |
| 9 | B | 601 | TA1 | C46-C45 | 2.92 | 1.60 | 1.53 |
| 9 | B | 601 | TA1 | C25-C24 | 2.98 | 1.39 | 1.34 |
| 8 | B | 600 | GDP | C8-N7 | 3.31 | 1.41 | 1.34 |
| 9 | B | 601 | TA1 | C45-C24 | 3.37 | 1.61 | 1.54 |
| 9 | B | 601 | TA1 | O02-C03 | 3.41 | 1.41 | 1.34 |
| 9 | B | 601 | TA1 | C36-C31 | 3.53 | 1.45 | 1.39 |
| 5 | N | 401 | ADP | PB-O3B | 3.97 | 1.68 | 1.54 |
| 8 | B | 600 | GDP | O6-C6 | 4.05 | 1.34 | 1.24 |
| 9 | B | 601 | TA1 | C18-C10 | 4.19 | 1.69 | 1.57 |
| 9 | B | 601 | TA1 | C05-C04 | 4.51 | 1.46 | 1.39 |
| 7 | B | 500 | GTP | C6-N1 | 4.82 | 1.41 | 1.33 |
| 9 | B | 601 | TA1 | C06-C05 | 5.70 | 1.50 | 1.38 |
| 8 | B | 600 | GDP | O4'-C1' | 6.02 | 1.49 | 1.41 |
| 8 | B | 600 | GDP | C2-N1 | 7.31 | 1.49 | 1.35 |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | B | 600 | GDP | C6-C5-C4 | -9.94 | 109.50 | 120.86 |
| 5 | N | 401 | ADP | N3-C2-N1 | -8.98 | 121.82 | 128.87 |
| 7 | B | 500 | GTP | C5-C6-N1 | -7.80 | 113.33 | 123.52 |
| 8 | B | 600 | GDP | N2-C2-N1 | -5.68 | 107.83 | 117.20 |
| 8 | B | 600 | GDP | N3-C2-N1 | -5.37 | 120.26 | 127.56 |
| 9 | B | 601 | TA1 | C06-C05-C04 | -4.82 | 114.60 | 120.35 |
| 9 | B | 601 | TA1 | C05-C04-C03 | -3.96 | 111.46 | 120.38 |
| 7 | B | 500 | GTP | N3-C2-N1 | -3.50 | 122.79 | 127.56 |
| 5 | N | 401 | ADP | O3'-C3'-C2' | -3.09 | 101.86 | 111.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | B | 600 | GDP | C1'-N9-C4 | -2.64 | 123.86 | 126.81 |
| 9 | B | 601 | TA1 | O04-C11-C14 | -2.48 | 101.77 | 108.08 |
| 5 | N | 401 | ADP | C2'-C3'-C4' | -2.20 | 98.13 | 102.64 |
| 7 | B | 500 | GTP | C6-C5-C4 | -2.13 | 118.42 | 120.86 |
| 8 | B | 600 | GDP | O2'-C2'-C3' | 2.25 | 119.13 | 111.86 |
| 5 | N | 401 | ADP | C4'-O4'-C1' | 2.44 | 112.23 | 109.64 |
| 9 | B | 601 | TA1 | O01-C01-C43 | 2.52 | 113.42 | 106.82 |
| 9 | B | 601 | TA1 | C17-C18-C20 | 2.57 | 109.83 | 102.14 |
| 9 | B | 601 | TA1 | C45-C01-C02 | 3.08 | 115.19 | 111.64 |
| 8 | B | 600 | GDP | C2'-C3'-C4' | 3.22 | 109.22 | 102.64 |
| 9 | B | 601 | TA1 | C09-C04-C03 | 3.54 | 128.36 | 120.38 |
| 8 | B | 600 | GDP | C4'-O4'-C1' | 4.11 | 114.00 | 109.64 |
| 9 | B | 601 | TA1 | C07-C08-C09 | 5.15 | 127.36 | 120.20 |
| 7 | B | 500 | GTP | C6-N1-C2 | 7.51 | 124.68 | 115.88 |
| 8 | B | 600 | GDP | N2-C2-N3 | 7.56 | 131.90 | 117.72 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | B | 500 | GTP | 4 | 0 |
| 8 | B | 600 | GDP | 1 | 0 |
| 9 | B | 601 | TA1 | 6 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.