# Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 09:34 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 4V5T |
| Title | : | X-ray structure of the Grapevine Fanleaf virus |
| Authors | : | Schellenberger, P.; Sauter, C.; Lorber, B.; Bron, P.; Trapani, S.; Bergdoll, M.; Marmonier, A.; Schmitt-Keichinger, C.; Lemaire, O.; Demangeat, G.; Ritzenthaler, C. |
| Deposited on | : | 2011-02-01 |
| Resolution | : | 3.00 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

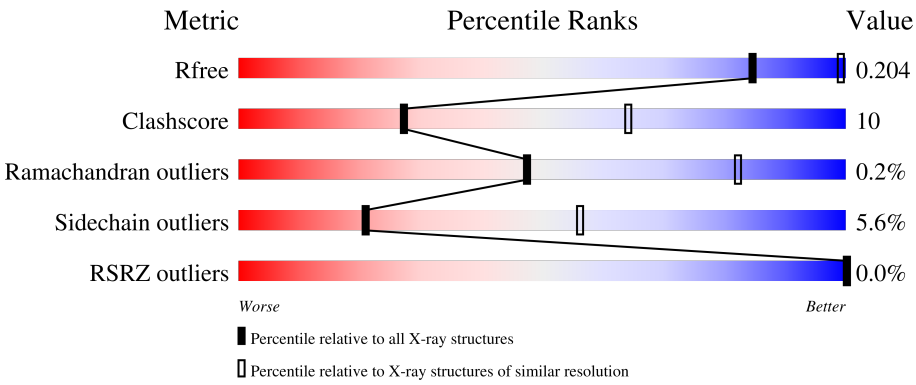
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AA | 504 | 79% 19% • |
| 1 | AB | 504 | 82% 16% • |
| 1 | AC | 504 | 81% 17% • |
| 1 | AD | 504 | 80% 17% • |
| 1 | AE | 504 | 83% 16% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AF | 504 | 81% 17% • |
| 1 | AG | 504 | 80% 16% • |
| 1 | AH | 504 | 81% 16% • |
| 1 | AI | 504 | 81% 16% • |
| 1 | AJ | 504 | 82% 16% • |
| 1 | AK | 504 | 80% 18% • |
| 1 | AL | 504 | 81% 17% • |
| 1 | AM | 504 | 82% 16% • |
| 1 | AN | 504 | 79% 19% • |
| 1 | AO | 504 | 80% 18% • |
| 1 | AP | 504 | 81% 17% • |
| 1 | AQ | 504 | 82% 16% • |
| 1 | AR | 504 | 81% 16% • |
| 1 | AS | 504 | 81% 16% • |
| 1 | AT | 504 | 80% 18% • |
| 1 | BA | 504 | 81% 17% • |
| 1 | BB | 504 | 81% 16% • |
| 1 | BC | 504 | 80% 17% • |
| 1 | BD | 504 | 83% 15% • |
| 1 | BE | 504 | 82% 16% • |
| 1 | BF | 504 | 79% 18% • |
| 1 | BG | 504 | 80% 18% • |
| 1 | BH | 504 | 80% 18% • |
| 1 | BI | 504 | 80% 18% • |
| 1 | BJ | 504 | 81% 17% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | BK | 504 | 82% 16% • |
| 1 | BL | 504 | 81% 16% • |
| 1 | BM | 504 | 81% 17% • |
| 1 | BN | 504 | 81% 16% • |
| 1 | BO | 504 | 80% 17% • |
| 1 | BP | 504 | 81% 16% • |
| 1 | BQ | 504 | 81% 17% • |
| 1 | BR | 504 | 81% 16% • |
| 1 | BS | 504 | 80% 18% • |
| 1 | BT | 504 | 80% 18% • |
| 1 | CA | 504 | 82% 15% • |
| 1 | CB | 504 | 81% 17% • |
| 1 | CC | 504 | 82% 15% • |
| 1 | CD | 504 | 81% 17% • |
| 1 | CE | 504 | 79% 19% • |
| 1 | CF | 504 | 80% 17% • |
| 1 | CG | 504 | 82% 16% • |
| 1 | CH | 504 | 80% 17% • |
| 1 | CI | 504 | 80% 17% • |
| 1 | CJ | 504 | 81% 17% • |
| 1 | CK | 504 | 81% 17% • |
| 1 | CL | 504 | 82% 16% • |
| 1 | CM | 504 | 79% 19% • |
| 1 | CN | 504 | 82% 16% • |
| 1 | CO | 504 | 80% 18% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | CP | 504 | 81% 16% • |
| 1 | CQ | 504 | 82% 16% • |
| 1 | CR | 504 | 81% 17% • |
| 1 | CS | 504 | 81% 17% • |
| 1 | CT | 504 | 82% 16% • |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 237060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COAT PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | AA | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AB | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AC | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AD | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AE | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AF | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AG | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AH | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AI | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AJ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AK | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AL | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AM | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AN | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AO | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AP | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | AQ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AR | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AS | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | AT | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BA | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BB | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BC | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BD | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BE | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BF | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BG | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BH | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BI | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BJ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BK | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BL | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BM | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BN | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BO | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BP | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BQ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | BR | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BS | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | BT | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CA | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CB | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CC | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CD | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CE | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CF | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CG | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CH | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CI | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CJ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CK | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CL | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CM | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CN | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CO | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CP | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CQ | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| 1 | CR | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | CS | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | CT | 504 | 3951 | 2555 | 653 | 721 | 22 | 0 | 0 | 0 |

# 3 Residue-property plots (i)

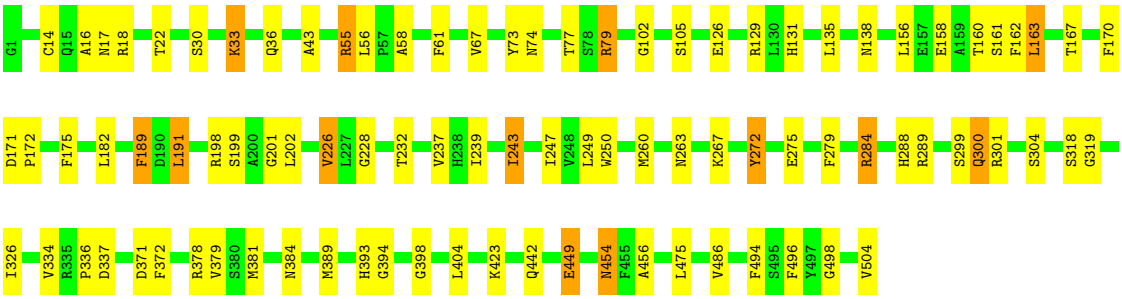
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain AA: 79% 19% •

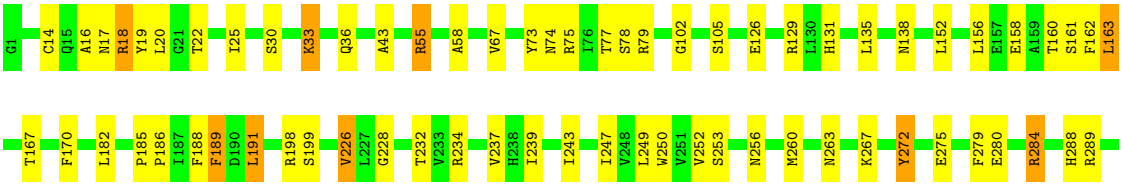
- Molecule 1: COAT PROTEIN

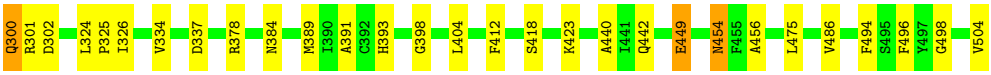
Chain AB: 82% 16% •




- Molecule 1: COAT PROTEIN

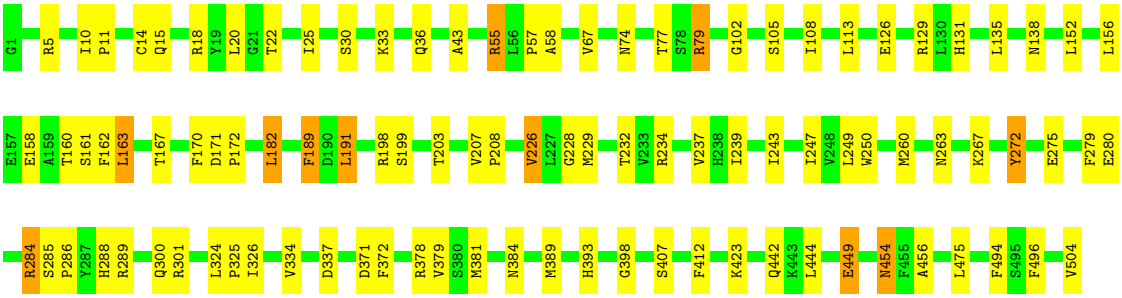
Chain AC: 81% 17% •





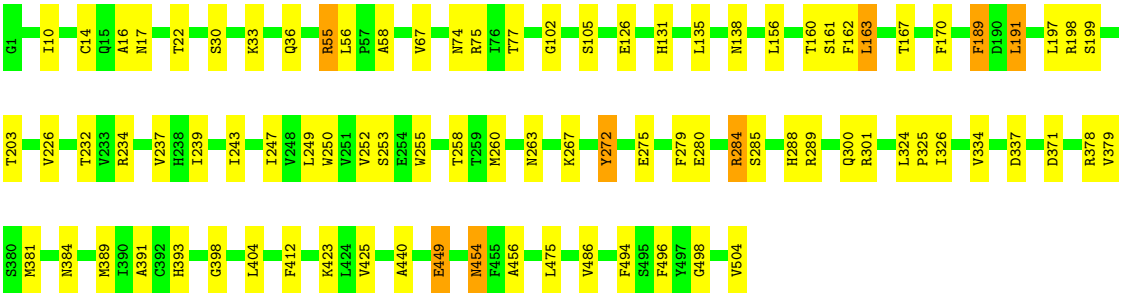

- Molecule 1: COAT PROTEIN

Chain AD:



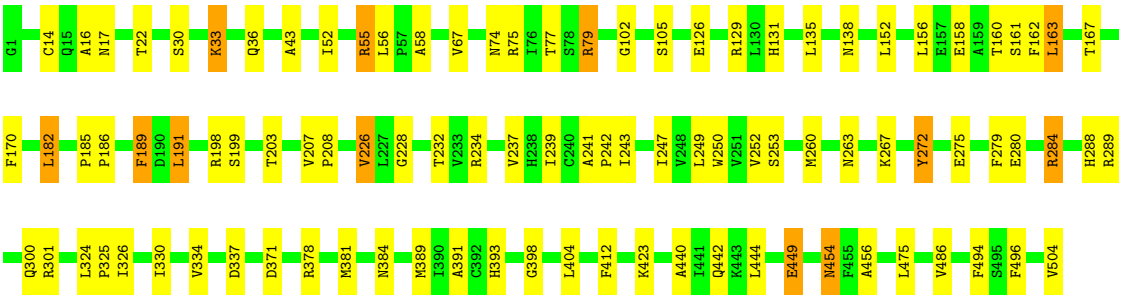

- Molecule 1: COAT PROTEIN

Chain AE:



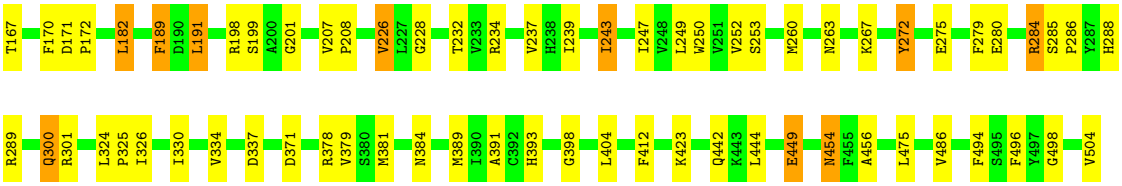

- Molecule 1: COAT PROTEIN

Chain AF:



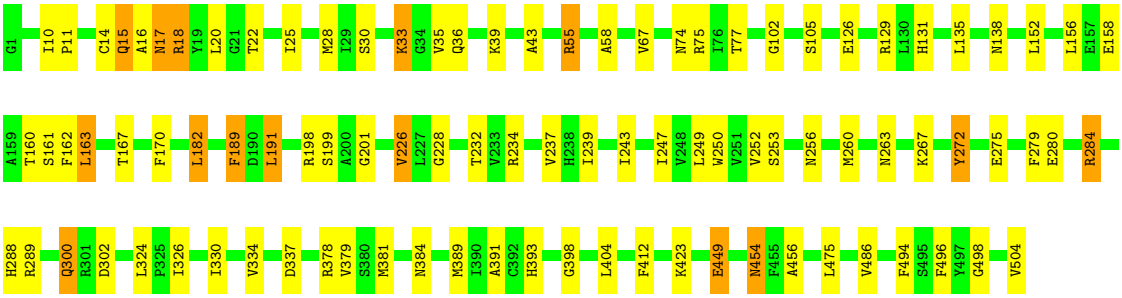

- Molecule 1: COAT PROTEIN

Chain AG:



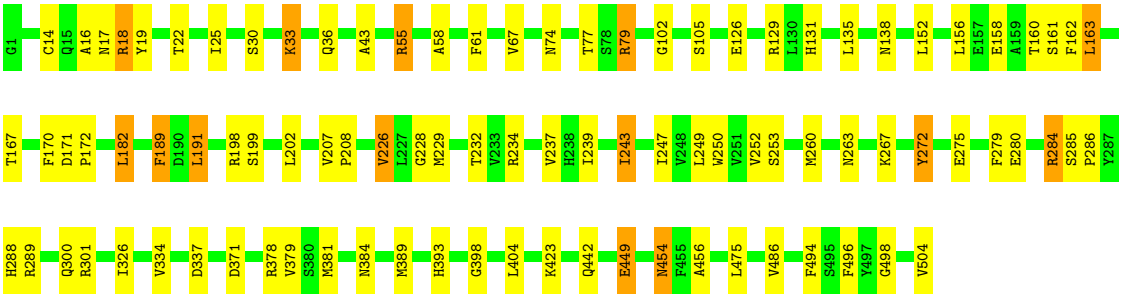

- Molecule 1: COAT PROTEIN

Chain AH:



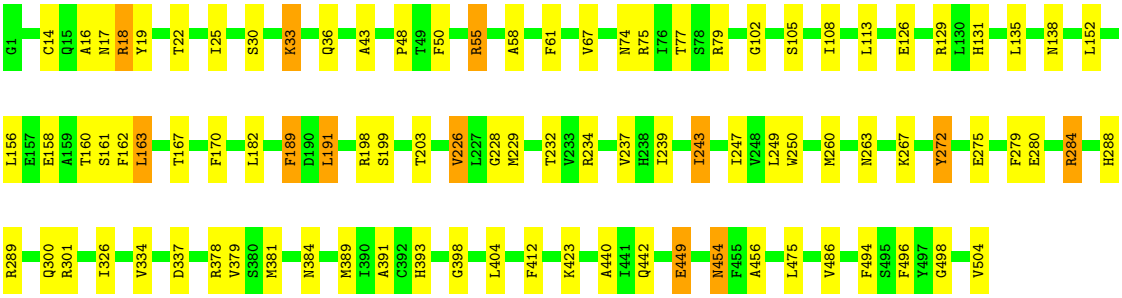

- Molecule 1: COAT PROTEIN

Chain AI:




- Molecule 1: COAT PROTEIN

Chain AJ:

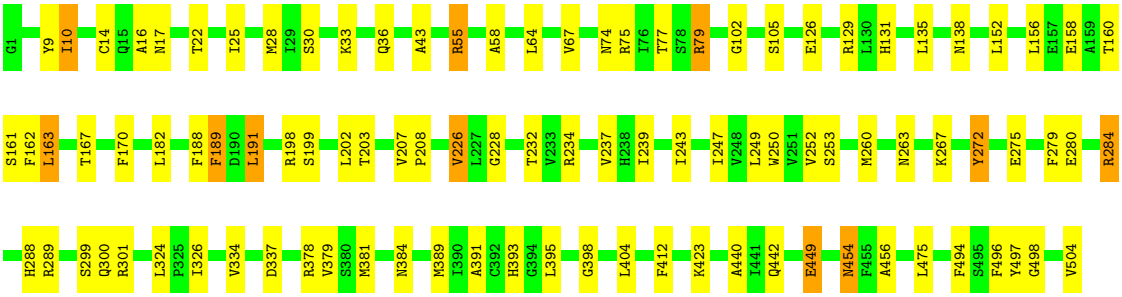



- Molecule 1: COAT PROTEIN

Chain AK:

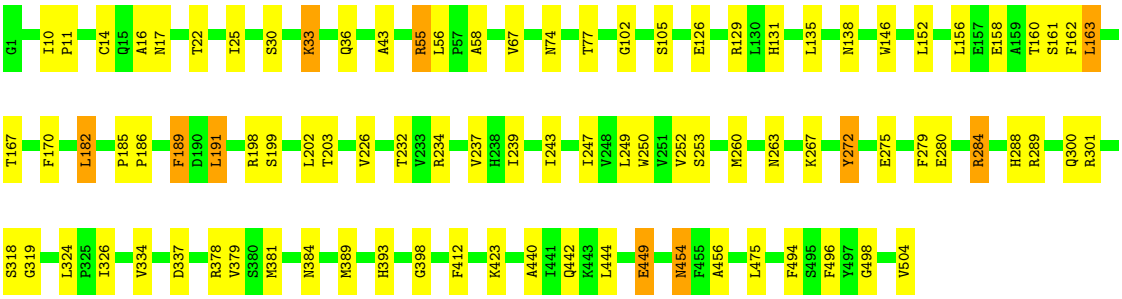
- Molecule 1: COAT PROTEIN

Chain AL:



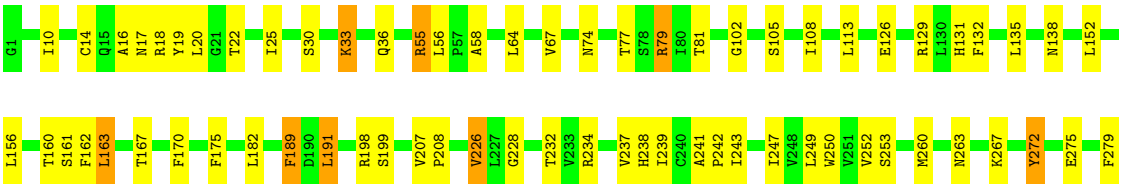

- Molecule 1: COAT PROTEIN

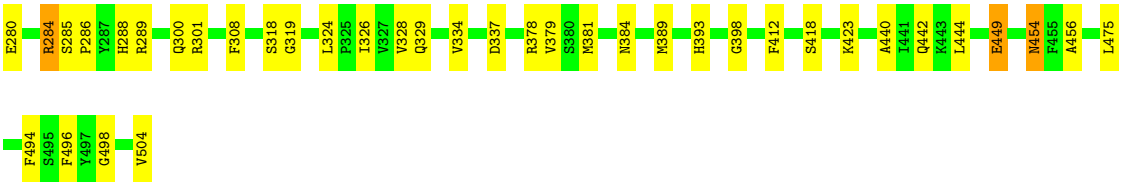
Chain AM:




- Molecule 1: COAT PROTEIN

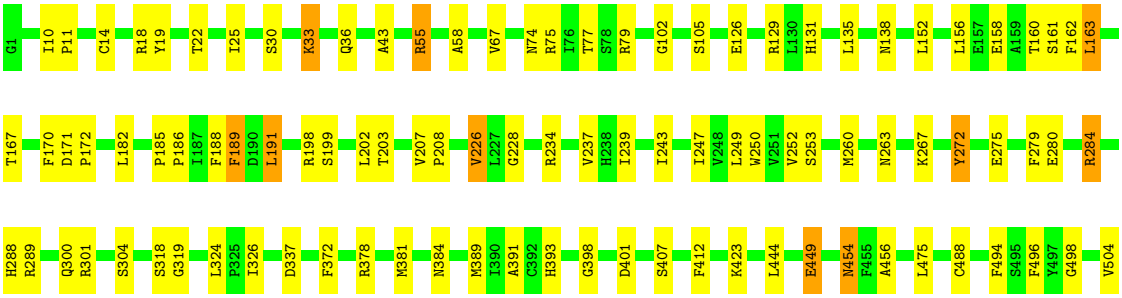
Chain AN:





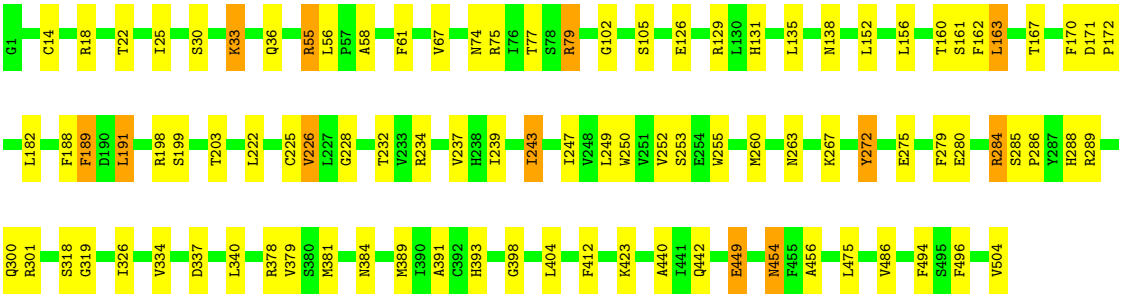

• Molecule 1: COAT PROTEIN

Chain AO:



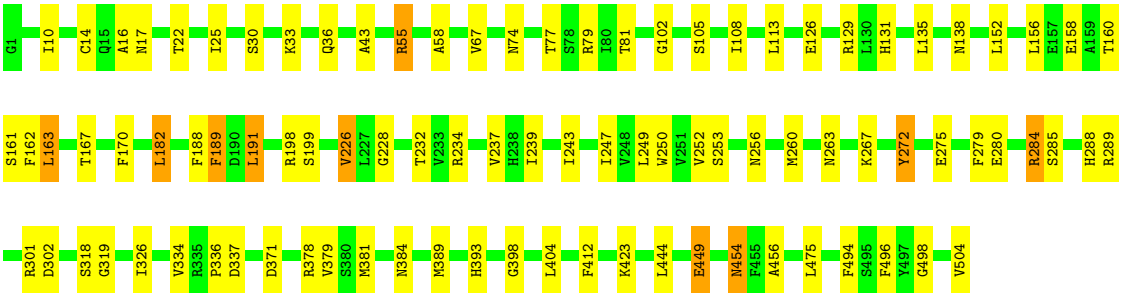

• Molecule 1: COAT PROTEIN

Chain AP:



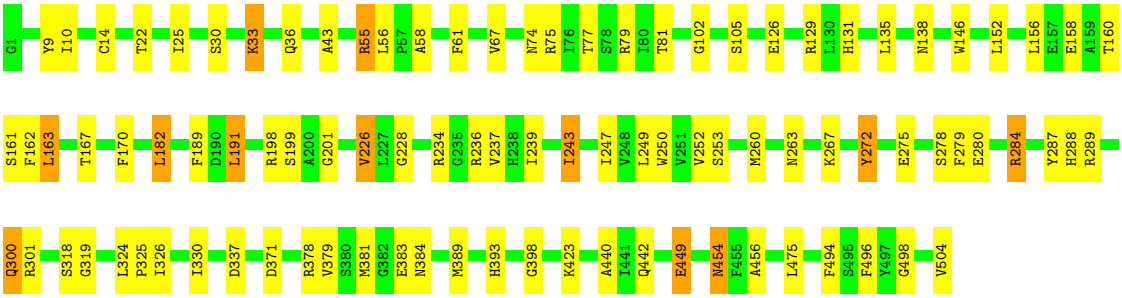

• Molecule 1: COAT PROTEIN

Chain AQ:



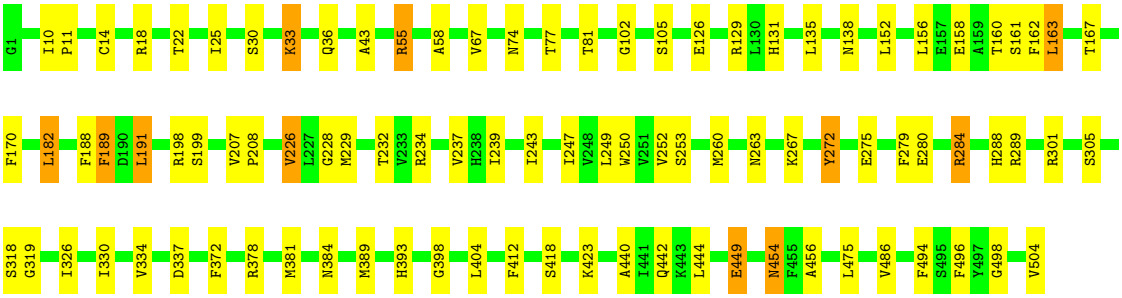

• Molecule 1: COAT PROTEIN

Chain AR:



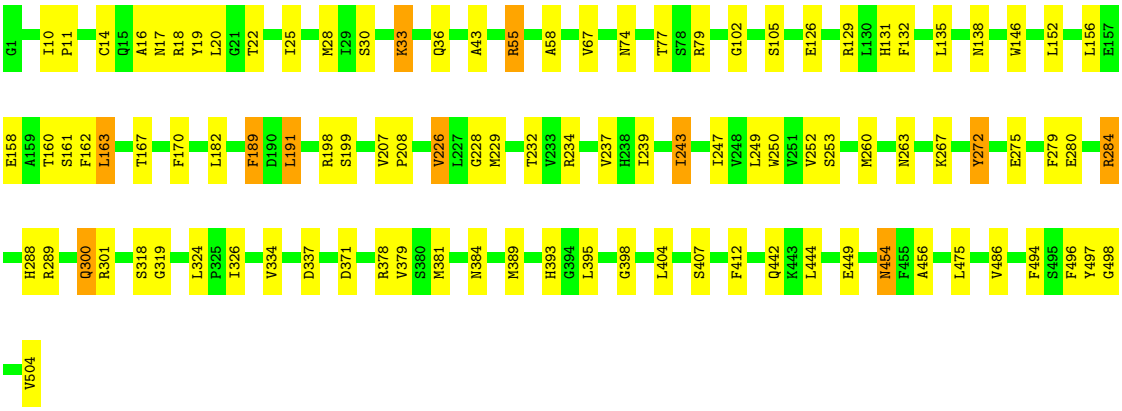

- Molecule 1: COAT PROTEIN

Chain AS:



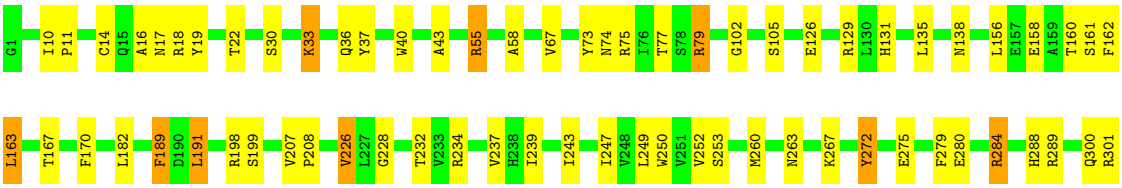

- Molecule 1: COAT PROTEIN

Chain AT:



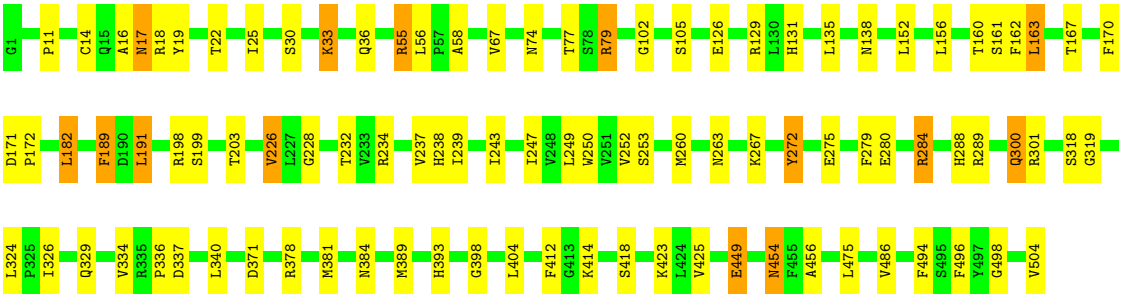

- Molecule 1: COAT PROTEIN

Chain BA:



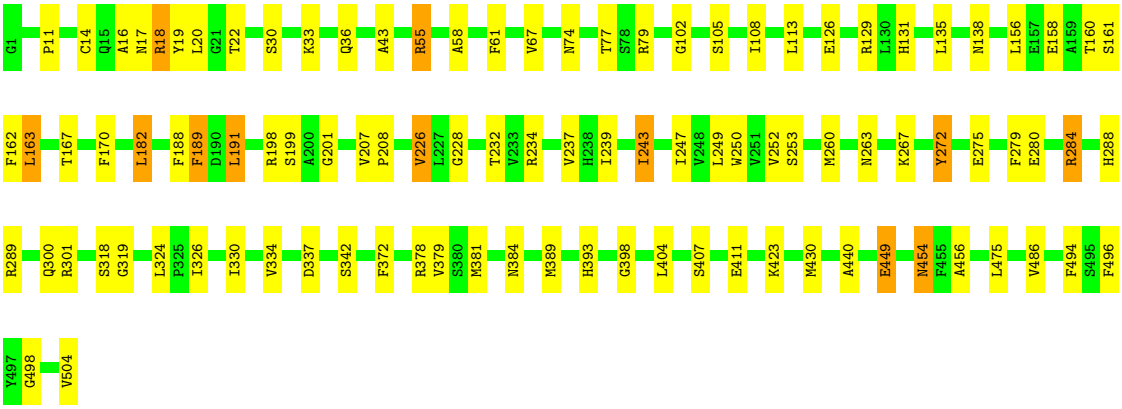
• Molecule 1: COAT PROTEIN

Chain BB:



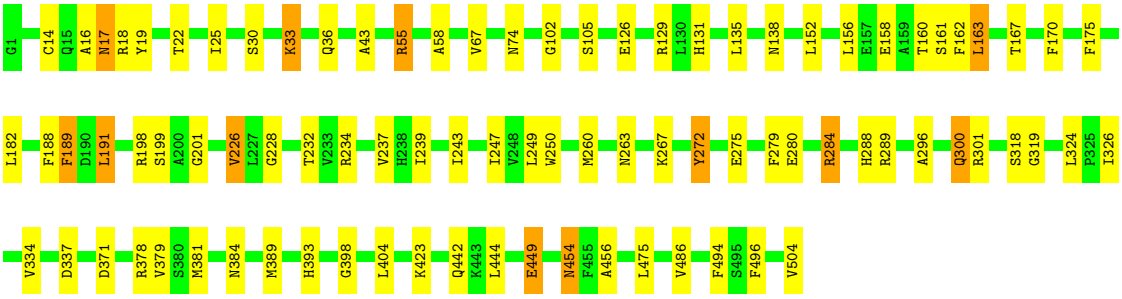

• Molecule 1: COAT PROTEIN

Chain BC:



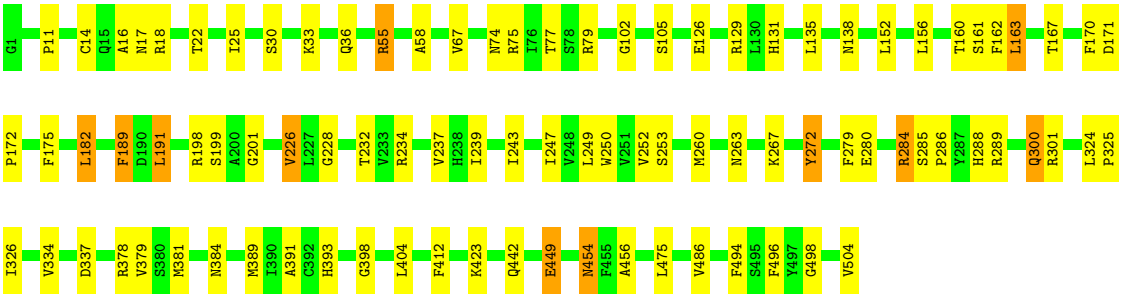

• Molecule 1: COAT PROTEIN

Chain BD:



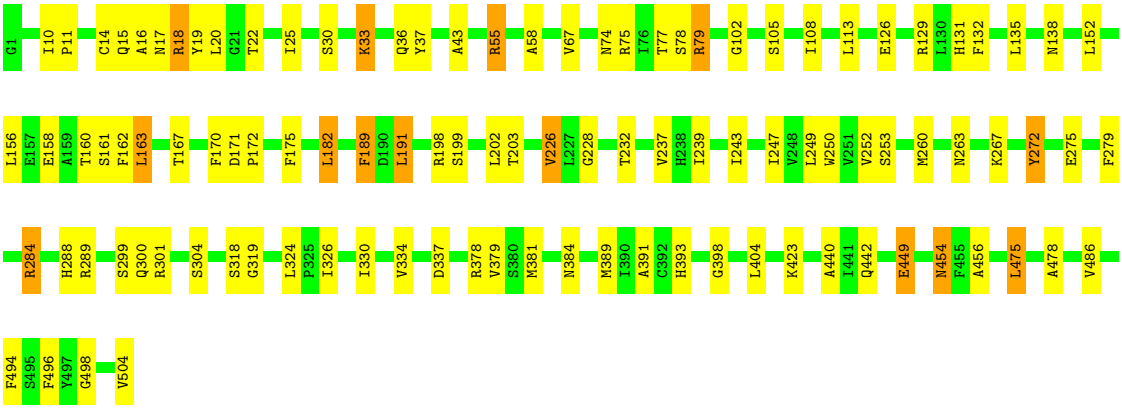

• Molecule 1: COAT PROTEIN

Chain BE:




- Molecule 1: COAT PROTEIN

Chain BF:

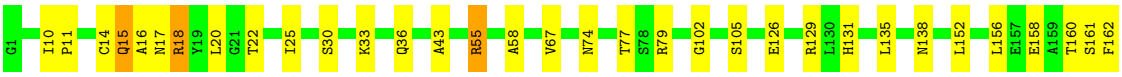


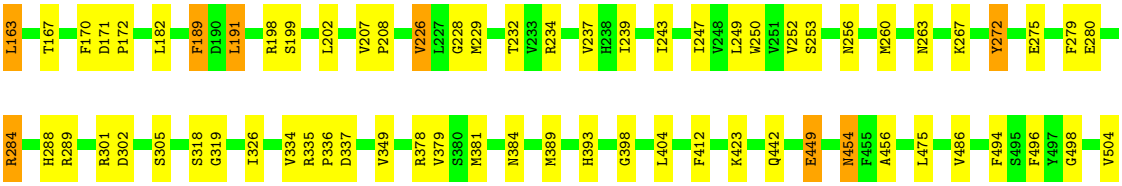

- Molecule 1: COAT PROTEIN

Chain BG:

- Molecule 1: COAT PROTEIN

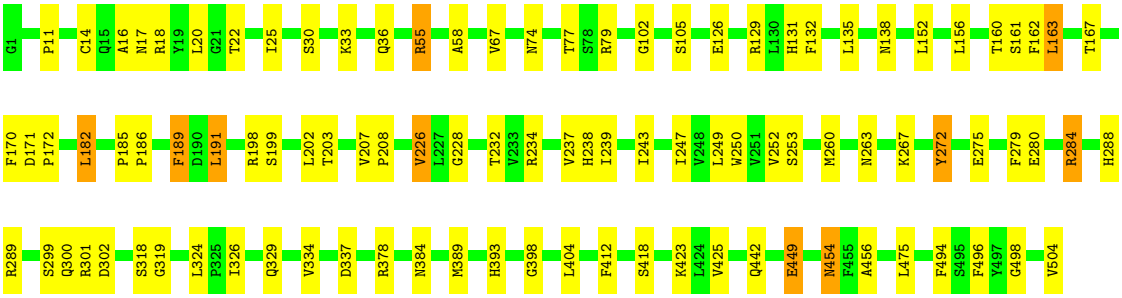
Chain BH:





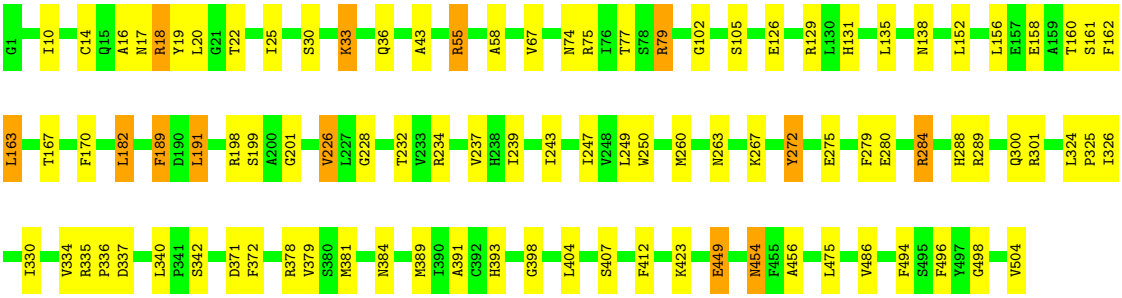

- Molecule 1: COAT PROTEIN

Chain BI:



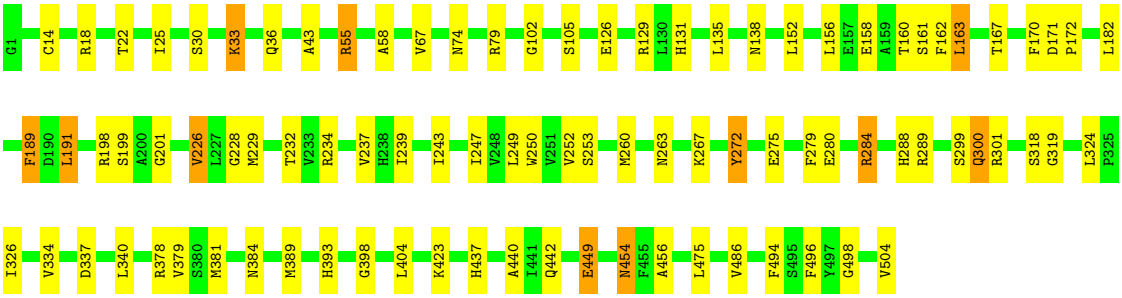

- Molecule 1: COAT PROTEIN

Chain BJ:




- Molecule 1: COAT PROTEIN

Chain BK:




- Molecule 1: COAT PROTEIN

Chain BL:

G1 Y9 C14 Q15 A16 N17 T22 I25 S30 K33 Q36 I52 R55 A58 V67 N74 T77 S78 R79 G102 S105 E126 R129 L130 H131 L135 N138 D145 L152 L156 T160 S161 F162 L163 T167

F170 D171 P172 L182 F189 D190 L191 R198 S199 A200 G201 V226 L227 G228 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 Y272 E275 F279 E280 R284 H288 R289 S299 Q300 R301 S318 G319 L324

P325 I326 Q329 V334 D337 D371 R378 V379 S380 M381 N384 M389 H393 G398 L404 Q405 F412 S418 K423 A440 I441 Q442 K443 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain BM: 81% 17% •

G1 P11 C14 Q15 A16 N17 R18 Y19 L20 G21 T22 I25 S30 K33 Q36 A43 R55 L56 P57 A58 V67 N74 R75 I76 T77 S78 R79 G102 S105 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160 S161

F162 L163 T167 F170 D171 P172 L182 F189 D190 L191 R198 S199 T203 V226 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 E254 W255 M260 N263 K267 Y272 E275 F279 E280 R284 S285 H288 R289

Q300 R301 S318 G319 I326 V334 D337 R378 V379 S380 M381 N384 M389 I390 A391 C392 H393 G398 L404 S407 F412 K423 Q442 K443 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 V504

- Molecule 1: COAT PROTEIN

Chain BN: 81% 16% •

G1 C14 Q15 A16 N17 R18 Y19 T22 I25 M28 I29 S30 K33 Q36 A43 R55 A58 L64 V67 N74 T77 G102 S105 I108 L113 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160

S161 F162 L163 T167 F170 D171 P172 L182 F189 D190 L191 R198 S199 T203 V207 P208 V226 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 W255 M260 N263 K267 Y272 E275 F279 E280 R284 S285

H288 R289 Q300 R301 I326 I330 V334 D337 D371 R378 M381 N384 M389 H393 G398 L404 F412 K423 A440 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain BO: 80% 17% •

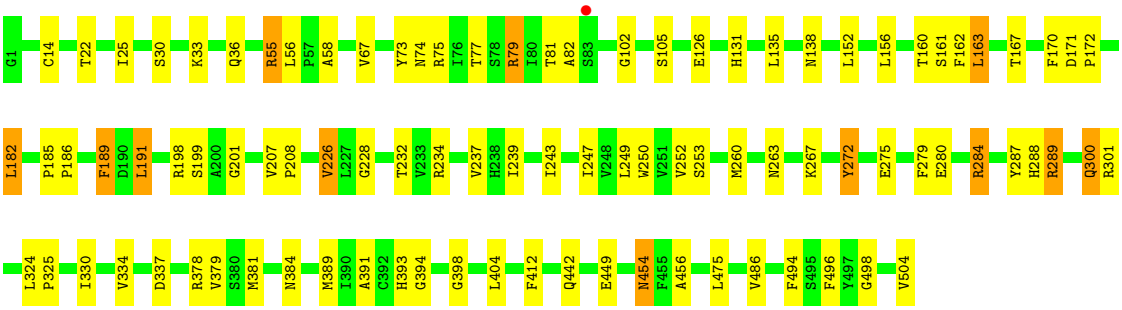
G1 I10 P11 C14 Q15 A16 N17 R18 T22 I25 S30 K33 Q36 M47 R55 A58 F61 V67 Y73 N74 R75 I76 T77 G102 S105 A117 E126 S127 P128 R129 L130 H131 L135 N138 L152 L156 T160 S161

F162 L163 T167 F170 D171 P172 F175 L182 P185 P186 F189 D190 L191 R198 S199 V226 L227 G228 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 N263 K267 Y272 E275 F279 E280 R284 H288 R289

R301 L324 P325 I326 I330 P336 D337 D371 R378 V379 S380 M381 G382 E383 N384 M389 I390 A391 C392 H393 G394 G398 D401 L404 K423 L444 E449 N454 F455 A456 L475 V486 L487 C488 F494 S495 F496 Y497 G498 V504

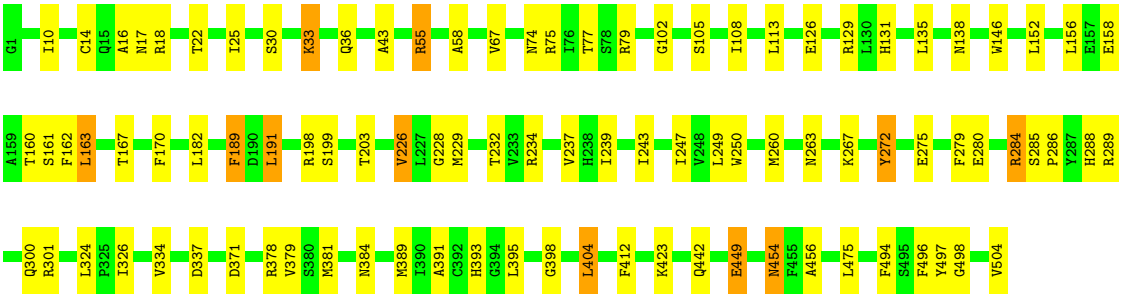
- Molecule 1: COAT PROTEIN

Chain BP: 81% 16% •



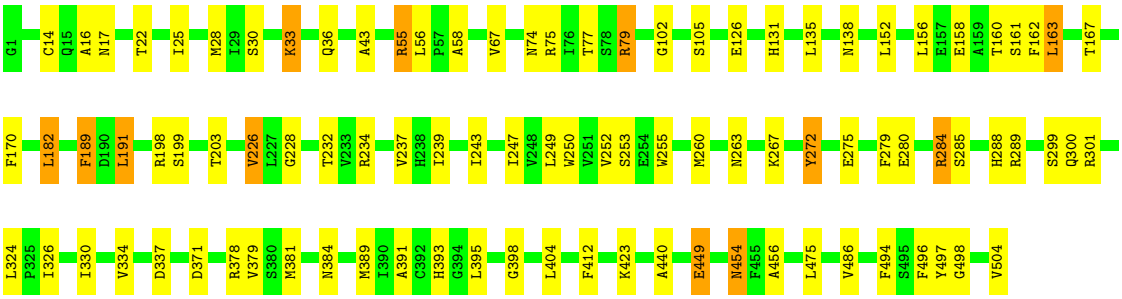

• Molecule 1: COAT PROTEIN

Chain BQ: 81% 17% •



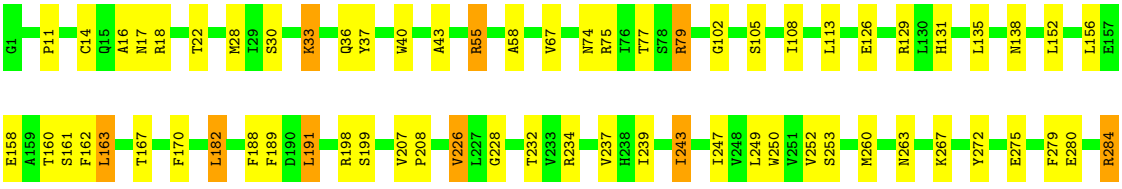

• Molecule 1: COAT PROTEIN

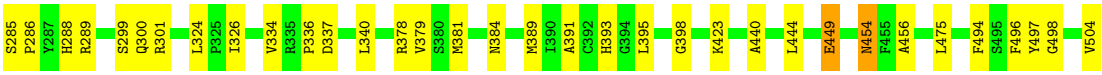
Chain BR: 81% 16% •




• Molecule 1: COAT PROTEIN

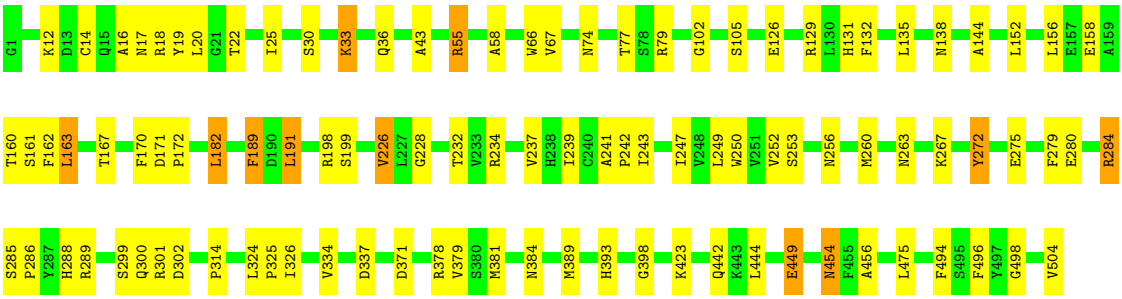
Chain BS: 80% 18% •





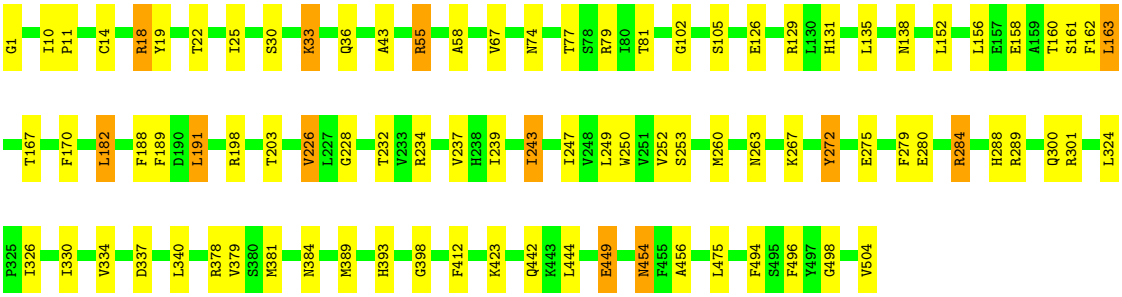

• Molecule 1: COAT PROTEIN

Chain BT: 80% 18%



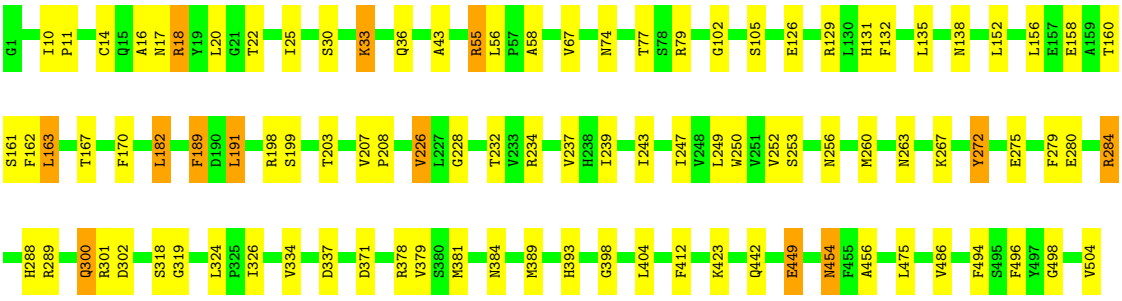

• Molecule 1: COAT PROTEIN

Chain CA: 82% 15%



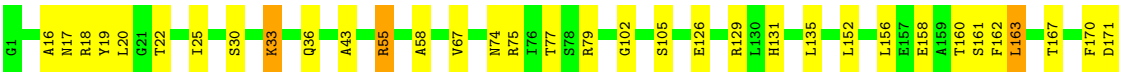

• Molecule 1: COAT PROTEIN

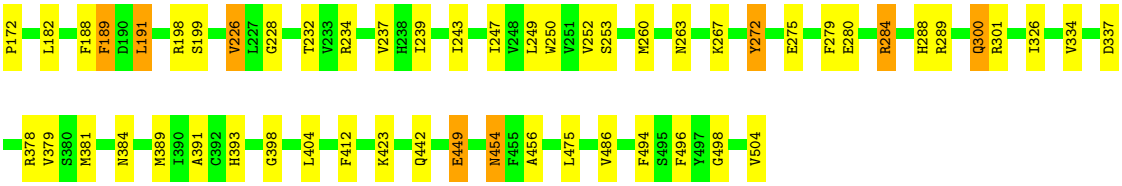
Chain CB: 81% 17%




• Molecule 1: COAT PROTEIN

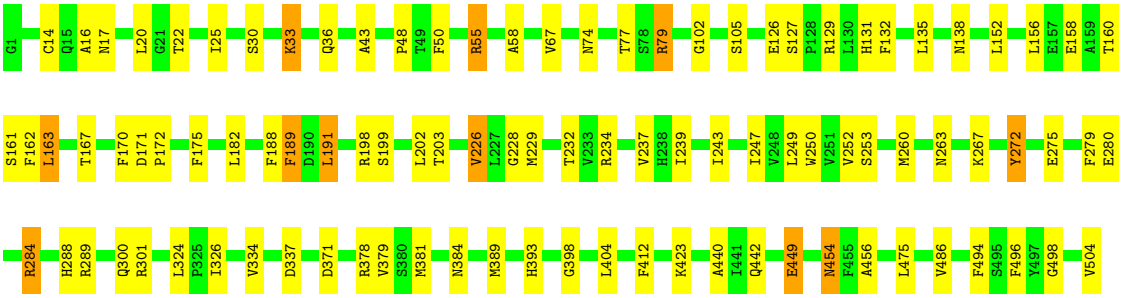
Chain CC: 82% 15%





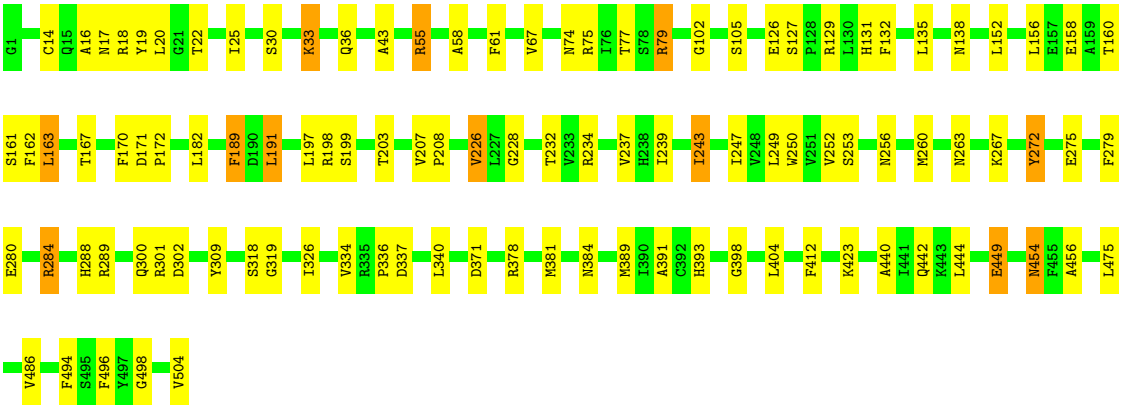

• Molecule 1: COAT PROTEIN

Chain CD:



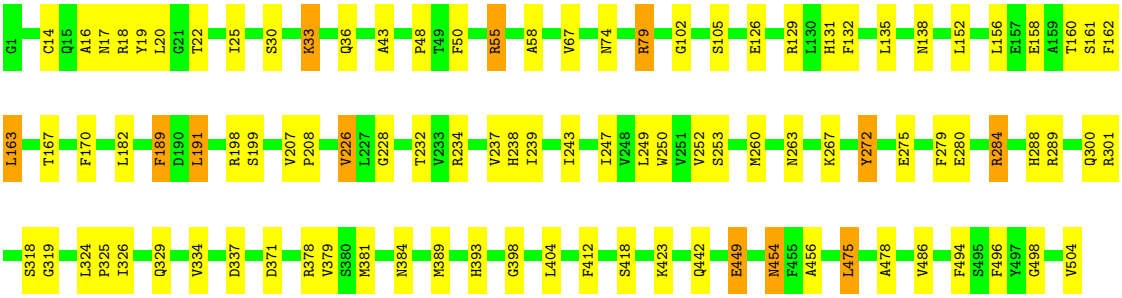

• Molecule 1: COAT PROTEIN

Chain CE:



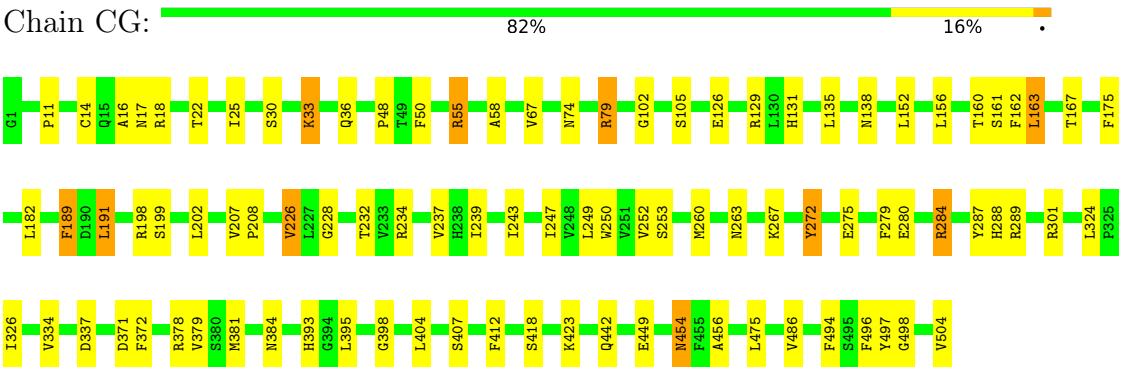

• Molecule 1: COAT PROTEIN

Chain CF:



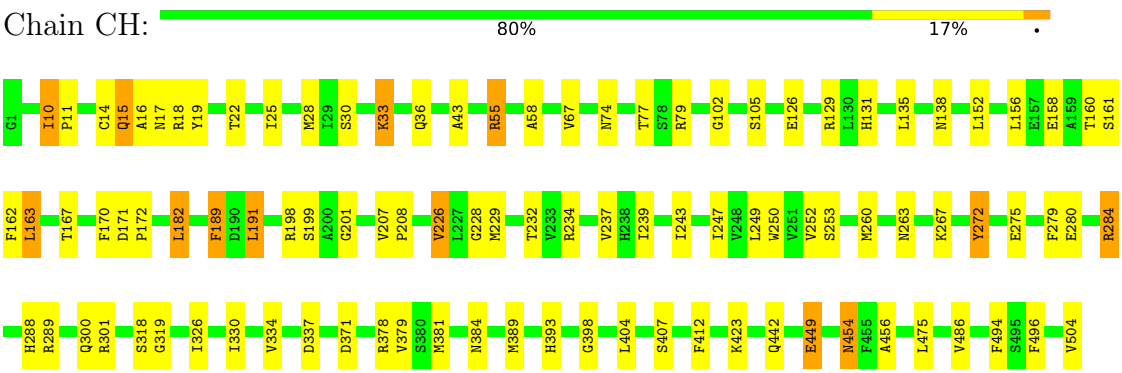

• Molecule 1: COAT PROTEIN

Chain CG:



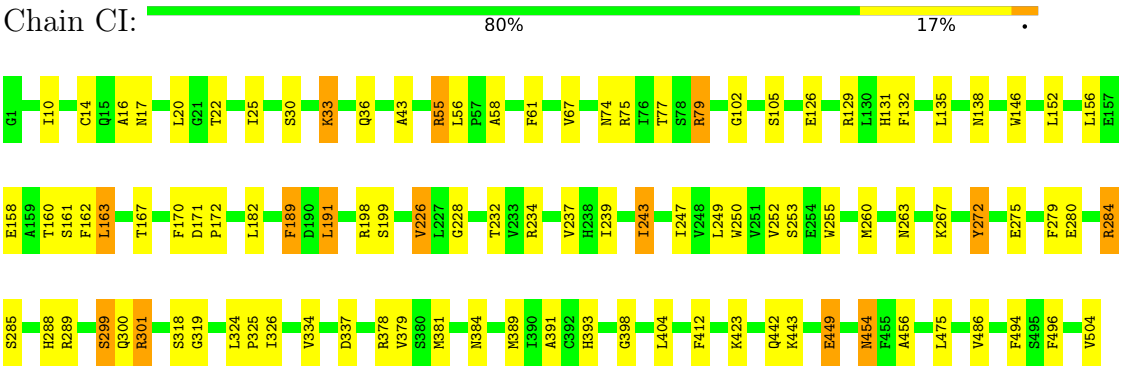

- Molecule 1: COAT PROTEIN

Chain CH:



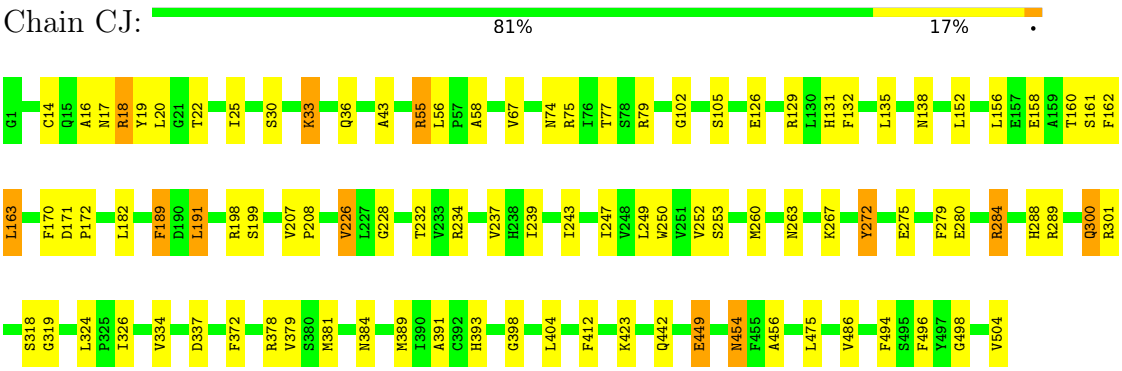

- Molecule 1: COAT PROTEIN

Chain CI:



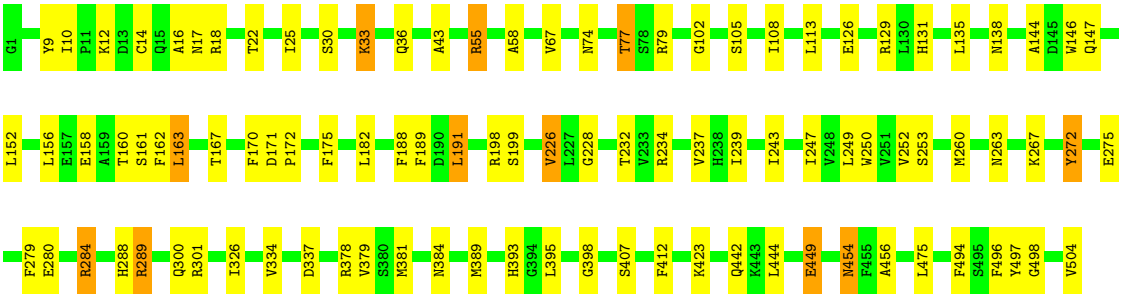

- Molecule 1: COAT PROTEIN

Chain CJ:



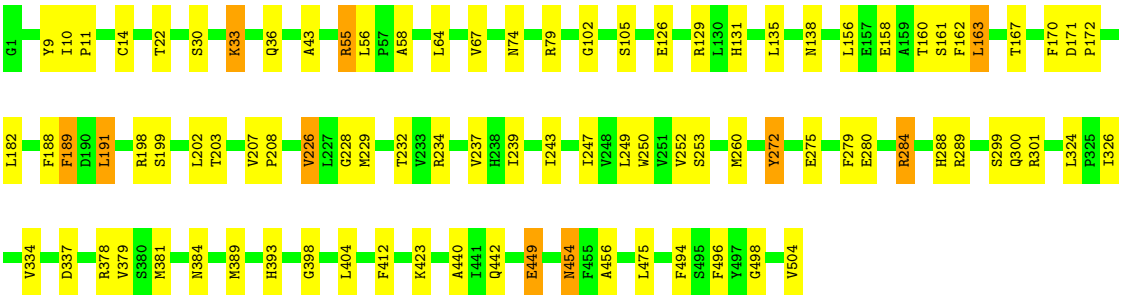
• Molecule 1: COAT PROTEIN

Chain CK: 81% 17%



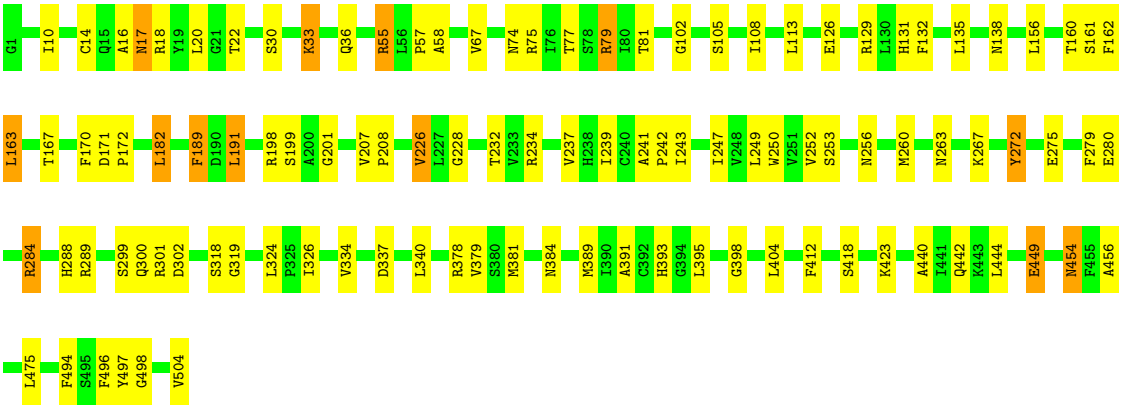

• Molecule 1: COAT PROTEIN

Chain CL: 82% 16%



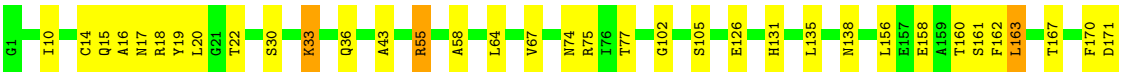

• Molecule 1: COAT PROTEIN

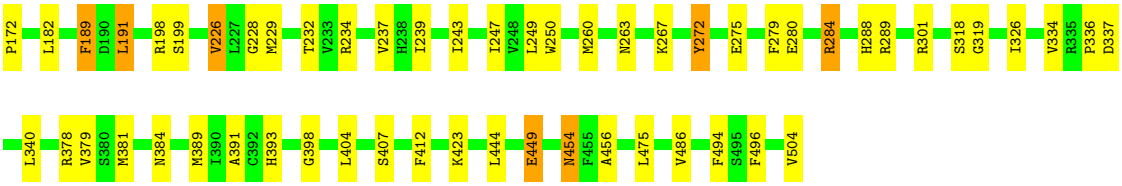
Chain CM: 79% 19%




• Molecule 1: COAT PROTEIN

Chain CN: 82% 16%



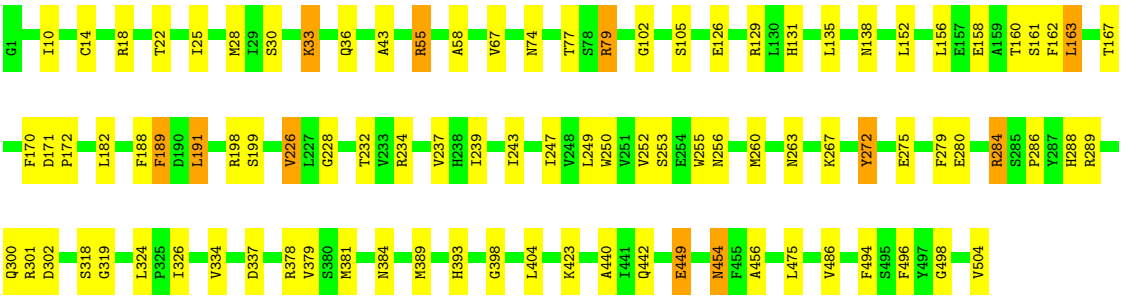



• Molecule 1: COAT PROTEIN

Chain CO: 80% 18% •

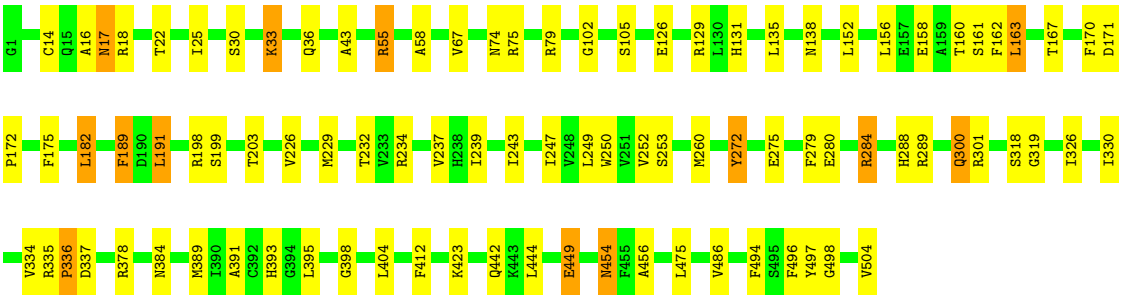
• Molecule 1: COAT PROTEIN

Chain CP: 81% 16% •



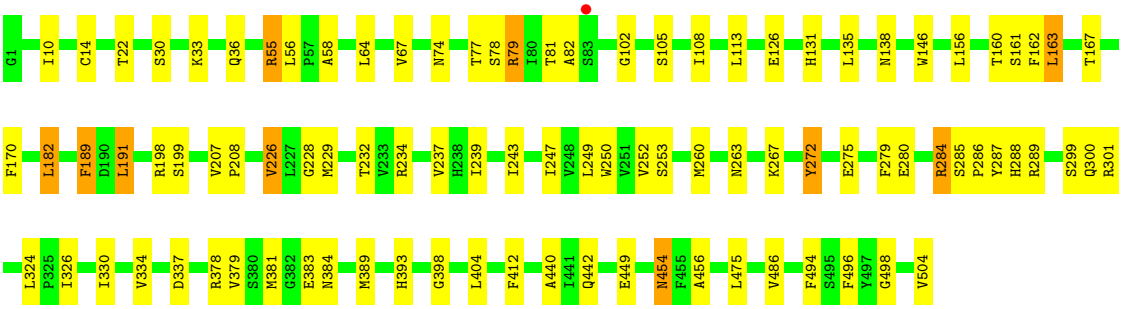

• Molecule 1: COAT PROTEIN

Chain CQ: 82% 16% •



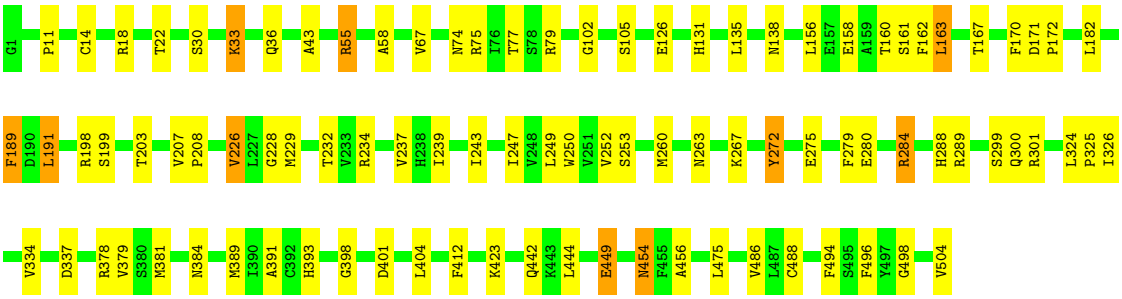

• Molecule 1: COAT PROTEIN

Chain CR:



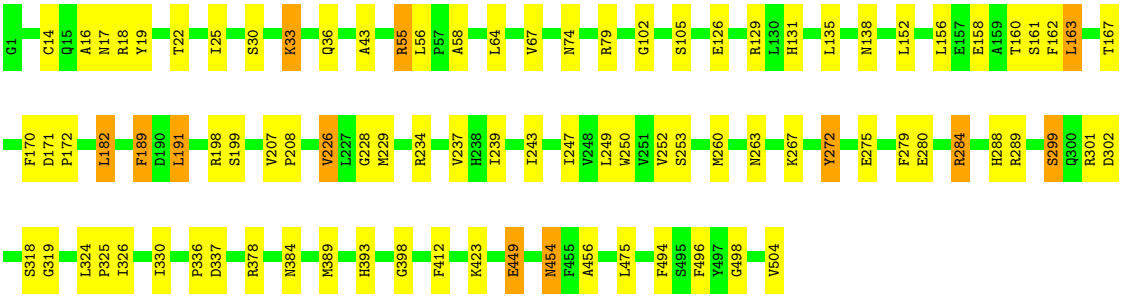

- Molecule 1: COAT PROTEIN

Chain CS:




- Molecule 1: COAT PROTEIN

Chain CT:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 279.40Å 279.60Å 293.30Å<br>102.40° 116.40° 108.20° | Depositor |
| Resolution (Å) | 135.43 – 3.00<br>135.43 – 3.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 88.3 (135.43-3.00)<br>96.3 (135.43-3.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.98 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, $R_{free}$ | 0.190 , 0.207<br>0.187 , 0.204 | Depositor<br>DCC |
| $R_{free}$ test set | 66376 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 42.7 | Xtriage |
| Anisotropy | 0.260 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 38.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.000 for k,h,-h-k-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 237060 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | AA | 0.50 | 0/4058 | 0.61 | 2/5517 (0.0%) |
| 1 | AB | 0.50 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | AC | 0.49 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AD | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AE | 0.53 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AF | 0.49 | 1/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | AG | 0.49 | 1/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | AH | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AI | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AJ | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AK | 0.48 | 2/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | AL | 0.53 | 2/4058 (0.0%) | 0.64 | 0/5517 |
| 1 | AM | 0.51 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | AN | 0.50 | 1/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AO | 0.52 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | AP | 0.51 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AQ | 0.50 | 1/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | AR | 0.52 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AS | 0.51 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AT | 0.49 | 1/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | BA | 0.49 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BB | 0.52 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | BC | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BD | 0.48 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BE | 0.50 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BF | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BG | 0.50 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | BH | 0.49 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BI | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BJ | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BK | 0.49 | 2/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | BL | 0.52 | 3/4058 (0.1%) | 0.62 | 0/5517 |
| 1 | BM | 0.53 | 3/4058 (0.1%) | 0.64 | 1/5517 (0.0%) |
| 1 | BN | 0.51 | 2/4058 (0.0%) | 0.63 | 0/5517 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | BO | 0.51 | 3/4058 (0.1%) | 0.63 | 0/5517 |
| 1 | BP | 0.53 | 2/4058 (0.0%) | 0.65 | 1/5517 (0.0%) |
| 1 | BQ | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BR | 0.51 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | BS | 0.50 | 0/4058 | 0.62 | 0/5517 |
| 1 | BT | 0.48 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CA | 0.51 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CB | 0.51 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | CC | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CD | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CE | 0.50 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CF | 0.48 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CG | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CH | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CI | 0.50 | 1/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | CJ | 0.50 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | CK | 0.48 | 0/4058 | 0.62 | 0/5517 |
| 1 | CL | 0.52 | 1/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | CM | 0.51 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CN | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CO | 0.51 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CP | 0.52 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CQ | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CR | 0.53 | 3/4058 (0.1%) | 0.64 | 1/5517 (0.0%) |
| 1 | CS | 0.52 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CT | 0.50 | 1/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| All | All | 0.50 | 95/243480 (0.0%) | 0.62 | 20/331020 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | AA | 0 | 2 |
| 1 | AB | 0 | 2 |
| 1 | AC | 0 | 2 |
| 1 | AD | 0 | 1 |
| 1 | AE | 0 | 1 |
| 1 | AF | 0 | 2 |
| 1 | AG | 0 | 2 |
| 1 | AH | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | AI | 0 | 2 |
| 1 | AJ | 0 | 2 |
| 1 | AK | 0 | 1 |
| 1 | AL | 0 | 1 |
| 1 | AM | 0 | 2 |
| 1 | AN | 0 | 2 |
| 1 | AO | 0 | 2 |
| 1 | AP | 0 | 2 |
| 1 | AQ | 0 | 1 |
| 1 | AR | 0 | 2 |
| 1 | AS | 0 | 2 |
| 1 | AT | 0 | 2 |
| 1 | BA | 0 | 2 |
| 1 | BB | 0 | 2 |
| 1 | BC | 0 | 1 |
| 1 | BD | 0 | 2 |
| 1 | BE | 0 | 1 |
| 1 | BF | 0 | 2 |
| 1 | BG | 0 | 2 |
| 1 | BH | 0 | 1 |
| 1 | BI | 0 | 1 |
| 1 | BJ | 0 | 2 |
| 1 | BK | 0 | 2 |
| 1 | BL | 0 | 2 |
| 1 | BM | 0 | 1 |
| 1 | BN | 0 | 2 |
| 1 | BO | 0 | 2 |
| 1 | BP | 0 | 1 |
| 1 | BQ | 0 | 2 |
| 1 | BR | 0 | 2 |
| 1 | BS | 0 | 2 |
| 1 | BT | 0 | 2 |
| 1 | CA | 0 | 2 |
| 1 | CB | 0 | 2 |
| 1 | CC | 0 | 2 |
| 1 | CD | 0 | 2 |
| 1 | CE | 0 | 2 |
| 1 | CF | 0 | 2 |
| 1 | CG | 0 | 2 |
| 1 | CH | 0 | 2 |
| 1 | CI | 0 | 2 |
| 1 | CJ | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | CK | 0 | 2 |
| 1 | CL | 0 | 2 |
| 1 | CM | 0 | 2 |
| 1 | CN | 0 | 2 |
| 1 | CO | 0 | 1 |
| 1 | CP | 0 | 2 |
| 1 | CQ | 0 | 2 |
| 1 | CR | 0 | 1 |
| 1 | CS | 0 | 2 |
| 1 | CT | 0 | 2 |
| All | All | 0 | 107 |

All (95) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | BM | 189 | PHE | CE1-CZ | -6.84 | 1.24 | 1.37 |
| 1 | AL | 189 | PHE | CE1-CZ | -6.45 | 1.25 | 1.37 |
| 1 | CJ | 189 | PHE | CE1-CZ | -6.29 | 1.25 | 1.37 |
| 1 | BL | 189 | PHE | CE1-CZ | -6.29 | 1.25 | 1.37 |
| 1 | BN | 189 | PHE | CE1-CZ | -6.23 | 1.25 | 1.37 |
| 1 | BR | 189 | PHE | CE1-CZ | -6.22 | 1.25 | 1.37 |
| 1 | CP | 189 | PHE | CE1-CZ | -6.21 | 1.25 | 1.37 |
| 1 | CS | 189 | PHE | CE1-CZ | -6.20 | 1.25 | 1.37 |
| 1 | BH | 189 | PHE | CE1-CZ | -6.17 | 1.25 | 1.37 |
| 1 | AG | 189 | PHE | CE1-CZ | -6.12 | 1.25 | 1.37 |
| 1 | BQ | 189 | PHE | CE1-CZ | -6.11 | 1.25 | 1.37 |
| 1 | BR | 189 | PHE | CE2-CZ | -6.08 | 1.25 | 1.37 |
| 1 | CA | 1 | GLY | N-CA | -6.08 | 1.36 | 1.46 |
| 1 | AP | 189 | PHE | CE1-CZ | -6.03 | 1.25 | 1.37 |
| 1 | BK | 189 | PHE | CE1-CZ | -6.03 | 1.25 | 1.37 |
| 1 | AK | 189 | PHE | CE1-CZ | -6.01 | 1.25 | 1.37 |
| 1 | BN | 189 | PHE | CE2-CZ | -5.99 | 1.25 | 1.37 |
| 1 | AI | 189 | PHE | CE1-CZ | -5.99 | 1.25 | 1.37 |
| 1 | AP | 189 | PHE | CE2-CZ | -5.95 | 1.26 | 1.37 |
| 1 | BM | 189 | PHE | CE2-CZ | -5.93 | 1.26 | 1.37 |
| 1 | CI | 189 | PHE | CE1-CZ | -5.92 | 1.26 | 1.37 |
| 1 | CN | 189 | PHE | CE1-CZ | -5.92 | 1.26 | 1.37 |
| 1 | AH | 189 | PHE | CE1-CZ | -5.88 | 1.26 | 1.37 |
| 1 | CQ | 189 | PHE | CE1-CZ | -5.87 | 1.26 | 1.37 |
| 1 | AM | 189 | PHE | CE1-CZ | -5.86 | 1.26 | 1.37 |
| 1 | AE | 189 | PHE | CE1-CZ | -5.83 | 1.26 | 1.37 |
| 1 | AD | 189 | PHE | CE1-CZ | -5.80 | 1.26 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | BO | 189 | PHE | CE1-CZ | -5.78 | 1.26 | 1.37 |
| 1 | CB | 189 | PHE | CE1-CZ | -5.78 | 1.26 | 1.37 |
| 1 | AC | 189 | PHE | CE1-CZ | -5.77 | 1.26 | 1.37 |
| 1 | BC | 189 | PHE | CE1-CZ | -5.73 | 1.26 | 1.37 |
| 1 | BG | 189 | PHE | CE2-CZ | -5.72 | 1.26 | 1.37 |
| 1 | BH | 189 | PHE | CE2-CZ | -5.70 | 1.26 | 1.37 |
| 1 | BK | 189 | PHE | CE2-CZ | -5.68 | 1.26 | 1.37 |
| 1 | CR | 189 | PHE | CE1-CZ | -5.68 | 1.26 | 1.37 |
| 1 | AO | 189 | PHE | CE1-CZ | -5.67 | 1.26 | 1.37 |
| 1 | AE | 189 | PHE | CE2-CZ | -5.66 | 1.26 | 1.37 |
| 1 | AM | 189 | PHE | CE2-CZ | -5.63 | 1.26 | 1.37 |
| 1 | BF | 189 | PHE | CE1-CZ | -5.60 | 1.26 | 1.37 |
| 1 | BI | 189 | PHE | CE1-CZ | -5.59 | 1.26 | 1.37 |
| 1 | CM | 189 | PHE | CE1-CZ | -5.59 | 1.26 | 1.37 |
| 1 | AO | 189 | PHE | CE2-CZ | -5.58 | 1.26 | 1.37 |
| 1 | CQ | 189 | PHE | CE2-CZ | -5.55 | 1.26 | 1.37 |
| 1 | BG | 189 | PHE | CE1-CZ | -5.55 | 1.26 | 1.37 |
| 1 | BL | 9 | TYR | CE2-CZ | 5.53 | 1.45 | 1.38 |
| 1 | BE | 189 | PHE | CE1-CZ | -5.50 | 1.26 | 1.37 |
| 1 | AI | 189 | PHE | CE2-CZ | -5.49 | 1.26 | 1.37 |
| 1 | AJ | 189 | PHE | CE1-CZ | -5.48 | 1.26 | 1.37 |
| 1 | BB | 189 | PHE | CE1-CZ | -5.48 | 1.26 | 1.37 |
| 1 | CP | 189 | PHE | CE2-CZ | -5.48 | 1.26 | 1.37 |
| 1 | CH | 189 | PHE | CE1-CZ | -5.48 | 1.26 | 1.37 |
| 1 | CT | 189 | PHE | CE1-CZ | -5.45 | 1.26 | 1.37 |
| 1 | AB | 189 | PHE | CE1-CZ | -5.45 | 1.26 | 1.37 |
| 1 | BJ | 189 | PHE | CE1-CZ | -5.44 | 1.27 | 1.37 |
| 1 | CF | 189 | PHE | CE1-CZ | -5.43 | 1.27 | 1.37 |
| 1 | BD | 189 | PHE | CE1-CZ | -5.42 | 1.27 | 1.37 |
| 1 | BB | 189 | PHE | CE2-CZ | -5.42 | 1.27 | 1.37 |
| 1 | AD | 189 | PHE | CE2-CZ | -5.37 | 1.27 | 1.37 |
| 1 | AS | 189 | PHE | CE2-CZ | -5.37 | 1.27 | 1.37 |
| 1 | AF | 189 | PHE | CE1-CZ | -5.35 | 1.27 | 1.37 |
| 1 | AN | 189 | PHE | CE1-CZ | -5.35 | 1.27 | 1.37 |
| 1 | BF | 189 | PHE | CE2-CZ | -5.33 | 1.27 | 1.37 |
| 1 | CR | 189 | PHE | CE2-CZ | -5.33 | 1.27 | 1.37 |
| 1 | BP | 189 | PHE | CE2-CZ | -5.33 | 1.27 | 1.37 |
| 1 | AT | 189 | PHE | CE1-CZ | -5.32 | 1.27 | 1.37 |
| 1 | CC | 189 | PHE | CE1-CZ | -5.30 | 1.27 | 1.37 |
| 1 | AL | 189 | PHE | CE2-CZ | -5.30 | 1.27 | 1.37 |
| 1 | CG | 189 | PHE | CE1-CZ | -5.30 | 1.27 | 1.37 |
| 1 | CB | 189 | PHE | CE2-CZ | -5.30 | 1.27 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | BP | 189 | PHE | CE1-CZ | -5.29 | 1.27 | 1.37 |
| 1 | AB | 189 | PHE | CE2-CZ | -5.28 | 1.27 | 1.37 |
| 1 | BL | 189 | PHE | CE2-CZ | -5.28 | 1.27 | 1.37 |
| 1 | AC | 189 | PHE | CE2-CZ | -5.26 | 1.27 | 1.37 |
| 1 | BE | 189 | PHE | CE2-CZ | -5.25 | 1.27 | 1.37 |
| 1 | BM | 189 | PHE | CG-CD1 | -5.25 | 1.30 | 1.38 |
| 1 | BD | 189 | PHE | CE2-CZ | -5.24 | 1.27 | 1.37 |
| 1 | CO | 189 | PHE | CE1-CZ | -5.23 | 1.27 | 1.37 |
| 1 | BQ | 189 | PHE | CE2-CZ | -5.22 | 1.27 | 1.37 |
| 1 | BA | 189 | PHE | CE1-CZ | -5.20 | 1.27 | 1.37 |
| 1 | BO | 383 | GLU | CG-CD | 5.18 | 1.59 | 1.51 |
| 1 | AH | 189 | PHE | CE2-CZ | -5.13 | 1.27 | 1.37 |
| 1 | CJ | 189 | PHE | CE2-CZ | -5.12 | 1.27 | 1.37 |
| 1 | AQ | 189 | PHE | CE1-CZ | -5.10 | 1.27 | 1.37 |
| 1 | CE | 189 | PHE | CE1-CZ | -5.10 | 1.27 | 1.37 |
| 1 | CD | 189 | PHE | CE1-CZ | -5.10 | 1.27 | 1.37 |
| 1 | BT | 189 | PHE | CE2-CZ | -5.09 | 1.27 | 1.37 |
| 1 | CD | 189 | PHE | CE2-CZ | -5.09 | 1.27 | 1.37 |
| 1 | BO | 189 | PHE | CE2-CZ | -5.09 | 1.27 | 1.37 |
| 1 | CL | 189 | PHE | CE2-CZ | -5.08 | 1.27 | 1.37 |
| 1 | CO | 189 | PHE | CE2-CZ | -5.08 | 1.27 | 1.37 |
| 1 | AK | 189 | PHE | CE2-CZ | -5.06 | 1.27 | 1.37 |
| 1 | CS | 189 | PHE | CE2-CZ | -5.06 | 1.27 | 1.37 |
| 1 | AR | 9 | TYR | CD1-CE1 | 5.06 | 1.47 | 1.39 |
| 1 | AR | 383 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |
| 1 | CR | 383 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 284 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 1 | CJ | 56 | LEU | CA-CB-CG | 5.46 | 127.86 | 115.30 |
| 1 | AF | 56 | LEU | CA-CB-CG | 5.34 | 127.57 | 115.30 |
| 1 | CT | 56 | LEU | CA-CB-CG | 5.29 | 127.46 | 115.30 |
| 1 | AR | 56 | LEU | CA-CB-CG | 5.25 | 127.36 | 115.30 |
| 1 | BR | 56 | LEU | CA-CB-CG | 5.24 | 127.36 | 115.30 |
| 1 | CR | 56 | LEU | CA-CB-CG | 5.24 | 127.34 | 115.30 |
| 1 | AM | 56 | LEU | CA-CB-CG | 5.24 | 127.34 | 115.30 |
| 1 | BP | 56 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 1 | BM | 56 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 1 | AE | 56 | LEU | CA-CB-CG | 5.20 | 127.27 | 115.30 |
| 1 | CI | 56 | LEU | CA-CB-CG | 5.20 | 127.27 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | BB | 56 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 1 | AB | 56 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 1 | CL | 56 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 1 | AP | 56 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | AA | 56 | LEU | CA-CB-CG | 5.09 | 127.01 | 115.30 |
| 1 | AN | 56 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 1 | BG | 56 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 |
| 1 | CB | 56 | LEU | CA-CB-CG | 5.01 | 126.82 | 115.30 |

There are no chirality outliers.

All (107) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 33 | LYS | Peptide |
| 1 | AA | 55 | ARG | Peptide |
| 1 | AB | 33 | LYS | Peptide |
| 1 | AB | 55 | ARG | Peptide |
| 1 | AC | 33 | LYS | Peptide |
| 1 | AC | 55 | ARG | Peptide |
| 1 | AD | 55 | ARG | Peptide |
| 1 | AE | 55 | ARG | Peptide |
| 1 | AF | 33 | LYS | Peptide |
| 1 | AF | 55 | ARG | Peptide |
| 1 | AG | 33 | LYS | Peptide |
| 1 | AG | 55 | ARG | Peptide |
| 1 | AH | 33 | LYS | Peptide |
| 1 | AH | 55 | ARG | Peptide |
| 1 | AI | 33 | LYS | Peptide |
| 1 | AI | 55 | ARG | Peptide |
| 1 | AJ | 33 | LYS | Peptide |
| 1 | AJ | 55 | ARG | Peptide |
| 1 | AK | 55 | ARG | Peptide |
| 1 | AL | 55 | ARG | Peptide |
| 1 | AM | 33 | LYS | Peptide |
| 1 | AM | 55 | ARG | Peptide |
| 1 | AN | 33 | LYS | Peptide |
| 1 | AN | 55 | ARG | Peptide |
| 1 | AO | 33 | LYS | Peptide |
| 1 | AO | 55 | ARG | Peptide |
| 1 | AP | 33 | LYS | Peptide |
| 1 | AP | 55 | ARG | Peptide |
| 1 | AQ | 55 | ARG | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AR | 33 | LYS | Peptide |
| 1 | AR | 55 | ARG | Peptide |
| 1 | AS | 33 | LYS | Peptide |
| 1 | AS | 55 | ARG | Peptide |
| 1 | AT | 33 | LYS | Peptide |
| 1 | AT | 55 | ARG | Peptide |
| 1 | BA | 33 | LYS | Peptide |
| 1 | BA | 55 | ARG | Peptide |
| 1 | BB | 33 | LYS | Peptide |
| 1 | BB | 55 | ARG | Peptide |
| 1 | BC | 55 | ARG | Peptide |
| 1 | BD | 33 | LYS | Peptide |
| 1 | BD | 55 | ARG | Peptide |
| 1 | BE | 55 | ARG | Peptide |
| 1 | BF | 33 | LYS | Peptide |
| 1 | BF | 55 | ARG | Peptide |
| 1 | BG | 33 | LYS | Peptide |
| 1 | BG | 55 | ARG | Peptide |
| 1 | BH | 55 | ARG | Peptide |
| 1 | BI | 55 | ARG | Peptide |
| 1 | BJ | 33 | LYS | Peptide |
| 1 | BJ | 55 | ARG | Peptide |
| 1 | BK | 33 | LYS | Peptide |
| 1 | BK | 55 | ARG | Peptide |
| 1 | BL | 33 | LYS | Peptide |
| 1 | BL | 55 | ARG | Peptide |
| 1 | BM | 55 | ARG | Peptide |
| 1 | BN | 33 | LYS | Peptide |
| 1 | BN | 55 | ARG | Peptide |
| 1 | BO | 33 | LYS | Peptide |
| 1 | BO | 55 | ARG | Peptide |
| 1 | BP | 55 | ARG | Peptide |
| 1 | BQ | 33 | LYS | Peptide |
| 1 | BQ | 55 | ARG | Peptide |
| 1 | BR | 33 | LYS | Peptide |
| 1 | BR | 55 | ARG | Peptide |
| 1 | BS | 33 | LYS | Peptide |
| 1 | BS | 55 | ARG | Peptide |
| 1 | BT | 33 | LYS | Peptide |
| 1 | BT | 55 | ARG | Peptide |
| 1 | CA | 33 | LYS | Peptide |
| 1 | CA | 55 | ARG | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | CB | 33 | LYS | Peptide |
| 1 | CB | 55 | ARG | Peptide |
| 1 | CC | 33 | LYS | Peptide |
| 1 | CC | 55 | ARG | Peptide |
| 1 | CD | 33 | LYS | Peptide |
| 1 | CD | 55 | ARG | Peptide |
| 1 | CE | 33 | LYS | Peptide |
| 1 | CE | 55 | ARG | Peptide |
| 1 | CF | 33 | LYS | Peptide |
| 1 | CF | 55 | ARG | Peptide |
| 1 | CG | 33 | LYS | Peptide |
| 1 | CG | 55 | ARG | Peptide |
| 1 | CH | 33 | LYS | Peptide |
| 1 | CH | 55 | ARG | Peptide |
| 1 | CI | 33 | LYS | Peptide |
| 1 | CI | 55 | ARG | Peptide |
| 1 | CJ | 33 | LYS | Peptide |
| 1 | CJ | 55 | ARG | Peptide |
| 1 | CK | 33 | LYS | Peptide |
| 1 | CK | 55 | ARG | Peptide |
| 1 | CL | 33 | LYS | Peptide |
| 1 | CL | 55 | ARG | Peptide |
| 1 | CM | 33 | LYS | Peptide |
| 1 | CM | 55 | ARG | Peptide |
| 1 | CN | 33 | LYS | Peptide |
| 1 | CN | 55 | ARG | Peptide |
| 1 | CO | 55 | ARG | Peptide |
| 1 | CP | 33 | LYS | Peptide |
| 1 | CP | 55 | ARG | Peptide |
| 1 | CQ | 33 | LYS | Peptide |
| 1 | CQ | 55 | ARG | Peptide |
| 1 | CR | 55 | ARG | Peptide |
| 1 | CS | 33 | LYS | Peptide |
| 1 | CS | 55 | ARG | Peptide |
| 1 | CT | 33 | LYS | Peptide |
| 1 | CT | 55 | ARG | Peptide |

## 5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | AA | 3951 | 0 | 3909 | 91 | 0 |
| 1 | AB | 3951 | 0 | 3909 | 89 | 0 |
| 1 | AC | 3951 | 0 | 3909 | 87 | 0 |
| 1 | AD | 3951 | 0 | 3909 | 93 | 0 |
| 1 | AE | 3951 | 0 | 3909 | 86 | 0 |
| 1 | AF | 3951 | 0 | 3909 | 92 | 0 |
| 1 | AG | 3951 | 0 | 3909 | 91 | 0 |
| 1 | AH | 3951 | 0 | 3909 | 90 | 0 |
| 1 | AI | 3951 | 0 | 3909 | 88 | 0 |
| 1 | AJ | 3951 | 0 | 3909 | 86 | 0 |
| 1 | AK | 3951 | 0 | 3909 | 88 | 0 |
| 1 | AL | 3951 | 0 | 3909 | 87 | 0 |
| 1 | AM | 3951 | 0 | 3909 | 83 | 0 |
| 1 | AN | 3951 | 0 | 3909 | 104 | 0 |
| 1 | AO | 3951 | 0 | 3909 | 91 | 0 |
| 1 | AP | 3951 | 0 | 3909 | 87 | 0 |
| 1 | AQ | 3951 | 0 | 3909 | 85 | 0 |
| 1 | AR | 3951 | 0 | 3909 | 88 | 0 |
| 1 | AS | 3951 | 0 | 3909 | 89 | 0 |
| 1 | AT | 3951 | 0 | 3909 | 91 | 0 |
| 1 | BA | 3951 | 0 | 3909 | 93 | 0 |
| 1 | BB | 3951 | 0 | 3909 | 97 | 0 |
| 1 | BC | 3951 | 0 | 3909 | 85 | 0 |
| 1 | BD | 3951 | 0 | 3909 | 78 | 0 |
| 1 | BE | 3951 | 0 | 3909 | 86 | 0 |
| 1 | BF | 3951 | 0 | 3909 | 92 | 0 |
| 1 | BG | 3951 | 0 | 3909 | 92 | 0 |
| 1 | BH | 3951 | 0 | 3909 | 97 | 0 |
| 1 | BI | 3951 | 0 | 3909 | 89 | 0 |
| 1 | BJ | 3951 | 0 | 3909 | 93 | 0 |
| 1 | BK | 3951 | 0 | 3909 | 81 | 0 |
| 1 | BL | 3951 | 0 | 3909 | 89 | 0 |
| 1 | BM | 3951 | 0 | 3909 | 89 | 0 |
| 1 | BN | 3951 | 0 | 3909 | 80 | 0 |
| 1 | BO | 3951 | 0 | 3909 | 93 | 0 |
| 1 | BP | 3951 | 0 | 3909 | 93 | 0 |
| 1 | BQ | 3951 | 0 | 3909 | 83 | 0 |
| 1 | BR | 3951 | 0 | 3909 | 90 | 0 |
| 1 | BS | 3951 | 0 | 3909 | 87 | 0 |
| 1 | BT | 3951 | 0 | 3909 | 87 | 0 |
| 1 | CA | 3951 | 0 | 3909 | 81 | 0 |
| 1 | CB | 3951 | 0 | 3909 | 87 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | CC | 3951 | 0 | 3909 | 84 | 0 |
| 1 | CD | 3951 | 0 | 3909 | 89 | 0 |
| 1 | CE | 3951 | 0 | 3909 | 97 | 0 |
| 1 | CF | 3951 | 0 | 3909 | 94 | 0 |
| 1 | CG | 3951 | 0 | 3909 | 92 | 0 |
| 1 | CH | 3951 | 0 | 3909 | 91 | 0 |
| 1 | CI | 3951 | 0 | 3909 | 92 | 0 |
| 1 | CJ | 3951 | 0 | 3909 | 94 | 0 |
| 1 | CK | 3951 | 0 | 3909 | 84 | 0 |
| 1 | CL | 3951 | 0 | 3909 | 81 | 0 |
| 1 | CM | 3951 | 0 | 3909 | 93 | 0 |
| 1 | CN | 3951 | 0 | 3909 | 81 | 0 |
| 1 | CO | 3951 | 0 | 3909 | 96 | 0 |
| 1 | CP | 3951 | 0 | 3909 | 85 | 0 |
| 1 | CQ | 3951 | 0 | 3909 | 85 | 0 |
| 1 | CR | 3951 | 0 | 3909 | 86 | 0 |
| 1 | CS | 3951 | 0 | 3909 | 86 | 0 |
| 1 | CT | 3951 | 0 | 3909 | 76 | 0 |
| All | All | 237060 | 0 | 234540 | 4775 | 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 10.

All (4775) 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:CF:79:ARG:HH11 | 1:CF:79:ARG:HG3 | 1.18 | 1.07 |
| 1:CC:250:TRP:CZ3 | 1:CC:272:TYR:HE1 | 1.77 | 1.02 |
| 1:BO:250:TRP:CZ3 | 1:BO:272:TYR:HE1 | 1.83 | 0.97 |
| 1:BS:79:ARG:HG3 | 1:BS:79:ARG:HH11 | 1.31 | 0.96 |
| 1:BJ:250:TRP:CZ3 | 1:BJ:272:TYR:HE1 | 1.85 | 0.94 |
| 1:CC:250:TRP:CZ3 | 1:CC:272:TYR:CE1 | 2.54 | 0.94 |
| 1:BP:250:TRP:CZ3 | 1:BP:272:TYR:HE1 | 1.85 | 0.94 |
| 1:CD:79:ARG:HG3 | 1:CD:79:ARG:HH11 | 1.34 | 0.93 |
| 1:AS:250:TRP:CZ3 | 1:AS:272:TYR:HE1 | 1.87 | 0.92 |
| 1:BJ:191:LEU:H | 1:BJ:191:LEU:HD23 | 1.34 | 0.92 |
| 1:BJ:250:TRP:CZ3 | 1:BJ:272:TYR:CE1 | 2.58 | 0.91 |
| 1:BO:250:TRP:CZ3 | 1:BO:272:TYR:CE1 | 2.58 | 0.91 |
| 1:BJ:79:ARG:HH11 | 1:BJ:79:ARG:HG3 | 1.35 | 0.91 |
| 1:AS:250:TRP:CZ3 | 1:AS:272:TYR:CE1 | 2.59 | 0.91 |
| 1:BE:191:LEU:HD23 | 1:BE:191:LEU:H | 1.36 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AJ:191:LEU:HD23 | 1:AJ:191:LEU:H | 1.34 | 0.90 |
| 1:AL:191:LEU:HD23 | 1:AL:191:LEU:H | 1.37 | 0.89 |
| 1:AP:191:LEU:HD23 | 1:AP:191:LEU:H | 1.36 | 0.89 |
| 1:AC:191:LEU:H | 1:AC:191:LEU:HD23 | 1.36 | 0.89 |
| 1:AM:191:LEU:HD23 | 1:AM:191:LEU:H | 1.38 | 0.89 |
| 1:AR:191:LEU:HD23 | 1:AR:191:LEU:H | 1.38 | 0.89 |
| 1:BP:250:TRP:CZ3 | 1:BP:272:TYR:CE1 | 2.60 | 0.89 |
| 1:AB:191:LEU:HD23 | 1:AB:191:LEU:H | 1.37 | 0.89 |
| 1:AG:79:ARG:HH11 | 1:AG:79:ARG:HG3 | 1.36 | 0.89 |
| 1:AO:191:LEU:HD23 | 1:AO:191:LEU:H | 1.37 | 0.89 |
| 1:AA:55:ARG:NE | 1:CC:272:TYR:HE2 | 1.71 | 0.89 |
| 1:BP:191:LEU:HD23 | 1:BP:191:LEU:H | 1.37 | 0.89 |
| 1:CC:191:LEU:HD23 | 1:CC:191:LEU:H | 1.38 | 0.89 |
| 1:AN:79:ARG:HH11 | 1:AN:79:ARG:HG3 | 1.38 | 0.88 |
| 1:AG:191:LEU:HD23 | 1:AG:191:LEU:H | 1.38 | 0.88 |
| 1:CP:191:LEU:HD23 | 1:CP:191:LEU:H | 1.38 | 0.88 |
| 1:CE:191:LEU:HD23 | 1:CE:191:LEU:H | 1.39 | 0.88 |
| 1:BH:15:GLN:HE21 | 1:BH:15:GLN:HA | 1.38 | 0.88 |
| 1:AE:191:LEU:HD23 | 1:AE:191:LEU:H | 1.39 | 0.88 |
| 1:BD:191:LEU:HD23 | 1:BD:191:LEU:H | 1.39 | 0.88 |
| 1:CI:191:LEU:H | 1:CI:191:LEU:HD23 | 1.37 | 0.88 |
| 1:BB:191:LEU:HD23 | 1:BB:191:LEU:H | 1.39 | 0.88 |
| 1:BM:191:LEU:H | 1:BM:191:LEU:HD23 | 1.38 | 0.88 |
| 1:CQ:191:LEU:HD23 | 1:CQ:191:LEU:H | 1.37 | 0.87 |
| 1:AQ:191:LEU:HD23 | 1:AQ:191:LEU:H | 1.39 | 0.87 |
| 1:CD:191:LEU:HD23 | 1:CD:191:LEU:H | 1.39 | 0.87 |
| 1:CO:250:TRP:CZ3 | 1:CO:272:TYR:CE1 | 2.63 | 0.87 |
| 1:AL:79:ARG:HG3 | 1:AL:79:ARG:HH11 | 1.39 | 0.87 |
| 1:CB:191:LEU:HD23 | 1:CB:191:LEU:H | 1.39 | 0.87 |
| 1:CL:191:LEU:H | 1:CL:191:LEU:HD23 | 1.39 | 0.87 |
| 1:AA:191:LEU:HD23 | 1:AA:191:LEU:H | 1.37 | 0.87 |
| 1:BQ:191:LEU:HD23 | 1:BQ:191:LEU:H | 1.40 | 0.87 |
| 1:AA:55:ARG:NE | 1:CC:272:TYR:CE2 | 2.42 | 0.87 |
| 1:BI:191:LEU:HD23 | 1:BI:191:LEU:H | 1.39 | 0.87 |
| 1:BF:191:LEU:HD23 | 1:BF:191:LEU:H | 1.40 | 0.87 |
| 1:BG:191:LEU:HD23 | 1:BG:191:LEU:H | 1.39 | 0.87 |
| 1:BO:272:TYR:HE2 | 1:BR:55:ARG:NE | 1.73 | 0.87 |
| 1:CM:191:LEU:HD23 | 1:CM:191:LEU:H | 1.39 | 0.86 |
| 1:AO:250:TRP:CZ3 | 1:AO:272:TYR:CE1 | 2.63 | 0.86 |
| 1:BO:191:LEU:HD23 | 1:BO:191:LEU:H | 1.38 | 0.86 |
| 1:BP:272:TYR:HE2 | 1:CE:55:ARG:NE | 1.72 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:191:LEU:HD23 | 1:AK:191:LEU:H | 1.38 | 0.86 |
| 1:CJ:250:TRP:CZ3 | 1:CJ:272:TYR:HE1 | 1.94 | 0.86 |
| 1:CK:191:LEU:HD23 | 1:CK:191:LEU:H | 1.40 | 0.86 |
| 1:CF:191:LEU:HD23 | 1:CF:191:LEU:H | 1.39 | 0.86 |
| 1:CR:191:LEU:HD23 | 1:CR:191:LEU:H | 1.41 | 0.86 |
| 1:BC:191:LEU:HD23 | 1:BC:191:LEU:H | 1.40 | 0.86 |
| 1:CQ:250:TRP:CZ3 | 1:CQ:272:TYR:CE1 | 2.64 | 0.86 |
| 1:AD:191:LEU:HD23 | 1:AD:191:LEU:H | 1.40 | 0.86 |
| 1:BH:191:LEU:HD23 | 1:BH:191:LEU:H | 1.40 | 0.86 |
| 1:BS:191:LEU:HD23 | 1:BS:191:LEU:H | 1.40 | 0.86 |
| 1:BT:191:LEU:HD23 | 1:BT:191:LEU:H | 1.40 | 0.86 |
| 1:CM:250:TRP:CZ3 | 1:CM:272:TYR:CE1 | 2.64 | 0.86 |
| 1:CN:189:PHE:HE1 | 1:CN:198:ARG:HG3 | 1.41 | 0.86 |
| 1:CJ:250:TRP:CZ3 | 1:CJ:272:TYR:CE1 | 2.63 | 0.86 |
| 1:AG:250:TRP:CZ3 | 1:AG:272:TYR:CE1 | 2.64 | 0.85 |
| 1:BJ:189:PHE:HE1 | 1:BJ:198:ARG:HG3 | 1.40 | 0.85 |
| 1:CH:191:LEU:HD23 | 1:CH:191:LEU:H | 1.39 | 0.85 |
| 1:AF:79:ARG:HG3 | 1:AF:79:ARG:HH11 | 1.38 | 0.85 |
| 1:BK:191:LEU:HD23 | 1:BK:191:LEU:H | 1.41 | 0.85 |
| 1:CO:191:LEU:HD23 | 1:CO:191:LEU:H | 1.42 | 0.85 |
| 1:BR:191:LEU:HD23 | 1:BR:191:LEU:H | 1.42 | 0.85 |
| 1:CP:250:TRP:CZ3 | 1:CP:272:TYR:CE1 | 2.65 | 0.85 |
| 1:BP:272:TYR:CE2 | 1:CE:55:ARG:NE | 2.44 | 0.85 |
| 1:CB:189:PHE:HE1 | 1:CB:198:ARG:CG | 1.90 | 0.85 |
| 1:CS:191:LEU:HD23 | 1:CS:191:LEU:H | 1.42 | 0.85 |
| 1:CR:189:PHE:HE1 | 1:CR:198:ARG:CG | 1.89 | 0.85 |
| 1:AT:191:LEU:HD23 | 1:AT:191:LEU:H | 1.42 | 0.85 |
| 1:AT:250:TRP:CZ3 | 1:AT:272:TYR:CE1 | 2.65 | 0.85 |
| 1:CG:189:PHE:HE1 | 1:CG:198:ARG:CG | 1.90 | 0.85 |
| 1:BT:250:TRP:CZ3 | 1:BT:272:TYR:CE1 | 2.65 | 0.84 |
| 1:AO:272:TYR:CE2 | 1:AR:55:ARG:NE | 2.45 | 0.84 |
| 1:CN:191:LEU:HD23 | 1:CN:191:LEU:H | 1.40 | 0.84 |
| 1:CO:250:TRP:CZ3 | 1:CO:272:TYR:HE1 | 1.95 | 0.84 |
| 1:AN:55:ARG:NE | 1:AS:272:TYR:CE2 | 2.45 | 0.84 |
| 1:BN:189:PHE:HE1 | 1:BN:198:ARG:CG | 1.91 | 0.84 |
| 1:BO:272:TYR:CE2 | 1:BR:55:ARG:NE | 2.45 | 0.84 |
| 1:BA:191:LEU:HD23 | 1:BA:191:LEU:H | 1.42 | 0.84 |
| 1:CG:191:LEU:HD23 | 1:CG:191:LEU:H | 1.40 | 0.84 |
| 1:AN:189:PHE:HE1 | 1:AN:198:ARG:CG | 1.91 | 0.84 |
| 1:CD:250:TRP:CZ3 | 1:CD:272:TYR:CE1 | 2.65 | 0.84 |
| 1:CM:189:PHE:HE1 | 1:CM:198:ARG:CG | 1.91 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AI:191:LEU:HD23 | 1:AI:191:LEU:H | 1.40 | 0.84 |
| 1:AF:189:PHE:HE1 | 1:AF:198:ARG:HG3 | 1.43 | 0.84 |
| 1:CJ:189:PHE:HE1 | 1:CJ:198:ARG:HG3 | 1.43 | 0.84 |
| 1:AM:454:ASN:HD22 | 1:AM:456:ALA:H | 1.26 | 0.83 |
| 1:AN:191:LEU:H | 1:AN:191:LEU:HD23 | 1.42 | 0.83 |
| 1:AR:189:PHE:HE1 | 1:AR:198:ARG:HG3 | 1.42 | 0.83 |
| 1:BP:79:ARG:CG | 1:BP:79:ARG:HH11 | 1.90 | 0.83 |
| 1:AH:191:LEU:HD23 | 1:AH:191:LEU:H | 1.43 | 0.83 |
| 1:AO:250:TRP:CZ3 | 1:AO:272:TYR:HE1 | 1.95 | 0.83 |
| 1:BB:454:ASN:HD22 | 1:BB:456:ALA:H | 1.26 | 0.83 |
| 1:BN:191:LEU:HD23 | 1:BN:191:LEU:H | 1.41 | 0.83 |
| 1:BO:15:GLN:HA | 1:BO:15:GLN:HE21 | 1.43 | 0.83 |
| 1:CT:191:LEU:HD23 | 1:CT:191:LEU:H | 1.41 | 0.83 |
| 1:AI:79:ARG:HG3 | 1:AI:79:ARG:HH11 | 1.43 | 0.83 |
| 1:CG:250:TRP:CZ3 | 1:CG:272:TYR:CE1 | 2.67 | 0.83 |
| 1:CQ:454:ASN:HD22 | 1:CQ:456:ALA:H | 1.27 | 0.83 |
| 1:CA:191:LEU:HD23 | 1:CA:191:LEU:H | 1.41 | 0.83 |
| 1:CF:250:TRP:CZ3 | 1:CF:272:TYR:CE1 | 2.66 | 0.83 |
| 1:AR:189:PHE:HE1 | 1:AR:198:ARG:CG | 1.91 | 0.83 |
| 1:BA:79:ARG:HH11 | 1:BA:79:ARG:HG3 | 1.43 | 0.83 |
| 1:CC:250:TRP:CE3 | 1:CC:272:TYR:CE1 | 2.66 | 0.83 |
| 1:AB:250:TRP:CZ3 | 1:AB:272:TYR:CE1 | 2.66 | 0.83 |
| 1:AI:189:PHE:HE1 | 1:AI:198:ARG:CG | 1.91 | 0.83 |
| 1:BA:250:TRP:CZ3 | 1:BA:272:TYR:CE1 | 2.67 | 0.83 |
| 1:CF:189:PHE:HE1 | 1:CF:198:ARG:CG | 1.92 | 0.83 |
| 1:AS:191:LEU:HD23 | 1:AS:191:LEU:H | 1.43 | 0.83 |
| 1:BE:189:PHE:HE1 | 1:BE:198:ARG:CG | 1.91 | 0.82 |
| 1:BI:454:ASN:HD22 | 1:BI:456:ALA:H | 1.26 | 0.82 |
| 1:CE:189:PHE:HE1 | 1:CE:198:ARG:HG3 | 1.44 | 0.82 |
| 1:BI:189:PHE:HE1 | 1:BI:198:ARG:HG3 | 1.44 | 0.82 |
| 1:AI:189:PHE:HE1 | 1:AI:198:ARG:HG3 | 1.42 | 0.82 |
| 1:AN:250:TRP:CZ3 | 1:AN:272:TYR:CE1 | 2.68 | 0.82 |
| 1:AR:250:TRP:CZ3 | 1:AR:272:TYR:CE1 | 2.67 | 0.82 |
| 1:CH:79:ARG:HH11 | 1:CH:79:ARG:HG3 | 1.45 | 0.82 |
| 1:CR:454:ASN:HD22 | 1:CR:456:ALA:H | 1.27 | 0.82 |
| 1:AE:189:PHE:HE1 | 1:AE:198:ARG:HG3 | 1.42 | 0.82 |
| 1:AF:454:ASN:HD22 | 1:AF:456:ALA:H | 1.27 | 0.82 |
| 1:BD:250:TRP:CZ3 | 1:BD:272:TYR:CE1 | 2.67 | 0.82 |
| 1:CG:189:PHE:HE1 | 1:CG:198:ARG:HG3 | 1.44 | 0.82 |
| 1:BB:189:PHE:HE1 | 1:BB:198:ARG:CG | 1.92 | 0.82 |
| 1:BB:250:TRP:CZ3 | 1:BB:272:TYR:CE1 | 2.68 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:250:TRP:CZ3 | 1:BG:272:TYR:CE1 | 2.67 | 0.82 |
| 1:BL:191:LEU:HD23 | 1:BL:191:LEU:H | 1.43 | 0.82 |
| 1:CH:250:TRP:CZ3 | 1:CH:272:TYR:CE1 | 2.68 | 0.82 |
| 1:CN:189:PHE:HE1 | 1:CN:198:ARG:CG | 1.92 | 0.82 |
| 1:CR:250:TRP:CZ3 | 1:CR:272:TYR:CE1 | 2.68 | 0.82 |
| 1:AN:189:PHE:HE1 | 1:AN:198:ARG:HG3 | 1.44 | 0.82 |
| 1:AC:250:TRP:CZ3 | 1:AC:272:TYR:CE1 | 2.67 | 0.82 |
| 1:CJ:189:PHE:HE1 | 1:CJ:198:ARG:CG | 1.92 | 0.82 |
| 1:AF:191:LEU:HD23 | 1:AF:191:LEU:H | 1.43 | 0.81 |
| 1:AJ:189:PHE:HE1 | 1:AJ:198:ARG:CG | 1.92 | 0.81 |
| 1:BH:189:PHE:HE1 | 1:BH:198:ARG:CG | 1.92 | 0.81 |
| 1:CE:250:TRP:CZ3 | 1:CE:272:TYR:CE1 | 2.67 | 0.81 |
| 1:CF:454:ASN:HD22 | 1:CF:456:ALA:H | 1.26 | 0.81 |
| 1:CB:189:PHE:HE1 | 1:CB:198:ARG:HG3 | 1.45 | 0.81 |
| 1:CK:250:TRP:CZ3 | 1:CK:272:TYR:CE1 | 2.68 | 0.81 |
| 1:AB:189:PHE:HE1 | 1:AB:198:ARG:CG | 1.93 | 0.81 |
| 1:BG:189:PHE:HE1 | 1:BG:198:ARG:HG3 | 1.45 | 0.81 |
| 1:CF:79:ARG:HH11 | 1:CF:79:ARG:CG | 1.91 | 0.81 |
| 1:CJ:191:LEU:HD23 | 1:CJ:191:LEU:H | 1.42 | 0.81 |
| 1:CJ:272:TYR:CE2 | 1:CQ:55:ARG:NE | 2.48 | 0.81 |
| 1:BN:250:TRP:CZ3 | 1:BN:272:TYR:CE1 | 2.69 | 0.81 |
| 1:BP:454:ASN:HD22 | 1:BP:456:ALA:H | 1.27 | 0.81 |
| 1:CN:250:TRP:CZ3 | 1:CN:272:TYR:CE1 | 2.67 | 0.81 |
| 1:AH:189:PHE:HE1 | 1:AH:198:ARG:CG | 1.93 | 0.81 |
| 1:AK:250:TRP:CZ3 | 1:AK:272:TYR:CE1 | 2.69 | 0.81 |
| 1:AH:250:TRP:CZ3 | 1:AH:272:TYR:CE1 | 2.68 | 0.81 |
| 1:CT:250:TRP:CZ3 | 1:CT:272:TYR:CE1 | 2.68 | 0.81 |
| 1:AE:250:TRP:CZ3 | 1:AE:272:TYR:CE1 | 2.69 | 0.81 |
| 1:AM:189:PHE:HE1 | 1:AM:198:ARG:CG | 1.94 | 0.81 |
| 1:BI:250:TRP:CZ3 | 1:BI:272:TYR:CE1 | 2.69 | 0.81 |
| 1:BR:79:ARG:HH11 | 1:BR:79:ARG:HG3 | 1.45 | 0.81 |
| 1:CK:454:ASN:HD22 | 1:CK:456:ALA:H | 1.28 | 0.81 |
| 1:AM:189:PHE:HE1 | 1:AM:198:ARG:HG3 | 1.45 | 0.80 |
| 1:AM:250:TRP:CZ3 | 1:AM:272:TYR:CE1 | 2.70 | 0.80 |
| 1:BK:250:TRP:CZ3 | 1:BK:272:TYR:CE1 | 2.68 | 0.80 |
| 1:BM:189:PHE:HE1 | 1:BM:198:ARG:CG | 1.94 | 0.80 |
| 1:AL:250:TRP:CZ3 | 1:AL:272:TYR:CE1 | 2.69 | 0.80 |
| 1:BM:250:TRP:CZ3 | 1:BM:272:TYR:CE1 | 2.69 | 0.80 |
| 1:BB:189:PHE:HE1 | 1:BB:198:ARG:HG3 | 1.45 | 0.80 |
| 1:CS:454:ASN:HD22 | 1:CS:456:ALA:H | 1.24 | 0.80 |
| 1:AR:454:ASN:HD22 | 1:AR:456:ALA:H | 1.29 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CF:189:PHE:HE1 | 1:CF:198:ARG:HG3 | 1.46 | 0.80 |
| 1:CM:189:PHE:HE1 | 1:CM:198:ARG:HG3 | 1.45 | 0.80 |
| 1:CM:454:ASN:HD22 | 1:CM:456:ALA:H | 1.29 | 0.80 |
| 1:CD:454:ASN:HD22 | 1:CD:456:ALA:H | 1.30 | 0.80 |
| 1:BL:250:TRP:CZ3 | 1:BL:272:TYR:CE1 | 2.70 | 0.80 |
| 1:CI:189:PHE:HE1 | 1:CI:198:ARG:HG3 | 1.45 | 0.80 |
| 1:CL:454:ASN:HD22 | 1:CL:456:ALA:H | 1.29 | 0.80 |
| 1:CS:250:TRP:CZ3 | 1:CS:272:TYR:CE1 | 2.69 | 0.80 |
| 1:AO:272:TYR:HE2 | 1:AR:55:ARG:NE | 1.80 | 0.80 |
| 1:AL:454:ASN:HD22 | 1:AL:456:ALA:H | 1.30 | 0.79 |
| 1:BF:189:PHE:HE1 | 1:BF:198:ARG:CG | 1.95 | 0.79 |
| 1:CH:189:PHE:HE1 | 1:CH:198:ARG:CG | 1.95 | 0.79 |
| 1:CI:250:TRP:CZ3 | 1:CI:272:TYR:CE1 | 2.69 | 0.79 |
| 1:AF:250:TRP:CZ3 | 1:AF:272:TYR:CE1 | 2.70 | 0.79 |
| 1:AG:189:PHE:HE1 | 1:AG:198:ARG:HG3 | 1.46 | 0.79 |
| 1:BK:454:ASN:HD22 | 1:BK:456:ALA:H | 1.27 | 0.79 |
| 1:BO:250:TRP:CE3 | 1:BO:272:TYR:CE1 | 2.70 | 0.79 |
| 1:CN:454:ASN:HD22 | 1:CN:456:ALA:H | 1.30 | 0.79 |
| 1:BF:250:TRP:CZ3 | 1:BF:272:TYR:CE1 | 2.70 | 0.79 |
| 1:BH:189:PHE:HE1 | 1:BH:198:ARG:HG3 | 1.45 | 0.79 |
| 1:BH:250:TRP:CZ3 | 1:BH:272:TYR:CE1 | 2.69 | 0.79 |
| 1:CP:250:TRP:CZ3 | 1:CP:272:TYR:HE1 | 2.01 | 0.79 |
| 1:BR:189:PHE:HE1 | 1:BR:198:ARG:HG3 | 1.46 | 0.79 |
| 1:BR:250:TRP:CZ3 | 1:BR:272:TYR:CE1 | 2.71 | 0.79 |
| 1:BT:454:ASN:HD22 | 1:BT:456:ALA:H | 1.31 | 0.79 |
| 1:CA:250:TRP:CZ3 | 1:CA:272:TYR:CE1 | 2.71 | 0.79 |
| 1:CB:250:TRP:CZ3 | 1:CB:272:TYR:CE1 | 2.70 | 0.79 |
| 1:CL:250:TRP:CZ3 | 1:CL:272:TYR:CE1 | 2.70 | 0.79 |
| 1:BJ:272:TYR:CE2 | 1:BQ:55:ARG:NE | 2.51 | 0.79 |
| 1:CR:189:PHE:HE1 | 1:CR:198:ARG:HG3 | 1.47 | 0.79 |
| 1:AJ:189:PHE:HE1 | 1:AJ:198:ARG:HG3 | 1.48 | 0.79 |
| 1:CI:189:PHE:HE1 | 1:CI:198:ARG:CG | 1.96 | 0.79 |
| 1:BE:189:PHE:HE1 | 1:BE:198:ARG:HG3 | 1.46 | 0.78 |
| 1:BQ:250:TRP:CZ3 | 1:BQ:272:TYR:CE1 | 2.71 | 0.78 |
| 1:CO:272:TYR:CE2 | 1:CR:55:ARG:NE | 2.51 | 0.78 |
| 1:AG:189:PHE:HE1 | 1:AG:198:ARG:CG | 1.95 | 0.78 |
| 1:AQ:250:TRP:CZ3 | 1:AQ:272:TYR:CE1 | 2.71 | 0.78 |
| 1:AN:454:ASN:HD22 | 1:AN:456:ALA:H | 1.30 | 0.78 |
| 1:BM:454:ASN:HD22 | 1:BM:456:ALA:H | 1.31 | 0.78 |
| 1:BF:454:ASN:HD22 | 1:BF:456:ALA:H | 1.30 | 0.78 |
| 1:AG:250:TRP:CZ3 | 1:AG:272:TYR:HE1 | 2.02 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:189:PHE:HE1 | 1:BJ:198:ARG:CG | 1.96 | 0.78 |
| 1:CD:250:TRP:CZ3 | 1:CD:272:TYR:HE1 | 2.01 | 0.78 |
| 1:AE:454:ASN:HD22 | 1:AE:456:ALA:H | 1.31 | 0.77 |
| 1:BJ:272:TYR:HE2 | 1:BQ:55:ARG:NE | 1.82 | 0.77 |
| 1:BA:189:PHE:HE1 | 1:BA:198:ARG:HG3 | 1.49 | 0.77 |
| 1:BS:250:TRP:CZ3 | 1:BS:272:TYR:CE1 | 2.73 | 0.77 |
| 1:CJ:454:ASN:HD22 | 1:CJ:456:ALA:H | 1.31 | 0.77 |
| 1:AA:454:ASN:HD22 | 1:AA:456:ALA:H | 1.30 | 0.77 |
| 1:AD:454:ASN:HD22 | 1:AD:456:ALA:H | 1.32 | 0.77 |
| 1:BG:189:PHE:HE1 | 1:BG:198:ARG:CG | 1.96 | 0.77 |
| 1:AP:22:THR:OG1 | 1:AP:131:HIS:HD2 | 1.67 | 0.77 |
| 1:CH:189:PHE:HE1 | 1:CH:198:ARG:HG3 | 1.46 | 0.77 |
| 1:BC:454:ASN:HD22 | 1:BC:456:ALA:H | 1.31 | 0.77 |
| 1:CO:79:ARG:HG3 | 1:CO:79:ARG:HH11 | 1.49 | 0.77 |
| 1:CT:454:ASN:HD22 | 1:CT:456:ALA:H | 1.33 | 0.77 |
| 1:AA:250:TRP:CZ3 | 1:AA:272:TYR:CE1 | 2.72 | 0.77 |
| 1:AD:250:TRP:CZ3 | 1:AD:272:TYR:CE1 | 2.72 | 0.77 |
| 1:AE:55:ARG:NE | 1:CP:272:TYR:CE2 | 2.52 | 0.77 |
| 1:CE:189:PHE:HE1 | 1:CE:198:ARG:CG | 1.98 | 0.77 |
| 1:BL:454:ASN:HD22 | 1:BL:456:ALA:H | 1.31 | 0.77 |
| 1:CD:22:THR:OG1 | 1:CD:131:HIS:HD2 | 1.68 | 0.77 |
| 1:BH:454:ASN:HD22 | 1:BH:456:ALA:H | 1.30 | 0.77 |
| 1:BQ:284:ARG:HH11 | 1:BQ:284:ARG:CG | 1.98 | 0.77 |
| 1:CO:189:PHE:HE1 | 1:CO:198:ARG:HG3 | 1.49 | 0.77 |
| 1:AK:55:ARG:NE | 1:CF:272:TYR:CE2 | 2.53 | 0.76 |
| 1:CD:272:TYR:CE2 | 1:CS:55:ARG:NE | 2.53 | 0.76 |
| 1:AK:454:ASN:HD22 | 1:AK:456:ALA:H | 1.34 | 0.76 |
| 1:BA:454:ASN:HD22 | 1:BA:456:ALA:H | 1.32 | 0.76 |
| 1:BQ:189:PHE:HE1 | 1:BQ:198:ARG:HG3 | 1.48 | 0.76 |
| 1:CE:250:TRP:CZ3 | 1:CE:272:TYR:HE1 | 2.03 | 0.76 |
| 1:BJ:250:TRP:CE3 | 1:BJ:272:TYR:CE1 | 2.73 | 0.76 |
| 1:BP:250:TRP:CE3 | 1:BP:272:TYR:CE1 | 2.73 | 0.76 |
| 1:AO:454:ASN:HD22 | 1:AO:456:ALA:H | 1.33 | 0.76 |
| 1:AP:250:TRP:CZ3 | 1:AP:272:TYR:CE1 | 2.73 | 0.76 |
| 1:AB:189:PHE:HE1 | 1:AB:198:ARG:HG3 | 1.49 | 0.76 |
| 1:BD:272:TYR:CE2 | 1:BS:55:ARG:NE | 2.54 | 0.76 |
| 1:BF:79:ARG:HH11 | 1:BF:79:ARG:HG3 | 1.48 | 0.76 |
| 1:BL:189:PHE:HE1 | 1:BL:198:ARG:HG3 | 1.51 | 0.76 |
| 1:BP:189:PHE:HE1 | 1:BP:198:ARG:HG3 | 1.50 | 0.76 |
| 1:BC:22:THR:OG1 | 1:BC:131:HIS:HD2 | 1.69 | 0.76 |
| 1:BP:22:THR:OG1 | 1:BP:131:HIS:HD2 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:33:LYS:HG2 | 1:AP:33:LYS:O | 1.86 | 0.76 |
| 1:BE:250:TRP:CZ3 | 1:BE:272:TYR:CE1 | 2.73 | 0.76 |
| 1:CA:454:ASN:HD22 | 1:CA:456:ALA:H | 1.34 | 0.76 |
| 1:AN:55:ARG:NE | 1:AS:272:TYR:HE2 | 1.83 | 0.76 |
| 1:AG:55:ARG:NE | 1:CG:272:TYR:CE2 | 2.53 | 0.75 |
| 1:BS:454:ASN:HD22 | 1:BS:456:ALA:H | 1.30 | 0.75 |
| 1:CC:79:ARG:HH11 | 1:CC:79:ARG:HG3 | 1.51 | 0.75 |
| 1:AB:55:ARG:NE | 1:BB:272:TYR:CE2 | 2.54 | 0.75 |
| 1:AF:189:PHE:HE1 | 1:AF:198:ARG:CG | 1.98 | 0.75 |
| 1:AJ:454:ASN:HD22 | 1:AJ:456:ALA:H | 1.35 | 0.75 |
| 1:AK:189:PHE:HE1 | 1:AK:198:ARG:HG3 | 1.51 | 0.75 |
| 1:AH:189:PHE:HE1 | 1:AH:198:ARG:HG3 | 1.49 | 0.75 |
| 1:BN:454:ASN:HD22 | 1:BN:456:ALA:H | 1.33 | 0.75 |
| 1:BR:454:ASN:HD22 | 1:BR:456:ALA:H | 1.31 | 0.75 |
| 1:CE:22:THR:OG1 | 1:CE:131:HIS:HD2 | 1.68 | 0.75 |
| 1:AO:272:TYR:HE2 | 1:AR:55:ARG:CD | 2.00 | 0.75 |
| 1:BS:189:PHE:HE1 | 1:BS:198:ARG:HG3 | 1.52 | 0.75 |
| 1:CJ:22:THR:OG1 | 1:CJ:131:HIS:HD2 | 1.69 | 0.75 |
| 1:AR:22:THR:OG1 | 1:AR:131:HIS:HD2 | 1.70 | 0.75 |
| 1:BR:189:PHE:HE1 | 1:BR:198:ARG:CG | 2.00 | 0.75 |
| 1:AC:454:ASN:HD22 | 1:AC:456:ALA:H | 1.31 | 0.75 |
| 1:BN:189:PHE:HE1 | 1:BN:198:ARG:HG3 | 1.51 | 0.75 |
| 1:AF:22:THR:OG1 | 1:AF:131:HIS:HD2 | 1.70 | 0.75 |
| 1:AH:454:ASN:HD22 | 1:AH:456:ALA:H | 1.35 | 0.75 |
| 1:BG:272:TYR:CE2 | 1:CG:55:ARG:CD | 2.68 | 0.75 |
| 1:BH:55:ARG:NE | 1:BK:272:TYR:CE2 | 2.54 | 0.75 |
| 1:BJ:454:ASN:HD22 | 1:BJ:456:ALA:H | 1.32 | 0.75 |
| 1:AJ:250:TRP:CZ3 | 1:AJ:272:TYR:CE1 | 2.75 | 0.74 |
| 1:BA:74:ASN:HB3 | 1:BA:126:GLU:HG2 | 1.69 | 0.74 |
| 1:AE:22:THR:OG1 | 1:AE:131:HIS:HD2 | 1.69 | 0.74 |
| 1:AP:454:ASN:HD22 | 1:AP:456:ALA:H | 1.32 | 0.74 |
| 1:BA:33:LYS:HG2 | 1:BA:33:LYS:O | 1.87 | 0.74 |
| 1:BA:22:THR:OG1 | 1:BA:131:HIS:HD2 | 1.70 | 0.74 |
| 1:BG:74:ASN:HB3 | 1:BG:126:GLU:HG2 | 1.68 | 0.74 |
| 1:CL:33:LYS:O | 1:CL:33:LYS:HG2 | 1.88 | 0.74 |
| 1:CB:454:ASN:HD22 | 1:CB:456:ALA:H | 1.35 | 0.74 |
| 1:CL:189:PHE:HE1 | 1:CL:198:ARG:HG3 | 1.52 | 0.74 |
| 1:CI:74:ASN:HB3 | 1:CI:126:GLU:HG2 | 1.68 | 0.74 |
| 1:AS:454:ASN:HD22 | 1:AS:456:ALA:H | 1.35 | 0.74 |
| 1:BB:33:LYS:O | 1:BB:33:LYS:HG2 | 1.87 | 0.74 |
| 1:BG:33:LYS:HG2 | 1:BG:33:LYS:O | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AB:272:TYR:CE2 | 1:CB:55:ARG:NE | 2.56 | 0.74 |
| 1:AS:250:TRP:CE3 | 1:AS:272:TYR:CE1 | 2.75 | 0.74 |
| 1:BQ:36:GLN:NE2 | 1:BQ:156:LEU:H | 1.85 | 0.74 |
| 1:BC:250:TRP:CZ3 | 1:BC:272:TYR:CE1 | 2.76 | 0.74 |
| 1:BE:33:LYS:O | 1:BE:33:LYS:HG2 | 1.88 | 0.74 |
| 1:BG:272:TYR:CE2 | 1:CG:55:ARG:HD3 | 2.23 | 0.74 |
| 1:BI:189:PHE:HE1 | 1:BI:198:ARG:CG | 2.00 | 0.74 |
| 1:CH:454:ASN:HD22 | 1:CH:456:ALA:H | 1.32 | 0.74 |
| 1:AE:189:PHE:HE1 | 1:AE:198:ARG:CG | 1.98 | 0.74 |
| 1:BL:33:LYS:HG2 | 1:BL:33:LYS:O | 1.87 | 0.74 |
| 1:BQ:284:ARG:HH11 | 1:BQ:284:ARG:HG2 | 1.52 | 0.74 |
| 1:BT:79:ARG:HH11 | 1:BT:79:ARG:HG3 | 1.51 | 0.74 |
| 1:AL:74:ASN:HB3 | 1:AL:126:GLU:HG2 | 1.70 | 0.73 |
| 1:AR:189:PHE:HE2 | 1:AR:249:LEU:HD21 | 1.53 | 0.73 |
| 1:CG:79:ARG:HG3 | 1:CG:79:ARG:HH11 | 1.52 | 0.73 |
| 1:CI:189:PHE:HE2 | 1:CI:249:LEU:HD21 | 1.53 | 0.73 |
| 1:AE:55:ARG:CD | 1:CP:272:TYR:HE2 | 2.01 | 0.73 |
| 1:CO:454:ASN:HD22 | 1:CO:456:ALA:H | 1.34 | 0.73 |
| 1:AD:55:ARG:NE | 1:AN:272:TYR:CE2 | 2.56 | 0.73 |
| 1:AR:33:LYS:O | 1:AR:33:LYS:HG2 | 1.88 | 0.73 |
| 1:AT:33:LYS:O | 1:AT:33:LYS:HG2 | 1.88 | 0.73 |
| 1:BE:454:ASN:HD22 | 1:BE:456:ALA:H | 1.35 | 0.73 |
| 1:BO:272:TYR:HE2 | 1:BR:55:ARG:CD | 2.01 | 0.73 |
| 1:CC:454:ASN:HD22 | 1:CC:456:ALA:H | 1.34 | 0.73 |
| 1:AF:33:LYS:O | 1:AF:33:LYS:HG2 | 1.88 | 0.73 |
| 1:BS:74:ASN:HB3 | 1:BS:126:GLU:HG2 | 1.70 | 0.73 |
| 1:BA:14:CYS:H | 1:BA:138:ASN:HD21 | 1.35 | 0.73 |
| 1:BG:272:TYR:CE2 | 1:CG:55:ARG:NE | 2.57 | 0.73 |
| 1:BM:284:ARG:CG | 1:BM:284:ARG:HH11 | 2.02 | 0.73 |
| 1:CE:33:LYS:O | 1:CE:33:LYS:HG2 | 1.89 | 0.73 |
| 1:CL:284:ARG:CG | 1:CL:284:ARG:HH11 | 2.01 | 0.73 |
| 1:CQ:250:TRP:CZ3 | 1:CQ:272:TYR:HE1 | 2.05 | 0.73 |
| 1:AM:284:ARG:HH11 | 1:AM:284:ARG:CG | 2.01 | 0.73 |
| 1:BK:189:PHE:HE1 | 1:BK:198:ARG:HG3 | 1.52 | 0.73 |
| 1:CG:22:THR:OG1 | 1:CG:131:HIS:HD2 | 1.70 | 0.73 |
| 1:BB:284:ARG:CG | 1:BB:284:ARG:HH11 | 2.02 | 0.73 |
| 1:BF:189:PHE:HE1 | 1:BF:198:ARG:HG3 | 1.52 | 0.73 |
| 1:BJ:189:PHE:CE1 | 1:BJ:198:ARG:HG3 | 2.23 | 0.73 |
| 1:BO:284:ARG:HG2 | 1:BO:284:ARG:HH11 | 1.54 | 0.73 |
| 1:CC:33:LYS:HG2 | 1:CC:33:LYS:O | 1.88 | 0.73 |
| 1:CN:189:PHE:CE1 | 1:CN:198:ARG:HG3 | 2.23 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AN:22:THR:OG1 | 1:AN:131:HIS:HD2 | 1.72 | 0.73 |
| 1:BE:16:ALA:O | 1:BE:17:ASN:HB2 | 1.89 | 0.73 |
| 1:BP:79:ARG:HH11 | 1:BP:79:ARG:HG3 | 1.52 | 0.73 |
| 1:CG:33:LYS:O | 1:CG:33:LYS:HG2 | 1.88 | 0.73 |
| 1:CG:454:ASN:HD22 | 1:CG:456:ALA:H | 1.34 | 0.73 |
| 1:AI:250:TRP:CZ3 | 1:AI:272:TYR:CE1 | 2.76 | 0.72 |
| 1:BD:250:TRP:CZ3 | 1:BD:272:TYR:HE1 | 2.06 | 0.72 |
| 1:BO:33:LYS:HG2 | 1:BO:33:LYS:O | 1.87 | 0.72 |
| 1:CT:33:LYS:HG2 | 1:CT:33:LYS:O | 1.88 | 0.72 |
| 1:AB:250:TRP:CZ3 | 1:AB:272:TYR:HE1 | 2.06 | 0.72 |
| 1:AC:284:ARG:CG | 1:AC:284:ARG:HH11 | 2.02 | 0.72 |
| 1:AD:79:ARG:HH11 | 1:AD:79:ARG:HG3 | 1.54 | 0.72 |
| 1:BJ:191:LEU:H | 1:BJ:191:LEU:CD2 | 2.02 | 0.72 |
| 1:CD:284:ARG:HG2 | 1:CD:284:ARG:HH11 | 1.55 | 0.72 |
| 1:CG:79:ARG:HH11 | 1:CG:79:ARG:CG | 2.02 | 0.72 |
| 1:CO:272:TYR:HE2 | 1:CR:55:ARG:CD | 2.03 | 0.72 |
| 1:BO:454:ASN:HD22 | 1:BO:456:ALA:H | 1.37 | 0.72 |
| 1:CI:454:ASN:HD22 | 1:CI:456:ALA:H | 1.35 | 0.72 |
| 1:AG:189:PHE:HE2 | 1:AG:249:LEU:HD21 | 1.54 | 0.72 |
| 1:AK:55:ARG:CD | 1:CF:272:TYR:CE2 | 2.71 | 0.72 |
| 1:AL:22:THR:OG1 | 1:AL:131:HIS:HD2 | 1.72 | 0.72 |
| 1:AM:22:THR:OG1 | 1:AM:131:HIS:HD2 | 1.72 | 0.72 |
| 1:AP:55:ARG:NE | 1:BM:272:TYR:CE2 | 2.57 | 0.72 |
| 1:BD:33:LYS:HG2 | 1:BD:33:LYS:O | 1.89 | 0.72 |
| 1:BK:33:LYS:O | 1:BK:33:LYS:HG2 | 1.88 | 0.72 |
| 1:CO:33:LYS:O | 1:CO:33:LYS:HG2 | 1.89 | 0.72 |
| 1:AQ:74:ASN:HB3 | 1:AQ:126:GLU:HG2 | 1.72 | 0.72 |
| 1:AD:189:PHE:HE1 | 1:AD:198:ARG:HG3 | 1.54 | 0.72 |
| 1:AE:189:PHE:HE2 | 1:AE:249:LEU:HD21 | 1.55 | 0.72 |
| 1:AM:284:ARG:HH11 | 1:AM:284:ARG:HG2 | 1.51 | 0.72 |
| 1:AT:454:ASN:HD22 | 1:AT:456:ALA:H | 1.36 | 0.72 |
| 1:BQ:33:LYS:O | 1:BQ:33:LYS:HG2 | 1.89 | 0.72 |
| 1:CK:33:LYS:HG2 | 1:CK:33:LYS:O | 1.90 | 0.72 |
| 1:AB:201:GLY:HA3 | 1:AB:300:GLN:HG2 | 1.70 | 0.72 |
| 1:BM:79:ARG:HH11 | 1:BM:79:ARG:HG3 | 1.55 | 0.72 |
| 1:AA:189:PHE:HE1 | 1:AA:198:ARG:HG3 | 1.53 | 0.72 |
| 1:AE:55:ARG:CD | 1:CP:272:TYR:CE2 | 2.72 | 0.72 |
| 1:AK:55:ARG:CD | 1:CF:272:TYR:HE2 | 2.03 | 0.72 |
| 1:AS:22:THR:OG1 | 1:AS:131:HIS:HD2 | 1.73 | 0.72 |
| 1:BH:33:LYS:O | 1:BH:33:LYS:HG2 | 1.90 | 0.72 |
| 1:CP:79:ARG:HH11 | 1:CP:79:ARG:HG3 | 1.54 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AQ:454:ASN:HD22 | 1:AQ:456:ALA:H | 1.36 | 0.72 |
| 1:AT:55:ARG:NE | 1:BA:272:TYR:CE2 | 2.57 | 0.72 |
| 1:BG:272:TYR:CD2 | 1:CG:55:ARG:HD3 | 2.24 | 0.72 |
| 1:AB:33:LYS:HG2 | 1:AB:33:LYS:O | 1.90 | 0.72 |
| 1:AF:74:ASN:HB3 | 1:AF:126:GLU:HG2 | 1.72 | 0.72 |
| 1:AT:189:PHE:HE1 | 1:AT:198:ARG:HG3 | 1.53 | 0.72 |
| 1:AT:250:TRP:CZ3 | 1:AT:272:TYR:HE1 | 2.06 | 0.72 |
| 1:BL:74:ASN:HB3 | 1:BL:126:GLU:HG2 | 1.71 | 0.72 |
| 1:BM:189:PHE:HE2 | 1:BM:249:LEU:HD21 | 1.54 | 0.72 |
| 1:AC:250:TRP:CZ3 | 1:AC:272:TYR:HE1 | 2.08 | 0.71 |
| 1:BF:55:ARG:NE | 1:CH:272:TYR:CE2 | 2.57 | 0.71 |
| 1:CL:74:ASN:HB3 | 1:CL:126:GLU:HG2 | 1.71 | 0.71 |
| 1:CN:36:GLN:NE2 | 1:CN:156:LEU:H | 1.88 | 0.71 |
| 1:AB:454:ASN:HD22 | 1:AB:456:ALA:H | 1.38 | 0.71 |
| 1:AC:33:LYS:O | 1:AC:33:LYS:HG2 | 1.90 | 0.71 |
| 1:AM:33:LYS:HG2 | 1:AM:33:LYS:O | 1.91 | 0.71 |
| 1:AN:55:ARG:CD | 1:AS:272:TYR:HE2 | 2.03 | 0.71 |
| 1:BR:74:ASN:HB3 | 1:BR:126:GLU:HG2 | 1.72 | 0.71 |
| 1:CC:284:ARG:HG2 | 1:CC:284:ARG:HH11 | 1.55 | 0.71 |
| 1:CR:79:ARG:CG | 1:CR:79:ARG:HH11 | 2.03 | 0.71 |
| 1:AC:55:ARG:NE | 1:AT:272:TYR:CE2 | 2.58 | 0.71 |
| 1:AJ:33:LYS:O | 1:AJ:33:LYS:HG2 | 1.90 | 0.71 |
| 1:AK:74:ASN:HB3 | 1:AK:126:GLU:HG2 | 1.72 | 0.71 |
| 1:BT:250:TRP:CZ3 | 1:BT:272:TYR:HE1 | 2.08 | 0.71 |
| 1:CC:55:ARG:NE | 1:CT:272:TYR:CE2 | 2.58 | 0.71 |
| 1:AN:33:LYS:HG2 | 1:AN:33:LYS:O | 1.90 | 0.71 |
| 1:AQ:33:LYS:O | 1:AQ:33:LYS:HG2 | 1.89 | 0.71 |
| 1:BP:55:ARG:NE | 1:CM:272:TYR:CE2 | 2.59 | 0.71 |
| 1:CJ:272:TYR:HE2 | 1:CQ:55:ARG:NE | 1.86 | 0.71 |
| 1:AQ:22:THR:OG1 | 1:AQ:131:HIS:HD2 | 1.72 | 0.71 |
| 1:BH:22:THR:OG1 | 1:BH:131:HIS:HD2 | 1.73 | 0.71 |
| 1:CL:22:THR:OG1 | 1:CL:131:HIS:HD2 | 1.73 | 0.71 |
| 1:CM:250:TRP:CZ3 | 1:CM:272:TYR:HE1 | 2.06 | 0.71 |
| 1:AF:189:PHE:HE2 | 1:AF:249:LEU:HD21 | 1.55 | 0.71 |
| 1:AG:454:ASN:HD22 | 1:AG:456:ALA:H | 1.36 | 0.71 |
| 1:BB:191:LEU:H | 1:BB:191:LEU:CD2 | 2.03 | 0.71 |
| 1:BC:36:GLN:NE2 | 1:BC:156:LEU:H | 1.89 | 0.71 |
| 1:BO:284:ARG:HH11 | 1:BO:284:ARG:CG | 2.02 | 0.71 |
| 1:CH:36:GLN:NE2 | 1:CH:156:LEU:H | 1.88 | 0.71 |
| 1:CS:74:ASN:HB3 | 1:CS:126:GLU:HG2 | 1.72 | 0.71 |
| 1:AJ:55:ARG:NE | 1:BL:272:TYR:CE2 | 2.59 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AN:55:ARG:CD | 1:AS:272:TYR:CE2 | 2.73 | 0.71 |
| 1:CE:272:TYR:CE2 | 1:CM:55:ARG:NE | 2.58 | 0.71 |
| 1:CK:36:GLN:NE2 | 1:CK:156:LEU:H | 1.88 | 0.71 |
| 1:AB:79:ARG:HH11 | 1:AB:79:ARG:HG3 | 1.56 | 0.71 |
| 1:AG:284:ARG:HH11 | 1:AG:284:ARG:CG | 2.04 | 0.71 |
| 1:AR:250:TRP:CZ3 | 1:AR:272:TYR:HE1 | 2.06 | 0.71 |
| 1:AT:55:ARG:CD | 1:BA:272:TYR:CE2 | 2.74 | 0.71 |
| 1:BB:55:ARG:NE | 1:CB:272:TYR:CE2 | 2.59 | 0.71 |
| 1:BG:272:TYR:HE2 | 1:CG:55:ARG:CD | 2.03 | 0.71 |
| 1:BS:22:THR:OG1 | 1:BS:131:HIS:HD2 | 1.74 | 0.71 |
| 1:CI:272:TYR:CE2 | 1:CO:55:ARG:NE | 2.59 | 0.71 |
| 1:CN:55:ARG:NE | 1:CS:272:TYR:CE2 | 2.59 | 0.71 |
| 1:CS:33:LYS:O | 1:CS:33:LYS:HG2 | 1.91 | 0.71 |
| 1:AA:272:TYR:CE2 | 1:CT:55:ARG:NE | 2.59 | 0.71 |
| 1:AB:284:ARG:HG2 | 1:AB:284:ARG:HH11 | 1.55 | 0.71 |
| 1:AC:272:TYR:CE2 | 1:BA:55:ARG:NE | 2.58 | 0.71 |
| 1:BA:284:ARG:HH11 | 1:BA:284:ARG:CG | 2.03 | 0.71 |
| 1:BC:189:PHE:HE1 | 1:BC:198:ARG:HG3 | 1.55 | 0.71 |
| 1:BI:33:LYS:O | 1:BI:33:LYS:HG2 | 1.90 | 0.71 |
| 1:BN:22:THR:OG1 | 1:BN:131:HIS:HD2 | 1.74 | 0.71 |
| 1:BR:33:LYS:HG2 | 1:BR:33:LYS:O | 1.90 | 0.71 |
| 1:CA:36:GLN:NE2 | 1:CA:156:LEU:H | 1.89 | 0.71 |
| 1:CI:22:THR:OG1 | 1:CI:131:HIS:HD2 | 1.72 | 0.71 |
| 1:CJ:14:CYS:H | 1:CJ:138:ASN:HD21 | 1.38 | 0.71 |
| 1:CJ:33:LYS:O | 1:CJ:33:LYS:HG2 | 1.91 | 0.71 |
| 1:CN:74:ASN:HB3 | 1:CN:126:GLU:HG2 | 1.73 | 0.71 |
| 1:CR:33:LYS:O | 1:CR:33:LYS:HG2 | 1.90 | 0.71 |
| 1:AE:272:TYR:CE2 | 1:AM:55:ARG:NE | 2.59 | 0.71 |
| 1:BC:33:LYS:O | 1:BC:33:LYS:HG2 | 1.91 | 0.71 |
| 1:BP:33:LYS:O | 1:BP:33:LYS:HG2 | 1.90 | 0.71 |
| 1:BT:22:THR:OG1 | 1:BT:131:HIS:HD2 | 1.74 | 0.71 |
| 1:CF:22:THR:OG1 | 1:CF:131:HIS:HD2 | 1.73 | 0.71 |
| 1:BJ:74:ASN:HB3 | 1:BJ:126:GLU:HG2 | 1.73 | 0.70 |
| 1:BP:284:ARG:HG2 | 1:BP:284:ARG:HH11 | 1.56 | 0.70 |
| 1:BQ:272:TYR:CE2 | 1:CL:55:ARG:NE | 2.58 | 0.70 |
| 1:CC:284:ARG:HH11 | 1:CC:284:ARG:CG | 2.04 | 0.70 |
| 1:CP:189:PHE:HE1 | 1:CP:198:ARG:HG3 | 1.56 | 0.70 |
| 1:CT:74:ASN:HB3 | 1:CT:126:GLU:HG2 | 1.73 | 0.70 |
| 1:AB:191:LEU:H | 1:AB:191:LEU:CD2 | 2.04 | 0.70 |
| 1:AK:14:CYS:H | 1:AK:138:ASN:HD21 | 1.38 | 0.70 |
| 1:AN:74:ASN:HB3 | 1:AN:126:GLU:HG2 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:272:TYR:CE2 | 1:BE:55:ARG:NE | 2.59 | 0.70 |
| 1:BQ:454:ASN:HD22 | 1:BQ:456:ALA:H | 1.37 | 0.70 |
| 1:BT:33:LYS:O | 1:BT:33:LYS:HG2 | 1.90 | 0.70 |
| 1:CJ:189:PHE:CE1 | 1:CJ:198:ARG:HG3 | 2.26 | 0.70 |
| 1:CJ:272:TYR:HE2 | 1:CQ:55:ARG:CD | 2.04 | 0.70 |
| 1:CM:22:THR:OG1 | 1:CM:131:HIS:HD2 | 1.73 | 0.70 |
| 1:AD:74:ASN:HB3 | 1:AD:126:GLU:HG2 | 1.73 | 0.70 |
| 1:AJ:79:ARG:HH11 | 1:AJ:79:ARG:HG3 | 1.56 | 0.70 |
| 1:AL:55:ARG:NE | 1:CQ:272:TYR:CE2 | 2.59 | 0.70 |
| 1:BL:22:THR:OG1 | 1:BL:131:HIS:HD2 | 1.74 | 0.70 |
| 1:CB:22:THR:OG1 | 1:CB:131:HIS:HD2 | 1.73 | 0.70 |
| 1:CN:284:ARG:HG2 | 1:CN:284:ARG:HH11 | 1.57 | 0.70 |
| 1:AE:14:CYS:H | 1:AE:138:ASN:HD21 | 1.39 | 0.70 |
| 1:AS:284:ARG:HH11 | 1:AS:284:ARG:CG | 2.04 | 0.70 |
| 1:BI:284:ARG:HH11 | 1:BI:284:ARG:CG | 2.04 | 0.70 |
| 1:CE:454:ASN:HD22 | 1:CE:456:ALA:H | 1.37 | 0.70 |
| 1:CN:33:LYS:HG2 | 1:CN:33:LYS:O | 1.91 | 0.70 |
| 1:CS:189:PHE:HE1 | 1:CS:198:ARG:HG3 | 1.56 | 0.70 |
| 1:CT:284:ARG:HH11 | 1:CT:284:ARG:CG | 2.04 | 0.70 |
| 1:AF:55:ARG:NE | 1:BH:272:TYR:CE2 | 2.59 | 0.70 |
| 1:AF:189:PHE:CE1 | 1:AF:198:ARG:HG3 | 2.26 | 0.70 |
| 1:AF:272:TYR:CE2 | 1:BK:55:ARG:NE | 2.59 | 0.70 |
| 1:AG:284:ARG:HH11 | 1:AG:284:ARG:HG2 | 1.56 | 0.70 |
| 1:BA:250:TRP:CZ3 | 1:BA:272:TYR:HE1 | 2.10 | 0.70 |
| 1:BF:284:ARG:HH11 | 1:BF:284:ARG:CG | 2.04 | 0.70 |
| 1:CA:33:LYS:O | 1:CA:33:LYS:HG2 | 1.90 | 0.70 |
| 1:CB:74:ASN:HB3 | 1:CB:126:GLU:HG2 | 1.74 | 0.70 |
| 1:CQ:191:LEU:H | 1:CQ:191:LEU:CD2 | 2.04 | 0.70 |
| 1:AA:33:LYS:O | 1:AA:33:LYS:HG2 | 1.92 | 0.70 |
| 1:AP:191:LEU:H | 1:AP:191:LEU:CD2 | 2.05 | 0.70 |
| 1:AS:33:LYS:HG2 | 1:AS:33:LYS:O | 1.90 | 0.70 |
| 1:BT:189:PHE:HE1 | 1:BT:198:ARG:HG3 | 1.56 | 0.70 |
| 1:CD:55:ARG:NE | 1:CN:272:TYR:CE2 | 2.59 | 0.70 |
| 1:CP:22:THR:OG1 | 1:CP:131:HIS:HD2 | 1.74 | 0.70 |
| 1:AL:284:ARG:HH11 | 1:AL:284:ARG:CG | 2.05 | 0.70 |
| 1:CH:55:ARG:NE | 1:CK:272:TYR:CE2 | 2.60 | 0.70 |
| 1:CT:284:ARG:HH11 | 1:CT:284:ARG:HG2 | 1.56 | 0.70 |
| 1:AI:22:THR:OG1 | 1:AI:131:HIS:HD2 | 1.75 | 0.70 |
| 1:BH:189:PHE:HE2 | 1:BH:249:LEU:HD21 | 1.56 | 0.70 |
| 1:BI:284:ARG:HH11 | 1:BI:284:ARG:HG2 | 1.57 | 0.70 |
| 1:BJ:22:THR:OG1 | 1:BJ:131:HIS:HD2 | 1.75 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:36:GLN:NE2 | 1:BJ:156:LEU:H | 1.89 | 0.70 |
| 1:CB:79:ARG:HH11 | 1:CB:79:ARG:HG3 | 1.56 | 0.70 |
| 1:CE:189:PHE:CE1 | 1:CE:198:ARG:HG3 | 2.27 | 0.70 |
| 1:CJ:74:ASN:HB3 | 1:CJ:126:GLU:HG2 | 1.74 | 0.70 |
| 1:CJ:250:TRP:CE3 | 1:CJ:272:TYR:CE1 | 2.80 | 0.70 |
| 1:AN:189:PHE:HE2 | 1:AN:249:LEU:HD21 | 1.56 | 0.70 |
| 1:AO:191:LEU:H | 1:AO:191:LEU:CD2 | 2.05 | 0.70 |
| 1:AR:189:PHE:CE1 | 1:AR:198:ARG:HG3 | 2.25 | 0.70 |
| 1:BD:272:TYR:HE2 | 1:BS:55:ARG:CD | 2.04 | 0.70 |
| 1:BI:55:ARG:NE | 1:BR:272:TYR:CE2 | 2.59 | 0.70 |
| 1:CO:272:TYR:HE2 | 1:CR:55:ARG:NE | 1.88 | 0.70 |
| 1:CP:33:LYS:O | 1:CP:33:LYS:HG2 | 1.89 | 0.70 |
| 1:CT:16:ALA:O | 1:CT:17:ASN:HB2 | 1.91 | 0.70 |
| 1:AA:55:ARG:CD | 1:CC:272:TYR:CE2 | 2.75 | 0.70 |
| 1:AB:284:ARG:HH11 | 1:AB:284:ARG:CG | 2.05 | 0.70 |
| 1:AH:33:LYS:HG2 | 1:AH:33:LYS:O | 1.92 | 0.70 |
| 1:AH:189:PHE:HE2 | 1:AH:249:LEU:HD21 | 1.56 | 0.70 |
| 1:AI:33:LYS:O | 1:AI:33:LYS:HG2 | 1.92 | 0.70 |
| 1:BD:284:ARG:HH11 | 1:BD:284:ARG:CG | 2.05 | 0.70 |
| 1:BF:22:THR:OG1 | 1:BF:131:HIS:HD2 | 1.74 | 0.70 |
| 1:BH:74:ASN:HB3 | 1:BH:126:GLU:HG2 | 1.74 | 0.70 |
| 1:BH:284:ARG:CG | 1:BH:284:ARG:HH11 | 2.04 | 0.70 |
| 1:BN:74:ASN:HB3 | 1:BN:126:GLU:HG2 | 1.74 | 0.70 |
| 1:AE:33:LYS:HG2 | 1:AE:33:LYS:O | 1.92 | 0.69 |
| 1:AE:189:PHE:CE1 | 1:AE:198:ARG:HG3 | 2.26 | 0.69 |
| 1:AK:191:LEU:H | 1:AK:191:LEU:CD2 | 2.05 | 0.69 |
| 1:BD:191:LEU:H | 1:BD:191:LEU:CD2 | 2.04 | 0.69 |
| 1:BL:79:ARG:HH11 | 1:BL:79:ARG:HG3 | 1.57 | 0.69 |
| 1:BM:189:PHE:HE1 | 1:BM:198:ARG:HG3 | 1.55 | 0.69 |
| 1:BS:33:LYS:O | 1:BS:33:LYS:HG2 | 1.92 | 0.69 |
| 1:CA:22:THR:OG1 | 1:CA:131:HIS:HD2 | 1.75 | 0.69 |
| 1:CO:189:PHE:CE1 | 1:CO:198:ARG:HG3 | 2.26 | 0.69 |
| 1:AA:55:ARG:CD | 1:CC:272:TYR:HE2 | 2.04 | 0.69 |
| 1:AJ:191:LEU:H | 1:AJ:191:LEU:CD2 | 2.04 | 0.69 |
| 1:AM:191:LEU:H | 1:AM:191:LEU:CD2 | 2.05 | 0.69 |
| 1:AN:189:PHE:CE1 | 1:AN:198:ARG:HG3 | 2.26 | 0.69 |
| 1:AT:55:ARG:CD | 1:BA:272:TYR:HE2 | 2.06 | 0.69 |
| 1:BO:22:THR:OG1 | 1:BO:131:HIS:HD2 | 1.75 | 0.69 |
| 1:CD:284:ARG:HH11 | 1:CD:284:ARG:CG | 2.04 | 0.69 |
| 1:AB:74:ASN:HB3 | 1:AB:126:GLU:HG2 | 1.73 | 0.69 |
| 1:AO:284:ARG:HG2 | 1:AO:284:ARG:HH11 | 1.57 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BD:22:THR:OG1 | 1:BD:131:HIS:HD2 | 1.73 | 0.69 |
| 1:CE:272:TYR:HE2 | 1:CM:55:ARG:CD | 2.05 | 0.69 |
| 1:AA:284:ARG:HH11 | 1:AA:284:ARG:CG | 2.06 | 0.69 |
| 1:AE:74:ASN:HB3 | 1:AE:126:GLU:HG2 | 1.74 | 0.69 |
| 1:AG:33:LYS:O | 1:AG:33:LYS:HG2 | 1.91 | 0.69 |
| 1:AK:33:LYS:HG2 | 1:AK:33:LYS:O | 1.93 | 0.69 |
| 1:AL:191:LEU:H | 1:AL:191:LEU:CD2 | 2.06 | 0.69 |
| 1:BB:284:ARG:HH11 | 1:BB:284:ARG:HG2 | 1.57 | 0.69 |
| 1:BC:55:ARG:NE | 1:BT:272:TYR:CE2 | 2.60 | 0.69 |
| 1:CF:74:ASN:HB3 | 1:CF:126:GLU:HG2 | 1.73 | 0.69 |
| 1:AD:55:ARG:CD | 1:AN:272:TYR:CE2 | 2.75 | 0.69 |
| 1:BN:33:LYS:O | 1:BN:33:LYS:HG2 | 1.93 | 0.69 |
| 1:BT:74:ASN:HB3 | 1:BT:126:GLU:HG2 | 1.74 | 0.69 |
| 1:CB:33:LYS:O | 1:CB:33:LYS:HG2 | 1.91 | 0.69 |
| 1:CL:189:PHE:CE1 | 1:CL:198:ARG:HG3 | 2.28 | 0.69 |
| 1:CO:284:ARG:HG2 | 1:CO:284:ARG:HH11 | 1.58 | 0.69 |
| 1:CQ:284:ARG:HH11 | 1:CQ:284:ARG:CG | 2.06 | 0.69 |
| 1:AI:454:ASN:HD22 | 1:AI:456:ALA:H | 1.39 | 0.69 |
| 1:BG:454:ASN:HD22 | 1:BG:456:ALA:H | 1.39 | 0.69 |
| 1:BI:191:LEU:H | 1:BI:191:LEU:CD2 | 2.05 | 0.69 |
| 1:BO:74:ASN:HB3 | 1:BO:126:GLU:HG2 | 1.73 | 0.69 |
| 1:CC:22:THR:OG1 | 1:CC:131:HIS:HD2 | 1.75 | 0.69 |
| 1:CI:33:LYS:HG2 | 1:CI:33:LYS:O | 1.90 | 0.69 |
| 1:CI:284:ARG:HH11 | 1:CI:284:ARG:CG | 2.06 | 0.69 |
| 1:CP:454:ASN:HD22 | 1:CP:456:ALA:H | 1.40 | 0.69 |
| 1:AH:250:TRP:CZ3 | 1:AH:272:TYR:HE1 | 2.11 | 0.69 |
| 1:AT:22:THR:OG1 | 1:AT:131:HIS:HD2 | 1.76 | 0.69 |
| 1:AT:79:ARG:HG3 | 1:AT:79:ARG:HH11 | 1.58 | 0.69 |
| 1:BI:22:THR:OG1 | 1:BI:131:HIS:HD2 | 1.73 | 0.69 |
| 1:BO:191:LEU:H | 1:BO:191:LEU:CD2 | 2.05 | 0.69 |
| 1:BP:191:LEU:H | 1:BP:191:LEU:CD2 | 2.05 | 0.69 |
| 1:BT:191:LEU:H | 1:BT:191:LEU:CD2 | 2.06 | 0.69 |
| 1:CG:189:PHE:HE2 | 1:CG:249:LEU:HD21 | 1.57 | 0.69 |
| 1:CG:189:PHE:CE1 | 1:CG:198:ARG:HG3 | 2.27 | 0.69 |
| 1:CT:14:CYS:H | 1:CT:138:ASN:HD21 | 1.39 | 0.69 |
| 1:AA:22:THR:OG1 | 1:AA:131:HIS:HD2 | 1.74 | 0.69 |
| 1:AC:22:THR:OG1 | 1:AC:131:HIS:HD2 | 1.76 | 0.69 |
| 1:AD:33:LYS:O | 1:AD:33:LYS:HG2 | 1.93 | 0.69 |
| 1:AF:284:ARG:CG | 1:AF:284:ARG:HH11 | 2.05 | 0.69 |
| 1:AI:189:PHE:CE1 | 1:AI:198:ARG:HG3 | 2.25 | 0.69 |
| 1:AM:189:PHE:HE2 | 1:AM:249:LEU:HD21 | 1.57 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AN:250:TRP:CZ3 | 1:AN:272:TYR:HE1 | 2.10 | 0.69 |
| 1:AP:284:ARG:HH11 | 1:AP:284:ARG:CG | 2.06 | 0.69 |
| 1:BB:189:PHE:HE2 | 1:BB:249:LEU:HD21 | 1.56 | 0.69 |
| 1:BH:55:ARG:CD | 1:BK:272:TYR:CE2 | 2.76 | 0.69 |
| 1:BN:284:ARG:HH11 | 1:BN:284:ARG:CG | 2.06 | 0.69 |
| 1:BP:189:PHE:CE1 | 1:BP:198:ARG:HG3 | 2.28 | 0.69 |
| 1:CB:191:LEU:H | 1:CB:191:LEU:CD2 | 2.06 | 0.69 |
| 1:CH:15:GLN:HA | 1:CH:15:GLN:HE21 | 1.57 | 0.69 |
| 1:CN:250:TRP:CZ3 | 1:CN:272:TYR:HE1 | 2.08 | 0.69 |
| 1:CN:284:ARG:HH11 | 1:CN:284:ARG:CG | 2.06 | 0.69 |
| 1:CQ:74:ASN:HB3 | 1:CQ:126:GLU:HG2 | 1.74 | 0.69 |
| 1:AG:36:GLN:NE2 | 1:AG:156:LEU:H | 1.91 | 0.69 |
| 1:AI:284:ARG:CG | 1:AI:284:ARG:HH11 | 2.05 | 0.69 |
| 1:AJ:74:ASN:HB3 | 1:AJ:126:GLU:HG2 | 1.73 | 0.69 |
| 1:BD:189:PHE:HE1 | 1:BD:198:ARG:HG3 | 1.58 | 0.69 |
| 1:BJ:55:ARG:NE | 1:CL:272:TYR:CE2 | 2.61 | 0.69 |
| 1:BK:284:ARG:HG2 | 1:BK:284:ARG:HH11 | 1.57 | 0.69 |
| 1:CB:189:PHE:CE1 | 1:CB:198:ARG:HG3 | 2.28 | 0.69 |
| 1:CF:250:TRP:CZ3 | 1:CF:272:TYR:HE1 | 2.09 | 0.69 |
| 1:AB:272:TYR:HE2 | 1:CB:55:ARG:CD | 2.06 | 0.69 |
| 1:AD:284:ARG:HH11 | 1:AD:284:ARG:CG | 2.05 | 0.69 |
| 1:AL:189:PHE:HE1 | 1:AL:198:ARG:HG3 | 1.58 | 0.69 |
| 1:AR:284:ARG:HH11 | 1:AR:284:ARG:CG | 2.06 | 0.69 |
| 1:BA:79:ARG:HH11 | 1:BA:79:ARG:CG | 2.06 | 0.69 |
| 1:BB:55:ARG:CD | 1:CB:272:TYR:CE2 | 2.76 | 0.69 |
| 1:CB:16:ALA:O | 1:CB:17:ASN:HB2 | 1.93 | 0.69 |
| 1:AH:284:ARG:HH11 | 1:AH:284:ARG:CG | 2.06 | 0.68 |
| 1:AK:189:PHE:CE1 | 1:AK:198:ARG:HG3 | 2.28 | 0.68 |
| 1:AL:272:TYR:CE2 | 1:CJ:55:ARG:NE | 2.61 | 0.68 |
| 1:AM:189:PHE:CE1 | 1:AM:198:ARG:HG3 | 2.28 | 0.68 |
| 1:AS:74:ASN:HB3 | 1:AS:126:GLU:HG2 | 1.74 | 0.68 |
| 1:BE:74:ASN:HB3 | 1:BE:126:GLU:HG2 | 1.74 | 0.68 |
| 1:CH:33:LYS:O | 1:CH:33:LYS:HG2 | 1.91 | 0.68 |
| 1:CL:284:ARG:HH11 | 1:CL:284:ARG:HG2 | 1.56 | 0.68 |
| 1:CN:55:ARG:CD | 1:CS:272:TYR:CE2 | 2.76 | 0.68 |
| 1:CO:22:THR:OG1 | 1:CO:131:HIS:HD2 | 1.75 | 0.68 |
| 1:CS:22:THR:OG1 | 1:CS:131:HIS:HD2 | 1.76 | 0.68 |
| 1:CT:189:PHE:HE1 | 1:CT:198:ARG:HG3 | 1.55 | 0.68 |
| 1:AL:33:LYS:O | 1:AL:33:LYS:HG2 | 1.94 | 0.68 |
| 1:AO:272:TYR:CE2 | 1:AR:55:ARG:CD | 2.76 | 0.68 |
| 1:AQ:272:TYR:CE2 | 1:BL:55:ARG:NE | 2.61 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AR:191:LEU:H | 1:AR:191:LEU:CD2 | 2.06 | 0.68 |
| 1:BF:191:LEU:H | 1:BF:191:LEU:CD2 | 2.05 | 0.68 |
| 1:BM:16:ALA:O | 1:BM:17:ASN:HB2 | 1.92 | 0.68 |
| 1:CM:189:PHE:HE2 | 1:CM:249:LEU:HD21 | 1.58 | 0.68 |
| 1:AA:36:GLN:NE2 | 1:AA:156:LEU:H | 1.92 | 0.68 |
| 1:AC:74:ASN:HB3 | 1:AC:126:GLU:HG2 | 1.75 | 0.68 |
| 1:BG:284:ARG:HH11 | 1:BG:284:ARG:CG | 2.07 | 0.68 |
| 1:CE:284:ARG:HH11 | 1:CE:284:ARG:CG | 2.06 | 0.68 |
| 1:CG:189:PHE:CE1 | 1:CG:198:ARG:CG | 2.77 | 0.68 |
| 1:CG:250:TRP:CZ3 | 1:CG:272:TYR:HE1 | 2.10 | 0.68 |
| 1:CI:189:PHE:CE1 | 1:CI:198:ARG:HG3 | 2.28 | 0.68 |
| 1:CI:191:LEU:H | 1:CI:191:LEU:CD2 | 2.05 | 0.68 |
| 1:CN:191:LEU:H | 1:CN:191:LEU:CD2 | 2.06 | 0.68 |
| 1:CR:189:PHE:HE2 | 1:CR:249:LEU:HD21 | 1.57 | 0.68 |
| 1:AA:191:LEU:H | 1:AA:191:LEU:CD2 | 2.05 | 0.68 |
| 1:AH:15:GLN:HA | 1:AH:15:GLN:HE21 | 1.57 | 0.68 |
| 1:AI:36:GLN:NE2 | 1:AI:156:LEU:H | 1.92 | 0.68 |
| 1:AM:16:ALA:O | 1:AM:17:ASN:HB2 | 1.92 | 0.68 |
| 1:AO:79:ARG:HH11 | 1:AO:79:ARG:HG3 | 1.56 | 0.68 |
| 1:AT:284:ARG:HG2 | 1:AT:284:ARG:HH11 | 1.59 | 0.68 |
| 1:BE:191:LEU:H | 1:BE:191:LEU:CD2 | 2.06 | 0.68 |
| 1:BI:189:PHE:CE1 | 1:BI:198:ARG:HG3 | 2.28 | 0.68 |
| 1:BK:36:GLN:NE2 | 1:BK:156:LEU:H | 1.89 | 0.68 |
| 1:BK:74:ASN:HB3 | 1:BK:126:GLU:HG2 | 1.74 | 0.68 |
| 1:CI:284:ARG:HH11 | 1:CI:284:ARG:HG2 | 1.57 | 0.68 |
| 1:CN:22:THR:OG1 | 1:CN:131:HIS:HD2 | 1.76 | 0.68 |
| 1:CN:189:PHE:HE2 | 1:CN:249:LEU:HD21 | 1.58 | 0.68 |
| 1:AO:284:ARG:HH11 | 1:AO:284:ARG:CG | 2.05 | 0.68 |
| 1:BI:272:TYR:CE2 | 1:BO:55:ARG:NE | 2.61 | 0.68 |
| 1:BO:272:TYR:CE2 | 1:BR:55:ARG:CD | 2.77 | 0.68 |
| 1:BT:284:ARG:HH11 | 1:BT:284:ARG:CG | 2.07 | 0.68 |
| 1:CB:250:TRP:CZ3 | 1:CB:272:TYR:HE1 | 2.11 | 0.68 |
| 1:CE:16:ALA:O | 1:CE:17:ASN:HB2 | 1.92 | 0.68 |
| 1:CF:33:LYS:HG2 | 1:CF:33:LYS:O | 1.94 | 0.68 |
| 1:CQ:33:LYS:HG2 | 1:CQ:33:LYS:O | 1.93 | 0.68 |
| 1:BD:272:TYR:CE2 | 1:BS:55:ARG:CD | 2.76 | 0.68 |
| 1:BR:284:ARG:HH11 | 1:BR:284:ARG:CG | 2.07 | 0.68 |
| 1:AC:191:LEU:H | 1:AC:191:LEU:CD2 | 2.06 | 0.68 |
| 1:AK:36:GLN:NE2 | 1:AK:156:LEU:H | 1.92 | 0.68 |
| 1:AS:284:ARG:HH11 | 1:AS:284:ARG:HG2 | 1.58 | 0.68 |
| 1:BC:272:TYR:CE2 | 1:CA:55:ARG:NE | 2.62 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:33:LYS:HG2 | 1:BJ:33:LYS:O | 1.94 | 0.68 |
| 1:BM:191:LEU:H | 1:BM:191:LEU:CD2 | 2.06 | 0.68 |
| 1:CM:191:LEU:H | 1:CM:191:LEU:CD2 | 2.06 | 0.68 |
| 1:AB:189:PHE:HE2 | 1:AB:249:LEU:HD21 | 1.59 | 0.68 |
| 1:AC:284:ARG:HH11 | 1:AC:284:ARG:HG2 | 1.59 | 0.68 |
| 1:AL:14:CYS:H | 1:AL:138:ASN:HD21 | 1.40 | 0.68 |
| 1:AT:74:ASN:HB3 | 1:AT:126:GLU:HG2 | 1.75 | 0.68 |
| 1:BL:284:ARG:HH11 | 1:BL:284:ARG:CG | 2.07 | 0.68 |
| 1:CA:79:ARG:HG3 | 1:CA:79:ARG:HH11 | 1.58 | 0.68 |
| 1:CA:284:ARG:HG2 | 1:CA:284:ARG:HH11 | 1.57 | 0.68 |
| 1:CH:74:ASN:HB3 | 1:CH:126:GLU:HG2 | 1.75 | 0.68 |
| 1:CM:284:ARG:HH11 | 1:CM:284:ARG:CG | 2.06 | 0.68 |
| 1:AG:22:THR:OG1 | 1:AG:131:HIS:HD2 | 1.77 | 0.68 |
| 1:AG:74:ASN:HB3 | 1:AG:126:GLU:HG2 | 1.75 | 0.68 |
| 1:AO:74:ASN:HB3 | 1:AO:126:GLU:HG2 | 1.75 | 0.68 |
| 1:AO:250:TRP:CE3 | 1:AO:272:TYR:CE1 | 2.81 | 0.68 |
| 1:BC:284:ARG:HH11 | 1:BC:284:ARG:CG | 2.07 | 0.68 |
| 1:BG:189:PHE:HE2 | 1:BG:249:LEU:HD21 | 1.57 | 0.68 |
| 1:BM:22:THR:OG1 | 1:BM:131:HIS:HD2 | 1.76 | 0.68 |
| 1:BQ:284:ARG:HG2 | 1:BQ:284:ARG:NH1 | 2.09 | 0.68 |
| 1:CH:189:PHE:HE2 | 1:CH:249:LEU:HD21 | 1.59 | 0.68 |
| 1:CO:284:ARG:HH11 | 1:CO:284:ARG:CG | 2.07 | 0.68 |
| 1:CP:74:ASN:HB3 | 1:CP:126:GLU:HG2 | 1.74 | 0.68 |
| 1:AK:284:ARG:HH11 | 1:AK:284:ARG:CG | 2.06 | 0.68 |
| 1:BM:33:LYS:HG2 | 1:BM:33:LYS:O | 1.93 | 0.68 |
| 1:CQ:22:THR:OG1 | 1:CQ:131:HIS:HD2 | 1.76 | 0.68 |
| 1:CH:250:TRP:CZ3 | 1:CH:272:TYR:HE1 | 2.12 | 0.67 |
| 1:CI:55:ARG:NE | 1:CR:272:TYR:CE2 | 2.62 | 0.67 |
| 1:CK:284:ARG:HH11 | 1:CK:284:ARG:CG | 2.06 | 0.67 |
| 1:CM:33:LYS:O | 1:CM:33:LYS:HG2 | 1.93 | 0.67 |
| 1:CP:191:LEU:H | 1:CP:191:LEU:CD2 | 2.05 | 0.67 |
| 1:CR:22:THR:OG1 | 1:CR:131:HIS:HD2 | 1.76 | 0.67 |
| 1:AA:284:ARG:HH11 | 1:AA:284:ARG:HG2 | 1.58 | 0.67 |
| 1:AD:272:TYR:CE2 | 1:AS:55:ARG:NE | 2.63 | 0.67 |
| 1:AG:191:LEU:H | 1:AG:191:LEU:CD2 | 2.07 | 0.67 |
| 1:AI:191:LEU:H | 1:AI:191:LEU:CD2 | 2.07 | 0.67 |
| 1:BC:189:PHE:CE1 | 1:BC:198:ARG:HG3 | 2.30 | 0.67 |
| 1:BE:284:ARG:CG | 1:BE:284:ARG:HH11 | 2.07 | 0.67 |
| 1:BR:284:ARG:HH11 | 1:BR:284:ARG:HG2 | 1.59 | 0.67 |
| 1:CC:189:PHE:HE1 | 1:CC:198:ARG:HG3 | 1.59 | 0.67 |
| 1:CD:272:TYR:CE2 | 1:CS:55:ARG:CD | 2.78 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CM:74:ASN:HB3 | 1:CM:126:GLU:HG2 | 1.76 | 0.67 |
| 1:CN:55:ARG:CD | 1:CS:272:TYR:HE2 | 2.07 | 0.67 |
| 1:AB:272:TYR:CE2 | 1:CB:55:ARG:CD | 2.78 | 0.67 |
| 1:AD:284:ARG:HH11 | 1:AD:284:ARG:HG2 | 1.58 | 0.67 |
| 1:AI:74:ASN:HB3 | 1:AI:126:GLU:HG2 | 1.76 | 0.67 |
| 1:BB:250:TRP:CZ3 | 1:BB:272:TYR:HE1 | 2.11 | 0.67 |
| 1:BK:284:ARG:HH11 | 1:BK:284:ARG:CG | 2.07 | 0.67 |
| 1:BM:11:PRO:HG2 | 1:BM:18:ARG:HD3 | 1.76 | 0.67 |
| 1:CJ:189:PHE:HE2 | 1:CJ:249:LEU:HD21 | 1.58 | 0.67 |
| 1:CM:189:PHE:CE1 | 1:CM:198:ARG:HG3 | 2.28 | 0.67 |
| 1:AF:272:TYR:CE2 | 1:BK:55:ARG:CD | 2.77 | 0.67 |
| 1:AH:272:TYR:CE2 | 1:CF:55:ARG:NE | 2.63 | 0.67 |
| 1:AI:189:PHE:HE2 | 1:AI:249:LEU:HD21 | 1.58 | 0.67 |
| 1:AJ:22:THR:OG1 | 1:AJ:131:HIS:HD2 | 1.76 | 0.67 |
| 1:AT:36:GLN:NE2 | 1:AT:156:LEU:H | 1.92 | 0.67 |
| 1:BE:189:PHE:HE2 | 1:BE:249:LEU:HD21 | 1.59 | 0.67 |
| 1:BF:284:ARG:HH11 | 1:BF:284:ARG:HG2 | 1.57 | 0.67 |
| 1:BH:189:PHE:CE1 | 1:BH:198:ARG:HG3 | 2.28 | 0.67 |
| 1:BM:284:ARG:HH11 | 1:BM:284:ARG:HG2 | 1.59 | 0.67 |
| 1:CA:191:LEU:H | 1:CA:191:LEU:CD2 | 2.06 | 0.67 |
| 1:CL:79:ARG:HG3 | 1:CL:79:ARG:HH11 | 1.59 | 0.67 |
| 1:AE:250:TRP:CZ3 | 1:AE:272:TYR:HE1 | 2.11 | 0.67 |
| 1:AN:284:ARG:HH11 | 1:AN:284:ARG:CG | 2.08 | 0.67 |
| 1:BE:22:THR:OG1 | 1:BE:131:HIS:HD2 | 1.76 | 0.67 |
| 1:BH:191:LEU:H | 1:BH:191:LEU:CD2 | 2.07 | 0.67 |
| 1:CL:191:LEU:H | 1:CL:191:LEU:CD2 | 2.06 | 0.67 |
| 1:AD:14:CYS:H | 1:AD:138:ASN:HD21 | 1.43 | 0.67 |
| 1:BC:284:ARG:HH11 | 1:BC:284:ARG:HG2 | 1.59 | 0.67 |
| 1:BK:22:THR:OG1 | 1:BK:131:HIS:HD2 | 1.76 | 0.67 |
| 1:BQ:191:LEU:H | 1:BQ:191:LEU:CD2 | 2.07 | 0.67 |
| 1:CA:189:PHE:HE1 | 1:CA:198:ARG:HG3 | 1.58 | 0.67 |
| 1:CD:33:LYS:O | 1:CD:33:LYS:HG2 | 1.95 | 0.67 |
| 1:CJ:272:TYR:CE2 | 1:CQ:55:ARG:CD | 2.78 | 0.67 |
| 1:CN:74:ASN:ND2 | 1:CN:77:THR:OG1 | 2.27 | 0.67 |
| 1:CO:250:TRP:CE3 | 1:CO:272:TYR:CE1 | 2.83 | 0.67 |
| 1:CO:272:TYR:CE2 | 1:CR:55:ARG:CD | 2.78 | 0.67 |
| 1:CT:22:THR:OG1 | 1:CT:131:HIS:HD2 | 1.78 | 0.67 |
| 1:AI:272:TYR:CE2 | 1:AO:55:ARG:CD | 2.76 | 0.67 |
| 1:AI:284:ARG:HH11 | 1:AI:284:ARG:HG2 | 1.58 | 0.67 |
| 1:BB:16:ALA:O | 1:BB:17:ASN:HB2 | 1.92 | 0.67 |
| 1:BC:191:LEU:H | 1:BC:191:LEU:CD2 | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BD:454:ASN:HD22 | 1:BD:456:ALA:H | 1.43 | 0.67 |
| 1:CD:74:ASN:HB3 | 1:CD:126:GLU:HG2 | 1.77 | 0.67 |
| 1:CG:284:ARG:CG | 1:CG:284:ARG:HH11 | 2.07 | 0.67 |
| 1:CT:191:LEU:H | 1:CT:191:LEU:CD2 | 2.08 | 0.67 |
| 1:AI:272:TYR:CE2 | 1:AO:55:ARG:NE | 2.63 | 0.67 |
| 1:AJ:189:PHE:HE2 | 1:AJ:249:LEU:HD21 | 1.59 | 0.67 |
| 1:AL:79:ARG:HH11 | 1:AL:79:ARG:CG | 2.06 | 0.67 |
| 1:AR:284:ARG:HH11 | 1:AR:284:ARG:HG2 | 1.60 | 0.67 |
| 1:BD:55:ARG:NE | 1:BN:272:TYR:CE2 | 2.63 | 0.67 |
| 1:BG:284:ARG:HH11 | 1:BG:284:ARG:HG2 | 1.60 | 0.67 |
| 1:BI:55:ARG:CD | 1:BR:272:TYR:CE2 | 2.77 | 0.67 |
| 1:BQ:189:PHE:CE1 | 1:BQ:198:ARG:HG3 | 2.29 | 0.67 |
| 1:CC:191:LEU:H | 1:CC:191:LEU:CD2 | 2.07 | 0.67 |
| 1:CR:189:PHE:CE1 | 1:CR:198:ARG:HG3 | 2.29 | 0.67 |
| 1:AD:191:LEU:H | 1:AD:191:LEU:CD2 | 2.07 | 0.67 |
| 1:AE:36:GLN:NE2 | 1:AE:156:LEU:H | 1.93 | 0.67 |
| 1:AS:189:PHE:HE1 | 1:AS:198:ARG:HG3 | 1.57 | 0.67 |
| 1:BQ:272:TYR:CE2 | 1:CL:55:ARG:CD | 2.78 | 0.67 |
| 1:CC:74:ASN:HB3 | 1:CC:126:GLU:HG2 | 1.75 | 0.67 |
| 1:CE:74:ASN:HB3 | 1:CE:126:GLU:HG2 | 1.76 | 0.67 |
| 1:CF:189:PHE:HE2 | 1:CF:249:LEU:HD21 | 1.59 | 0.67 |
| 1:AB:55:ARG:CD | 1:BB:272:TYR:CE2 | 2.78 | 0.66 |
| 1:AO:36:GLN:NE2 | 1:AO:156:LEU:H | 1.92 | 0.66 |
| 1:AT:191:LEU:H | 1:AT:191:LEU:CD2 | 2.08 | 0.66 |
| 1:BB:55:ARG:CD | 1:CB:272:TYR:HE2 | 2.08 | 0.66 |
| 1:CB:36:GLN:NE2 | 1:CB:156:LEU:H | 1.93 | 0.66 |
| 1:CB:284:ARG:HH11 | 1:CB:284:ARG:CG | 2.08 | 0.66 |
| 1:AT:284:ARG:HH11 | 1:AT:284:ARG:CG | 2.08 | 0.66 |
| 1:BB:189:PHE:CE1 | 1:BB:198:ARG:HG3 | 2.28 | 0.66 |
| 1:BI:189:PHE:HE2 | 1:BI:249:LEU:HD21 | 1.59 | 0.66 |
| 1:BS:191:LEU:H | 1:BS:191:LEU:CD2 | 2.08 | 0.66 |
| 1:CE:189:PHE:HE2 | 1:CE:249:LEU:HD21 | 1.59 | 0.66 |
| 1:CM:16:ALA:O | 1:CM:17:ASN:HB2 | 1.95 | 0.66 |
| 1:CG:191:LEU:H | 1:CG:191:LEU:CD2 | 2.06 | 0.66 |
| 1:CK:191:LEU:H | 1:CK:191:LEU:CD2 | 2.07 | 0.66 |
| 1:AA:272:TYR:CE2 | 1:CT:55:ARG:CD | 2.79 | 0.66 |
| 1:AM:284:ARG:HG2 | 1:AM:284:ARG:NH1 | 2.09 | 0.66 |
| 1:BE:189:PHE:CE1 | 1:BE:198:ARG:HG3 | 2.29 | 0.66 |
| 1:BF:33:LYS:O | 1:BF:33:LYS:HG2 | 1.96 | 0.66 |
| 1:BR:189:PHE:CE1 | 1:BR:198:ARG:HG3 | 2.29 | 0.66 |
| 1:CG:16:ALA:O | 1:CG:17:ASN:HB2 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CO:74:ASN:HB3 | 1:CO:126:GLU:HG2 | 1.77 | 0.66 |
| 1:CR:191:LEU:H | 1:CR:191:LEU:CD2 | 2.08 | 0.66 |
| 1:AH:36:GLN:NE2 | 1:AH:156:LEU:H | 1.93 | 0.66 |
| 1:AH:55:ARG:NE | 1:AK:272:TYR:CE2 | 2.64 | 0.66 |
| 1:CE:79:ARG:HH11 | 1:CE:79:ARG:HG3 | 1.60 | 0.66 |
| 1:CF:191:LEU:H | 1:CF:191:LEU:CD2 | 2.07 | 0.66 |
| 1:CH:284:ARG:HG2 | 1:CH:284:ARG:HH11 | 1.59 | 0.66 |
| 1:BA:189:PHE:CE1 | 1:BA:198:ARG:HG3 | 2.29 | 0.66 |
| 1:BB:189:PHE:CE1 | 1:BB:198:ARG:CG | 2.78 | 0.66 |
| 1:BC:55:ARG:CD | 1:BT:272:TYR:CE2 | 2.79 | 0.66 |
| 1:CD:36:GLN:NE2 | 1:CD:156:LEU:H | 1.93 | 0.66 |
| 1:CE:191:LEU:H | 1:CE:191:LEU:CD2 | 2.09 | 0.66 |
| 1:CN:14:CYS:H | 1:CN:138:ASN:HD21 | 1.41 | 0.66 |
| 1:CP:284:ARG:HH11 | 1:CP:284:ARG:CG | 2.07 | 0.66 |
| 1:CR:250:TRP:CZ3 | 1:CR:272:TYR:HE1 | 2.14 | 0.66 |
| 1:AM:272:TYR:CE2 | 1:CP:55:ARG:NE | 2.63 | 0.66 |
| 1:AO:33:LYS:O | 1:AO:33:LYS:HG2 | 1.94 | 0.66 |
| 1:BA:191:LEU:H | 1:BA:191:LEU:CD2 | 2.08 | 0.66 |
| 1:CE:272:TYR:CE2 | 1:CM:55:ARG:CD | 2.79 | 0.66 |
| 1:CK:74:ASN:HB3 | 1:CK:126:GLU:HG2 | 1.76 | 0.66 |
| 1:CK:284:ARG:HH11 | 1:CK:284:ARG:HG2 | 1.59 | 0.66 |
| 1:CM:284:ARG:HH11 | 1:CM:284:ARG:HG2 | 1.60 | 0.66 |
| 1:CQ:16:ALA:O | 1:CQ:17:ASN:HB2 | 1.96 | 0.66 |
| 1:AE:55:ARG:HD3 | 1:CP:272:TYR:CD2 | 2.31 | 0.66 |
| 1:AR:14:CYS:H | 1:AR:138:ASN:HD21 | 1.42 | 0.66 |
| 1:AT:55:ARG:HD3 | 1:BA:272:TYR:CD2 | 2.31 | 0.66 |
| 1:BC:74:ASN:HB3 | 1:BC:126:GLU:HG2 | 1.78 | 0.66 |
| 1:CD:272:TYR:HE2 | 1:CS:55:ARG:CD | 2.09 | 0.66 |
| 1:CS:284:ARG:HH11 | 1:CS:284:ARG:CG | 2.09 | 0.66 |
| 1:AI:14:CYS:H | 1:AI:138:ASN:HD21 | 1.42 | 0.66 |
| 1:AN:189:PHE:HE2 | 1:AN:249:LEU:CD2 | 2.08 | 0.66 |
| 1:AP:74:ASN:HB3 | 1:AP:126:GLU:HG2 | 1.76 | 0.66 |
| 1:AQ:36:GLN:NE2 | 1:AQ:156:LEU:H | 1.94 | 0.66 |
| 1:BH:55:ARG:CD | 1:BK:272:TYR:HE2 | 2.09 | 0.66 |
| 1:BN:189:PHE:HE2 | 1:BN:249:LEU:HD21 | 1.61 | 0.66 |
| 1:BP:272:TYR:CE2 | 1:CE:55:ARG:CZ | 2.79 | 0.66 |
| 1:BS:284:ARG:CG | 1:BS:284:ARG:HH11 | 2.08 | 0.66 |
| 1:CI:272:TYR:CE2 | 1:CO:55:ARG:CD | 2.79 | 0.66 |
| 1:CO:191:LEU:H | 1:CO:191:LEU:CD2 | 2.07 | 0.66 |
| 1:AQ:189:PHE:HE1 | 1:AQ:198:ARG:HG3 | 1.60 | 0.66 |
| 1:AQ:272:TYR:CE2 | 1:BL:55:ARG:CD | 2.79 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BK:250:TRP:CZ3 | 1:BK:272:TYR:HE1 | 2.13 | 0.66 |
| 1:AF:272:TYR:CD2 | 1:BK:55:ARG:HD3 | 2.31 | 0.65 |
| 1:AG:16:ALA:O | 1:AG:17:ASN:HB2 | 1.94 | 0.65 |
| 1:AK:55:ARG:HD3 | 1:CF:272:TYR:CD2 | 2.31 | 0.65 |
| 1:AL:250:TRP:CZ3 | 1:AL:272:TYR:HE1 | 2.14 | 0.65 |
| 1:AL:284:ARG:HH11 | 1:AL:284:ARG:HG2 | 1.60 | 0.65 |
| 1:BO:189:PHE:HE1 | 1:BO:198:ARG:HG3 | 1.62 | 0.65 |
| 1:CD:191:LEU:H | 1:CD:191:LEU:CD2 | 2.09 | 0.65 |
| 1:CH:191:LEU:H | 1:CH:191:LEU:CD2 | 2.07 | 0.65 |
| 1:AK:55:ARG:HD3 | 1:CF:272:TYR:CE2 | 2.31 | 0.65 |
| 1:BE:272:TYR:CE2 | 1:BM:55:ARG:NE | 2.65 | 0.65 |
| 1:BN:36:GLN:NE2 | 1:BN:156:LEU:H | 1.94 | 0.65 |
| 1:CI:36:GLN:NE2 | 1:CI:156:LEU:H | 1.94 | 0.65 |
| 1:CQ:284:ARG:HH11 | 1:CQ:284:ARG:HG2 | 1.62 | 0.65 |
| 1:AQ:272:TYR:CD2 | 1:BL:55:ARG:HD3 | 2.31 | 0.65 |
| 1:AR:189:PHE:HE2 | 1:AR:249:LEU:CD2 | 2.09 | 0.65 |
| 1:BG:191:LEU:H | 1:BG:191:LEU:CD2 | 2.08 | 0.65 |
| 1:BT:55:ARG:NE | 1:CA:272:TYR:CE2 | 2.64 | 0.65 |
| 1:CA:284:ARG:HH11 | 1:CA:284:ARG:CG | 2.09 | 0.65 |
| 1:AM:74:ASN:HB3 | 1:AM:126:GLU:HG2 | 1.78 | 0.65 |
| 1:AN:191:LEU:H | 1:AN:191:LEU:CD2 | 2.10 | 0.65 |
| 1:BJ:284:ARG:HH11 | 1:BJ:284:ARG:CG | 2.08 | 0.65 |
| 1:BS:79:ARG:HH11 | 1:BS:79:ARG:CG | 2.04 | 0.65 |
| 1:CB:284:ARG:HH11 | 1:CB:284:ARG:HG2 | 1.59 | 0.65 |
| 1:CH:284:ARG:HH11 | 1:CH:284:ARG:CG | 2.08 | 0.65 |
| 1:CP:250:TRP:CE3 | 1:CP:272:TYR:CE1 | 2.84 | 0.65 |
| 1:AB:22:THR:OG1 | 1:AB:131:HIS:HD2 | 1.78 | 0.65 |
| 1:AB:55:ARG:CD | 1:BB:272:TYR:HE2 | 2.10 | 0.65 |
| 1:AP:284:ARG:HH11 | 1:AP:284:ARG:HG2 | 1.62 | 0.65 |
| 1:BL:74:ASN:CB | 1:BL:126:GLU:HG2 | 2.27 | 0.65 |
| 1:CF:189:PHE:CE1 | 1:CF:198:ARG:HG3 | 2.29 | 0.65 |
| 1:CQ:189:PHE:HE1 | 1:CQ:198:ARG:HG3 | 1.61 | 0.65 |
| 1:AP:55:ARG:CD | 1:BM:272:TYR:HE2 | 2.10 | 0.65 |
| 1:AE:284:ARG:HH11 | 1:AE:284:ARG:CG | 2.08 | 0.65 |
| 1:AF:189:PHE:HE2 | 1:AF:249:LEU:CD2 | 2.10 | 0.65 |
| 1:AJ:55:ARG:CD | 1:BL:272:TYR:CE2 | 2.79 | 0.65 |
| 1:BD:74:ASN:HB3 | 1:BD:126:GLU:HG2 | 1.77 | 0.65 |
| 1:BL:191:LEU:H | 1:BL:191:LEU:CD2 | 2.09 | 0.65 |
| 1:CH:22:THR:OG1 | 1:CH:131:HIS:HD2 | 1.78 | 0.65 |
| 1:CJ:191:LEU:H | 1:CJ:191:LEU:CD2 | 2.10 | 0.65 |
| 1:CN:16:ALA:O | 1:CN:17:ASN:HB2 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AB:36:GLN:NE2 | 1:AB:156:LEU:H | 1.94 | 0.65 |
| 1:AP:250:TRP:CZ3 | 1:AP:272:TYR:HE1 | 2.14 | 0.65 |
| 1:BJ:55:ARG:CD | 1:CL:272:TYR:CE2 | 2.80 | 0.65 |
| 1:BS:189:PHE:CE1 | 1:BS:198:ARG:HG3 | 2.31 | 0.65 |
| 1:AA:74:ASN:HB3 | 1:AA:126:GLU:HG2 | 1.78 | 0.65 |
| 1:AD:36:GLN:NE2 | 1:AD:156:LEU:H | 1.95 | 0.65 |
| 1:AF:284:ARG:HH11 | 1:AF:284:ARG:HG2 | 1.61 | 0.65 |
| 1:AS:189:PHE:CE1 | 1:AS:198:ARG:HG3 | 2.32 | 0.65 |
| 1:BB:14:CYS:H | 1:BB:138:ASN:HD21 | 1.45 | 0.65 |
| 1:BB:239:ILE:HG12 | 1:BB:326:ILE:CD1 | 2.27 | 0.65 |
| 1:BI:74:ASN:HB3 | 1:BI:126:GLU:HG2 | 1.79 | 0.65 |
| 1:BN:250:TRP:CZ3 | 1:BN:272:TYR:HE1 | 2.15 | 0.65 |
| 1:CF:288:HIS:HD2 | 1:CF:337:ASP:OD2 | 1.79 | 0.65 |
| 1:CG:74:ASN:HB3 | 1:CG:126:GLU:HG2 | 1.78 | 0.65 |
| 1:CQ:14:CYS:H | 1:CQ:138:ASN:HD21 | 1.43 | 0.65 |
| 1:BF:36:GLN:NE2 | 1:BF:156:LEU:H | 1.94 | 0.65 |
| 1:BI:55:ARG:CD | 1:BR:272:TYR:HE2 | 2.10 | 0.65 |
| 1:BK:189:PHE:CE1 | 1:BK:198:ARG:HG3 | 2.32 | 0.65 |
| 1:CB:189:PHE:HE2 | 1:CB:249:LEU:HD21 | 1.61 | 0.65 |
| 1:CD:272:TYR:CD2 | 1:CS:55:ARG:HD3 | 2.32 | 0.65 |
| 1:CG:284:ARG:HH11 | 1:CG:284:ARG:HG2 | 1.62 | 0.65 |
| 1:CK:189:PHE:HE1 | 1:CK:198:ARG:HG3 | 1.59 | 0.65 |
| 1:CM:189:PHE:CE1 | 1:CM:198:ARG:CG | 2.79 | 0.65 |
| 1:CS:191:LEU:H | 1:CS:191:LEU:CD2 | 2.10 | 0.65 |
| 1:AA:14:CYS:H | 1:AA:138:ASN:HD21 | 1.45 | 0.64 |
| 1:AD:22:THR:OG1 | 1:AD:131:HIS:HD2 | 1.79 | 0.64 |
| 1:AH:189:PHE:CE1 | 1:AH:198:ARG:HG3 | 2.31 | 0.64 |
| 1:AJ:284:ARG:HH11 | 1:AJ:284:ARG:CG | 2.10 | 0.64 |
| 1:BA:284:ARG:HH11 | 1:BA:284:ARG:HG2 | 1.61 | 0.64 |
| 1:BB:55:ARG:HD3 | 1:CB:272:TYR:CD2 | 2.32 | 0.64 |
| 1:BF:250:TRP:CZ3 | 1:BF:272:TYR:HE1 | 2.14 | 0.64 |
| 1:BH:250:TRP:CZ3 | 1:BH:272:TYR:HE1 | 2.15 | 0.64 |
| 1:AD:55:ARG:HD3 | 1:AN:272:TYR:CD2 | 2.32 | 0.64 |
| 1:AG:272:TYR:CE2 | 1:BG:55:ARG:NE | 2.65 | 0.64 |
| 1:AK:250:TRP:CZ3 | 1:AK:272:TYR:HE1 | 2.14 | 0.64 |
| 1:AT:189:PHE:CE1 | 1:AT:198:ARG:HG3 | 2.32 | 0.64 |
| 1:BE:272:TYR:CE2 | 1:BM:55:ARG:CD | 2.80 | 0.64 |
| 1:BJ:189:PHE:HE2 | 1:BJ:249:LEU:HD21 | 1.61 | 0.64 |
| 1:BJ:284:ARG:HH11 | 1:BJ:284:ARG:HG2 | 1.62 | 0.64 |
| 1:CJ:284:ARG:HH11 | 1:CJ:284:ARG:CG | 2.10 | 0.64 |
| 1:CR:74:ASN:HB3 | 1:CR:126:GLU:HG2 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AH:74:ASN:HB3 | 1:AH:126:GLU:HG2 | 1.79 | 0.64 |
| 1:AI:272:TYR:CD2 | 1:AO:55:ARG:HD3 | 2.32 | 0.64 |
| 1:AI:272:TYR:HE2 | 1:AO:55:ARG:CD | 2.09 | 0.64 |
| 1:AP:55:ARG:CD | 1:BM:272:TYR:CE2 | 2.80 | 0.64 |
| 1:BP:55:ARG:CD | 1:CM:272:TYR:HE2 | 2.10 | 0.64 |
| 1:BP:55:ARG:CD | 1:CM:272:TYR:CE2 | 2.81 | 0.64 |
| 1:CC:189:PHE:CE1 | 1:CC:198:ARG:HG3 | 2.32 | 0.64 |
| 1:CI:74:ASN:CB | 1:CI:126:GLU:HG2 | 2.26 | 0.64 |
| 1:CL:14:CYS:H | 1:CL:138:ASN:HD21 | 1.45 | 0.64 |
| 1:CR:189:PHE:CE1 | 1:CR:198:ARG:CG | 2.78 | 0.64 |
| 1:AD:55:ARG:CD | 1:AN:272:TYR:HE2 | 2.08 | 0.64 |
| 1:AN:55:ARG:HD3 | 1:AS:272:TYR:CD2 | 2.31 | 0.64 |
| 1:AS:36:GLN:NE2 | 1:AS:156:LEU:H | 1.95 | 0.64 |
| 1:BE:189:PHE:CE1 | 1:BE:198:ARG:CG | 2.78 | 0.64 |
| 1:BG:36:GLN:NE2 | 1:BG:156:LEU:H | 1.96 | 0.64 |
| 1:BG:189:PHE:CE1 | 1:BG:198:ARG:HG3 | 2.29 | 0.64 |
| 1:BJ:189:PHE:CE1 | 1:BJ:198:ARG:CG | 2.81 | 0.64 |
| 1:AN:16:ALA:O | 1:AN:17:ASN:HB2 | 1.97 | 0.64 |
| 1:AT:55:ARG:HD3 | 1:BA:272:TYR:CE2 | 2.33 | 0.64 |
| 1:BM:189:PHE:HE2 | 1:BM:249:LEU:CD2 | 2.10 | 0.64 |
| 1:BN:284:ARG:HH11 | 1:BN:284:ARG:HG2 | 1.62 | 0.64 |
| 1:BQ:272:TYR:HE2 | 1:CL:55:ARG:CD | 2.10 | 0.64 |
| 1:CF:284:ARG:HH11 | 1:CF:284:ARG:CG | 2.10 | 0.64 |
| 1:AD:250:TRP:CZ3 | 1:AD:272:TYR:HE1 | 2.14 | 0.64 |
| 1:AE:191:LEU:H | 1:AE:191:LEU:CD2 | 2.08 | 0.64 |
| 1:AF:250:TRP:CZ3 | 1:AF:272:TYR:HE1 | 2.15 | 0.64 |
| 1:AG:189:PHE:CE1 | 1:AG:198:ARG:HG3 | 2.29 | 0.64 |
| 1:AK:22:THR:OG1 | 1:AK:131:HIS:HD2 | 1.79 | 0.64 |
| 1:AL:36:GLN:NE2 | 1:AL:156:LEU:H | 1.95 | 0.64 |
| 1:AQ:191:LEU:H | 1:AQ:191:LEU:CD2 | 2.08 | 0.64 |
| 1:BF:272:TYR:CE2 | 1:CK:55:ARG:NE | 2.66 | 0.64 |
| 1:BH:284:ARG:HH11 | 1:BH:284:ARG:HG2 | 1.61 | 0.64 |
| 1:CH:189:PHE:HE2 | 1:CH:249:LEU:CD2 | 2.10 | 0.64 |
| 1:CK:22:THR:OG1 | 1:CK:131:HIS:HD2 | 1.81 | 0.64 |
| 1:CK:250:TRP:CZ3 | 1:CK:272:TYR:HE1 | 2.13 | 0.64 |
| 1:CP:189:PHE:CE1 | 1:CP:198:ARG:HG3 | 2.33 | 0.64 |
| 1:CS:250:TRP:CZ3 | 1:CS:272:TYR:HE1 | 2.12 | 0.64 |
| 1:AO:189:PHE:HE1 | 1:AO:198:ARG:HG3 | 1.61 | 0.64 |
| 1:BB:22:THR:OG1 | 1:BB:131:HIS:HD2 | 1.80 | 0.64 |
| 1:BE:284:ARG:HH11 | 1:BE:284:ARG:HG2 | 1.61 | 0.64 |
| 1:BF:189:PHE:HE2 | 1:BF:249:LEU:HD21 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:55:ARG:HD3 | 1:BK:272:TYR:CD2 | 2.32 | 0.64 |
| 1:BR:189:PHE:HE2 | 1:BR:249:LEU:HD21 | 1.61 | 0.64 |
| 1:CK:14:CYS:H | 1:CK:138:ASN:HD21 | 1.44 | 0.64 |
| 1:CN:55:ARG:HD3 | 1:CS:272:TYR:CE2 | 2.32 | 0.64 |
| 1:AB:189:PHE:CE1 | 1:AB:198:ARG:HG3 | 2.31 | 0.64 |
| 1:AQ:284:ARG:CG | 1:AQ:284:ARG:HH11 | 2.11 | 0.64 |
| 1:BF:55:ARG:CD | 1:CH:272:TYR:CE2 | 2.81 | 0.64 |
| 1:CI:272:TYR:HE2 | 1:CO:55:ARG:CD | 2.11 | 0.64 |
| 1:AL:55:ARG:CD | 1:CQ:272:TYR:CE2 | 2.81 | 0.64 |
| 1:AM:189:PHE:CE1 | 1:AM:198:ARG:CG | 2.80 | 0.64 |
| 1:AM:250:TRP:CZ3 | 1:AM:272:TYR:HE1 | 2.16 | 0.64 |
| 1:AN:74:ASN:CB | 1:AN:126:GLU:HG2 | 2.28 | 0.64 |
| 1:AN:284:ARG:HH11 | 1:AN:284:ARG:HG2 | 1.63 | 0.64 |
| 1:BG:79:ARG:HH11 | 1:BG:79:ARG:HG3 | 1.62 | 0.64 |
| 1:BH:36:GLN:NE2 | 1:BH:156:LEU:H | 1.96 | 0.64 |
| 1:BL:189:PHE:CE1 | 1:BL:198:ARG:HG3 | 2.31 | 0.64 |
| 1:BN:55:ARG:NE | 1:BS:272:TYR:CE2 | 2.65 | 0.64 |
| 1:BO:284:ARG:HG2 | 1:BO:284:ARG:NH1 | 2.12 | 0.64 |
| 1:BQ:22:THR:OG1 | 1:BQ:131:HIS:HD2 | 1.81 | 0.64 |
| 1:BS:74:ASN:CB | 1:BS:126:GLU:HG2 | 2.28 | 0.64 |
| 1:CH:189:PHE:CE1 | 1:CH:198:ARG:HG3 | 2.30 | 0.64 |
| 1:AR:36:GLN:NE2 | 1:AR:156:LEU:H | 1.95 | 0.64 |
| 1:BA:189:PHE:HE1 | 1:BA:198:ARG:CG | 2.11 | 0.64 |
| 1:BF:67:VAL:HG23 | 1:BF:135:LEU:HB2 | 1.80 | 0.64 |
| 1:BO:36:GLN:NE2 | 1:BO:156:LEU:H | 1.96 | 0.64 |
| 1:BQ:272:TYR:CD2 | 1:CL:55:ARG:HD3 | 2.33 | 0.64 |
| 1:BR:191:LEU:H | 1:BR:191:LEU:CD2 | 2.09 | 0.64 |
| 1:CA:67:VAL:HG23 | 1:CA:135:LEU:HB2 | 1.79 | 0.64 |
| 1:CE:250:TRP:CE3 | 1:CE:272:TYR:CE1 | 2.86 | 0.64 |
| 1:CK:189:PHE:CE1 | 1:CK:198:ARG:HG3 | 2.33 | 0.64 |
| 1:AC:55:ARG:CD | 1:AT:272:TYR:CE2 | 2.81 | 0.63 |
| 1:AC:272:TYR:CE2 | 1:BA:55:ARG:CD | 2.81 | 0.63 |
| 1:AG:250:TRP:CE3 | 1:AG:272:TYR:CE1 | 2.86 | 0.63 |
| 1:AI:55:ARG:NE | 1:AR:272:TYR:CE2 | 2.66 | 0.63 |
| 1:AJ:189:PHE:CE1 | 1:AJ:198:ARG:HG3 | 2.30 | 0.63 |
| 1:AR:74:ASN:HB3 | 1:AR:126:GLU:HG2 | 1.80 | 0.63 |
| 1:BN:55:ARG:CD | 1:BS:272:TYR:CE2 | 2.80 | 0.63 |
| 1:BT:14:CYS:H | 1:BT:138:ASN:HD21 | 1.46 | 0.63 |
| 1:AE:272:TYR:CE2 | 1:AM:55:ARG:CD | 2.81 | 0.63 |
| 1:AF:55:ARG:CD | 1:BH:272:TYR:CE2 | 2.81 | 0.63 |
| 1:BA:74:ASN:CB | 1:BA:126:GLU:HG2 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BF:55:ARG:CD | 1:CH:272:TYR:HE2 | 2.10 | 0.63 |
| 1:BG:22:THR:OG1 | 1:BG:131:HIS:HD2 | 1.80 | 0.63 |
| 1:BG:250:TRP:CZ3 | 1:BG:272:TYR:HE1 | 2.13 | 0.63 |
| 1:BO:272:TYR:CE2 | 1:BR:55:ARG:CZ | 2.81 | 0.63 |
| 1:CC:55:ARG:CD | 1:CT:272:TYR:CE2 | 2.82 | 0.63 |
| 1:CH:55:ARG:CD | 1:CK:272:TYR:CE2 | 2.81 | 0.63 |
| 1:AA:55:ARG:CZ | 1:CC:272:TYR:CE2 | 2.82 | 0.63 |
| 1:AL:272:TYR:CE2 | 1:CJ:55:ARG:CD | 2.82 | 0.63 |
| 1:BE:36:GLN:NE2 | 1:BE:156:LEU:H | 1.96 | 0.63 |
| 1:BH:189:PHE:CE1 | 1:BH:198:ARG:CG | 2.80 | 0.63 |
| 1:CB:189:PHE:CE1 | 1:CB:198:ARG:CG | 2.79 | 0.63 |
| 1:CN:18:ARG:HG3 | 1:CN:19:TYR:N | 2.12 | 0.63 |
| 1:AD:189:PHE:CE1 | 1:AD:198:ARG:HG3 | 2.34 | 0.63 |
| 1:AE:55:ARG:HD3 | 1:CP:272:TYR:CE2 | 2.34 | 0.63 |
| 1:AG:284:ARG:HG2 | 1:AG:284:ARG:NH1 | 2.12 | 0.63 |
| 1:BB:74:ASN:HB3 | 1:BB:126:GLU:HG2 | 1.79 | 0.63 |
| 1:BN:189:PHE:CE1 | 1:BN:198:ARG:HG3 | 2.34 | 0.63 |
| 1:BP:272:TYR:CD2 | 1:CE:55:ARG:CZ | 2.82 | 0.63 |
| 1:CD:250:TRP:CE3 | 1:CD:272:TYR:CE1 | 2.86 | 0.63 |
| 1:CE:189:PHE:CE1 | 1:CE:198:ARG:CG | 2.81 | 0.63 |
| 1:CI:14:CYS:H | 1:CI:138:ASN:HD21 | 1.47 | 0.63 |
| 1:AI:272:TYR:CE2 | 1:AO:55:ARG:HD3 | 2.34 | 0.63 |
| 1:BF:272:TYR:CE2 | 1:CK:55:ARG:CD | 2.81 | 0.63 |
| 1:BR:36:GLN:NE2 | 1:BR:156:LEU:H | 1.97 | 0.63 |
| 1:CJ:189:PHE:CE1 | 1:CJ:198:ARG:CG | 2.80 | 0.63 |
| 1:CM:79:ARG:HH11 | 1:CM:79:ARG:HG3 | 1.64 | 0.63 |
| 1:AF:191:LEU:H | 1:AF:191:LEU:CD2 | 2.11 | 0.63 |
| 1:AF:272:TYR:HE2 | 1:BK:55:ARG:CD | 2.12 | 0.63 |
| 1:BL:284:ARG:HH11 | 1:BL:284:ARG:HG2 | 1.63 | 0.63 |
| 1:BN:189:PHE:CE1 | 1:BN:198:ARG:CG | 2.79 | 0.63 |
| 1:BQ:74:ASN:HB3 | 1:BQ:126:GLU:HG2 | 1.81 | 0.63 |
| 1:CD:284:ARG:HG2 | 1:CD:284:ARG:NH1 | 2.12 | 0.63 |
| 1:AB:74:ASN:CB | 1:AB:126:GLU:HG2 | 2.29 | 0.63 |
| 1:AL:189:PHE:CE1 | 1:AL:198:ARG:HG3 | 2.34 | 0.63 |
| 1:AR:79:ARG:HH11 | 1:AR:79:ARG:HG3 | 1.63 | 0.63 |
| 1:AR:189:PHE:CE1 | 1:AR:198:ARG:CG | 2.79 | 0.63 |
| 1:BJ:272:TYR:HE2 | 1:BQ:55:ARG:CD | 2.10 | 0.63 |
| 1:BP:74:ASN:HB3 | 1:BP:126:GLU:HG2 | 1.80 | 0.63 |
| 1:BP:284:ARG:HH11 | 1:BP:284:ARG:CG | 2.12 | 0.63 |
| 1:CS:284:ARG:HH11 | 1:CS:284:ARG:HG2 | 1.63 | 0.63 |
| 1:AA:272:TYR:HE2 | 1:CT:55:ARG:CD | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BM:250:TRP:CZ3 | 1:BM:272:TYR:HE1 | 2.17 | 0.63 |
| 1:CA:74:ASN:HB3 | 1:CA:126:GLU:HG2 | 1.81 | 0.63 |
| 1:CF:284:ARG:HH11 | 1:CF:284:ARG:HG2 | 1.63 | 0.63 |
| 1:AO:203:THR:HB | 1:AO:300:GLN:HG3 | 1.81 | 0.63 |
| 1:CA:250:TRP:CZ3 | 1:CA:272:TYR:HE1 | 2.14 | 0.63 |
| 1:CD:14:CYS:H | 1:CD:138:ASN:HD21 | 1.46 | 0.63 |
| 1:CM:189:PHE:HE2 | 1:CM:249:LEU:CD2 | 2.11 | 0.63 |
| 1:CT:36:GLN:NE2 | 1:CT:156:LEU:H | 1.97 | 0.63 |
| 1:AC:55:ARG:CD | 1:AT:272:TYR:HE2 | 2.11 | 0.62 |
| 1:BB:79:ARG:HG3 | 1:BB:79:ARG:HH11 | 1.64 | 0.62 |
| 1:BC:74:ASN:ND2 | 1:BC:77:THR:OG1 | 2.32 | 0.62 |
| 1:BD:284:ARG:HH11 | 1:BD:284:ARG:HG2 | 1.64 | 0.62 |
| 1:BM:74:ASN:HB3 | 1:BM:126:GLU:HG2 | 1.80 | 0.62 |
| 1:CD:79:ARG:HH11 | 1:CD:79:ARG:CG | 2.07 | 0.62 |
| 1:AA:189:PHE:CE1 | 1:AA:198:ARG:HG3 | 2.34 | 0.62 |
| 1:AG:55:ARG:CD | 1:CG:272:TYR:HE2 | 2.12 | 0.62 |
| 1:AG:79:ARG:HG3 | 1:AG:79:ARG:NH1 | 2.09 | 0.62 |
| 1:AL:272:TYR:HE2 | 1:CJ:55:ARG:CD | 2.12 | 0.62 |
| 1:AM:36:GLN:NE2 | 1:AM:156:LEU:H | 1.97 | 0.62 |
| 1:AM:272:TYR:CE2 | 1:CP:55:ARG:CD | 2.82 | 0.62 |
| 1:BI:55:ARG:HD3 | 1:BR:272:TYR:CD2 | 2.33 | 0.62 |
| 1:BL:16:ALA:O | 1:BL:17:ASN:HB2 | 1.98 | 0.62 |
| 1:BS:36:GLN:NE2 | 1:BS:156:LEU:H | 1.95 | 0.62 |
| 1:BT:284:ARG:HH11 | 1:BT:284:ARG:HG2 | 1.63 | 0.62 |
| 1:AN:36:GLN:NE2 | 1:AN:156:LEU:H | 1.96 | 0.62 |
| 1:BB:36:GLN:NE2 | 1:BB:156:LEU:H | 1.96 | 0.62 |
| 1:CE:36:GLN:NE2 | 1:CE:156:LEU:H | 1.97 | 0.62 |
| 1:CN:55:ARG:HD3 | 1:CS:272:TYR:CD2 | 2.34 | 0.62 |
| 1:AH:284:ARG:HH11 | 1:AH:284:ARG:HG2 | 1.63 | 0.62 |
| 1:BE:79:ARG:HG3 | 1:BE:79:ARG:HH11 | 1.63 | 0.62 |
| 1:BI:189:PHE:HE2 | 1:BI:249:LEU:CD2 | 2.12 | 0.62 |
| 1:CG:189:PHE:HE2 | 1:CG:249:LEU:CD2 | 2.12 | 0.62 |
| 1:AC:284:ARG:HG2 | 1:AC:284:ARG:NH1 | 2.13 | 0.62 |
| 1:BD:272:TYR:CD2 | 1:BS:55:ARG:HD3 | 2.35 | 0.62 |
| 1:BJ:55:ARG:CD | 1:CL:272:TYR:HE2 | 2.11 | 0.62 |
| 1:BL:239:ILE:HG12 | 1:BL:326:ILE:CD1 | 2.29 | 0.62 |
| 1:BP:14:CYS:H | 1:BP:138:ASN:HD21 | 1.47 | 0.62 |
| 1:BT:74:ASN:CB | 1:BT:126:GLU:HG2 | 2.28 | 0.62 |
| 1:CR:79:ARG:HH11 | 1:CR:79:ARG:HG2 | 1.64 | 0.62 |
| 1:CT:284:ARG:HG2 | 1:CT:284:ARG:NH1 | 2.14 | 0.62 |
| 1:AA:250:TRP:CZ3 | 1:AA:272:TYR:HE1 | 2.17 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AM:454:ASN:HD22 | 1:AM:456:ALA:N | 1.97 | 0.62 |
| 1:BC:55:ARG:CD | 1:BT:272:TYR:HE2 | 2.12 | 0.62 |
| 1:BD:272:TYR:CE2 | 1:BS:55:ARG:HD3 | 2.34 | 0.62 |
| 1:BF:74:ASN:HB3 | 1:BF:126:GLU:HG2 | 1.80 | 0.62 |
| 1:BN:55:ARG:CD | 1:BS:272:TYR:HE2 | 2.13 | 0.62 |
| 1:BS:284:ARG:HH11 | 1:BS:284:ARG:HG2 | 1.64 | 0.62 |
| 1:CD:189:PHE:HE1 | 1:CD:198:ARG:HG3 | 1.64 | 0.62 |
| 1:AJ:36:GLN:NE2 | 1:AJ:156:LEU:H | 1.96 | 0.62 |
| 1:BC:55:ARG:HD3 | 1:BT:272:TYR:CD2 | 2.35 | 0.62 |
| 1:BF:284:ARG:HG2 | 1:BF:284:ARG:NH1 | 2.13 | 0.62 |
| 1:BG:15:GLN:HA | 1:BG:15:GLN:HE21 | 1.64 | 0.62 |
| 1:BI:272:TYR:HE2 | 1:BO:55:ARG:CD | 2.13 | 0.62 |
| 1:BR:22:THR:OG1 | 1:BR:131:HIS:HD2 | 1.82 | 0.62 |
| 1:AC:189:PHE:HE1 | 1:AC:198:ARG:HG3 | 1.63 | 0.62 |
| 1:AH:272:TYR:CE2 | 1:CF:55:ARG:CD | 2.83 | 0.62 |
| 1:AO:22:THR:OG1 | 1:AO:131:HIS:HD2 | 1.82 | 0.62 |
| 1:AO:272:TYR:CE2 | 1:AR:55:ARG:CZ | 2.82 | 0.62 |
| 1:CA:189:PHE:CE1 | 1:CA:198:ARG:HG3 | 2.34 | 0.62 |
| 1:CF:454:ASN:HD22 | 1:CF:456:ALA:N | 1.96 | 0.62 |
| 1:AR:201:GLY:HA3 | 1:AR:300:GLN:HG2 | 1.81 | 0.62 |
| 1:BB:288:HIS:HD2 | 1:BB:337:ASP:OD2 | 1.82 | 0.62 |
| 1:BK:191:LEU:H | 1:BK:191:LEU:CD2 | 2.09 | 0.62 |
| 1:CL:36:GLN:NE2 | 1:CL:156:LEU:H | 1.97 | 0.62 |
| 1:CQ:36:GLN:NE2 | 1:CQ:156:LEU:H | 1.98 | 0.62 |
| 1:AE:272:TYR:HE2 | 1:AM:55:ARG:CD | 2.13 | 0.62 |
| 1:AF:74:ASN:CB | 1:AF:126:GLU:HG2 | 2.30 | 0.62 |
| 1:AH:22:THR:OG1 | 1:AH:131:HIS:HD2 | 1.81 | 0.62 |
| 1:AK:284:ARG:HH11 | 1:AK:284:ARG:HG2 | 1.64 | 0.62 |
| 1:AN:189:PHE:CE1 | 1:AN:198:ARG:CG | 2.79 | 0.62 |
| 1:AS:191:LEU:H | 1:AS:191:LEU:CD2 | 2.12 | 0.62 |
| 1:BB:55:ARG:HD3 | 1:CB:272:TYR:CE2 | 2.35 | 0.62 |
| 1:BH:14:CYS:H | 1:BH:138:ASN:HD21 | 1.46 | 0.62 |
| 1:BI:272:TYR:CE2 | 1:BO:55:ARG:CD | 2.82 | 0.62 |
| 1:CF:189:PHE:CE1 | 1:CF:198:ARG:CG | 2.79 | 0.62 |
| 1:CL:250:TRP:CZ3 | 1:CL:272:TYR:HE1 | 2.14 | 0.62 |
| 1:CT:189:PHE:CE1 | 1:CT:198:ARG:HG3 | 2.33 | 0.62 |
| 1:AG:189:PHE:HE2 | 1:AG:249:LEU:CD2 | 2.12 | 0.61 |
| 1:AH:191:LEU:H | 1:AH:191:LEU:CD2 | 2.10 | 0.61 |
| 1:AL:55:ARG:CD | 1:CQ:272:TYR:HE2 | 2.13 | 0.61 |
| 1:AQ:79:ARG:HG3 | 1:AQ:79:ARG:HH11 | 1.64 | 0.61 |
| 1:BA:288:HIS:HD2 | 1:BA:337:ASP:OD2 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:189:PHE:CE1 | 1:BG:198:ARG:CG | 2.81 | 0.61 |
| 1:BJ:272:TYR:CE2 | 1:BQ:55:ARG:CD | 2.83 | 0.61 |
| 1:CE:14:CYS:H | 1:CE:138:ASN:HD21 | 1.45 | 0.61 |
| 1:CI:250:TRP:CZ3 | 1:CI:272:TYR:HE1 | 2.16 | 0.61 |
| 1:AH:67:VAL:HG23 | 1:AH:135:LEU:HB2 | 1.81 | 0.61 |
| 1:AK:74:ASN:CB | 1:AK:126:GLU:HG2 | 2.29 | 0.61 |
| 1:AM:189:PHE:HE2 | 1:AM:249:LEU:CD2 | 2.13 | 0.61 |
| 1:BD:36:GLN:NE2 | 1:BD:156:LEU:H | 1.98 | 0.61 |
| 1:BI:239:ILE:HG12 | 1:BI:326:ILE:CD1 | 2.30 | 0.61 |
| 1:BQ:250:TRP:CZ3 | 1:BQ:272:TYR:HE1 | 2.17 | 0.61 |
| 1:CJ:36:GLN:NE2 | 1:CJ:156:LEU:H | 1.98 | 0.61 |
| 1:CS:189:PHE:CE1 | 1:CS:198:ARG:HG3 | 2.34 | 0.61 |
| 1:CS:454:ASN:ND2 | 1:CS:456:ALA:H | 1.98 | 0.61 |
| 1:AL:16:ALA:O | 1:AL:17:ASN:HB2 | 1.98 | 0.61 |
| 1:AP:36:GLN:NE2 | 1:AP:156:LEU:H | 1.98 | 0.61 |
| 1:AR:284:ARG:HG2 | 1:AR:284:ARG:NH1 | 2.16 | 0.61 |
| 1:AT:250:TRP:CE3 | 1:AT:272:TYR:CE1 | 2.88 | 0.61 |
| 1:CB:74:ASN:CB | 1:CB:126:GLU:HG2 | 2.30 | 0.61 |
| 1:CI:284:ARG:HG2 | 1:CI:284:ARG:NH1 | 2.15 | 0.61 |
| 1:CJ:74:ASN:CB | 1:CJ:126:GLU:HG2 | 2.31 | 0.61 |
| 1:CT:250:TRP:CZ3 | 1:CT:272:TYR:HE1 | 2.14 | 0.61 |
| 1:AA:272:TYR:CD2 | 1:CT:55:ARG:HD3 | 2.36 | 0.61 |
| 1:AN:288:HIS:HD2 | 1:AN:337:ASP:OD2 | 1.83 | 0.61 |
| 1:BB:284:ARG:HG2 | 1:BB:284:ARG:NH1 | 2.14 | 0.61 |
| 1:CH:189:PHE:CE1 | 1:CH:198:ARG:CG | 2.81 | 0.61 |
| 1:CR:284:ARG:CG | 1:CR:284:ARG:HH11 | 2.12 | 0.61 |
| 1:AA:189:PHE:HE1 | 1:AA:198:ARG:CG | 2.13 | 0.61 |
| 1:AI:284:ARG:HG2 | 1:AI:284:ARG:NH1 | 2.15 | 0.61 |
| 1:BC:74:ASN:CB | 1:BC:126:GLU:HG2 | 2.30 | 0.61 |
| 1:BJ:79:ARG:HH11 | 1:BJ:79:ARG:CG | 2.10 | 0.61 |
| 1:BN:55:ARG:HD3 | 1:BS:272:TYR:CE2 | 2.35 | 0.61 |
| 1:BR:250:TRP:CZ3 | 1:BR:272:TYR:HE1 | 2.15 | 0.61 |
| 1:CH:55:ARG:CD | 1:CK:272:TYR:HE2 | 2.13 | 0.61 |
| 1:CH:74:ASN:CB | 1:CH:126:GLU:HG2 | 2.29 | 0.61 |
| 1:CI:189:PHE:HE2 | 1:CI:249:LEU:CD2 | 2.12 | 0.61 |
| 1:CP:36:GLN:NE2 | 1:CP:156:LEU:H | 1.98 | 0.61 |
| 1:CQ:250:TRP:CE3 | 1:CQ:272:TYR:CE1 | 2.89 | 0.61 |
| 1:AB:58:ALA:HB2 | 1:AB:102:GLY:HA3 | 1.83 | 0.61 |
| 1:AC:272:TYR:HE2 | 1:BA:55:ARG:CD | 2.13 | 0.61 |
| 1:AF:36:GLN:NE2 | 1:AF:156:LEU:H | 1.97 | 0.61 |
| 1:BD:250:TRP:CE3 | 1:BD:272:TYR:CE1 | 2.88 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BM:284:ARG:HG2 | 1:BM:284:ARG:NH1 | 2.15 | 0.61 |
| 1:CG:14:CYS:H | 1:CG:138:ASN:HD21 | 1.48 | 0.61 |
| 1:CN:189:PHE:CE1 | 1:CN:198:ARG:CG | 2.79 | 0.61 |
| 1:CS:454:ASN:HD22 | 1:CS:456:ALA:N | 1.98 | 0.61 |
| 1:AE:74:ASN:CB | 1:AE:126:GLU:HG2 | 2.31 | 0.61 |
| 1:AI:189:PHE:HE2 | 1:AI:249:LEU:CD2 | 2.14 | 0.61 |
| 1:AJ:203:THR:HB | 1:AJ:300:GLN:HG3 | 1.82 | 0.61 |
| 1:AJ:284:ARG:HH11 | 1:AJ:284:ARG:HG2 | 1.65 | 0.61 |
| 1:AQ:250:TRP:CZ3 | 1:AQ:272:TYR:HE1 | 2.17 | 0.61 |
| 1:BB:189:PHE:HE2 | 1:BB:249:LEU:CD2 | 2.13 | 0.61 |
| 1:BC:272:TYR:CE2 | 1:CA:55:ARG:CD | 2.84 | 0.61 |
| 1:BE:74:ASN:CB | 1:BE:126:GLU:HG2 | 2.30 | 0.61 |
| 1:BE:272:TYR:HE2 | 1:BM:55:ARG:CD | 2.13 | 0.61 |
| 1:CC:36:GLN:NE2 | 1:CC:156:LEU:H | 1.98 | 0.61 |
| 1:AM:454:ASN:ND2 | 1:AM:456:ALA:H | 1.96 | 0.61 |
| 1:BO:14:CYS:H | 1:BO:138:ASN:HD21 | 1.48 | 0.61 |
| 1:CN:189:PHE:HE2 | 1:CN:249:LEU:CD2 | 2.12 | 0.61 |
| 1:CP:74:ASN:CB | 1:CP:126:GLU:HG2 | 2.30 | 0.61 |
| 1:CR:284:ARG:HH11 | 1:CR:284:ARG:HG2 | 1.64 | 0.61 |
| 1:AC:36:GLN:NE2 | 1:AC:156:LEU:H | 1.98 | 0.61 |
| 1:AO:67:VAL:HG23 | 1:AO:135:LEU:HB2 | 1.83 | 0.61 |
| 1:BI:250:TRP:CZ3 | 1:BI:272:TYR:HE1 | 2.16 | 0.61 |
| 1:CD:189:PHE:CE1 | 1:CD:198:ARG:HG3 | 2.36 | 0.61 |
| 1:AB:250:TRP:CE3 | 1:AB:272:TYR:CE1 | 2.89 | 0.61 |
| 1:BQ:74:ASN:ND2 | 1:BQ:77:THR:OG1 | 2.34 | 0.61 |
| 1:CM:74:ASN:CB | 1:CM:126:GLU:HG2 | 2.31 | 0.61 |
| 1:AA:55:ARG:CZ | 1:CC:272:TYR:CD2 | 2.84 | 0.60 |
| 1:BJ:189:PHE:HE2 | 1:BJ:249:LEU:CD2 | 2.14 | 0.60 |
| 1:BT:36:GLN:NE2 | 1:BT:156:LEU:H | 1.99 | 0.60 |
| 1:BA:36:GLN:NE2 | 1:BA:156:LEU:H | 1.99 | 0.60 |
| 1:BD:189:PHE:CE1 | 1:BD:198:ARG:HG3 | 2.34 | 0.60 |
| 1:BF:14:CYS:H | 1:BF:138:ASN:HD21 | 1.47 | 0.60 |
| 1:BN:191:LEU:H | 1:BN:191:LEU:CD2 | 2.10 | 0.60 |
| 1:CB:284:ARG:HG2 | 1:CB:284:ARG:NH1 | 2.16 | 0.60 |
| 1:CE:189:PHE:HE2 | 1:CE:249:LEU:CD2 | 2.13 | 0.60 |
| 1:CE:284:ARG:HH11 | 1:CE:284:ARG:HG2 | 1.66 | 0.60 |
| 1:CJ:284:ARG:HH11 | 1:CJ:284:ARG:HG2 | 1.66 | 0.60 |
| 1:AB:55:ARG:HD3 | 1:BB:272:TYR:CD2 | 2.35 | 0.60 |
| 1:AP:189:PHE:HE1 | 1:AP:198:ARG:HG3 | 1.66 | 0.60 |
| 1:BE:272:TYR:CE2 | 1:BM:55:ARG:HD3 | 2.35 | 0.60 |
| 1:BH:74:ASN:CB | 1:BH:126:GLU:HG2 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:284:ARG:HG2 | 1:BH:284:ARG:NH1 | 2.16 | 0.60 |
| 1:CC:55:ARG:CD | 1:CT:272:TYR:HE2 | 2.13 | 0.60 |
| 1:CC:284:ARG:HG2 | 1:CC:284:ARG:NH1 | 2.12 | 0.60 |
| 1:CN:284:ARG:HG2 | 1:CN:284:ARG:NH1 | 2.15 | 0.60 |
| 1:AD:272:TYR:CE2 | 1:AS:55:ARG:CD | 2.85 | 0.60 |
| 1:AF:55:ARG:CD | 1:BH:272:TYR:HE2 | 2.13 | 0.60 |
| 1:AJ:55:ARG:HD3 | 1:BL:272:TYR:CD2 | 2.37 | 0.60 |
| 1:AM:272:TYR:HE2 | 1:CP:55:ARG:CD | 2.14 | 0.60 |
| 1:BG:74:ASN:CB | 1:BG:126:GLU:HG2 | 2.31 | 0.60 |
| 1:BO:74:ASN:CB | 1:BO:126:GLU:HG2 | 2.31 | 0.60 |
| 1:BP:272:TYR:HE2 | 1:CE:55:ARG:CD | 2.14 | 0.60 |
| 1:CS:14:CYS:H | 1:CS:138:ASN:HD21 | 1.49 | 0.60 |
| 1:AH:74:ASN:ND2 | 1:AH:77:THR:OG1 | 2.34 | 0.60 |
| 1:AH:272:TYR:CD2 | 1:CF:55:ARG:HD3 | 2.36 | 0.60 |
| 1:AH:398:GLY:HA3 | 1:AH:494:PHE:CD2 | 2.37 | 0.60 |
| 1:AO:272:TYR:CE2 | 1:AR:55:ARG:HD3 | 2.37 | 0.60 |
| 1:BC:272:TYR:HE2 | 1:CA:55:ARG:CD | 2.14 | 0.60 |
| 1:BG:189:PHE:HE2 | 1:BG:249:LEU:CD2 | 2.14 | 0.60 |
| 1:CD:55:ARG:CD | 1:CN:272:TYR:HE2 | 2.14 | 0.60 |
| 1:CQ:74:ASN:CB | 1:CQ:126:GLU:HG2 | 2.31 | 0.60 |
| 1:AD:74:ASN:CB | 1:AD:126:GLU:HG2 | 2.31 | 0.60 |
| 1:CM:284:ARG:HG2 | 1:CM:284:ARG:NH1 | 2.15 | 0.60 |
| 1:AB:189:PHE:CE1 | 1:AB:198:ARG:CG | 2.81 | 0.60 |
| 1:AQ:74:ASN:CB | 1:AQ:126:GLU:HG2 | 2.31 | 0.60 |
| 1:BE:272:TYR:CD2 | 1:BM:55:ARG:HD3 | 2.37 | 0.60 |
| 1:BO:16:ALA:O | 1:BO:17:ASN:HB2 | 2.00 | 0.60 |
| 1:BT:250:TRP:CE3 | 1:BT:272:TYR:CE1 | 2.90 | 0.60 |
| 1:AF:189:PHE:CE1 | 1:AF:198:ARG:CG | 2.82 | 0.60 |
| 1:AG:55:ARG:NE | 1:CG:272:TYR:HE2 | 1.99 | 0.60 |
| 1:AS:284:ARG:HG2 | 1:AS:284:ARG:NH1 | 2.15 | 0.60 |
| 1:BF:189:PHE:CE1 | 1:BF:198:ARG:HG3 | 2.36 | 0.60 |
| 1:BF:272:TYR:HE2 | 1:CK:55:ARG:CD | 2.14 | 0.60 |
| 1:CD:55:ARG:CD | 1:CN:272:TYR:CE2 | 2.85 | 0.60 |
| 1:CI:272:TYR:CD2 | 1:CO:55:ARG:HD3 | 2.36 | 0.60 |
| 1:CL:74:ASN:CB | 1:CL:126:GLU:HG2 | 2.32 | 0.60 |
| 1:CL:284:ARG:HG2 | 1:CL:284:ARG:NH1 | 2.14 | 0.60 |
| 1:AJ:191:LEU:HD23 | 1:AJ:191:LEU:N | 2.12 | 0.60 |
| 1:AN:454:ASN:HD22 | 1:AN:456:ALA:N | 2.00 | 0.60 |
| 1:AS:74:ASN:CB | 1:AS:126:GLU:HG2 | 2.31 | 0.60 |
| 1:BR:74:ASN:CB | 1:BR:126:GLU:HG2 | 2.31 | 0.60 |
| 1:CM:454:ASN:HD22 | 1:CM:456:ALA:N | 1.99 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AC:272:TYR:CD2 | 1:BA:55:ARG:HD3 | 2.37 | 0.60 |
| 1:AG:14:CYS:H | 1:AG:138:ASN:HD21 | 1.49 | 0.60 |
| 1:AK:284:ARG:HG2 | 1:AK:284:ARG:NH1 | 2.17 | 0.60 |
| 1:BR:284:ARG:HG2 | 1:BR:284:ARG:NH1 | 2.16 | 0.60 |
| 1:AF:79:ARG:HH11 | 1:AF:79:ARG:CG | 2.10 | 0.59 |
| 1:AI:189:PHE:CE1 | 1:AI:198:ARG:CG | 2.79 | 0.59 |
| 1:AO:454:ASN:HD22 | 1:AO:456:ALA:N | 2.00 | 0.59 |
| 1:AT:74:ASN:CB | 1:AT:126:GLU:HG2 | 2.31 | 0.59 |
| 1:BC:454:ASN:HD22 | 1:BC:456:ALA:N | 2.00 | 0.59 |
| 1:BI:55:ARG:HD3 | 1:BR:272:TYR:CE2 | 2.37 | 0.59 |
| 1:BR:189:PHE:CE1 | 1:BR:198:ARG:CG | 2.84 | 0.59 |
| 1:CE:74:ASN:ND2 | 1:CE:77:THR:OG1 | 2.35 | 0.59 |
| 1:CF:74:ASN:CB | 1:CF:126:GLU:HG2 | 2.31 | 0.59 |
| 1:CG:36:GLN:NE2 | 1:CG:156:LEU:H | 1.99 | 0.59 |
| 1:CQ:454:ASN:HD22 | 1:CQ:456:ALA:N | 1.99 | 0.59 |
| 1:AA:55:ARG:HD3 | 1:CC:272:TYR:CD2 | 2.38 | 0.59 |
| 1:AB:189:PHE:HE2 | 1:AB:249:LEU:CD2 | 2.14 | 0.59 |
| 1:AL:74:ASN:CB | 1:AL:126:GLU:HG2 | 2.32 | 0.59 |
| 1:AL:284:ARG:HG2 | 1:AL:284:ARG:NH1 | 2.16 | 0.59 |
| 1:BE:284:ARG:HG2 | 1:BE:284:ARG:NH1 | 2.17 | 0.59 |
| 1:CE:74:ASN:CB | 1:CE:126:GLU:HG2 | 2.32 | 0.59 |
| 1:CE:272:TYR:CE2 | 1:CM:55:ARG:HD3 | 2.37 | 0.59 |
| 1:CF:189:PHE:HE2 | 1:CF:249:LEU:CD2 | 2.15 | 0.59 |
| 1:CK:284:ARG:HG2 | 1:CK:284:ARG:NH1 | 2.15 | 0.59 |
| 1:CQ:189:PHE:CE1 | 1:CQ:198:ARG:HG3 | 2.37 | 0.59 |
| 1:CQ:284:ARG:HG2 | 1:CQ:284:ARG:NH1 | 2.17 | 0.59 |
| 1:CT:74:ASN:CB | 1:CT:126:GLU:HG2 | 2.31 | 0.59 |
| 1:AA:454:ASN:HD22 | 1:AA:456:ALA:N | 1.99 | 0.59 |
| 1:AB:16:ALA:O | 1:AB:17:ASN:HB2 | 2.02 | 0.59 |
| 1:AG:74:ASN:CB | 1:AG:126:GLU:HG2 | 2.32 | 0.59 |
| 1:BG:284:ARG:HG2 | 1:BG:284:ARG:NH1 | 2.15 | 0.59 |
| 1:BI:454:ASN:HD22 | 1:BI:456:ALA:N | 1.99 | 0.59 |
| 1:BL:189:PHE:HE1 | 1:BL:198:ARG:CG | 2.14 | 0.59 |
| 1:CA:284:ARG:HG2 | 1:CA:284:ARG:NH1 | 2.15 | 0.59 |
| 1:AG:189:PHE:CE1 | 1:AG:198:ARG:CG | 2.81 | 0.59 |
| 1:AO:284:ARG:HG2 | 1:AO:284:ARG:NH1 | 2.15 | 0.59 |
| 1:BB:454:ASN:HD22 | 1:BB:456:ALA:N | 1.99 | 0.59 |
| 1:BE:250:TRP:CZ3 | 1:BE:272:TYR:HE1 | 2.18 | 0.59 |
| 1:BH:55:ARG:HD3 | 1:BK:272:TYR:CE2 | 2.38 | 0.59 |
| 1:BH:79:ARG:HG3 | 1:BH:79:ARG:HH11 | 1.67 | 0.59 |
| 1:BH:398:GLY:HA3 | 1:BH:494:PHE:CD2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BK:74:ASN:CB | 1:BK:126:GLU:HG2 | 2.32 | 0.59 |
| 1:BR:16:ALA:O | 1:BR:17:ASN:HB2 | 2.02 | 0.59 |
| 1:CI:189:PHE:CE1 | 1:CI:198:ARG:CG | 2.83 | 0.59 |
| 1:AA:272:TYR:CE2 | 1:CT:55:ARG:HD3 | 2.37 | 0.59 |
| 1:AE:203:THR:HB | 1:AE:300:GLN:HG3 | 1.83 | 0.59 |
| 1:AG:55:ARG:CD | 1:CG:272:TYR:CE2 | 2.86 | 0.59 |
| 1:AP:79:ARG:HH11 | 1:AP:79:ARG:HG3 | 1.66 | 0.59 |
| 1:BK:189:PHE:HE1 | 1:BK:198:ARG:CG | 2.15 | 0.59 |
| 1:BK:284:ARG:HG2 | 1:BK:284:ARG:NH1 | 2.15 | 0.59 |
| 1:BM:239:ILE:HG12 | 1:BM:326:ILE:CD1 | 2.32 | 0.59 |
| 1:CD:74:ASN:CB | 1:CD:126:GLU:HG2 | 2.32 | 0.59 |
| 1:CD:454:ASN:HD22 | 1:CD:456:ALA:N | 1.98 | 0.59 |
| 1:CN:74:ASN:CB | 1:CN:126:GLU:HG2 | 2.32 | 0.59 |
| 1:CN:454:ASN:HD22 | 1:CN:456:ALA:N | 2.00 | 0.59 |
| 1:CR:189:PHE:HE2 | 1:CR:249:LEU:CD2 | 2.15 | 0.59 |
| 1:AD:55:ARG:HD3 | 1:AN:272:TYR:CE2 | 2.37 | 0.59 |
| 1:AJ:55:ARG:CD | 1:BL:272:TYR:HE2 | 2.13 | 0.59 |
| 1:AJ:189:PHE:HE2 | 1:AJ:249:LEU:CD2 | 2.15 | 0.59 |
| 1:BI:284:ARG:HG2 | 1:BI:284:ARG:NH1 | 2.15 | 0.59 |
| 1:BK:14:CYS:H | 1:BK:138:ASN:HD21 | 1.49 | 0.59 |
| 1:BQ:67:VAL:HG23 | 1:BQ:135:LEU:HB2 | 1.84 | 0.59 |
| 1:CF:250:TRP:CE3 | 1:CF:272:TYR:CE1 | 2.91 | 0.59 |
| 1:AJ:189:PHE:CE1 | 1:AJ:198:ARG:CG | 2.79 | 0.59 |
| 1:AT:74:ASN:ND2 | 1:AT:77:THR:OG1 | 2.35 | 0.59 |
| 1:BC:239:ILE:HG12 | 1:BC:326:ILE:CD1 | 2.33 | 0.59 |
| 1:CF:250:TRP:HZ3 | 1:CF:272:TYR:CE1 | 2.20 | 0.59 |
| 1:CP:284:ARG:HH11 | 1:CP:284:ARG:HG2 | 1.66 | 0.59 |
| 1:AB:272:TYR:CE2 | 1:CB:55:ARG:HD3 | 2.38 | 0.59 |
| 1:AC:74:ASN:CB | 1:AC:126:GLU:HG2 | 2.32 | 0.59 |
| 1:AF:284:ARG:HG2 | 1:AF:284:ARG:NH1 | 2.17 | 0.59 |
| 1:AJ:74:ASN:CB | 1:AJ:126:GLU:HG2 | 2.32 | 0.59 |
| 1:AP:284:ARG:HG2 | 1:AP:284:ARG:NH1 | 2.17 | 0.59 |
| 1:BA:284:ARG:HG2 | 1:BA:284:ARG:NH1 | 2.15 | 0.59 |
| 1:BJ:55:ARG:HD3 | 1:CL:272:TYR:CD2 | 2.38 | 0.59 |
| 1:BL:250:TRP:CZ3 | 1:BL:272:TYR:HE1 | 2.20 | 0.59 |
| 1:BN:16:ALA:O | 1:BN:17:ASN:HB2 | 2.01 | 0.59 |
| 1:BQ:189:PHE:HE1 | 1:BQ:198:ARG:CG | 2.13 | 0.59 |
| 1:BT:189:PHE:CE1 | 1:BT:198:ARG:HG3 | 2.36 | 0.59 |
| 1:CC:74:ASN:CB | 1:CC:126:GLU:HG2 | 2.32 | 0.59 |
| 1:AA:398:GLY:HA3 | 1:AA:494:PHE:CD2 | 2.38 | 0.59 |
| 1:AE:189:PHE:HE2 | 1:AE:249:LEU:CD2 | 2.14 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AE:284:ARG:HH11 | 1:AE:284:ARG:HG2 | 1.66 | 0.59 |
| 1:BS:250:TRP:CZ3 | 1:BS:272:TYR:HE1 | 2.19 | 0.59 |
| 1:CO:74:ASN:CB | 1:CO:126:GLU:HG2 | 2.31 | 0.59 |
| 1:CS:288:HIS:HD2 | 1:CS:337:ASP:OD2 | 1.86 | 0.59 |
| 1:AC:250:TRP:CE3 | 1:AC:272:TYR:CE1 | 2.90 | 0.59 |
| 1:AH:189:PHE:HE2 | 1:AH:249:LEU:CD2 | 2.15 | 0.59 |
| 1:BF:74:ASN:CB | 1:BF:126:GLU:HG2 | 2.33 | 0.59 |
| 1:BM:454:ASN:HD22 | 1:BM:456:ALA:N | 2.00 | 0.59 |
| 1:AD:272:TYR:HE2 | 1:AS:55:ARG:CD | 2.16 | 0.58 |
| 1:BD:55:ARG:CD | 1:BN:272:TYR:CE2 | 2.86 | 0.58 |
| 1:BI:189:PHE:CE1 | 1:BI:198:ARG:CG | 2.83 | 0.58 |
| 1:BJ:55:ARG:HD3 | 1:CL:272:TYR:CE2 | 2.38 | 0.58 |
| 1:BM:189:PHE:CE1 | 1:BM:198:ARG:CG | 2.82 | 0.58 |
| 1:AL:55:ARG:HD3 | 1:CQ:272:TYR:CD2 | 2.37 | 0.58 |
| 1:AP:189:PHE:CE1 | 1:AP:198:ARG:HG3 | 2.38 | 0.58 |
| 1:BF:272:TYR:CE2 | 1:CK:55:ARG:HD3 | 2.38 | 0.58 |
| 1:BP:272:TYR:CE2 | 1:CE:55:ARG:CD | 2.86 | 0.58 |
| 1:CG:250:TRP:CE3 | 1:CG:272:TYR:CE1 | 2.92 | 0.58 |
| 1:AJ:272:TYR:CE2 | 1:AQ:55:ARG:NE | 2.71 | 0.58 |
| 1:AO:239:ILE:HG12 | 1:AO:326:ILE:CD1 | 2.33 | 0.58 |
| 1:AP:272:TYR:CE2 | 1:BE:55:ARG:CD | 2.87 | 0.58 |
| 1:AR:250:TRP:CE3 | 1:AR:272:TYR:CE1 | 2.91 | 0.58 |
| 1:BD:284:ARG:HG2 | 1:BD:284:ARG:NH1 | 2.18 | 0.58 |
| 1:BG:16:ALA:O | 1:BG:17:ASN:HB2 | 2.03 | 0.58 |
| 1:BI:74:ASN:CB | 1:BI:126:GLU:HG2 | 2.32 | 0.58 |
| 1:CF:79:ARG:HG3 | 1:CF:79:ARG:NH1 | 2.00 | 0.58 |
| 1:CI:79:ARG:HH11 | 1:CI:79:ARG:HG3 | 1.68 | 0.58 |
| 1:AC:454:ASN:HD22 | 1:AC:456:ALA:N | 2.00 | 0.58 |
| 1:AE:272:TYR:CD2 | 1:AM:55:ARG:HD3 | 2.39 | 0.58 |
| 1:AI:74:ASN:CB | 1:AI:126:GLU:HG2 | 2.33 | 0.58 |
| 1:AQ:272:TYR:HE2 | 1:BL:55:ARG:CD | 2.17 | 0.58 |
| 1:AQ:284:ARG:HH11 | 1:AQ:284:ARG:HG2 | 1.68 | 0.58 |
| 1:BA:189:PHE:CE1 | 1:BA:198:ARG:CG | 2.86 | 0.58 |
| 1:BA:189:PHE:HE2 | 1:BA:249:LEU:HD21 | 1.67 | 0.58 |
| 1:BH:189:PHE:HE2 | 1:BH:249:LEU:CD2 | 2.16 | 0.58 |
| 1:BN:189:PHE:HE2 | 1:BN:249:LEU:CD2 | 2.16 | 0.58 |
| 1:BP:189:PHE:HE1 | 1:BP:198:ARG:CG | 2.16 | 0.58 |
| 1:AA:74:ASN:ND2 | 1:AA:77:THR:OG1 | 2.36 | 0.58 |
| 1:AH:14:CYS:H | 1:AH:138:ASN:HD21 | 1.50 | 0.58 |
| 1:BB:74:ASN:CB | 1:BB:126:GLU:HG2 | 2.34 | 0.58 |
| 1:BJ:74:ASN:CB | 1:BJ:126:GLU:HG2 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BQ:43:ALA:HB1 | 1:BQ:158:GLU:HA | 1.86 | 0.58 |
| 1:BS:189:PHE:HE1 | 1:BS:198:ARG:CG | 2.16 | 0.58 |
| 1:CO:272:TYR:CE2 | 1:CR:55:ARG:HD3 | 2.38 | 0.58 |
| 1:AA:74:ASN:CB | 1:AA:126:GLU:HG2 | 2.34 | 0.58 |
| 1:AB:272:TYR:CD2 | 1:CB:55:ARG:HD3 | 2.39 | 0.58 |
| 1:AB:284:ARG:HG2 | 1:AB:284:ARG:NH1 | 2.13 | 0.58 |
| 1:AP:74:ASN:CB | 1:AP:126:GLU:HG2 | 2.34 | 0.58 |
| 1:BF:272:TYR:CD2 | 1:CK:55:ARG:HD3 | 2.39 | 0.58 |
| 1:BF:454:ASN:HD22 | 1:BF:456:ALA:N | 2.00 | 0.58 |
| 1:BS:454:ASN:HD22 | 1:BS:456:ALA:N | 2.01 | 0.58 |
| 1:CK:74:ASN:CB | 1:CK:126:GLU:HG2 | 2.32 | 0.58 |
| 1:AA:67:VAL:HG23 | 1:AA:135:LEU:HB2 | 1.85 | 0.58 |
| 1:AA:189:PHE:CE1 | 1:AA:198:ARG:CG | 2.87 | 0.58 |
| 1:AA:284:ARG:HG2 | 1:AA:284:ARG:NH1 | 2.15 | 0.58 |
| 1:AD:189:PHE:HE1 | 1:AD:198:ARG:CG | 2.15 | 0.58 |
| 1:AF:203:THR:HB | 1:AF:300:GLN:HG3 | 1.85 | 0.58 |
| 1:AP:58:ALA:HB2 | 1:AP:102:GLY:HA3 | 1.84 | 0.58 |
| 1:AR:454:ASN:HD22 | 1:AR:456:ALA:N | 2.01 | 0.58 |
| 1:BC:55:ARG:HD3 | 1:BT:272:TYR:CE2 | 2.37 | 0.58 |
| 1:BC:284:ARG:HG2 | 1:BC:284:ARG:NH1 | 2.16 | 0.58 |
| 1:BO:398:GLY:HA3 | 1:BO:494:PHE:CD2 | 2.37 | 0.58 |
| 1:BS:14:CYS:H | 1:BS:138:ASN:HD21 | 1.52 | 0.58 |
| 1:BT:55:ARG:CD | 1:CA:272:TYR:CE2 | 2.86 | 0.58 |
| 1:CM:36:GLN:NE2 | 1:CM:156:LEU:H | 2.02 | 0.58 |
| 1:CN:250:TRP:CE3 | 1:CN:272:TYR:CE1 | 2.91 | 0.58 |
| 1:AD:189:PHE:HE2 | 1:AD:249:LEU:CD2 | 2.17 | 0.58 |
| 1:AH:284:ARG:HG2 | 1:AH:284:ARG:NH1 | 2.17 | 0.58 |
| 1:AN:442:GLN:HE21 | 1:AO:412:PHE:HB2 | 1.68 | 0.58 |
| 1:AP:55:ARG:HD3 | 1:BM:272:TYR:CE2 | 2.39 | 0.58 |
| 1:BF:189:PHE:CE1 | 1:BF:198:ARG:CG | 2.81 | 0.58 |
| 1:BN:67:VAL:HG23 | 1:BN:135:LEU:HB2 | 1.86 | 0.58 |
| 1:BN:454:ASN:HD22 | 1:BN:456:ALA:N | 2.02 | 0.58 |
| 1:BP:55:ARG:HD3 | 1:CM:272:TYR:CD2 | 2.39 | 0.58 |
| 1:CI:454:ASN:HD22 | 1:CI:456:ALA:N | 2.02 | 0.58 |
| 1:CM:250:TRP:CE3 | 1:CM:272:TYR:CE1 | 2.91 | 0.58 |
| 1:CR:36:GLN:NE2 | 1:CR:156:LEU:H | 2.02 | 0.58 |
| 1:CS:74:ASN:CB | 1:CS:126:GLU:HG2 | 2.32 | 0.58 |
| 1:AC:189:PHE:CE1 | 1:AC:198:ARG:HG3 | 2.39 | 0.58 |
| 1:AE:454:ASN:HD22 | 1:AE:456:ALA:N | 2.01 | 0.58 |
| 1:AF:55:ARG:HD3 | 1:BH:272:TYR:CD2 | 2.39 | 0.58 |
| 1:AO:162:PHE:CD2 | 1:AO:163:LEU:HD13 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:74:ASN:ND2 | 1:AP:77:THR:OG1 | 2.37 | 0.58 |
| 1:AP:272:TYR:HE2 | 1:BE:55:ARG:CD | 2.16 | 0.58 |
| 1:BD:272:TYR:HE2 | 1:BS:55:ARG:NE | 2.02 | 0.58 |
| 1:BP:284:ARG:HG2 | 1:BP:284:ARG:NH1 | 2.17 | 0.58 |
| 1:CF:454:ASN:ND2 | 1:CF:456:ALA:H | 2.00 | 0.58 |
| 1:CI:272:TYR:CE2 | 1:CO:55:ARG:HD3 | 2.39 | 0.58 |
| 1:CS:36:GLN:NE2 | 1:CS:156:LEU:H | 2.01 | 0.58 |
| 1:AD:284:ARG:HG2 | 1:AD:284:ARG:NH1 | 2.14 | 0.58 |
| 1:AG:272:TYR:CE2 | 1:BG:55:ARG:CD | 2.87 | 0.58 |
| 1:AJ:55:ARG:HD3 | 1:BL:272:TYR:CE2 | 2.39 | 0.58 |
| 1:AN:250:TRP:CE3 | 1:AN:272:TYR:CE1 | 2.92 | 0.58 |
| 1:AT:189:PHE:HE1 | 1:AT:198:ARG:CG | 2.16 | 0.58 |
| 1:BA:189:PHE:HE2 | 1:BA:249:LEU:CD2 | 2.16 | 0.58 |
| 1:BH:454:ASN:HD22 | 1:BH:456:ALA:N | 2.02 | 0.58 |
| 1:BL:284:ARG:HG2 | 1:BL:284:ARG:NH1 | 2.19 | 0.58 |
| 1:BM:250:TRP:HZ3 | 1:BM:272:TYR:CE1 | 2.20 | 0.58 |
| 1:CK:454:ASN:HD22 | 1:CK:456:ALA:N | 1.98 | 0.58 |
| 1:CQ:250:TRP:HZ3 | 1:CQ:272:TYR:CE1 | 2.19 | 0.58 |
| 1:AM:398:GLY:HA3 | 1:AM:494:PHE:CD2 | 2.39 | 0.57 |
| 1:BA:250:TRP:HZ3 | 1:BA:272:TYR:CE1 | 2.22 | 0.57 |
| 1:BG:11:PRO:HG2 | 1:BG:18:ARG:HD2 | 1.85 | 0.57 |
| 1:BP:36:GLN:NE2 | 1:BP:156:LEU:H | 2.02 | 0.57 |
| 1:BP:454:ASN:HD22 | 1:BP:456:ALA:N | 1.99 | 0.57 |
| 1:BQ:272:TYR:CE2 | 1:CL:55:ARG:HD3 | 2.37 | 0.57 |
| 1:BQ:288:HIS:HD2 | 1:BQ:337:ASP:OD2 | 1.87 | 0.57 |
| 1:CG:454:ASN:HD22 | 1:CG:456:ALA:N | 2.01 | 0.57 |
| 1:CH:79:ARG:HG3 | 1:CH:79:ARG:NH1 | 2.17 | 0.57 |
| 1:CJ:272:TYR:CD2 | 1:CQ:55:ARG:HD3 | 2.39 | 0.57 |
| 1:AH:272:TYR:HE2 | 1:CF:55:ARG:CD | 2.18 | 0.57 |
| 1:AR:74:ASN:CB | 1:AR:126:GLU:HG2 | 2.34 | 0.57 |
| 1:AT:189:PHE:CE1 | 1:AT:198:ARG:CG | 2.87 | 0.57 |
| 1:BK:454:ASN:HD22 | 1:BK:456:ALA:N | 1.99 | 0.57 |
| 1:BP:454:ASN:ND2 | 1:BP:456:ALA:H | 2.00 | 0.57 |
| 1:BT:284:ARG:HG2 | 1:BT:284:ARG:NH1 | 2.18 | 0.57 |
| 1:CA:43:ALA:HB1 | 1:CA:158:GLU:HA | 1.86 | 0.57 |
| 1:CG:284:ARG:HG2 | 1:CG:284:ARG:NH1 | 2.17 | 0.57 |
| 1:AJ:14:CYS:H | 1:AJ:138:ASN:HD21 | 1.51 | 0.57 |
| 1:AN:55:ARG:CZ | 1:AS:272:TYR:CD2 | 2.87 | 0.57 |
| 1:AN:284:ARG:HG2 | 1:AN:284:ARG:NH1 | 2.18 | 0.57 |
| 1:BB:454:ASN:ND2 | 1:BB:456:ALA:H | 2.00 | 0.57 |
| 1:BO:15:GLN:HA | 1:BO:15:GLN:NE2 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BP:189:PHE:CE1 | 1:BP:198:ARG:CG | 2.88 | 0.57 |
| 1:CC:191:LEU:HD23 | 1:CC:191:LEU:N | 2.16 | 0.57 |
| 1:AH:16:ALA:O | 1:AH:17:ASN:HB2 | 2.04 | 0.57 |
| 1:BD:14:CYS:H | 1:BD:138:ASN:HD21 | 1.50 | 0.57 |
| 1:BK:288:HIS:HD2 | 1:BK:337:ASP:OD2 | 1.86 | 0.57 |
| 1:BS:284:ARG:HG2 | 1:BS:284:ARG:NH1 | 2.19 | 0.57 |
| 1:CH:43:ALA:HB1 | 1:CH:158:GLU:HA | 1.86 | 0.57 |
| 1:BL:189:PHE:CE1 | 1:BL:198:ARG:CG | 2.87 | 0.57 |
| 1:BN:74:ASN:CB | 1:BN:126:GLU:HG2 | 2.34 | 0.57 |
| 1:BO:189:PHE:CE1 | 1:BO:198:ARG:HG3 | 2.39 | 0.57 |
| 1:BP:55:ARG:HD3 | 1:CM:272:TYR:CE2 | 2.39 | 0.57 |
| 1:CK:74:ASN:ND2 | 1:CK:77:THR:OG1 | 2.38 | 0.57 |
| 1:AB:288:HIS:HD2 | 1:AB:337:ASP:OD2 | 1.86 | 0.57 |
| 1:AC:191:LEU:HD23 | 1:AC:191:LEU:N | 2.15 | 0.57 |
| 1:AH:55:ARG:CD | 1:AK:272:TYR:HE2 | 2.17 | 0.57 |
| 1:AM:272:TYR:CD2 | 1:CP:55:ARG:HD3 | 2.40 | 0.57 |
| 1:AT:284:ARG:HG2 | 1:AT:284:ARG:NH1 | 2.16 | 0.57 |
| 1:BC:14:CYS:H | 1:BC:138:ASN:HD21 | 1.52 | 0.57 |
| 1:BD:55:ARG:CD | 1:BN:272:TYR:HE2 | 2.17 | 0.57 |
| 1:BL:250:TRP:HZ3 | 1:BL:272:TYR:CE1 | 2.22 | 0.57 |
| 1:CO:14:CYS:H | 1:CO:138:ASN:HD21 | 1.53 | 0.57 |
| 1:CS:284:ARG:HG2 | 1:CS:284:ARG:NH1 | 2.18 | 0.57 |
| 1:AL:272:TYR:CE2 | 1:CJ:55:ARG:HD3 | 2.40 | 0.57 |
| 1:BA:250:TRP:CE3 | 1:BA:272:TYR:CE1 | 2.93 | 0.57 |
| 1:BF:189:PHE:HE2 | 1:BF:249:LEU:CD2 | 2.17 | 0.57 |
| 1:BI:272:TYR:CE2 | 1:BO:55:ARG:HD3 | 2.40 | 0.57 |
| 1:BQ:14:CYS:H | 1:BQ:138:ASN:HD21 | 1.53 | 0.57 |
| 1:BS:189:PHE:CE1 | 1:BS:198:ARG:CG | 2.88 | 0.57 |
| 1:CB:189:PHE:HE2 | 1:CB:249:LEU:CD2 | 2.17 | 0.57 |
| 1:CL:189:PHE:CE1 | 1:CL:198:ARG:CG | 2.88 | 0.57 |
| 1:CS:250:TRP:CE3 | 1:CS:272:TYR:CE1 | 2.93 | 0.57 |
| 1:AF:272:TYR:CE2 | 1:BK:55:ARG:HD3 | 2.40 | 0.57 |
| 1:AG:250:TRP:HZ3 | 1:AG:272:TYR:CE1 | 2.21 | 0.57 |
| 1:AN:239:ILE:HG12 | 1:AN:326:ILE:CD1 | 2.34 | 0.57 |
| 1:BK:189:PHE:HE2 | 1:BK:249:LEU:CD2 | 2.18 | 0.57 |
| 1:CR:14:CYS:H | 1:CR:138:ASN:HD21 | 1.50 | 0.57 |
| 1:CR:189:PHE:HE1 | 1:CR:198:ARG:HG2 | 1.67 | 0.57 |
| 1:AB:14:CYS:H | 1:AB:138:ASN:HD21 | 1.52 | 0.57 |
| 1:AN:14:CYS:H | 1:AN:138:ASN:HD21 | 1.53 | 0.57 |
| 1:AQ:189:PHE:HE2 | 1:AQ:249:LEU:CD2 | 2.17 | 0.57 |
| 1:AS:398:GLY:HA3 | 1:AS:494:PHE:CD2 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:250:TRP:HZ3 | 1:BI:272:TYR:CE1 | 2.23 | 0.57 |
| 1:CC:250:TRP:CE3 | 1:CC:272:TYR:CD1 | 2.92 | 0.57 |
| 1:CF:284:ARG:HG2 | 1:CF:284:ARG:NH1 | 2.19 | 0.57 |
| 1:CH:284:ARG:HG2 | 1:CH:284:ARG:NH1 | 2.16 | 0.57 |
| 1:CM:14:CYS:H | 1:CM:138:ASN:HD21 | 1.51 | 0.57 |
| 1:AG:272:TYR:HE2 | 1:BG:55:ARG:CD | 2.17 | 0.57 |
| 1:AH:189:PHE:CE1 | 1:AH:198:ARG:CG | 2.81 | 0.57 |
| 1:BK:454:ASN:ND2 | 1:BK:456:ALA:H | 2.02 | 0.57 |
| 1:BP:74:ASN:CB | 1:BP:126:GLU:HG2 | 2.35 | 0.57 |
| 1:BR:454:ASN:ND2 | 1:BR:456:ALA:H | 2.03 | 0.57 |
| 1:CJ:18:ARG:HD2 | 1:CJ:19:TYR:O | 2.05 | 0.57 |
| 1:CM:239:ILE:HG12 | 1:CM:326:ILE:CD1 | 2.35 | 0.57 |
| 1:CP:79:ARG:HH11 | 1:CP:79:ARG:CG | 2.16 | 0.57 |
| 1:BB:250:TRP:CE3 | 1:BB:272:TYR:CE1 | 2.92 | 0.56 |
| 1:BT:288:HIS:HD2 | 1:BT:337:ASP:OD2 | 1.88 | 0.56 |
| 1:CJ:454:ASN:HD22 | 1:CJ:456:ALA:N | 2.00 | 0.56 |
| 1:AB:55:ARG:HD3 | 1:BB:272:TYR:CE2 | 2.40 | 0.56 |
| 1:AH:250:TRP:CE3 | 1:AH:272:TYR:CE1 | 2.93 | 0.56 |
| 1:AJ:79:ARG:HG3 | 1:AJ:79:ARG:NH1 | 2.20 | 0.56 |
| 1:AQ:189:PHE:CE1 | 1:AQ:198:ARG:HG3 | 2.39 | 0.56 |
| 1:BA:14:CYS:H | 1:BA:138:ASN:ND2 | 2.03 | 0.56 |
| 1:BB:191:LEU:HD23 | 1:BB:191:LEU:N | 2.17 | 0.56 |
| 1:BE:74:ASN:ND2 | 1:BE:77:THR:OG1 | 2.38 | 0.56 |
| 1:BF:55:ARG:HD3 | 1:CH:272:TYR:CD2 | 2.40 | 0.56 |
| 1:BH:250:TRP:HZ3 | 1:BH:272:TYR:CE1 | 2.22 | 0.56 |
| 1:BM:14:CYS:H | 1:BM:138:ASN:HD21 | 1.53 | 0.56 |
| 1:CF:239:ILE:HG12 | 1:CF:326:ILE:CD1 | 2.35 | 0.56 |
| 1:AF:79:ARG:HG3 | 1:AF:79:ARG:NH1 | 2.17 | 0.56 |
| 1:AH:55:ARG:CD | 1:AK:272:TYR:CE2 | 2.88 | 0.56 |
| 1:AH:75:ARG:NH2 | 1:AH:391:ALA:O | 2.37 | 0.56 |
| 1:AI:454:ASN:HD22 | 1:AI:456:ALA:N | 2.03 | 0.56 |
| 1:AR:10:ILE:HG21 | 1:AR:146:TRP:CZ2 | 2.41 | 0.56 |
| 1:BA:454:ASN:HD22 | 1:BA:456:ALA:N | 2.01 | 0.56 |
| 1:BJ:79:ARG:HG3 | 1:BJ:79:ARG:NH1 | 2.13 | 0.56 |
| 1:BM:36:GLN:NE2 | 1:BM:156:LEU:H | 2.02 | 0.56 |
| 1:BN:189:PHE:CE1 | 1:BN:198:ARG:HG2 | 2.41 | 0.56 |
| 1:CE:272:TYR:CD2 | 1:CM:55:ARG:HD3 | 2.40 | 0.56 |
| 1:CF:36:GLN:NE2 | 1:CF:156:LEU:H | 2.03 | 0.56 |
| 1:CG:250:TRP:HZ3 | 1:CG:272:TYR:CE1 | 2.23 | 0.56 |
| 1:CI:250:TRP:HZ3 | 1:CI:272:TYR:CE1 | 2.22 | 0.56 |
| 1:CO:239:ILE:HG12 | 1:CO:326:ILE:CD1 | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CO:284:ARG:HG2 | 1:CO:284:ARG:NH1 | 2.15 | 0.56 |
| 1:CT:14:CYS:H | 1:CT:138:ASN:ND2 | 2.04 | 0.56 |
| 1:AJ:272:TYR:CE2 | 1:AQ:55:ARG:CD | 2.88 | 0.56 |
| 1:BE:454:ASN:HD22 | 1:BE:456:ALA:N | 2.02 | 0.56 |
| 1:CS:398:GLY:HA3 | 1:CS:494:PHE:CD2 | 2.40 | 0.56 |
| 1:AA:189:PHE:HE2 | 1:AA:249:LEU:CD2 | 2.18 | 0.56 |
| 1:AQ:288:HIS:HD2 | 1:AQ:337:ASP:OD2 | 1.88 | 0.56 |
| 1:AT:454:ASN:HD22 | 1:AT:456:ALA:N | 2.02 | 0.56 |
| 1:BM:398:GLY:HA3 | 1:BM:494:PHE:CD2 | 2.40 | 0.56 |
| 1:BN:284:ARG:HG2 | 1:BN:284:ARG:NH1 | 2.17 | 0.56 |
| 1:BR:189:PHE:HE2 | 1:BR:249:LEU:CD2 | 2.18 | 0.56 |
| 1:BS:58:ALA:HB2 | 1:BS:102:GLY:HA3 | 1.88 | 0.56 |
| 1:CM:250:TRP:HZ3 | 1:CM:272:TYR:CE1 | 2.18 | 0.56 |
| 1:CO:36:GLN:NE2 | 1:CO:156:LEU:H | 2.03 | 0.56 |
| 1:AC:55:ARG:HD3 | 1:AT:272:TYR:CD2 | 2.41 | 0.56 |
| 1:AN:250:TRP:HZ3 | 1:AN:272:TYR:CE1 | 2.24 | 0.56 |
| 1:BH:15:GLN:HA | 1:BH:15:GLN:NE2 | 2.15 | 0.56 |
| 1:BM:67:VAL:HG23 | 1:BM:135:LEU:HB2 | 1.88 | 0.56 |
| 1:BO:272:TYR:CD2 | 1:BR:55:ARG:CZ | 2.88 | 0.56 |
| 1:BQ:189:PHE:CE1 | 1:BQ:198:ARG:CG | 2.88 | 0.56 |
| 1:BR:454:ASN:HD22 | 1:BR:456:ALA:N | 2.01 | 0.56 |
| 1:BT:189:PHE:HE1 | 1:BT:198:ARG:CG | 2.18 | 0.56 |
| 1:BT:454:ASN:HD22 | 1:BT:456:ALA:N | 2.01 | 0.56 |
| 1:CF:18:ARG:HG3 | 1:CF:19:TYR:N | 2.19 | 0.56 |
| 1:CH:250:TRP:CE3 | 1:CH:272:TYR:CE1 | 2.93 | 0.56 |
| 1:CJ:189:PHE:HE2 | 1:CJ:249:LEU:CD2 | 2.19 | 0.56 |
| 1:CP:284:ARG:HG2 | 1:CP:284:ARG:NH1 | 2.20 | 0.56 |
| 1:AD:272:TYR:CD2 | 1:AS:55:ARG:HD3 | 2.41 | 0.56 |
| 1:AD:398:GLY:HA3 | 1:AD:494:PHE:CD2 | 2.40 | 0.56 |
| 1:AE:189:PHE:CE1 | 1:AE:198:ARG:CG | 2.83 | 0.56 |
| 1:AE:250:TRP:CE3 | 1:AE:272:TYR:CE1 | 2.94 | 0.56 |
| 1:AP:250:TRP:CE3 | 1:AP:272:TYR:CE1 | 2.93 | 0.56 |
| 1:AQ:189:PHE:HE2 | 1:AQ:249:LEU:HD21 | 1.71 | 0.56 |
| 1:BJ:284:ARG:HG2 | 1:BJ:284:ARG:NH1 | 2.18 | 0.56 |
| 1:BK:398:GLY:HA3 | 1:BK:494:PHE:CD2 | 2.40 | 0.56 |
| 1:CH:191:LEU:HD23 | 1:CH:191:LEU:N | 2.18 | 0.56 |
| 1:AM:74:ASN:CB | 1:AM:126:GLU:HG2 | 2.35 | 0.56 |
| 1:CE:284:ARG:HG2 | 1:CE:284:ARG:NH1 | 2.21 | 0.56 |
| 1:CG:398:GLY:HA3 | 1:CG:494:PHE:CD2 | 2.41 | 0.56 |
| 1:CH:454:ASN:HD22 | 1:CH:456:ALA:N | 2.02 | 0.56 |
| 1:CK:9:TYR:HE1 | 1:CK:147:GLN:HE21 | 1.53 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AE:284:ARG:HG2 | 1:AE:284:ARG:NH1 | 2.20 | 0.56 |
| 1:AL:288:HIS:HD2 | 1:AL:337:ASP:OD2 | 1.89 | 0.56 |
| 1:AM:288:HIS:HD2 | 1:AM:337:ASP:OD2 | 1.88 | 0.56 |
| 1:AT:288:HIS:HD2 | 1:AT:337:ASP:OD2 | 1.88 | 0.56 |
| 1:BD:67:VAL:HG23 | 1:BD:135:LEU:HB2 | 1.88 | 0.56 |
| 1:BF:74:ASN:ND2 | 1:BF:77:THR:OG1 | 2.38 | 0.56 |
| 1:BI:398:GLY:HA3 | 1:BI:494:PHE:CD2 | 2.41 | 0.56 |
| 1:BN:250:TRP:HZ3 | 1:BN:272:TYR:CE1 | 2.24 | 0.56 |
| 1:BS:79:ARG:HG3 | 1:BS:79:ARG:NH1 | 2.10 | 0.56 |
| 1:BT:55:ARG:CD | 1:CA:272:TYR:HE2 | 2.19 | 0.56 |
| 1:CH:288:HIS:HD2 | 1:CH:337:ASP:OD2 | 1.88 | 0.56 |
| 1:CR:284:ARG:HG2 | 1:CR:284:ARG:NH1 | 2.20 | 0.56 |
| 1:CT:189:PHE:HE2 | 1:CT:249:LEU:CD2 | 2.19 | 0.56 |
| 1:AD:67:VAL:HG23 | 1:AD:135:LEU:HB2 | 1.88 | 0.56 |
| 1:AH:288:HIS:HD2 | 1:AH:337:ASP:OD2 | 1.88 | 0.56 |
| 1:AP:55:ARG:HD3 | 1:BM:272:TYR:CD2 | 2.41 | 0.56 |
| 1:BJ:18:ARG:HD2 | 1:BJ:19:TYR:O | 2.06 | 0.56 |
| 1:CJ:272:TYR:CE2 | 1:CQ:55:ARG:CZ | 2.89 | 0.56 |
| 1:CR:74:ASN:CB | 1:CR:126:GLU:HG2 | 2.35 | 0.56 |
| 1:AN:79:ARG:HH11 | 1:AN:79:ARG:CG | 2.11 | 0.55 |
| 1:AO:189:PHE:CE1 | 1:AO:198:ARG:HG3 | 2.40 | 0.55 |
| 1:BJ:454:ASN:HD22 | 1:BJ:456:ALA:N | 2.02 | 0.55 |
| 1:BK:189:PHE:CE1 | 1:BK:198:ARG:CG | 2.89 | 0.55 |
| 1:BK:250:TRP:CE3 | 1:BK:272:TYR:CE1 | 2.94 | 0.55 |
| 1:CC:55:ARG:HD3 | 1:CT:272:TYR:CD2 | 2.40 | 0.55 |
| 1:CL:454:ASN:HD22 | 1:CL:456:ALA:N | 2.01 | 0.55 |
| 1:AL:272:TYR:CD2 | 1:CJ:55:ARG:HD3 | 2.42 | 0.55 |
| 1:AM:272:TYR:CE2 | 1:CP:55:ARG:HD3 | 2.40 | 0.55 |
| 1:AR:58:ALA:HB2 | 1:AR:102:GLY:HA3 | 1.88 | 0.55 |
| 1:BE:288:HIS:HD2 | 1:BE:337:ASP:OD2 | 1.89 | 0.55 |
| 1:BF:55:ARG:HD3 | 1:CH:272:TYR:CE2 | 2.41 | 0.55 |
| 1:BP:75:ARG:NH2 | 1:BP:391:ALA:O | 2.39 | 0.55 |
| 1:AH:11:PRO:HG2 | 1:AH:18:ARG:HD2 | 1.87 | 0.55 |
| 1:AL:55:ARG:HD3 | 1:CQ:272:TYR:CE2 | 2.41 | 0.55 |
| 1:AL:250:TRP:HZ3 | 1:AL:272:TYR:CE1 | 2.22 | 0.55 |
| 1:AN:454:ASN:ND2 | 1:AN:456:ALA:H | 2.03 | 0.55 |
| 1:BC:79:ARG:HH11 | 1:BC:79:ARG:HG3 | 1.70 | 0.55 |
| 1:BK:250:TRP:HZ3 | 1:BK:272:TYR:CE1 | 2.23 | 0.55 |
| 1:BL:288:HIS:HD2 | 1:BL:337:ASP:OD2 | 1.89 | 0.55 |
| 1:BP:77:THR:O | 1:BP:81:THR:HG23 | 2.07 | 0.55 |
| 1:CB:67:VAL:HG23 | 1:CB:135:LEU:HB2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CB:454:ASN:HD22 | 1:CB:456:ALA:N | 2.01 | 0.55 |
| 1:CC:454:ASN:HD22 | 1:CC:456:ALA:N | 2.02 | 0.55 |
| 1:CQ:288:HIS:HD2 | 1:CQ:337:ASP:OD2 | 1.89 | 0.55 |
| 1:AD:189:PHE:CE1 | 1:AD:198:ARG:CG | 2.89 | 0.55 |
| 1:BB:11:PRO:HG2 | 1:BB:18:ARG:HD2 | 1.88 | 0.55 |
| 1:BI:191:LEU:HD23 | 1:BI:191:LEU:N | 2.18 | 0.55 |
| 1:BJ:67:VAL:HG23 | 1:BJ:135:LEU:HB2 | 1.88 | 0.55 |
| 1:BQ:398:GLY:HA3 | 1:BQ:494:PHE:CD2 | 2.41 | 0.55 |
| 1:BT:55:ARG:HD3 | 1:CA:272:TYR:CD2 | 2.42 | 0.55 |
| 1:CJ:79:ARG:HH11 | 1:CJ:79:ARG:HG3 | 1.72 | 0.55 |
| 1:CJ:284:ARG:HG2 | 1:CJ:284:ARG:NH1 | 2.20 | 0.55 |
| 1:CO:189:PHE:CE1 | 1:CO:198:ARG:CG | 2.90 | 0.55 |
| 1:CO:272:TYR:CD2 | 1:CR:55:ARG:HD3 | 2.41 | 0.55 |
| 1:CQ:454:ASN:ND2 | 1:CQ:456:ALA:H | 2.00 | 0.55 |
| 1:AA:16:ALA:O | 1:AA:17:ASN:HB2 | 2.07 | 0.55 |
| 1:AS:67:VAL:HG23 | 1:AS:135:LEU:HB2 | 1.88 | 0.55 |
| 1:BA:74:ASN:ND2 | 1:BA:77:THR:OG1 | 2.40 | 0.55 |
| 1:BA:232:THR:HB | 1:BA:334:VAL:HG23 | 1.87 | 0.55 |
| 1:BB:67:VAL:HG23 | 1:BB:135:LEU:HB2 | 1.89 | 0.55 |
| 1:BB:74:ASN:ND2 | 1:BB:77:THR:OG1 | 2.39 | 0.55 |
| 1:BD:74:ASN:CB | 1:BD:126:GLU:HG2 | 2.36 | 0.55 |
| 1:BD:398:GLY:HA3 | 1:BD:494:PHE:CD2 | 2.40 | 0.55 |
| 1:BM:74:ASN:CB | 1:BM:126:GLU:HG2 | 2.36 | 0.55 |
| 1:CB:250:TRP:CE3 | 1:CB:272:TYR:CE1 | 2.93 | 0.55 |
| 1:CD:272:TYR:HE2 | 1:CS:55:ARG:NE | 2.01 | 0.55 |
| 1:CE:454:ASN:HD22 | 1:CE:456:ALA:N | 2.03 | 0.55 |
| 1:CG:74:ASN:CB | 1:CG:126:GLU:HG2 | 2.37 | 0.55 |
| 1:CH:55:ARG:HD3 | 1:CK:272:TYR:CD2 | 2.41 | 0.55 |
| 1:CM:75:ARG:NH2 | 1:CM:391:ALA:O | 2.38 | 0.55 |
| 1:AD:250:TRP:CE3 | 1:AD:272:TYR:CE1 | 2.95 | 0.55 |
| 1:AE:55:ARG:NE | 1:CP:272:TYR:HE2 | 2.00 | 0.55 |
| 1:AG:55:ARG:CZ | 1:CG:272:TYR:CE2 | 2.89 | 0.55 |
| 1:AR:398:GLY:HA3 | 1:AR:494:PHE:CD2 | 2.42 | 0.55 |
| 1:BF:250:TRP:CE3 | 1:BF:272:TYR:CE1 | 2.95 | 0.55 |
| 1:BN:55:ARG:HD3 | 1:BS:272:TYR:CD2 | 2.41 | 0.55 |
| 1:CA:74:ASN:CB | 1:CA:126:GLU:HG2 | 2.37 | 0.55 |
| 1:CQ:189:PHE:HE2 | 1:CQ:249:LEU:CD2 | 2.20 | 0.55 |
| 1:CR:454:ASN:HD22 | 1:CR:456:ALA:N | 2.02 | 0.55 |
| 1:CT:189:PHE:HE1 | 1:CT:198:ARG:CG | 2.19 | 0.55 |
| 1:AB:191:LEU:HD23 | 1:AB:191:LEU:N | 2.16 | 0.55 |
| 1:AF:14:CYS:H | 1:AF:138:ASN:HD21 | 1.52 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AH:74:ASN:CB | 1:AH:126:GLU:HG2 | 2.37 | 0.55 |
| 1:AQ:284:ARG:HG2 | 1:AQ:284:ARG:NH1 | 2.20 | 0.55 |
| 1:BC:16:ALA:O | 1:BC:17:ASN:HB2 | 2.06 | 0.55 |
| 1:BO:250:TRP:CE3 | 1:BO:272:TYR:CD1 | 2.95 | 0.55 |
| 1:BQ:189:PHE:HE2 | 1:BQ:249:LEU:CD2 | 2.20 | 0.55 |
| 1:BS:189:PHE:HE2 | 1:BS:249:LEU:CD2 | 2.20 | 0.55 |
| 1:BS:288:HIS:HD2 | 1:BS:337:ASP:OD2 | 1.89 | 0.55 |
| 1:BS:454:ASN:ND2 | 1:BS:456:ALA:H | 2.03 | 0.55 |
| 1:CS:203:THR:HB | 1:CS:300:GLN:HG3 | 1.88 | 0.55 |
| 1:AQ:67:VAL:HG23 | 1:AQ:135:LEU:HB2 | 1.88 | 0.55 |
| 1:AS:250:TRP:HZ3 | 1:AS:272:TYR:CE1 | 2.23 | 0.55 |
| 1:BJ:272:TYR:CE2 | 1:BQ:55:ARG:CZ | 2.90 | 0.55 |
| 1:BQ:74:ASN:CB | 1:BQ:126:GLU:HG2 | 2.35 | 0.55 |
| 1:BT:189:PHE:HE2 | 1:BT:249:LEU:CD2 | 2.20 | 0.55 |
| 1:CE:288:HIS:HD2 | 1:CE:337:ASP:OD2 | 1.90 | 0.55 |
| 1:CN:250:TRP:HZ3 | 1:CN:272:TYR:CE1 | 2.23 | 0.55 |
| 1:AE:14:CYS:H | 1:AE:138:ASN:ND2 | 2.05 | 0.55 |
| 1:AF:16:ALA:O | 1:AF:17:ASN:HB2 | 2.07 | 0.55 |
| 1:AT:43:ALA:HB1 | 1:AT:158:GLU:HA | 1.89 | 0.55 |
| 1:BI:454:ASN:ND2 | 1:BI:456:ALA:H | 2.01 | 0.55 |
| 1:BJ:14:CYS:H | 1:BJ:138:ASN:HD21 | 1.55 | 0.55 |
| 1:CK:250:TRP:CE3 | 1:CK:272:TYR:CE1 | 2.94 | 0.55 |
| 1:CR:250:TRP:CE3 | 1:CR:272:TYR:CE1 | 2.94 | 0.55 |
| 1:CS:189:PHE:CE1 | 1:CS:198:ARG:CG | 2.90 | 0.55 |
| 1:AI:43:ALA:HB1 | 1:AI:158:GLU:HA | 1.89 | 0.55 |
| 1:AJ:191:LEU:CD2 | 1:AJ:191:LEU:N | 2.70 | 0.55 |
| 1:BE:189:PHE:HE2 | 1:BE:249:LEU:CD2 | 2.18 | 0.55 |
| 1:BG:67:VAL:HG23 | 1:BG:135:LEU:HB2 | 1.88 | 0.55 |
| 1:BG:250:TRP:CE3 | 1:BG:272:TYR:CE1 | 2.95 | 0.55 |
| 1:BM:189:PHE:CE1 | 1:BM:198:ARG:HG3 | 2.38 | 0.55 |
| 1:BQ:454:ASN:HD22 | 1:BQ:456:ALA:N | 2.03 | 0.55 |
| 1:CH:11:PRO:HG2 | 1:CH:18:ARG:HD2 | 1.88 | 0.55 |
| 1:CI:288:HIS:HD2 | 1:CI:337:ASP:OD2 | 1.90 | 0.55 |
| 1:CT:454:ASN:HD22 | 1:CT:456:ALA:N | 2.02 | 0.55 |
| 1:AB:250:TRP:HZ3 | 1:AB:272:TYR:CE1 | 2.23 | 0.54 |
| 1:AD:454:ASN:HD22 | 1:AD:456:ALA:N | 2.02 | 0.54 |
| 1:AN:55:ARG:HD3 | 1:AS:272:TYR:CE2 | 2.42 | 0.54 |
| 1:AO:398:GLY:HA3 | 1:AO:494:PHE:CD2 | 2.42 | 0.54 |
| 1:BQ:189:PHE:HE2 | 1:BQ:249:LEU:HD21 | 1.72 | 0.54 |
| 1:BT:67:VAL:HG23 | 1:BT:135:LEU:HB2 | 1.89 | 0.54 |
| 1:CJ:58:ALA:HB2 | 1:CJ:102:GLY:HA3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CM:288:HIS:HD2 | 1:CM:337:ASP:OD2 | 1.90 | 0.54 |
| 1:AB:398:GLY:HA3 | 1:AB:494:PHE:CD2 | 2.43 | 0.54 |
| 1:AJ:284:ARG:HG2 | 1:AJ:284:ARG:NH1 | 2.21 | 0.54 |
| 1:AK:250:TRP:CE3 | 1:AK:272:TYR:CE1 | 2.96 | 0.54 |
| 1:AM:74:ASN:ND2 | 1:AM:77:THR:OG1 | 2.39 | 0.54 |
| 1:AQ:272:TYR:CE2 | 1:BL:55:ARG:HD3 | 2.42 | 0.54 |
| 1:AB:454:ASN:HD22 | 1:AB:456:ALA:N | 2.04 | 0.54 |
| 1:AG:79:ARG:HH11 | 1:AG:79:ARG:CG | 2.13 | 0.54 |
| 1:AG:398:GLY:HA3 | 1:AG:494:PHE:CD2 | 2.43 | 0.54 |
| 1:AH:43:ALA:HB1 | 1:AH:158:GLU:HA | 1.88 | 0.54 |
| 1:AI:74:ASN:ND2 | 1:AI:77:THR:OG1 | 2.39 | 0.54 |
| 1:AK:454:ASN:HD22 | 1:AK:456:ALA:N | 2.03 | 0.54 |
| 1:AO:272:TYR:CD2 | 1:AR:55:ARG:CZ | 2.91 | 0.54 |
| 1:BA:398:GLY:HA3 | 1:BA:494:PHE:CD2 | 2.42 | 0.54 |
| 1:BD:288:HIS:HD2 | 1:BD:337:ASP:OD2 | 1.90 | 0.54 |
| 1:BH:288:HIS:HD2 | 1:BH:337:ASP:OD2 | 1.90 | 0.54 |
| 1:BL:36:GLN:NE2 | 1:BL:156:LEU:H | 2.05 | 0.54 |
| 1:CP:288:HIS:HD2 | 1:CP:337:ASP:OD2 | 1.90 | 0.54 |
| 1:CS:189:PHE:HE1 | 1:CS:198:ARG:CG | 2.19 | 0.54 |
| 1:AC:398:GLY:HA3 | 1:AC:494:PHE:CD2 | 2.42 | 0.54 |
| 1:AF:454:ASN:HD22 | 1:AF:456:ALA:N | 1.99 | 0.54 |
| 1:AG:5:ARG:HD3 | 1:CG:263:ASN:HD22 | 1.73 | 0.54 |
| 1:AG:288:HIS:HD2 | 1:AG:337:ASP:OD2 | 1.89 | 0.54 |
| 1:AJ:250:TRP:CZ3 | 1:AJ:272:TYR:HE1 | 2.23 | 0.54 |
| 1:AP:454:ASN:HD22 | 1:AP:456:ALA:N | 2.02 | 0.54 |
| 1:BI:14:CYS:H | 1:BI:138:ASN:HD21 | 1.55 | 0.54 |
| 1:CD:55:ARG:HD3 | 1:CN:272:TYR:CD2 | 2.43 | 0.54 |
| 1:CD:272:TYR:CE2 | 1:CS:55:ARG:HD3 | 2.41 | 0.54 |
| 1:CH:67:VAL:HG23 | 1:CH:135:LEU:HB2 | 1.90 | 0.54 |
| 1:CL:250:TRP:CE3 | 1:CL:272:TYR:CE1 | 2.95 | 0.54 |
| 1:CS:189:PHE:HE2 | 1:CS:249:LEU:CD2 | 2.21 | 0.54 |
| 1:AI:250:TRP:CZ3 | 1:AI:272:TYR:HE1 | 2.22 | 0.54 |
| 1:AJ:67:VAL:HG23 | 1:AJ:135:LEU:HB2 | 1.90 | 0.54 |
| 1:AK:14:CYS:H | 1:AK:138:ASN:ND2 | 2.05 | 0.54 |
| 1:BA:189:PHE:HD2 | 1:BA:247:ILE:HD11 | 1.72 | 0.54 |
| 1:BA:232:THR:HB | 1:BA:334:VAL:CG2 | 2.37 | 0.54 |
| 1:BG:14:CYS:H | 1:BG:138:ASN:HD21 | 1.54 | 0.54 |
| 1:BM:189:PHE:CE1 | 1:BM:198:ARG:HG2 | 2.43 | 0.54 |
| 1:BP:79:ARG:HH11 | 1:BP:79:ARG:HG2 | 1.70 | 0.54 |
| 1:BP:398:GLY:HA3 | 1:BP:494:PHE:CD2 | 2.43 | 0.54 |
| 1:CB:398:GLY:HA3 | 1:CB:494:PHE:CD2 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CF:30:SER:O | 1:CF:33:LYS:HB2 | 2.08 | 0.54 |
| 1:CR:398:GLY:HA3 | 1:CR:494:PHE:CD2 | 2.42 | 0.54 |
| 1:AC:67:VAL:HG23 | 1:AC:135:LEU:HB2 | 1.90 | 0.54 |
| 1:AD:454:ASN:ND2 | 1:AD:456:ALA:H | 2.04 | 0.54 |
| 1:AR:454:ASN:HD21 | 1:AR:456:ALA:HB3 | 1.73 | 0.54 |
| 1:BD:454:ASN:HD22 | 1:BD:456:ALA:N | 2.06 | 0.54 |
| 1:BG:454:ASN:HD22 | 1:BG:456:ALA:N | 2.04 | 0.54 |
| 1:CF:79:ARG:CG | 1:CF:79:ARG:NH1 | 2.60 | 0.54 |
| 1:CG:67:VAL:HG23 | 1:CG:135:LEU:HB2 | 1.90 | 0.54 |
| 1:CO:272:TYR:CE2 | 1:CR:55:ARG:CZ | 2.91 | 0.54 |
| 1:CT:189:PHE:CE1 | 1:CT:198:ARG:CG | 2.91 | 0.54 |
| 1:CT:250:TRP:CE3 | 1:CT:272:TYR:CE1 | 2.96 | 0.54 |
| 1:AA:58:ALA:HB2 | 1:AA:102:GLY:HA3 | 1.89 | 0.54 |
| 1:AL:14:CYS:H | 1:AL:138:ASN:ND2 | 2.03 | 0.54 |
| 1:AQ:454:ASN:HD22 | 1:AQ:456:ALA:N | 2.04 | 0.54 |
| 1:AR:189:PHE:CE2 | 1:AR:249:LEU:HD21 | 2.41 | 0.54 |
| 1:BC:398:GLY:HA3 | 1:BC:494:PHE:CD2 | 2.43 | 0.54 |
| 1:BG:250:TRP:HZ3 | 1:BG:272:TYR:CE1 | 2.20 | 0.54 |
| 1:BJ:74:ASN:ND2 | 1:BJ:77:THR:OG1 | 2.40 | 0.54 |
| 1:BP:189:PHE:HE2 | 1:BP:249:LEU:CD2 | 2.20 | 0.54 |
| 1:CA:250:TRP:CE3 | 1:CA:272:TYR:CE1 | 2.95 | 0.54 |
| 1:CB:14:CYS:H | 1:CB:138:ASN:HD21 | 1.54 | 0.54 |
| 1:CC:67:VAL:HG23 | 1:CC:135:LEU:HB2 | 1.90 | 0.54 |
| 1:CD:67:VAL:HG23 | 1:CD:135:LEU:HB2 | 1.89 | 0.54 |
| 1:CT:250:TRP:HZ3 | 1:CT:272:TYR:CE1 | 2.23 | 0.54 |
| 1:AE:288:HIS:HD2 | 1:AE:337:ASP:OD2 | 1.90 | 0.54 |
| 1:AE:454:ASN:ND2 | 1:AE:456:ALA:H | 2.03 | 0.54 |
| 1:AI:170:PHE:HD1 | 1:AI:389:MET:HE2 | 1.73 | 0.54 |
| 1:AM:67:VAL:HG23 | 1:AM:135:LEU:HB2 | 1.89 | 0.54 |
| 1:AO:272:TYR:CD2 | 1:AR:55:ARG:HD3 | 2.43 | 0.54 |
| 1:AP:14:CYS:H | 1:AP:138:ASN:HD21 | 1.53 | 0.54 |
| 1:AT:11:PRO:HG2 | 1:AT:18:ARG:HD2 | 1.89 | 0.54 |
| 1:AT:14:CYS:H | 1:AT:138:ASN:HD21 | 1.56 | 0.54 |
| 1:AT:189:PHE:HE2 | 1:AT:249:LEU:CD2 | 2.21 | 0.54 |
| 1:BR:398:GLY:HA3 | 1:BR:494:PHE:CD2 | 2.43 | 0.54 |
| 1:CE:454:ASN:HD21 | 1:CE:456:ALA:HB3 | 1.73 | 0.54 |
| 1:CH:14:CYS:H | 1:CH:138:ASN:HD21 | 1.55 | 0.54 |
| 1:CI:74:ASN:ND2 | 1:CI:77:THR:OG1 | 2.40 | 0.54 |
| 1:CQ:454:ASN:HD21 | 1:CQ:456:ALA:HB3 | 1.72 | 0.54 |
| 1:CS:239:ILE:HG12 | 1:CS:326:ILE:CD1 | 2.37 | 0.54 |
| 1:CT:67:VAL:HG23 | 1:CT:135:LEU:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:288:HIS:HD2 | 1:AK:337:ASP:OD2 | 1.90 | 0.54 |
| 1:AO:288:HIS:HD2 | 1:AO:337:ASP:OD2 | 1.91 | 0.54 |
| 1:AT:398:GLY:HA3 | 1:AT:494:PHE:CD2 | 2.42 | 0.54 |
| 1:BD:189:PHE:HE2 | 1:BD:249:LEU:CD2 | 2.20 | 0.54 |
| 1:BO:272:TYR:CE2 | 1:BR:55:ARG:HD3 | 2.43 | 0.54 |
| 1:BQ:162:PHE:CD2 | 1:BQ:163:LEU:HD13 | 2.43 | 0.54 |
| 1:BR:250:TRP:CE3 | 1:BR:272:TYR:CE1 | 2.96 | 0.54 |
| 1:BS:79:ARG:CG | 1:BS:79:ARG:NH1 | 2.66 | 0.54 |
| 1:CL:454:ASN:ND2 | 1:CL:456:ALA:H | 2.03 | 0.54 |
| 1:CN:454:ASN:ND2 | 1:CN:456:ALA:H | 2.02 | 0.54 |
| 1:CT:189:PHE:HD2 | 1:CT:247:ILE:HD11 | 1.73 | 0.54 |
| 1:AF:67:VAL:HG23 | 1:AF:135:LEU:HB2 | 1.90 | 0.54 |
| 1:AL:74:ASN:ND2 | 1:AL:77:THR:OG1 | 2.41 | 0.54 |
| 1:AM:250:TRP:CE3 | 1:AM:272:TYR:CE1 | 2.96 | 0.54 |
| 1:AR:288:HIS:HD2 | 1:AR:337:ASP:OD2 | 1.91 | 0.54 |
| 1:BB:30:SER:O | 1:BB:33:LYS:HB2 | 2.08 | 0.54 |
| 1:BJ:191:LEU:HD23 | 1:BJ:191:LEU:N | 2.13 | 0.54 |
| 1:BK:67:VAL:HG23 | 1:BK:135:LEU:HB2 | 1.90 | 0.54 |
| 1:BT:170:PHE:HD1 | 1:BT:389:MET:HE2 | 1.72 | 0.54 |
| 1:BT:250:TRP:HZ3 | 1:BT:272:TYR:CE1 | 2.22 | 0.54 |
| 1:CC:79:ARG:HG3 | 1:CC:79:ARG:NH1 | 2.21 | 0.54 |
| 1:CI:55:ARG:CD | 1:CR:272:TYR:CE2 | 2.91 | 0.54 |
| 1:CK:67:VAL:HG23 | 1:CK:135:LEU:HB2 | 1.89 | 0.54 |
| 1:AC:55:ARG:HD3 | 1:AT:272:TYR:CE2 | 2.43 | 0.53 |
| 1:AI:67:VAL:HG23 | 1:AI:135:LEU:HB2 | 1.89 | 0.53 |
| 1:AN:55:ARG:CZ | 1:AS:272:TYR:CE2 | 2.91 | 0.53 |
| 1:AO:74:ASN:CB | 1:AO:126:GLU:HG2 | 2.37 | 0.53 |
| 1:CL:189:PHE:HE1 | 1:CL:198:ARG:CG | 2.19 | 0.53 |
| 1:AG:454:ASN:HD22 | 1:AG:456:ALA:N | 2.04 | 0.53 |
| 1:AH:250:TRP:HZ3 | 1:AH:272:TYR:CE1 | 2.24 | 0.53 |
| 1:BJ:272:TYR:N | 1:BJ:272:TYR:HD1 | 2.06 | 0.53 |
| 1:BT:74:ASN:ND2 | 1:BT:77:THR:OG1 | 2.41 | 0.53 |
| 1:BT:398:GLY:HA3 | 1:BT:494:PHE:CD2 | 2.43 | 0.53 |
| 1:CE:203:THR:HB | 1:CE:300:GLN:HG3 | 1.90 | 0.53 |
| 1:CJ:288:HIS:HD2 | 1:CJ:337:ASP:OD2 | 1.91 | 0.53 |
| 1:CO:67:VAL:HG23 | 1:CO:135:LEU:HB2 | 1.90 | 0.53 |
| 1:AA:189:PHE:HE2 | 1:AA:249:LEU:HD21 | 1.74 | 0.53 |
| 1:AF:288:HIS:HD2 | 1:AF:337:ASP:OD2 | 1.91 | 0.53 |
| 1:AO:75:ARG:NH2 | 1:AO:391:ALA:O | 2.41 | 0.53 |
| 1:AS:454:ASN:HD22 | 1:AS:456:ALA:N | 2.03 | 0.53 |
| 1:BM:25:ILE:HG23 | 1:BM:152:LEU:HD11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CC:75:ARG:NH2 | 1:CC:391:ALA:O | 2.41 | 0.53 |
| 1:CO:189:PHE:HE2 | 1:CO:249:LEU:CD2 | 2.22 | 0.53 |
| 1:AI:55:ARG:CD | 1:AR:272:TYR:CE2 | 2.91 | 0.53 |
| 1:AL:250:TRP:CE3 | 1:AL:272:TYR:CE1 | 2.95 | 0.53 |
| 1:AN:398:GLY:HA3 | 1:AN:494:PHE:CD2 | 2.43 | 0.53 |
| 1:BJ:398:GLY:HA3 | 1:BJ:494:PHE:CD2 | 2.44 | 0.53 |
| 1:CR:189:PHE:CE1 | 1:CR:198:ARG:HG2 | 2.43 | 0.53 |
| 1:CS:75:ARG:NH2 | 1:CS:391:ALA:O | 2.42 | 0.53 |
| 1:AD:272:TYR:CE2 | 1:AS:55:ARG:HD3 | 2.43 | 0.53 |
| 1:AQ:16:ALA:O | 1:AQ:17:ASN:HB2 | 2.07 | 0.53 |
| 1:BD:55:ARG:HD3 | 1:BN:272:TYR:CD2 | 2.44 | 0.53 |
| 1:BR:43:ALA:HB1 | 1:BR:158:GLU:HA | 1.91 | 0.53 |
| 1:BT:189:PHE:CE1 | 1:BT:198:ARG:CG | 2.91 | 0.53 |
| 1:CA:11:PRO:HG2 | 1:CA:18:ARG:HD2 | 1.90 | 0.53 |
| 1:CB:288:HIS:HD2 | 1:CB:337:ASP:OD2 | 1.91 | 0.53 |
| 1:CC:288:HIS:HD2 | 1:CC:337:ASP:OD2 | 1.92 | 0.53 |
| 1:AG:272:TYR:N | 1:AG:272:TYR:HD1 | 2.07 | 0.53 |
| 1:AK:74:ASN:ND2 | 1:AK:77:THR:OG1 | 2.42 | 0.53 |
| 1:AK:191:LEU:HD23 | 1:AK:191:LEU:N | 2.17 | 0.53 |
| 1:BC:191:LEU:HD23 | 1:BC:191:LEU:N | 2.19 | 0.53 |
| 1:BI:272:TYR:CD2 | 1:BO:55:ARG:HD3 | 2.43 | 0.53 |
| 1:BM:454:ASN:ND2 | 1:BM:456:ALA:H | 2.04 | 0.53 |
| 1:BN:250:TRP:CE3 | 1:BN:272:TYR:CE1 | 2.96 | 0.53 |
| 1:CE:67:VAL:HG23 | 1:CE:135:LEU:HB2 | 1.91 | 0.53 |
| 1:CO:189:PHE:HE1 | 1:CO:198:ARG:CG | 2.19 | 0.53 |
| 1:CR:67:VAL:HG23 | 1:CR:135:LEU:HB2 | 1.89 | 0.53 |
| 1:AC:239:ILE:HG12 | 1:AC:326:ILE:CD1 | 2.38 | 0.53 |
| 1:AG:58:ALA:HB2 | 1:AG:102:GLY:HA3 | 1.90 | 0.53 |
| 1:AH:162:PHE:CD2 | 1:AH:163:LEU:HD13 | 2.43 | 0.53 |
| 1:AI:55:ARG:CD | 1:AR:272:TYR:HE2 | 2.21 | 0.53 |
| 1:AJ:272:TYR:HE2 | 1:AQ:55:ARG:CD | 2.22 | 0.53 |
| 1:AK:58:ALA:HB2 | 1:AK:102:GLY:HA3 | 1.89 | 0.53 |
| 1:AL:454:ASN:HD22 | 1:AL:456:ALA:N | 2.01 | 0.53 |
| 1:AQ:250:TRP:CE3 | 1:AQ:272:TYR:CE1 | 2.97 | 0.53 |
| 1:AR:250:TRP:HZ3 | 1:AR:272:TYR:CE1 | 2.23 | 0.53 |
| 1:BO:67:VAL:HG23 | 1:BO:135:LEU:HB2 | 1.90 | 0.53 |
| 1:BQ:250:TRP:CE3 | 1:BQ:272:TYR:CE1 | 2.97 | 0.53 |
| 1:BR:79:ARG:HH11 | 1:BR:79:ARG:CG | 2.16 | 0.53 |
| 1:AA:239:ILE:HG12 | 1:AA:326:ILE:CD1 | 2.39 | 0.53 |
| 1:AF:454:ASN:ND2 | 1:AF:456:ALA:H | 2.01 | 0.53 |
| 1:AO:30:SER:O | 1:AO:33:LYS:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AO:191:LEU:CD2 | 1:AO:191:LEU:N | 2.72 | 0.53 |
| 1:BB:162:PHE:CD2 | 1:BB:163:LEU:HD13 | 2.44 | 0.53 |
| 1:BE:189:PHE:CE1 | 1:BE:198:ARG:HG2 | 2.43 | 0.53 |
| 1:BG:191:LEU:HD23 | 1:BG:191:LEU:N | 2.19 | 0.53 |
| 1:BJ:250:TRP:CE3 | 1:BJ:272:TYR:CD1 | 2.97 | 0.53 |
| 1:BM:288:HIS:HD2 | 1:BM:337:ASP:OD2 | 1.90 | 0.53 |
| 1:CG:189:PHE:CE1 | 1:CG:198:ARG:HG2 | 2.43 | 0.53 |
| 1:AA:288:HIS:HD2 | 1:AA:337:ASP:OD2 | 1.92 | 0.53 |
| 1:AC:250:TRP:HZ3 | 1:AC:272:TYR:CE1 | 2.26 | 0.53 |
| 1:AJ:272:TYR:CD2 | 1:AQ:55:ARG:HD3 | 2.44 | 0.53 |
| 1:AJ:454:ASN:HD22 | 1:AJ:456:ALA:N | 2.03 | 0.53 |
| 1:BD:250:TRP:HZ3 | 1:BD:272:TYR:CE1 | 2.27 | 0.53 |
| 1:BF:191:LEU:HD23 | 1:BF:191:LEU:N | 2.18 | 0.53 |
| 1:BN:18:ARG:HG3 | 1:BN:19:TYR:N | 2.22 | 0.53 |
| 1:BP:250:TRP:CE3 | 1:BP:272:TYR:CD1 | 2.97 | 0.53 |
| 1:CP:189:PHE:HE2 | 1:CP:249:LEU:CD2 | 2.22 | 0.53 |
| 1:AA:454:ASN:ND2 | 1:AA:456:ALA:H | 2.03 | 0.53 |
| 1:AC:272:TYR:CE2 | 1:BA:55:ARG:HD3 | 2.44 | 0.53 |
| 1:AK:398:GLY:HA3 | 1:AK:494:PHE:CD2 | 2.43 | 0.53 |
| 1:BC:272:TYR:CE2 | 1:CA:55:ARG:HD3 | 2.43 | 0.53 |
| 1:BK:189:PHE:HD2 | 1:BK:247:ILE:HD11 | 1.74 | 0.53 |
| 1:BM:203:THR:HB | 1:BM:300:GLN:HG3 | 1.91 | 0.53 |
| 1:BN:454:ASN:ND2 | 1:BN:456:ALA:H | 2.05 | 0.53 |
| 1:BP:58:ALA:HB2 | 1:BP:102:GLY:HA3 | 1.91 | 0.53 |
| 1:CK:454:ASN:ND2 | 1:CK:456:ALA:H | 2.01 | 0.53 |
| 1:CO:79:ARG:HH11 | 1:CO:79:ARG:CG | 2.20 | 0.53 |
| 1:AC:162:PHE:CD2 | 1:AC:163:LEU:HD13 | 2.44 | 0.52 |
| 1:AM:250:TRP:HZ3 | 1:AM:272:TYR:CE1 | 2.24 | 0.52 |
| 1:AO:43:ALA:HB1 | 1:AO:158:GLU:HA | 1.91 | 0.52 |
| 1:AS:189:PHE:HE2 | 1:AS:249:LEU:CD2 | 2.22 | 0.52 |
| 1:BA:239:ILE:HG12 | 1:BA:326:ILE:CD1 | 2.39 | 0.52 |
| 1:BF:189:PHE:CE1 | 1:BF:198:ARG:HG2 | 2.43 | 0.52 |
| 1:BN:189:PHE:HE1 | 1:BN:198:ARG:HG2 | 1.68 | 0.52 |
| 1:BN:288:HIS:HD2 | 1:BN:337:ASP:OD2 | 1.92 | 0.52 |
| 1:BO:288:HIS:HD2 | 1:BO:337:ASP:OD2 | 1.92 | 0.52 |
| 1:CF:14:CYS:H | 1:CF:138:ASN:HD21 | 1.57 | 0.52 |
| 1:CI:404:LEU:HD22 | 1:CI:486:VAL:HG22 | 1.91 | 0.52 |
| 1:CP:74:ASN:ND2 | 1:CP:77:THR:OG1 | 2.42 | 0.52 |
| 1:AD:288:HIS:HD2 | 1:AD:337:ASP:OD2 | 1.92 | 0.52 |
| 1:AK:189:PHE:CE1 | 1:AK:198:ARG:CG | 2.92 | 0.52 |
| 1:BA:454:ASN:ND2 | 1:BA:456:ALA:H | 2.05 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:36:GLN:NE2 | 1:BI:156:LEU:H | 2.07 | 0.52 |
| 1:BI:250:TRP:CE3 | 1:BI:272:TYR:CE1 | 2.96 | 0.52 |
| 1:BM:79:ARG:HH11 | 1:BM:79:ARG:CG | 2.22 | 0.52 |
| 1:CA:30:SER:O | 1:CA:33:LYS:HB2 | 2.10 | 0.52 |
| 1:CC:55:ARG:HD3 | 1:CT:272:TYR:CE2 | 2.44 | 0.52 |
| 1:CE:226:VAL:HG13 | 1:CE:228:GLY:H | 1.73 | 0.52 |
| 1:CH:250:TRP:HZ3 | 1:CH:272:TYR:CE1 | 2.22 | 0.52 |
| 1:AC:191:LEU:CD2 | 1:AC:191:LEU:N | 2.73 | 0.52 |
| 1:AG:272:TYR:CD2 | 1:BG:55:ARG:HD3 | 2.44 | 0.52 |
| 1:AH:454:ASN:HD22 | 1:AH:456:ALA:N | 2.03 | 0.52 |
| 1:AK:75:ARG:NH2 | 1:AK:391:ALA:O | 2.42 | 0.52 |
| 1:AL:189:PHE:HE2 | 1:AL:249:LEU:CD2 | 2.22 | 0.52 |
| 1:AQ:189:PHE:HE1 | 1:AQ:198:ARG:CG | 2.22 | 0.52 |
| 1:BF:30:SER:O | 1:BF:33:LYS:HB2 | 2.09 | 0.52 |
| 1:BF:398:GLY:HA3 | 1:BF:494:PHE:CD2 | 2.45 | 0.52 |
| 1:BN:170:PHE:HD1 | 1:BN:389:MET:CE | 2.21 | 0.52 |
| 1:BN:398:GLY:HA3 | 1:BN:494:PHE:CD2 | 2.45 | 0.52 |
| 1:BP:191:LEU:CD2 | 1:BP:191:LEU:N | 2.73 | 0.52 |
| 1:BR:162:PHE:CD2 | 1:BR:163:LEU:HD13 | 2.44 | 0.52 |
| 1:CA:454:ASN:HD22 | 1:CA:456:ALA:N | 2.04 | 0.52 |
| 1:CD:288:HIS:HD2 | 1:CD:337:ASP:OD2 | 1.92 | 0.52 |
| 1:CE:398:GLY:HA3 | 1:CE:494:PHE:CD2 | 2.44 | 0.52 |
| 1:CH:16:ALA:O | 1:CH:17:ASN:HB2 | 2.08 | 0.52 |
| 1:CJ:454:ASN:ND2 | 1:CJ:456:ALA:H | 2.04 | 0.52 |
| 1:CL:250:TRP:HZ3 | 1:CL:272:TYR:CE1 | 2.24 | 0.52 |
| 1:CM:67:VAL:HG23 | 1:CM:135:LEU:HB2 | 1.91 | 0.52 |
| 1:CO:398:GLY:HA3 | 1:CO:494:PHE:CD2 | 2.44 | 0.52 |
| 1:AF:250:TRP:CE3 | 1:AF:272:TYR:CE1 | 2.97 | 0.52 |
| 1:AM:203:THR:HB | 1:AM:300:GLN:HG3 | 1.91 | 0.52 |
| 1:AQ:256:ASN:HD22 | 1:AQ:302:ASP:HA | 1.73 | 0.52 |
| 1:BH:232:THR:HB | 1:BH:334:VAL:CG2 | 2.40 | 0.52 |
| 1:BJ:30:SER:O | 1:BJ:33:LYS:HB2 | 2.09 | 0.52 |
| 1:BM:43:ALA:HB1 | 1:BM:158:GLU:HA | 1.92 | 0.52 |
| 1:CA:189:PHE:CE1 | 1:CA:198:ARG:CG | 2.93 | 0.52 |
| 1:CF:398:GLY:HA3 | 1:CF:494:PHE:CD2 | 2.45 | 0.52 |
| 1:CI:250:TRP:CE3 | 1:CI:272:TYR:CE1 | 2.97 | 0.52 |
| 1:CL:398:GLY:HA3 | 1:CL:494:PHE:CD2 | 2.44 | 0.52 |
| 1:AA:250:TRP:CE3 | 1:AA:272:TYR:CE1 | 2.97 | 0.52 |
| 1:AB:191:LEU:CD2 | 1:AB:191:LEU:N | 2.72 | 0.52 |
| 1:AS:288:HIS:HD2 | 1:AS:337:ASP:OD2 | 1.91 | 0.52 |
| 1:BE:189:PHE:HE1 | 1:BE:198:ARG:HG2 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:288:HIS:HD2 | 1:BG:337:ASP:OD2 | 1.92 | 0.52 |
| 1:BJ:272:TYR:CD2 | 1:BQ:55:ARG:HD3 | 2.45 | 0.52 |
| 1:BS:250:TRP:HZ3 | 1:BS:272:TYR:CE1 | 2.27 | 0.52 |
| 1:BT:170:PHE:HD1 | 1:BT:389:MET:CE | 2.22 | 0.52 |
| 1:CI:55:ARG:CD | 1:CR:272:TYR:HE2 | 2.22 | 0.52 |
| 1:CM:454:ASN:HD21 | 1:CM:456:ALA:HB3 | 1.73 | 0.52 |
| 1:CM:454:ASN:ND2 | 1:CM:456:ALA:H | 2.02 | 0.52 |
| 1:CS:67:VAL:HG23 | 1:CS:135:LEU:HB2 | 1.91 | 0.52 |
| 1:AJ:16:ALA:O | 1:AJ:17:ASN:HB2 | 2.10 | 0.52 |
| 1:AL:189:PHE:CE1 | 1:AL:198:ARG:CG | 2.92 | 0.52 |
| 1:AM:191:LEU:CD2 | 1:AM:191:LEU:N | 2.73 | 0.52 |
| 1:AQ:239:ILE:HG12 | 1:AQ:326:ILE:CD1 | 2.40 | 0.52 |
| 1:BC:189:PHE:CE1 | 1:BC:198:ARG:CG | 2.92 | 0.52 |
| 1:BC:288:HIS:HD2 | 1:BC:337:ASP:OD2 | 1.92 | 0.52 |
| 1:BE:58:ALA:HB2 | 1:BE:102:GLY:HA3 | 1.92 | 0.52 |
| 1:BJ:43:ALA:HB1 | 1:BJ:158:GLU:HA | 1.92 | 0.52 |
| 1:BJ:272:TYR:N | 1:BJ:272:TYR:CD1 | 2.78 | 0.52 |
| 1:BK:79:ARG:HH11 | 1:BK:79:ARG:HG3 | 1.75 | 0.52 |
| 1:CA:288:HIS:HD2 | 1:CA:337:ASP:OD2 | 1.92 | 0.52 |
| 1:CC:398:GLY:HA3 | 1:CC:494:PHE:CD2 | 2.44 | 0.52 |
| 1:CC:404:LEU:HD22 | 1:CC:486:VAL:HG22 | 1.92 | 0.52 |
| 1:CD:398:GLY:HA3 | 1:CD:494:PHE:CD2 | 2.45 | 0.52 |
| 1:AA:30:SER:O | 1:AA:33:LYS:HB2 | 2.09 | 0.52 |
| 1:AL:79:ARG:CG | 1:AL:79:ARG:NH1 | 2.71 | 0.52 |
| 1:BA:58:ALA:HB2 | 1:BA:102:GLY:HA3 | 1.90 | 0.52 |
| 1:BH:250:TRP:CE3 | 1:BH:272:TYR:CE1 | 2.97 | 0.52 |
| 1:BI:58:ALA:HB2 | 1:BI:102:GLY:HA3 | 1.92 | 0.52 |
| 1:BJ:454:ASN:HD21 | 1:BJ:456:ALA:HB3 | 1.73 | 0.52 |
| 1:CC:74:ASN:ND2 | 1:CC:77:THR:OG1 | 2.43 | 0.52 |
| 1:CT:43:ALA:HB1 | 1:CT:158:GLU:HA | 1.90 | 0.52 |
| 1:AI:398:GLY:HA3 | 1:AI:494:PHE:CD2 | 2.45 | 0.52 |
| 1:AL:58:ALA:HB2 | 1:AL:102:GLY:HA3 | 1.92 | 0.52 |
| 1:BH:74:ASN:ND2 | 1:BH:77:THR:OG1 | 2.42 | 0.52 |
| 1:BQ:16:ALA:O | 1:BQ:17:ASN:HB2 | 2.10 | 0.52 |
| 1:CA:74:ASN:ND2 | 1:CA:77:THR:OG1 | 2.43 | 0.52 |
| 1:CL:189:PHE:HE2 | 1:CL:249:LEU:CD2 | 2.22 | 0.52 |
| 1:CT:58:ALA:HB2 | 1:CT:102:GLY:HA3 | 1.92 | 0.52 |
| 1:AD:263:ASN:O | 1:AD:267:LYS:HG3 | 2.10 | 0.52 |
| 1:AP:226:VAL:HG13 | 1:AP:228:GLY:H | 1.75 | 0.52 |
| 1:AQ:25:ILE:HG23 | 1:AQ:152:LEU:HD11 | 1.92 | 0.52 |
| 1:BE:14:CYS:H | 1:BE:138:ASN:HD21 | 1.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:288:HIS:HD2 | 1:BJ:337:ASP:OD2 | 1.91 | 0.52 |
| 1:BL:398:GLY:HA3 | 1:BL:494:PHE:CD2 | 2.44 | 0.52 |
| 1:BL:454:ASN:HD22 | 1:BL:456:ALA:N | 2.03 | 0.52 |
| 1:BR:288:HIS:HD2 | 1:BR:337:ASP:OD2 | 1.93 | 0.52 |
| 1:BT:79:ARG:HG3 | 1:BT:79:ARG:NH1 | 2.21 | 0.52 |
| 1:BT:454:ASN:ND2 | 1:BT:456:ALA:H | 2.03 | 0.52 |
| 1:CA:170:PHE:HD1 | 1:CA:389:MET:CE | 2.23 | 0.52 |
| 1:CD:58:ALA:HB2 | 1:CD:102:GLY:HA3 | 1.91 | 0.52 |
| 1:CN:288:HIS:HD2 | 1:CN:337:ASP:OD2 | 1.92 | 0.52 |
| 1:CP:189:PHE:CE1 | 1:CP:198:ARG:CG | 2.93 | 0.52 |
| 1:CR:250:TRP:HZ3 | 1:CR:272:TYR:CE1 | 2.23 | 0.52 |
| 1:CS:79:ARG:HH11 | 1:CS:79:ARG:HG3 | 1.73 | 0.52 |
| 1:AC:288:HIS:HD2 | 1:AC:337:ASP:OD2 | 1.92 | 0.52 |
| 1:AG:272:TYR:N | 1:AG:272:TYR:CD1 | 2.77 | 0.52 |
| 1:AN:189:PHE:CE2 | 1:AN:249:LEU:HD21 | 2.42 | 0.52 |
| 1:AO:79:ARG:HG3 | 1:AO:79:ARG:NH1 | 2.24 | 0.52 |
| 1:BR:67:VAL:HG23 | 1:BR:135:LEU:HB2 | 1.91 | 0.52 |
| 1:CC:272:TYR:N | 1:CC:272:TYR:HD1 | 2.07 | 0.52 |
| 1:CG:191:LEU:HD23 | 1:CG:191:LEU:N | 2.19 | 0.52 |
| 1:CJ:272:TYR:CE2 | 1:CQ:55:ARG:HD3 | 2.45 | 0.52 |
| 1:CR:74:ASN:ND2 | 1:CR:77:THR:OG1 | 2.44 | 0.52 |
| 1:AA:8:ILE:HG22 | 1:AA:10:ILE:HD11 | 1.91 | 0.51 |
| 1:AO:189:PHE:HE2 | 1:AO:249:LEU:CD2 | 2.24 | 0.51 |
| 1:AQ:191:LEU:HD23 | 1:AQ:191:LEU:N | 2.18 | 0.51 |
| 1:AR:67:VAL:HG23 | 1:AR:135:LEU:HB2 | 1.91 | 0.51 |
| 1:BF:379:VAL:HG11 | 1:BF:381:MET:HE1 | 1.92 | 0.51 |
| 1:BJ:250:TRP:HZ3 | 1:BJ:272:TYR:CE1 | 2.22 | 0.51 |
| 1:BL:250:TRP:CE3 | 1:BL:272:TYR:CE1 | 2.98 | 0.51 |
| 1:CK:288:HIS:HD2 | 1:CK:337:ASP:OD2 | 1.92 | 0.51 |
| 1:CN:170:PHE:HD1 | 1:CN:389:MET:CE | 2.23 | 0.51 |
| 1:AC:454:ASN:HD21 | 1:AC:456:ALA:HB3 | 1.75 | 0.51 |
| 1:AJ:170:PHE:HD1 | 1:AJ:389:MET:HE2 | 1.76 | 0.51 |
| 1:AS:43:ALA:HB1 | 1:AS:158:GLU:HA | 1.92 | 0.51 |
| 1:AS:232:THR:HB | 1:AS:334:VAL:HG23 | 1.92 | 0.51 |
| 1:BO:272:TYR:CD2 | 1:BR:55:ARG:HD3 | 2.45 | 0.51 |
| 1:BQ:25:ILE:HG23 | 1:BQ:152:LEU:HD11 | 1.91 | 0.51 |
| 1:CA:189:PHE:HE2 | 1:CA:249:LEU:CD2 | 2.23 | 0.51 |
| 1:CH:55:ARG:HD3 | 1:CK:272:TYR:CE2 | 2.45 | 0.51 |
| 1:CR:288:HIS:HD2 | 1:CR:337:ASP:OD2 | 1.92 | 0.51 |
| 1:CT:191:LEU:HD23 | 1:CT:191:LEU:N | 2.20 | 0.51 |
| 1:AH:272:TYR:CE2 | 1:CF:55:ARG:HD3 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AJ:288:HIS:HD2 | 1:AJ:337:ASP:OD2 | 1.93 | 0.51 |
| 1:AR:239:ILE:HG12 | 1:AR:326:ILE:CD1 | 2.41 | 0.51 |
| 1:AS:272:TYR:N | 1:AS:272:TYR:HD1 | 2.08 | 0.51 |
| 1:BC:454:ASN:ND2 | 1:BC:456:ALA:H | 2.03 | 0.51 |
| 1:BD:55:ARG:HD3 | 1:BN:272:TYR:CE2 | 2.45 | 0.51 |
| 1:BL:79:ARG:HH11 | 1:BL:79:ARG:CG | 2.23 | 0.51 |
| 1:CG:162:PHE:CD2 | 1:CG:163:LEU:HD13 | 2.45 | 0.51 |
| 1:CH:398:GLY:HA3 | 1:CH:494:PHE:CD2 | 2.45 | 0.51 |
| 1:CI:191:LEU:CD2 | 1:CI:191:LEU:N | 2.73 | 0.51 |
| 1:CJ:75:ARG:NH2 | 1:CJ:391:ALA:O | 2.42 | 0.51 |
| 1:AD:170:PHE:HD1 | 1:AD:389:MET:CE | 2.24 | 0.51 |
| 1:AD:454:ASN:HD21 | 1:AD:456:ALA:HB3 | 1.75 | 0.51 |
| 1:AF:58:ALA:HB2 | 1:AF:102:GLY:HA3 | 1.93 | 0.51 |
| 1:AH:454:ASN:HD21 | 1:AH:456:ALA:HB3 | 1.76 | 0.51 |
| 1:AI:14:CYS:H | 1:AI:138:ASN:ND2 | 2.08 | 0.51 |
| 1:BA:189:PHE:CE2 | 1:BA:249:LEU:HD21 | 2.45 | 0.51 |
| 1:BC:58:ALA:HB2 | 1:BC:102:GLY:HA3 | 1.92 | 0.51 |
| 1:BE:162:PHE:CD2 | 1:BE:163:LEU:HD13 | 2.46 | 0.51 |
| 1:BE:250:TRP:CE3 | 1:BE:272:TYR:CE1 | 2.98 | 0.51 |
| 1:BJ:226:VAL:HG13 | 1:BJ:228:GLY:H | 1.75 | 0.51 |
| 1:BQ:75:ARG:NH2 | 1:BQ:391:ALA:O | 2.43 | 0.51 |
| 1:CG:239:ILE:HG12 | 1:CG:326:ILE:CD1 | 2.40 | 0.51 |
| 1:CJ:170:PHE:HD1 | 1:CJ:389:MET:CE | 2.23 | 0.51 |
| 1:CN:43:ALA:HB1 | 1:CN:158:GLU:HA | 1.93 | 0.51 |
| 1:AD:79:ARG:HH11 | 1:AD:79:ARG:CG | 2.21 | 0.51 |
| 1:AD:239:ILE:HG12 | 1:AD:326:ILE:CD1 | 2.41 | 0.51 |
| 1:AJ:189:PHE:CE1 | 1:AJ:198:ARG:HG2 | 2.45 | 0.51 |
| 1:AL:189:PHE:HE2 | 1:AL:249:LEU:HD21 | 1.76 | 0.51 |
| 1:AR:379:VAL:HG11 | 1:AR:381:MET:HE1 | 1.91 | 0.51 |
| 1:BH:58:ALA:HB2 | 1:BH:102:GLY:HA3 | 1.92 | 0.51 |
| 1:BH:442:GLN:HE21 | 1:BI:412:PHE:HB2 | 1.76 | 0.51 |
| 1:BO:30:SER:O | 1:BO:33:LYS:HB2 | 2.11 | 0.51 |
| 1:CF:67:VAL:HG23 | 1:CF:135:LEU:HB2 | 1.91 | 0.51 |
| 1:CK:454:ASN:HD21 | 1:CK:456:ALA:HB3 | 1.75 | 0.51 |
| 1:CP:189:PHE:HE1 | 1:CP:198:ARG:CG | 2.23 | 0.51 |
| 1:CS:250:TRP:HZ3 | 1:CS:272:TYR:CE1 | 2.26 | 0.51 |
| 1:CT:288:HIS:HD2 | 1:CT:337:ASP:OD2 | 1.92 | 0.51 |
| 1:AE:58:ALA:HB2 | 1:AE:102:GLY:HA3 | 1.92 | 0.51 |
| 1:AO:226:VAL:HG13 | 1:AO:228:GLY:H | 1.74 | 0.51 |
| 1:AQ:398:GLY:HA3 | 1:AQ:494:PHE:CD2 | 2.44 | 0.51 |
| 1:BD:30:SER:O | 1:BD:33:LYS:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BF:191:LEU:CD2 | 1:BF:191:LEU:N | 2.74 | 0.51 |
| 1:BO:272:TYR:N | 1:BO:272:TYR:HD1 | 2.08 | 0.51 |
| 1:BQ:239:ILE:HG12 | 1:BQ:326:ILE:CD1 | 2.41 | 0.51 |
| 1:CB:43:ALA:HB1 | 1:CB:158:GLU:HA | 1.92 | 0.51 |
| 1:CE:272:TYR:N | 1:CE:272:TYR:HD1 | 2.08 | 0.51 |
| 1:CK:250:TRP:HZ3 | 1:CK:272:TYR:CE1 | 2.22 | 0.51 |
| 1:CS:191:LEU:HD23 | 1:CS:191:LEU:N | 2.21 | 0.51 |
| 1:AB:272:TYR:N | 1:AB:272:TYR:HD1 | 2.09 | 0.51 |
| 1:AJ:74:ASN:ND2 | 1:AJ:77:THR:OG1 | 2.44 | 0.51 |
| 1:AT:250:TRP:HZ3 | 1:AT:272:TYR:CE1 | 2.20 | 0.51 |
| 1:BD:18:ARG:HG3 | 1:BD:19:TYR:N | 2.26 | 0.51 |
| 1:BF:43:ALA:HB1 | 1:BF:158:GLU:HA | 1.92 | 0.51 |
| 1:BF:55:ARG:NE | 1:CH:272:TYR:HE2 | 2.08 | 0.51 |
| 1:BI:226:VAL:HG13 | 1:BI:228:GLY:H | 1.76 | 0.51 |
| 1:BN:43:ALA:HB1 | 1:BN:158:GLU:HA | 1.91 | 0.51 |
| 1:CB:74:ASN:ND2 | 1:CB:77:THR:OG1 | 2.44 | 0.51 |
| 1:CB:232:THR:HB | 1:CB:334:VAL:CG2 | 2.41 | 0.51 |
| 1:CG:25:ILE:HG23 | 1:CG:152:LEU:HD11 | 1.93 | 0.51 |
| 1:CK:412:PHE:HB2 | 1:CO:442:GLN:HE21 | 1.75 | 0.51 |
| 1:CQ:398:GLY:HA3 | 1:CQ:494:PHE:CD2 | 2.46 | 0.51 |
| 1:CS:11:PRO:HG2 | 1:CS:18:ARG:HD2 | 1.93 | 0.51 |
| 1:AB:79:ARG:HH11 | 1:AB:79:ARG:CG | 2.22 | 0.51 |
| 1:AE:197:LEU:HD12 | 1:AE:198:ARG:N | 2.26 | 0.51 |
| 1:AK:189:PHE:HE2 | 1:AK:249:LEU:CD2 | 2.23 | 0.51 |
| 1:AL:398:GLY:HA3 | 1:AL:494:PHE:CD2 | 2.46 | 0.51 |
| 1:AP:272:TYR:CD2 | 1:BE:55:ARG:HD3 | 2.46 | 0.51 |
| 1:AP:442:GLN:HE21 | 1:AQ:412:PHE:HB2 | 1.75 | 0.51 |
| 1:BB:18:ARG:HG3 | 1:BB:19:TYR:N | 2.25 | 0.51 |
| 1:BB:250:TRP:HZ3 | 1:BB:272:TYR:CE1 | 2.23 | 0.51 |
| 1:BC:250:TRP:CZ3 | 1:BC:272:TYR:HE1 | 2.26 | 0.51 |
| 1:BF:170:PHE:HD1 | 1:BF:389:MET:CE | 2.24 | 0.51 |
| 1:BH:284:ARG:CG | 1:BH:284:ARG:NH1 | 2.69 | 0.51 |
| 1:BJ:272:TYR:CD2 | 1:BQ:55:ARG:CZ | 2.94 | 0.51 |
| 1:BR:79:ARG:HG3 | 1:BR:79:ARG:NH1 | 2.22 | 0.51 |
| 1:BT:30:SER:O | 1:BT:33:LYS:HB2 | 2.11 | 0.51 |
| 1:CA:250:TRP:HZ3 | 1:CA:272:TYR:CE1 | 2.26 | 0.51 |
| 1:CB:189:PHE:CE1 | 1:CB:198:ARG:HG2 | 2.46 | 0.51 |
| 1:CF:162:PHE:CD2 | 1:CF:163:LEU:HD13 | 2.45 | 0.51 |
| 1:CG:226:VAL:HG13 | 1:CG:228:GLY:H | 1.75 | 0.51 |
| 1:CI:226:VAL:HG13 | 1:CI:228:GLY:H | 1.76 | 0.51 |
| 1:CJ:191:LEU:HD23 | 1:CJ:191:LEU:N | 2.21 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CO:75:ARG:NH2 | 1:CO:391:ALA:O | 2.43 | 0.51 |
| 1:CP:191:LEU:CD2 | 1:CP:191:LEU:N | 2.73 | 0.51 |
| 1:CQ:239:ILE:HG12 | 1:CQ:326:ILE:CD1 | 2.41 | 0.51 |
| 1:AE:67:VAL:HG23 | 1:AE:135:LEU:HB2 | 1.93 | 0.51 |
| 1:AF:239:ILE:HG12 | 1:AF:326:ILE:CD1 | 2.41 | 0.51 |
| 1:AI:170:PHE:HD1 | 1:AI:389:MET:CE | 2.24 | 0.51 |
| 1:AP:272:TYR:HE2 | 1:BE:55:ARG:NE | 2.07 | 0.51 |
| 1:AQ:43:ALA:HB1 | 1:AQ:158:GLU:HA | 1.91 | 0.51 |
| 1:AQ:189:PHE:HD2 | 1:AQ:247:ILE:HD11 | 1.76 | 0.51 |
| 1:AS:250:TRP:CE3 | 1:AS:272:TYR:CD1 | 2.99 | 0.51 |
| 1:BI:288:HIS:HD2 | 1:BI:337:ASP:OD2 | 1.93 | 0.51 |
| 1:BL:9:TYR:HE2 | 1:BL:145:ASP:HB3 | 1.75 | 0.51 |
| 1:BS:250:TRP:CE3 | 1:BS:272:TYR:CE1 | 2.98 | 0.51 |
| 1:CI:284:ARG:CG | 1:CI:284:ARG:NH1 | 2.71 | 0.51 |
| 1:CJ:272:TYR:N | 1:CJ:272:TYR:HD1 | 2.07 | 0.51 |
| 1:CN:189:PHE:HD2 | 1:CN:247:ILE:CD1 | 2.24 | 0.51 |
| 1:AD:250:TRP:HZ3 | 1:AD:272:TYR:CE1 | 2.29 | 0.51 |
| 1:BA:16:ALA:O | 1:BA:17:ASN:HB2 | 2.11 | 0.51 |
| 1:BB:189:PHE:HD2 | 1:BB:247:ILE:CD1 | 2.24 | 0.51 |
| 1:BH:232:THR:HB | 1:BH:334:VAL:HG23 | 1.93 | 0.51 |
| 1:BI:30:SER:O | 1:BI:33:LYS:HB2 | 2.10 | 0.51 |
| 1:BO:189:PHE:HE2 | 1:BO:249:LEU:CD2 | 2.24 | 0.51 |
| 1:CG:30:SER:O | 1:CG:33:LYS:HB2 | 2.11 | 0.51 |
| 1:CM:191:LEU:CD2 | 1:CM:191:LEU:N | 2.74 | 0.51 |
| 1:CO:250:TRP:HZ3 | 1:CO:272:TYR:CE1 | 2.23 | 0.51 |
| 1:AE:191:LEU:CD2 | 1:AE:191:LEU:N | 2.74 | 0.50 |
| 1:AF:398:GLY:HA3 | 1:AF:494:PHE:CD2 | 2.46 | 0.50 |
| 1:AI:58:ALA:HB2 | 1:AI:102:GLY:HA3 | 1.92 | 0.50 |
| 1:AK:170:PHE:HD1 | 1:AK:389:MET:CE | 2.24 | 0.50 |
| 1:AL:67:VAL:HG23 | 1:AL:135:LEU:HB2 | 1.94 | 0.50 |
| 1:AQ:189:PHE:CE1 | 1:AQ:198:ARG:CG | 2.94 | 0.50 |
| 1:AQ:250:TRP:HZ3 | 1:AQ:272:TYR:CE1 | 2.26 | 0.50 |
| 1:BC:43:ALA:HB1 | 1:BC:158:GLU:HA | 1.92 | 0.50 |
| 1:BH:170:PHE:HD1 | 1:BH:389:MET:CE | 2.23 | 0.50 |
| 1:BK:239:ILE:HG12 | 1:BK:326:ILE:CD1 | 2.41 | 0.50 |
| 1:BL:189:PHE:HE2 | 1:BL:249:LEU:CD2 | 2.24 | 0.50 |
| 1:BQ:191:LEU:HD23 | 1:BQ:191:LEU:N | 2.20 | 0.50 |
| 1:BS:162:PHE:CD2 | 1:BS:163:LEU:HD13 | 2.46 | 0.50 |
| 1:CD:454:ASN:ND2 | 1:CD:456:ALA:H | 2.02 | 0.50 |
| 1:CH:191:LEU:CD2 | 1:CH:191:LEU:N | 2.75 | 0.50 |
| 1:CJ:16:ALA:O | 1:CJ:17:ASN:HB2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CJ:74:ASN:ND2 | 1:CJ:77:THR:OG1 | 2.44 | 0.50 |
| 1:CJ:272:TYR:N | 1:CJ:272:TYR:CD1 | 2.79 | 0.50 |
| 1:CK:189:PHE:HE2 | 1:CK:249:LEU:CD2 | 2.24 | 0.50 |
| 1:CN:14:CYS:H | 1:CN:138:ASN:ND2 | 2.09 | 0.50 |
| 1:AA:55:ARG:HD3 | 1:CC:272:TYR:CE2 | 2.46 | 0.50 |
| 1:AA:75:ARG:NH2 | 1:AA:391:ALA:O | 2.45 | 0.50 |
| 1:AH:189:PHE:HE1 | 1:AH:198:ARG:HG2 | 1.75 | 0.50 |
| 1:AJ:272:TYR:CE2 | 1:AQ:55:ARG:HD3 | 2.46 | 0.50 |
| 1:AO:203:THR:CB | 1:AO:300:GLN:HG3 | 2.40 | 0.50 |
| 1:AP:288:HIS:HD2 | 1:AP:337:ASP:OD2 | 1.94 | 0.50 |
| 1:BL:454:ASN:ND2 | 1:BL:456:ALA:H | 2.05 | 0.50 |
| 1:BO:189:PHE:CE1 | 1:BO:198:ARG:CG | 2.94 | 0.50 |
| 1:BT:234:ARG:HG2 | 1:BT:280:GLU:HG2 | 1.94 | 0.50 |
| 1:CB:454:ASN:ND2 | 1:CB:456:ALA:H | 2.08 | 0.50 |
| 1:CF:16:ALA:O | 1:CF:17:ASN:HB2 | 2.12 | 0.50 |
| 1:CK:14:CYS:H | 1:CK:138:ASN:ND2 | 2.08 | 0.50 |
| 1:CT:263:ASN:O | 1:CT:267:LYS:HG3 | 2.11 | 0.50 |
| 1:AB:272:TYR:N | 1:AB:272:TYR:CD1 | 2.78 | 0.50 |
| 1:AC:79:ARG:HG3 | 1:AC:79:ARG:HH11 | 1.77 | 0.50 |
| 1:AF:250:TRP:HZ3 | 1:AF:272:TYR:CE1 | 2.25 | 0.50 |
| 1:AJ:189:PHE:HD2 | 1:AJ:247:ILE:CD1 | 2.25 | 0.50 |
| 1:AL:191:LEU:CD2 | 1:AL:191:LEU:N | 2.72 | 0.50 |
| 1:AN:67:VAL:HG23 | 1:AN:135:LEU:HB2 | 1.94 | 0.50 |
| 1:AT:162:PHE:CD2 | 1:AT:163:LEU:HD13 | 2.47 | 0.50 |
| 1:BB:189:PHE:CE2 | 1:BB:249:LEU:HD21 | 2.43 | 0.50 |
| 1:BF:162:PHE:CD2 | 1:BF:163:LEU:HD13 | 2.47 | 0.50 |
| 1:BG:30:SER:O | 1:BG:33:LYS:HB2 | 2.10 | 0.50 |
| 1:BI:67:VAL:HG23 | 1:BI:135:LEU:HB2 | 1.93 | 0.50 |
| 1:BI:79:ARG:HH11 | 1:BI:79:ARG:HG3 | 1.75 | 0.50 |
| 1:BM:250:TRP:CE3 | 1:BM:272:TYR:CE1 | 2.99 | 0.50 |
| 1:BS:74:ASN:ND2 | 1:BS:77:THR:OG1 | 2.44 | 0.50 |
| 1:CC:454:ASN:ND2 | 1:CC:456:ALA:H | 2.06 | 0.50 |
| 1:CE:30:SER:O | 1:CE:33:LYS:HB2 | 2.11 | 0.50 |
| 1:CH:18:ARG:HG3 | 1:CH:19:TYR:N | 2.26 | 0.50 |
| 1:CO:16:ALA:O | 1:CO:17:ASN:HB2 | 2.11 | 0.50 |
| 1:CO:77:THR:O | 1:CO:81:THR:HG23 | 2.11 | 0.50 |
| 1:CS:30:SER:O | 1:CS:33:LYS:HB2 | 2.12 | 0.50 |
| 1:AB:239:ILE:HG12 | 1:AB:326:ILE:CD1 | 2.41 | 0.50 |
| 1:AF:30:SER:O | 1:AF:33:LYS:HB2 | 2.12 | 0.50 |
| 1:AG:79:ARG:NH1 | 1:AG:79:ARG:CG | 2.72 | 0.50 |
| 1:AI:288:HIS:HD2 | 1:AI:337:ASP:OD2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AJ:170:PHE:HD1 | 1:AJ:389:MET:CE | 2.24 | 0.50 |
| 1:AN:14:CYS:HB3 | 1:AN:64:LEU:HD21 | 1.94 | 0.50 |
| 1:AN:232:THR:HB | 1:AN:334:VAL:CG2 | 2.40 | 0.50 |
| 1:AN:239:ILE:HG23 | 1:AN:324:LEU:HD21 | 1.93 | 0.50 |
| 1:AQ:239:ILE:HD12 | 1:AQ:275:GLU:HA | 1.94 | 0.50 |
| 1:AR:162:PHE:CD2 | 1:AR:163:LEU:HD13 | 2.46 | 0.50 |
| 1:AS:162:PHE:CD2 | 1:AS:163:LEU:HD13 | 2.45 | 0.50 |
| 1:BA:75:ARG:NH2 | 1:BA:391:ALA:O | 2.44 | 0.50 |
| 1:BC:250:TRP:HZ3 | 1:BC:272:TYR:CE1 | 2.28 | 0.50 |
| 1:BO:58:ALA:HB2 | 1:BO:102:GLY:HA3 | 1.93 | 0.50 |
| 1:CA:14:CYS:H | 1:CA:138:ASN:HD21 | 1.57 | 0.50 |
| 1:CA:189:PHE:HE1 | 1:CA:198:ARG:CG | 2.24 | 0.50 |
| 1:CD:250:TRP:HZ3 | 1:CD:272:TYR:CE1 | 2.26 | 0.50 |
| 1:CE:272:TYR:N | 1:CE:272:TYR:CD1 | 2.80 | 0.50 |
| 1:CF:170:PHE:HD1 | 1:CF:389:MET:HE2 | 1.76 | 0.50 |
| 1:CP:189:PHE:HD2 | 1:CP:247:ILE:HD11 | 1.77 | 0.50 |
| 1:AD:14:CYS:H | 1:AD:138:ASN:ND2 | 2.09 | 0.50 |
| 1:AD:191:LEU:CD2 | 1:AD:191:LEU:N | 2.74 | 0.50 |
| 1:AF:412:PHE:HB2 | 1:AJ:442:GLN:HE21 | 1.76 | 0.50 |
| 1:AG:75:ARG:NH2 | 1:AG:391:ALA:O | 2.45 | 0.50 |
| 1:AG:191:LEU:CD2 | 1:AG:191:LEU:N | 2.74 | 0.50 |
| 1:AN:191:LEU:HD23 | 1:AN:191:LEU:N | 2.20 | 0.50 |
| 1:AO:272:TYR:N | 1:AO:272:TYR:HD1 | 2.10 | 0.50 |
| 1:BH:454:ASN:ND2 | 1:BH:456:ALA:H | 2.04 | 0.50 |
| 1:BM:162:PHE:CD2 | 1:BM:163:LEU:HD13 | 2.46 | 0.50 |
| 1:CB:250:TRP:HZ3 | 1:CB:272:TYR:CE1 | 2.25 | 0.50 |
| 1:CM:189:PHE:CE1 | 1:CM:198:ARG:HG2 | 2.46 | 0.50 |
| 1:CR:454:ASN:ND2 | 1:CR:456:ALA:H | 2.02 | 0.50 |
| 1:AD:442:GLN:HE21 | 1:AE:412:PHE:HB2 | 1.77 | 0.50 |
| 1:AF:55:ARG:HD3 | 1:BH:272:TYR:CE2 | 2.46 | 0.50 |
| 1:AF:191:LEU:HD23 | 1:AF:191:LEU:N | 2.21 | 0.50 |
| 1:AI:191:LEU:HD23 | 1:AI:191:LEU:N | 2.19 | 0.50 |
| 1:AI:226:VAL:HG13 | 1:AI:228:GLY:H | 1.76 | 0.50 |
| 1:AO:189:PHE:CE1 | 1:AO:198:ARG:CG | 2.95 | 0.50 |
| 1:BB:398:GLY:HA3 | 1:BB:494:PHE:CD2 | 2.47 | 0.50 |
| 1:BO:189:PHE:HE1 | 1:BO:198:ARG:CG | 2.24 | 0.50 |
| 1:BS:170:PHE:HD1 | 1:BS:389:MET:CE | 2.25 | 0.50 |
| 1:BS:398:GLY:HA3 | 1:BS:494:PHE:CD2 | 2.47 | 0.50 |
| 1:CE:18:ARG:HG3 | 1:CE:19:TYR:N | 2.25 | 0.50 |
| 1:CI:398:GLY:HA3 | 1:CI:494:PHE:CD2 | 2.47 | 0.50 |
| 1:CJ:30:SER:O | 1:CJ:33:LYS:HB2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CP:239:ILE:HG12 | 1:CP:326:ILE:CD1 | 2.41 | 0.50 |
| 1:CQ:232:THR:HB | 1:CQ:334:VAL:HG23 | 1.93 | 0.50 |
| 1:CR:58:ALA:HB2 | 1:CR:102:GLY:HA3 | 1.94 | 0.50 |
| 1:AC:58:ALA:HB2 | 1:AC:102:GLY:HA3 | 1.94 | 0.50 |
| 1:AH:170:PHE:HD1 | 1:AH:389:MET:HE2 | 1.76 | 0.50 |
| 1:AI:79:ARG:HH11 | 1:AI:79:ARG:CG | 2.19 | 0.50 |
| 1:AM:58:ALA:HB2 | 1:AM:102:GLY:HA3 | 1.93 | 0.50 |
| 1:BI:189:PHE:HD2 | 1:BI:247:ILE:HD11 | 1.76 | 0.50 |
| 1:CC:250:TRP:HZ3 | 1:CC:272:TYR:CE1 | 2.20 | 0.50 |
| 1:CH:189:PHE:HD2 | 1:CH:247:ILE:CD1 | 2.25 | 0.50 |
| 1:CH:239:ILE:HG12 | 1:CH:326:ILE:CD1 | 2.42 | 0.50 |
| 1:CI:58:ALA:HB2 | 1:CI:102:GLY:HA3 | 1.93 | 0.50 |
| 1:CM:272:TYR:N | 1:CM:272:TYR:HD1 | 2.09 | 0.50 |
| 1:CR:189:PHE:HD2 | 1:CR:247:ILE:CD1 | 2.25 | 0.50 |
| 1:AC:239:ILE:HD12 | 1:AC:275:GLU:HA | 1.94 | 0.50 |
| 1:AE:250:TRP:HZ3 | 1:AE:272:TYR:CE1 | 2.28 | 0.50 |
| 1:AP:67:VAL:HG23 | 1:AP:135:LEU:HB2 | 1.93 | 0.50 |
| 1:BA:454:ASN:HD21 | 1:BA:456:ALA:HB3 | 1.77 | 0.50 |
| 1:BB:272:TYR:N | 1:BB:272:TYR:CD1 | 2.79 | 0.50 |
| 1:BC:226:VAL:HG13 | 1:BC:228:GLY:H | 1.76 | 0.50 |
| 1:BG:191:LEU:CD2 | 1:BG:191:LEU:N | 2.75 | 0.50 |
| 1:BJ:239:ILE:HG12 | 1:BJ:326:ILE:CD1 | 2.41 | 0.50 |
| 1:BJ:404:LEU:HD22 | 1:BJ:486:VAL:HG22 | 1.93 | 0.50 |
| 1:BN:170:PHE:HD1 | 1:BN:389:MET:HE2 | 1.77 | 0.50 |
| 1:BP:67:VAL:HG23 | 1:BP:135:LEU:HB2 | 1.93 | 0.50 |
| 1:BQ:58:ALA:HB2 | 1:BQ:102:GLY:HA3 | 1.94 | 0.50 |
| 1:CB:454:ASN:HD21 | 1:CB:456:ALA:HB3 | 1.77 | 0.50 |
| 1:CJ:272:TYR:CD2 | 1:CQ:55:ARG:CZ | 2.93 | 0.50 |
| 1:CK:43:ALA:HB1 | 1:CK:158:GLU:HA | 1.93 | 0.50 |
| 1:CM:272:TYR:N | 1:CM:272:TYR:CD1 | 2.79 | 0.50 |
| 1:CQ:14:CYS:H | 1:CQ:138:ASN:ND2 | 2.09 | 0.50 |
| 1:AC:30:SER:O | 1:AC:33:LYS:HB2 | 2.11 | 0.50 |
| 1:AD:189:PHE:HE2 | 1:AD:249:LEU:HD21 | 1.75 | 0.50 |
| 1:AE:272:TYR:CE2 | 1:AM:55:ARG:HD3 | 2.46 | 0.50 |
| 1:AK:43:ALA:HB1 | 1:AK:158:GLU:HA | 1.93 | 0.50 |
| 1:AL:226:VAL:HG13 | 1:AL:228:GLY:H | 1.77 | 0.50 |
| 1:AQ:170:PHE:HD1 | 1:AQ:389:MET:CE | 2.25 | 0.50 |
| 1:AR:454:ASN:ND2 | 1:AR:456:ALA:H | 2.03 | 0.50 |
| 1:AT:379:VAL:HG11 | 1:AT:381:MET:HE1 | 1.94 | 0.50 |
| 1:BB:58:ALA:HB2 | 1:BB:102:GLY:HA3 | 1.92 | 0.50 |
| 1:BB:189:PHE:CE1 | 1:BB:198:ARG:HG2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BD:170:PHE:HD1 | 1:BD:389:MET:CE | 2.24 | 0.50 |
| 1:BG:398:GLY:HA3 | 1:BG:494:PHE:CD2 | 2.47 | 0.50 |
| 1:BK:454:ASN:HD21 | 1:BK:456:ALA:HB3 | 1.76 | 0.50 |
| 1:CJ:67:VAL:HG23 | 1:CJ:135:LEU:HB2 | 1.92 | 0.50 |
| 1:CK:189:PHE:CE1 | 1:CK:198:ARG:CG | 2.94 | 0.50 |
| 1:CL:189:PHE:HD2 | 1:CL:247:ILE:HD11 | 1.76 | 0.50 |
| 1:CL:454:ASN:HD21 | 1:CL:456:ALA:HB3 | 1.77 | 0.50 |
| 1:CN:30:SER:O | 1:CN:33:LYS:HB2 | 2.11 | 0.50 |
| 1:CP:454:ASN:HD22 | 1:CP:456:ALA:N | 2.06 | 0.50 |
| 1:CQ:191:LEU:CD2 | 1:CQ:191:LEU:N | 2.73 | 0.50 |
| 1:AD:170:PHE:HD1 | 1:AD:389:MET:HE2 | 1.77 | 0.49 |
| 1:AP:239:ILE:HG12 | 1:AP:326:ILE:CD1 | 2.42 | 0.49 |
| 1:AR:30:SER:O | 1:AR:33:LYS:HB2 | 2.12 | 0.49 |
| 1:BD:170:PHE:HD1 | 1:BD:389:MET:HE2 | 1.76 | 0.49 |
| 1:BI:284:ARG:CG | 1:BI:284:ARG:NH1 | 2.70 | 0.49 |
| 1:BJ:191:LEU:CD2 | 1:BJ:191:LEU:N | 2.70 | 0.49 |
| 1:BM:189:PHE:HE1 | 1:BM:198:ARG:HG2 | 1.70 | 0.49 |
| 1:BS:189:PHE:HE2 | 1:BS:249:LEU:HD21 | 1.77 | 0.49 |
| 1:BT:189:PHE:HD2 | 1:BT:247:ILE:HD11 | 1.77 | 0.49 |
| 1:CB:232:THR:HB | 1:CB:334:VAL:HG23 | 1.93 | 0.49 |
| 1:CE:272:TYR:HE2 | 1:CM:55:ARG:NE | 2.03 | 0.49 |
| 1:CF:170:PHE:HD1 | 1:CF:389:MET:CE | 2.25 | 0.49 |
| 1:CR:191:LEU:CD2 | 1:CR:191:LEU:N | 2.75 | 0.49 |
| 1:AA:226:VAL:HG13 | 1:AA:228:GLY:H | 1.77 | 0.49 |
| 1:AJ:404:LEU:HD22 | 1:AJ:486:VAL:HG22 | 1.94 | 0.49 |
| 1:AL:30:SER:O | 1:AL:33:LYS:HB2 | 2.12 | 0.49 |
| 1:AO:189:PHE:HE1 | 1:AO:198:ARG:CG | 2.25 | 0.49 |
| 1:AP:404:LEU:HD22 | 1:AP:486:VAL:HG22 | 1.94 | 0.49 |
| 1:AT:170:PHE:HD1 | 1:AT:389:MET:CE | 2.25 | 0.49 |
| 1:BD:272:TYR:N | 1:BD:272:TYR:HD1 | 2.11 | 0.49 |
| 1:BL:189:PHE:HD2 | 1:BL:247:ILE:HD11 | 1.76 | 0.49 |
| 1:BT:189:PHE:HE2 | 1:BT:249:LEU:HD21 | 1.76 | 0.49 |
| 1:CB:25:ILE:HG23 | 1:CB:152:LEU:HD11 | 1.94 | 0.49 |
| 1:CD:79:ARG:CG | 1:CD:79:ARG:NH1 | 2.71 | 0.49 |
| 1:CG:189:PHE:CE2 | 1:CG:249:LEU:HD21 | 2.44 | 0.49 |
| 1:CL:67:VAL:HG23 | 1:CL:135:LEU:HB2 | 1.93 | 0.49 |
| 1:CR:30:SER:O | 1:CR:33:LYS:HB2 | 2.12 | 0.49 |
| 1:AJ:203:THR:CB | 1:AJ:300:GLN:HG3 | 2.42 | 0.49 |
| 1:AK:67:VAL:HG23 | 1:AK:135:LEU:HB2 | 1.92 | 0.49 |
| 1:AL:454:ASN:ND2 | 1:AL:456:ALA:H | 2.05 | 0.49 |
| 1:AN:58:ALA:HB2 | 1:AN:102:GLY:HA3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AO:25:ILE:HG23 | 1:AO:152:LEU:HD11 | 1.93 | 0.49 |
| 1:BB:272:TYR:N | 1:BB:272:TYR:HD1 | 2.11 | 0.49 |
| 1:BC:272:TYR:CD2 | 1:CA:55:ARG:HD3 | 2.47 | 0.49 |
| 1:BM:191:LEU:CD2 | 1:BM:191:LEU:N | 2.74 | 0.49 |
| 1:BN:14:CYS:H | 1:BN:138:ASN:HD21 | 1.58 | 0.49 |
| 1:BO:454:ASN:HD22 | 1:BO:456:ALA:N | 2.06 | 0.49 |
| 1:CE:22:THR:OG1 | 1:CE:131:HIS:CD2 | 2.58 | 0.49 |
| 1:CE:191:LEU:CD2 | 1:CE:191:LEU:N | 2.76 | 0.49 |
| 1:CI:189:PHE:HD2 | 1:CI:247:ILE:CD1 | 2.25 | 0.49 |
| 1:CL:288:HIS:HD2 | 1:CL:337:ASP:OD2 | 1.94 | 0.49 |
| 1:CM:189:PHE:HD2 | 1:CM:247:ILE:CD1 | 2.25 | 0.49 |
| 1:CN:67:VAL:HG23 | 1:CN:135:LEU:HB2 | 1.94 | 0.49 |
| 1:CQ:79:ARG:HH11 | 1:CQ:79:ARG:HG3 | 1.77 | 0.49 |
| 1:CQ:232:THR:HB | 1:CQ:334:VAL:CG2 | 2.42 | 0.49 |
| 1:CR:404:LEU:HD22 | 1:CR:486:VAL:HG22 | 1.94 | 0.49 |
| 1:AD:284:ARG:CG | 1:AD:284:ARG:NH1 | 2.70 | 0.49 |
| 1:AF:162:PHE:CD2 | 1:AF:163:LEU:HD13 | 2.47 | 0.49 |
| 1:AH:30:SER:O | 1:AH:33:LYS:HB2 | 2.12 | 0.49 |
| 1:AJ:250:TRP:HZ3 | 1:AJ:272:TYR:CE1 | 2.28 | 0.49 |
| 1:AP:191:LEU:CD2 | 1:AP:191:LEU:N | 2.72 | 0.49 |
| 1:BA:67:VAL:HG23 | 1:BA:135:LEU:HB2 | 1.94 | 0.49 |
| 1:BB:18:ARG:NH1 | 1:BB:18:ARG:HB2 | 2.27 | 0.49 |
| 1:BB:454:ASN:HD21 | 1:BB:456:ALA:HB3 | 1.77 | 0.49 |
| 1:BF:16:ALA:O | 1:BF:17:ASN:HB2 | 2.11 | 0.49 |
| 1:BJ:79:ARG:CG | 1:BJ:79:ARG:NH1 | 2.73 | 0.49 |
| 1:BK:189:PHE:HE2 | 1:BK:249:LEU:HD21 | 1.78 | 0.49 |
| 1:BN:263:ASN:O | 1:BN:267:LYS:HG3 | 2.12 | 0.49 |
| 1:BO:75:ARG:NH2 | 1:BO:391:ALA:O | 2.45 | 0.49 |
| 1:CE:189:PHE:CE2 | 1:CE:249:LEU:HD21 | 2.45 | 0.49 |
| 1:CL:14:CYS:HB3 | 1:CL:64:LEU:HD21 | 1.93 | 0.49 |
| 1:CO:288:HIS:HD2 | 1:CO:337:ASP:OD2 | 1.95 | 0.49 |
| 1:CO:454:ASN:HD22 | 1:CO:456:ALA:N | 2.06 | 0.49 |
| 1:CP:28:MET:HE2 | 1:CP:152:LEU:HG | 1.95 | 0.49 |
| 1:AB:30:SER:O | 1:AB:33:LYS:HB2 | 2.12 | 0.49 |
| 1:AE:16:ALA:O | 1:AE:17:ASN:HB2 | 2.11 | 0.49 |
| 1:AH:226:VAL:HG13 | 1:AH:228:GLY:H | 1.77 | 0.49 |
| 1:AI:239:ILE:HG12 | 1:AI:326:ILE:CD1 | 2.42 | 0.49 |
| 1:AJ:239:ILE:HD12 | 1:AJ:275:GLU:HA | 1.94 | 0.49 |
| 1:AJ:398:GLY:HA3 | 1:AJ:494:PHE:CD2 | 2.48 | 0.49 |
| 1:AQ:232:THR:HB | 1:AQ:334:VAL:HG23 | 1.94 | 0.49 |
| 1:AS:189:PHE:CE1 | 1:AS:198:ARG:CG | 2.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BB:284:ARG:CG | 1:BB:284:ARG:NH1 | 2.67 | 0.49 |
| 1:BE:67:VAL:HG23 | 1:BE:135:LEU:HB2 | 1.94 | 0.49 |
| 1:BE:398:GLY:HA3 | 1:BE:494:PHE:CD2 | 2.48 | 0.49 |
| 1:BI:162:PHE:CD2 | 1:BI:163:LEU:HD13 | 2.47 | 0.49 |
| 1:BI:191:LEU:CD2 | 1:BI:191:LEU:N | 2.74 | 0.49 |
| 1:BN:74:ASN:ND2 | 1:BN:77:THR:OG1 | 2.45 | 0.49 |
| 1:BN:454:ASN:HD21 | 1:BN:456:ALA:HB3 | 1.78 | 0.49 |
| 1:BO:272:TYR:CD1 | 1:BO:272:TYR:N | 2.79 | 0.49 |
| 1:BQ:30:SER:O | 1:BQ:33:LYS:HB2 | 2.11 | 0.49 |
| 1:CD:189:PHE:CE1 | 1:CD:198:ARG:CG | 2.96 | 0.49 |
| 1:CF:58:ALA:HB2 | 1:CF:102:GLY:HA3 | 1.94 | 0.49 |
| 1:CG:288:HIS:HD2 | 1:CG:337:ASP:OD2 | 1.95 | 0.49 |
| 1:CK:239:ILE:HD12 | 1:CK:275:GLU:HA | 1.94 | 0.49 |
| 1:CP:272:TYR:N | 1:CP:272:TYR:HD1 | 2.10 | 0.49 |
| 1:AB:61:PHE:CD2 | 1:AB:243:ILE:HD11 | 2.47 | 0.49 |
| 1:AG:74:ASN:ND2 | 1:AG:77:THR:OG1 | 2.46 | 0.49 |
| 1:AI:191:LEU:CD2 | 1:AI:191:LEU:N | 2.76 | 0.49 |
| 1:AK:16:ALA:O | 1:AK:17:ASN:HB2 | 2.12 | 0.49 |
| 1:AL:189:PHE:HE1 | 1:AL:198:ARG:CG | 2.24 | 0.49 |
| 1:BC:67:VAL:HG23 | 1:BC:135:LEU:HB2 | 1.94 | 0.49 |
| 1:BI:189:PHE:CE2 | 1:BI:249:LEU:HD21 | 2.45 | 0.49 |
| 1:BJ:58:ALA:HB2 | 1:BJ:102:GLY:HA3 | 1.94 | 0.49 |
| 1:BJ:170:PHE:HD1 | 1:BJ:389:MET:CE | 2.25 | 0.49 |
| 1:BP:162:PHE:CD2 | 1:BP:163:LEU:HD13 | 2.47 | 0.49 |
| 1:CF:232:THR:HB | 1:CF:334:VAL:CG2 | 2.43 | 0.49 |
| 1:CJ:239:ILE:HG12 | 1:CJ:326:ILE:CD1 | 2.43 | 0.49 |
| 1:CN:191:LEU:CD2 | 1:CN:191:LEU:N | 2.75 | 0.49 |
| 1:CR:454:ASN:HD21 | 1:CR:456:ALA:HB3 | 1.77 | 0.49 |
| 1:AB:162:PHE:CD2 | 1:AB:163:LEU:HD13 | 2.48 | 0.49 |
| 1:AB:272:TYR:CE2 | 1:CB:55:ARG:CZ | 2.96 | 0.49 |
| 1:AG:170:PHE:HD1 | 1:AG:389:MET:HE2 | 1.77 | 0.49 |
| 1:AI:263:ASN:O | 1:AI:267:LYS:HG3 | 2.13 | 0.49 |
| 1:AK:79:ARG:HH11 | 1:AK:79:ARG:HG3 | 1.77 | 0.49 |
| 1:BA:191:LEU:HD23 | 1:BA:191:LEU:N | 2.21 | 0.49 |
| 1:BD:43:ALA:HB1 | 1:BD:158:GLU:HA | 1.94 | 0.49 |
| 1:BK:43:ALA:HB1 | 1:BK:158:GLU:HA | 1.95 | 0.49 |
| 1:BO:74:ASN:ND2 | 1:BO:77:THR:OG1 | 2.45 | 0.49 |
| 1:BP:79:ARG:CG | 1:BP:79:ARG:NH1 | 2.61 | 0.49 |
| 1:BP:263:ASN:O | 1:BP:267:LYS:HG3 | 2.13 | 0.49 |
| 1:CA:239:ILE:HG12 | 1:CA:326:ILE:CD1 | 2.43 | 0.49 |
| 1:CD:170:PHE:HD1 | 1:CD:389:MET:CE | 2.25 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CF:189:PHE:HD2 | 1:CF:247:ILE:CD1 | 2.26 | 0.49 |
| 1:CG:189:PHE:HD2 | 1:CG:247:ILE:HD11 | 1.77 | 0.49 |
| 1:CI:454:ASN:ND2 | 1:CI:456:ALA:H | 2.08 | 0.49 |
| 1:CO:162:PHE:CD2 | 1:CO:163:LEU:HD13 | 2.47 | 0.49 |
| 1:CQ:189:PHE:HE2 | 1:CQ:249:LEU:HD21 | 1.77 | 0.49 |
| 1:AC:189:PHE:CE1 | 1:AC:198:ARG:CG | 2.95 | 0.49 |
| 1:AE:398:GLY:HA3 | 1:AE:494:PHE:CD2 | 2.48 | 0.49 |
| 1:AG:272:TYR:CE2 | 1:BG:55:ARG:HD3 | 2.47 | 0.49 |
| 1:AM:191:LEU:HD23 | 1:AM:191:LEU:N | 2.16 | 0.49 |
| 1:AO:454:ASN:ND2 | 1:AO:456:ALA:H | 2.06 | 0.49 |
| 1:AP:454:ASN:HD21 | 1:AP:456:ALA:HB3 | 1.78 | 0.49 |
| 1:AS:189:PHE:HD2 | 1:AS:247:ILE:HD11 | 1.78 | 0.49 |
| 1:AT:58:ALA:HB2 | 1:AT:102:GLY:HA3 | 1.93 | 0.49 |
| 1:BA:272:TYR:CD1 | 1:BA:272:TYR:N | 2.80 | 0.49 |
| 1:BE:170:PHE:HD1 | 1:BE:389:MET:HE2 | 1.77 | 0.49 |
| 1:BQ:191:LEU:CD2 | 1:BQ:191:LEU:N | 2.76 | 0.49 |
| 1:CC:189:PHE:HE2 | 1:CC:249:LEU:CD2 | 2.26 | 0.49 |
| 1:CE:232:THR:HB | 1:CE:334:VAL:HG23 | 1.95 | 0.49 |
| 1:CG:79:ARG:CG | 1:CG:79:ARG:NH1 | 2.70 | 0.49 |
| 1:CK:239:ILE:HG12 | 1:CK:326:ILE:CD1 | 2.42 | 0.49 |
| 1:AH:55:ARG:HD3 | 1:AK:272:TYR:CD2 | 2.48 | 0.49 |
| 1:AL:75:ARG:NH2 | 1:AL:391:ALA:O | 2.46 | 0.49 |
| 1:AL:284:ARG:CG | 1:AL:284:ARG:NH1 | 2.70 | 0.49 |
| 1:AQ:14:CYS:H | 1:AQ:138:ASN:HD21 | 1.58 | 0.49 |
| 1:AQ:454:ASN:HD21 | 1:AQ:456:ALA:HB3 | 1.78 | 0.49 |
| 1:AT:67:VAL:HG23 | 1:AT:135:LEU:HB2 | 1.93 | 0.49 |
| 1:BH:239:ILE:HG12 | 1:BH:326:ILE:CD1 | 2.42 | 0.49 |
| 1:BJ:16:ALA:O | 1:BJ:17:ASN:HB2 | 2.11 | 0.49 |
| 1:BP:250:TRP:HZ3 | 1:BP:272:TYR:CE1 | 2.27 | 0.49 |
| 1:CC:58:ALA:HB2 | 1:CC:102:GLY:HA3 | 1.94 | 0.49 |
| 1:CD:272:TYR:N | 1:CD:272:TYR:HD1 | 2.11 | 0.49 |
| 1:CE:284:ARG:CG | 1:CE:284:ARG:NH1 | 2.71 | 0.49 |
| 1:CI:16:ALA:O | 1:CI:17:ASN:HB2 | 2.13 | 0.49 |
| 1:CI:272:TYR:N | 1:CI:272:TYR:CD1 | 2.81 | 0.49 |
| 1:CJ:189:PHE:HD2 | 1:CJ:247:ILE:CD1 | 2.26 | 0.49 |
| 1:CM:239:ILE:HD12 | 1:CM:275:GLU:HA | 1.94 | 0.49 |
| 1:CT:398:GLY:HA3 | 1:CT:494:PHE:CD2 | 2.47 | 0.49 |
| 1:AG:55:ARG:CZ | 1:CG:272:TYR:CD2 | 2.96 | 0.49 |
| 1:AH:55:ARG:HD3 | 1:AK:272:TYR:CE2 | 2.48 | 0.49 |
| 1:AK:272:TYR:N | 1:AK:272:TYR:CD1 | 2.81 | 0.49 |
| 1:AR:442:GLN:HE21 | 1:AS:412:PHE:HB2 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BA:30:SER:O | 1:BA:33:LYS:HB2 | 2.13 | 0.49 |
| 1:BE:239:ILE:HG12 | 1:BE:326:ILE:CD1 | 2.42 | 0.49 |
| 1:BE:250:TRP:HZ3 | 1:BE:272:TYR:CE1 | 2.29 | 0.49 |
| 1:BK:284:ARG:CG | 1:BK:284:ARG:NH1 | 2.72 | 0.49 |
| 1:BO:189:PHE:HD2 | 1:BO:247:ILE:HD11 | 1.77 | 0.49 |
| 1:BR:74:ASN:ND2 | 1:BR:77:THR:OG1 | 2.46 | 0.49 |
| 1:CB:263:ASN:O | 1:CB:267:LYS:HG3 | 2.12 | 0.49 |
| 1:CC:30:SER:O | 1:CC:33:LYS:HB2 | 2.13 | 0.49 |
| 1:CG:14:CYS:H | 1:CG:138:ASN:ND2 | 2.10 | 0.49 |
| 1:CG:239:ILE:HD12 | 1:CG:275:GLU:HA | 1.94 | 0.49 |
| 1:CQ:67:VAL:HG23 | 1:CQ:135:LEU:HB2 | 1.94 | 0.49 |
| 1:AB:189:PHE:HD2 | 1:AB:247:ILE:CD1 | 2.25 | 0.48 |
| 1:AG:189:PHE:HD2 | 1:AG:247:ILE:CD1 | 2.25 | 0.48 |
| 1:AN:79:ARG:CG | 1:AN:79:ARG:NH1 | 2.74 | 0.48 |
| 1:AO:250:TRP:HZ3 | 1:AO:272:TYR:CE1 | 2.25 | 0.48 |
| 1:BA:284:ARG:CG | 1:BA:284:ARG:NH1 | 2.68 | 0.48 |
| 1:BP:30:SER:O | 1:BP:33:LYS:HB2 | 2.14 | 0.48 |
| 1:BP:272:TYR:N | 1:BP:272:TYR:HD1 | 2.11 | 0.48 |
| 1:BR:191:LEU:HD23 | 1:BR:191:LEU:N | 2.21 | 0.48 |
| 1:CA:284:ARG:CG | 1:CA:284:ARG:NH1 | 2.74 | 0.48 |
| 1:CG:189:PHE:HE1 | 1:CG:198:ARG:HG2 | 1.75 | 0.48 |
| 1:CJ:14:CYS:H | 1:CJ:138:ASN:ND2 | 2.07 | 0.48 |
| 1:CK:170:PHE:HD1 | 1:CK:389:MET:CE | 2.26 | 0.48 |
| 1:CP:272:TYR:N | 1:CP:272:TYR:CD1 | 2.81 | 0.48 |
| 1:CP:398:GLY:HA3 | 1:CP:494:PHE:CD2 | 2.48 | 0.48 |
| 1:CR:379:VAL:HG11 | 1:CR:381:MET:HE1 | 1.95 | 0.48 |
| 1:CT:299:SER:O | 1:CT:302:ASP:HB2 | 2.13 | 0.48 |
| 1:AC:454:ASN:ND2 | 1:AC:456:ALA:H | 2.06 | 0.48 |
| 1:AH:189:PHE:CE1 | 1:AH:198:ARG:HG2 | 2.48 | 0.48 |
| 1:AH:189:PHE:HD2 | 1:AH:247:ILE:CD1 | 2.26 | 0.48 |
| 1:AJ:250:TRP:CE3 | 1:AJ:272:TYR:CE1 | 3.01 | 0.48 |
| 1:AL:189:PHE:HD2 | 1:AL:247:ILE:HD11 | 1.78 | 0.48 |
| 1:AM:162:PHE:CD2 | 1:AM:163:LEU:HD13 | 2.48 | 0.48 |
| 1:AQ:234:ARG:HG2 | 1:AQ:280:GLU:HG2 | 1.94 | 0.48 |
| 1:AR:14:CYS:H | 1:AR:138:ASN:ND2 | 2.07 | 0.48 |
| 1:AR:189:PHE:HD2 | 1:AR:247:ILE:CD1 | 2.25 | 0.48 |
| 1:AR:263:ASN:O | 1:AR:267:LYS:HG3 | 2.13 | 0.48 |
| 1:AS:272:TYR:N | 1:AS:272:TYR:CD1 | 2.80 | 0.48 |
| 1:AT:189:PHE:HD2 | 1:AT:247:ILE:HD11 | 1.78 | 0.48 |
| 1:BH:454:ASN:HD21 | 1:BH:456:ALA:HB3 | 1.78 | 0.48 |
| 1:BO:250:TRP:HZ3 | 1:BO:272:TYR:CE1 | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BP:14:CYS:H | 1:BP:138:ASN:ND2 | 2.11 | 0.48 |
| 1:CC:189:PHE:CE1 | 1:CC:198:ARG:CG | 2.96 | 0.48 |
| 1:CF:189:PHE:CE1 | 1:CF:198:ARG:HG2 | 2.46 | 0.48 |
| 1:CI:189:PHE:CE2 | 1:CI:249:LEU:HD21 | 2.41 | 0.48 |
| 1:CO:18:ARG:HG3 | 1:CO:19:TYR:N | 2.27 | 0.48 |
| 1:CR:237:VAL:HG23 | 1:CR:279:PHE:CD2 | 2.48 | 0.48 |
| 1:CS:74:ASN:ND2 | 1:CS:77:THR:OG1 | 2.46 | 0.48 |
| 1:AG:454:ASN:ND2 | 1:AG:456:ALA:H | 2.08 | 0.48 |
| 1:AJ:30:SER:O | 1:AJ:33:LYS:HB2 | 2.13 | 0.48 |
| 1:BC:252:VAL:HG22 | 1:BC:253:SER:N | 2.28 | 0.48 |
| 1:BD:189:PHE:HD2 | 1:BD:247:ILE:HD11 | 1.78 | 0.48 |
| 1:BD:191:LEU:CD2 | 1:BD:191:LEU:N | 2.73 | 0.48 |
| 1:BS:239:ILE:HG12 | 1:BS:326:ILE:CD1 | 2.44 | 0.48 |
| 1:BT:239:ILE:HG12 | 1:BT:326:ILE:CD1 | 2.43 | 0.48 |
| 1:CE:239:ILE:HG12 | 1:CE:326:ILE:CD1 | 2.44 | 0.48 |
| 1:CF:442:GLN:HE21 | 1:CG:412:PHE:HB2 | 1.78 | 0.48 |
| 1:CG:189:PHE:HD2 | 1:CG:247:ILE:CD1 | 2.26 | 0.48 |
| 1:CS:11:PRO:HG2 | 1:CS:18:ARG:CD | 2.43 | 0.48 |
| 1:CS:189:PHE:HE2 | 1:CS:249:LEU:HD21 | 1.77 | 0.48 |
| 1:AB:442:GLN:HE21 | 1:AC:412:PHE:HB2 | 1.77 | 0.48 |
| 1:AG:189:PHE:CE2 | 1:AG:249:LEU:HD21 | 2.42 | 0.48 |
| 1:AK:189:PHE:HD2 | 1:AK:247:ILE:HD11 | 1.77 | 0.48 |
| 1:AN:232:THR:HB | 1:AN:334:VAL:HG23 | 1.96 | 0.48 |
| 1:AT:191:LEU:CD2 | 1:AT:191:LEU:N | 2.76 | 0.48 |
| 1:AT:454:ASN:ND2 | 1:AT:456:ALA:H | 2.09 | 0.48 |
| 1:BC:189:PHE:HE2 | 1:BC:249:LEU:CD2 | 2.26 | 0.48 |
| 1:BD:201:GLY:HA3 | 1:BD:300:GLN:HG2 | 1.96 | 0.48 |
| 1:BG:189:PHE:CE2 | 1:BG:249:LEU:HD21 | 2.44 | 0.48 |
| 1:BI:454:ASN:HD21 | 1:BI:456:ALA:HB3 | 1.78 | 0.48 |
| 1:BO:239:ILE:HG12 | 1:BO:326:ILE:CD1 | 2.44 | 0.48 |
| 1:CD:191:LEU:CD2 | 1:CD:191:LEU:N | 2.77 | 0.48 |
| 1:CM:398:GLY:HA3 | 1:CM:494:PHE:CD2 | 2.48 | 0.48 |
| 1:AH:189:PHE:CE2 | 1:AH:249:LEU:HD21 | 2.44 | 0.48 |
| 1:AI:250:TRP:CE3 | 1:AI:272:TYR:CE1 | 3.01 | 0.48 |
| 1:AJ:18:ARG:HD2 | 1:AJ:19:TYR:O | 2.13 | 0.48 |
| 1:AO:18:ARG:HG3 | 1:AO:19:TYR:N | 2.28 | 0.48 |
| 1:AQ:272:TYR:HD2 | 1:BL:55:ARG:HD3 | 1.76 | 0.48 |
| 1:BA:43:ALA:HB1 | 1:BA:158:GLU:HA | 1.95 | 0.48 |
| 1:BB:234:ARG:HG2 | 1:BB:280:GLU:HG2 | 1.95 | 0.48 |
| 1:BC:191:LEU:CD2 | 1:BC:191:LEU:N | 2.76 | 0.48 |
| 1:BD:272:TYR:N | 1:BD:272:TYR:CD1 | 2.81 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:226:VAL:HG13 | 1:BG:228:GLY:H | 1.78 | 0.48 |
| 1:BG:272:TYR:N | 1:BG:272:TYR:CD1 | 2.82 | 0.48 |
| 1:BH:189:PHE:CE1 | 1:BH:198:ARG:HG2 | 2.48 | 0.48 |
| 1:BJ:284:ARG:CG | 1:BJ:284:ARG:NH1 | 2.73 | 0.48 |
| 1:BM:272:TYR:N | 1:BM:272:TYR:CD1 | 2.82 | 0.48 |
| 1:BQ:454:ASN:ND2 | 1:BQ:456:ALA:H | 2.10 | 0.48 |
| 1:BS:454:ASN:HD21 | 1:BS:456:ALA:HB3 | 1.79 | 0.48 |
| 1:CD:55:ARG:HD3 | 1:CN:272:TYR:CE2 | 2.49 | 0.48 |
| 1:CN:10:ILE:HD13 | 1:CN:20:LEU:HD13 | 1.95 | 0.48 |
| 1:CO:393:HIS:CG | 1:CO:496:PHE:HB3 | 2.48 | 0.48 |
| 1:CS:272:TYR:N | 1:CS:272:TYR:CD1 | 2.81 | 0.48 |
| 1:AC:16:ALA:O | 1:AC:17:ASN:HB2 | 2.13 | 0.48 |
| 1:AG:67:VAL:HG23 | 1:AG:135:LEU:HB2 | 1.96 | 0.48 |
| 1:AJ:189:PHE:CE2 | 1:AJ:249:LEU:HD21 | 2.46 | 0.48 |
| 1:AP:22:THR:OG1 | 1:AP:131:HIS:CD2 | 2.58 | 0.48 |
| 1:AR:272:TYR:N | 1:AR:272:TYR:CD1 | 2.80 | 0.48 |
| 1:AR:272:TYR:N | 1:AR:272:TYR:HD1 | 2.12 | 0.48 |
| 1:BF:250:TRP:HZ3 | 1:BF:272:TYR:CE1 | 2.26 | 0.48 |
| 1:CG:272:TYR:N | 1:CG:272:TYR:CD1 | 2.82 | 0.48 |
| 1:CK:398:GLY:HA3 | 1:CK:494:PHE:CD2 | 2.48 | 0.48 |
| 1:CL:203:THR:HB | 1:CL:300:GLN:HG3 | 1.94 | 0.48 |
| 1:CN:189:PHE:HD2 | 1:CN:247:ILE:HD11 | 1.77 | 0.48 |
| 1:CN:454:ASN:HD21 | 1:CN:456:ALA:HB3 | 1.77 | 0.48 |
| 1:CQ:189:PHE:CE1 | 1:CQ:198:ARG:CG | 2.96 | 0.48 |
| 1:CS:234:ARG:HG2 | 1:CS:280:GLU:HG2 | 1.94 | 0.48 |
| 1:CS:272:TYR:N | 1:CS:272:TYR:HD1 | 2.11 | 0.48 |
| 1:CT:189:PHE:HE2 | 1:CT:249:LEU:HD21 | 1.79 | 0.48 |
| 1:AA:252:VAL:HG22 | 1:AA:253:SER:N | 2.28 | 0.48 |
| 1:AF:226:VAL:HG13 | 1:AF:228:GLY:H | 1.78 | 0.48 |
| 1:AI:379:VAL:HG11 | 1:AI:381:MET:HE1 | 1.95 | 0.48 |
| 1:AQ:232:THR:HB | 1:AQ:334:VAL:CG2 | 2.43 | 0.48 |
| 1:AR:189:PHE:HD2 | 1:AR:247:ILE:HD11 | 1.79 | 0.48 |
| 1:BF:454:ASN:HD21 | 1:BF:456:ALA:HB3 | 1.78 | 0.48 |
| 1:BG:58:ALA:HB2 | 1:BG:102:GLY:HA3 | 1.95 | 0.48 |
| 1:BH:43:ALA:HB1 | 1:BH:158:GLU:HA | 1.95 | 0.48 |
| 1:BP:189:PHE:HE2 | 1:BP:249:LEU:HD21 | 1.79 | 0.48 |
| 1:CB:20:LEU:HB2 | 1:CB:132:PHE:O | 2.14 | 0.48 |
| 1:CC:239:ILE:HG12 | 1:CC:326:ILE:CD1 | 2.44 | 0.48 |
| 1:CF:191:LEU:CD2 | 1:CF:191:LEU:N | 2.75 | 0.48 |
| 1:CH:454:ASN:ND2 | 1:CH:456:ALA:H | 2.06 | 0.48 |
| 1:CL:252:VAL:HG22 | 1:CL:253:SER:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CO:189:PHE:HD2 | 1:CO:247:ILE:HD11 | 1.78 | 0.48 |
| 1:CR:170:PHE:HD1 | 1:CR:389:MET:CE | 2.25 | 0.48 |
| 1:CS:284:ARG:CG | 1:CS:284:ARG:NH1 | 2.73 | 0.48 |
| 1:CT:272:TYR:N | 1:CT:272:TYR:CD1 | 2.82 | 0.48 |
| 1:AH:25:ILE:HG23 | 1:AH:152:LEU:HD11 | 1.96 | 0.48 |
| 1:AP:55:ARG:CZ | 1:BM:272:TYR:CE2 | 2.97 | 0.48 |
| 1:AP:454:ASN:ND2 | 1:AP:456:ALA:H | 2.05 | 0.48 |
| 1:AS:232:THR:HB | 1:AS:334:VAL:CG2 | 2.43 | 0.48 |
| 1:BB:239:ILE:HG23 | 1:BB:324:LEU:HD21 | 1.96 | 0.48 |
| 1:BC:404:LEU:HD22 | 1:BC:486:VAL:HG22 | 1.95 | 0.48 |
| 1:BF:239:ILE:HG12 | 1:BF:326:ILE:CD1 | 2.44 | 0.48 |
| 1:BN:239:ILE:HG12 | 1:BN:326:ILE:CD1 | 2.44 | 0.48 |
| 1:BR:75:ARG:NH2 | 1:BR:391:ALA:O | 2.46 | 0.48 |
| 1:BT:189:PHE:CE2 | 1:BT:249:LEU:HD21 | 2.49 | 0.48 |
| 1:CD:22:THR:OG1 | 1:CD:131:HIS:CD2 | 2.58 | 0.48 |
| 1:CD:74:ASN:ND2 | 1:CD:77:THR:OG1 | 2.46 | 0.48 |
| 1:CQ:170:PHE:HD1 | 1:CQ:389:MET:CE | 2.26 | 0.48 |
| 1:CR:10:ILE:HG21 | 1:CR:146:TRP:CZ2 | 2.49 | 0.48 |
| 1:AF:252:VAL:HG22 | 1:AF:253:SER:N | 2.29 | 0.48 |
| 1:AF:272:TYR:HD2 | 1:BK:55:ARG:HD3 | 1.77 | 0.48 |
| 1:AK:250:TRP:HZ3 | 1:AK:272:TYR:CE1 | 2.23 | 0.48 |
| 1:AN:440:ALA:CB | 1:AO:444:LEU:HD13 | 2.43 | 0.48 |
| 1:AO:14:CYS:H | 1:AO:138:ASN:HD21 | 1.60 | 0.48 |
| 1:AR:22:THR:OG1 | 1:AR:131:HIS:CD2 | 2.60 | 0.48 |
| 1:BA:170:PHE:HD1 | 1:BA:389:MET:CE | 2.26 | 0.48 |
| 1:BH:189:PHE:HD2 | 1:BH:247:ILE:CD1 | 2.27 | 0.48 |
| 1:BM:170:PHE:HD1 | 1:BM:389:MET:CE | 2.27 | 0.48 |
| 1:BN:239:ILE:HD12 | 1:BN:275:GLU:HA | 1.95 | 0.48 |
| 1:BR:263:ASN:O | 1:BR:267:LYS:HG3 | 2.14 | 0.48 |
| 1:BS:189:PHE:HD2 | 1:BS:247:ILE:HD11 | 1.79 | 0.48 |
| 1:BT:16:ALA:O | 1:BT:17:ASN:HB2 | 2.14 | 0.48 |
| 1:CB:30:SER:O | 1:CB:33:LYS:HB2 | 2.14 | 0.48 |
| 1:CG:191:LEU:CD2 | 1:CG:191:LEU:N | 2.75 | 0.48 |
| 1:CH:189:PHE:HD2 | 1:CH:247:ILE:HD11 | 1.79 | 0.48 |
| 1:CJ:43:ALA:HB1 | 1:CJ:158:GLU:HA | 1.95 | 0.48 |
| 1:CO:79:ARG:HG3 | 1:CO:79:ARG:NH1 | 2.23 | 0.48 |
| 1:CO:191:LEU:HD23 | 1:CO:191:LEU:N | 2.21 | 0.48 |
| 1:CP:162:PHE:CD2 | 1:CP:163:LEU:HD13 | 2.48 | 0.48 |
| 1:CR:239:ILE:HD12 | 1:CR:275:GLU:HA | 1.96 | 0.48 |
| 1:AB:189:PHE:CE1 | 1:AB:198:ARG:HG2 | 2.49 | 0.48 |
| 1:AI:162:PHE:CD2 | 1:AI:163:LEU:HD13 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:454:ASN:ND2 | 1:AK:456:ALA:H | 2.07 | 0.48 |
| 1:AP:272:TYR:CE2 | 1:BE:55:ARG:HD3 | 2.49 | 0.48 |
| 1:AS:239:ILE:HG12 | 1:AS:326:ILE:CD1 | 2.44 | 0.48 |
| 1:BD:189:PHE:CE1 | 1:BD:198:ARG:CG | 2.95 | 0.48 |
| 1:BH:263:ASN:O | 1:BH:267:LYS:HG3 | 2.14 | 0.48 |
| 1:BJ:393:HIS:CG | 1:BJ:496:PHE:HB3 | 2.49 | 0.48 |
| 1:BJ:454:ASN:ND2 | 1:BJ:456:ALA:H | 2.06 | 0.48 |
| 1:BL:440:ALA:CB | 1:BM:444:LEU:HD13 | 2.44 | 0.48 |
| 1:BN:237:VAL:HG23 | 1:BN:279:PHE:CD2 | 2.49 | 0.48 |
| 1:BQ:442:GLN:HE21 | 1:BR:412:PHE:HB2 | 1.78 | 0.48 |
| 1:CC:162:PHE:CD2 | 1:CC:163:LEU:HD13 | 2.49 | 0.48 |
| 1:CD:393:HIS:CG | 1:CD:496:PHE:HB3 | 2.48 | 0.48 |
| 1:CE:58:ALA:HB2 | 1:CE:102:GLY:HA3 | 1.96 | 0.48 |
| 1:CK:170:PHE:HD1 | 1:CK:389:MET:HE2 | 1.78 | 0.48 |
| 1:AA:250:TRP:HZ3 | 1:AA:272:TYR:CE1 | 2.28 | 0.47 |
| 1:AD:272:TYR:HD1 | 1:AD:272:TYR:N | 2.12 | 0.47 |
| 1:AF:237:VAL:HG23 | 1:AF:279:PHE:CD2 | 2.49 | 0.47 |
| 1:AH:189:PHE:HD2 | 1:AH:247:ILE:HD11 | 1.79 | 0.47 |
| 1:AN:442:GLN:NE2 | 1:AO:412:PHE:HB2 | 2.29 | 0.47 |
| 1:AP:30:SER:O | 1:AP:33:LYS:HB2 | 2.14 | 0.47 |
| 1:AS:234:ARG:HG2 | 1:AS:280:GLU:HG2 | 1.96 | 0.47 |
| 1:BH:191:LEU:CD2 | 1:BH:191:LEU:N | 2.76 | 0.47 |
| 1:BR:239:ILE:HD12 | 1:BR:275:GLU:HA | 1.95 | 0.47 |
| 1:CD:188:PHE:C | 1:CD:189:PHE:HD1 | 2.17 | 0.47 |
| 1:CH:170:PHE:HD1 | 1:CH:389:MET:CE | 2.27 | 0.47 |
| 1:CH:239:ILE:HD12 | 1:CH:275:GLU:HA | 1.96 | 0.47 |
| 1:CK:16:ALA:O | 1:CK:17:ASN:HB2 | 2.14 | 0.47 |
| 1:AB:67:VAL:HG23 | 1:AB:135:LEU:HB2 | 1.95 | 0.47 |
| 1:AI:30:SER:O | 1:AI:33:LYS:HB2 | 2.14 | 0.47 |
| 1:AN:189:PHE:CE1 | 1:AN:198:ARG:HG2 | 2.49 | 0.47 |
| 1:BE:11:PRO:HG2 | 1:BE:18:ARG:HD3 | 1.95 | 0.47 |
| 1:BH:67:VAL:HG23 | 1:BH:135:LEU:HB2 | 1.96 | 0.47 |
| 1:BL:201:GLY:HA3 | 1:BL:300:GLN:HG2 | 1.96 | 0.47 |
| 1:BN:189:PHE:HD2 | 1:BN:247:ILE:CD1 | 2.26 | 0.47 |
| 1:BT:162:PHE:CD2 | 1:BT:163:LEU:HD13 | 2.48 | 0.47 |
| 1:CA:25:ILE:HG23 | 1:CA:152:LEU:HD11 | 1.96 | 0.47 |
| 1:CF:379:VAL:HG11 | 1:CF:381:MET:HE1 | 1.95 | 0.47 |
| 1:CH:58:ALA:HB2 | 1:CH:102:GLY:HA3 | 1.96 | 0.47 |
| 1:CJ:226:VAL:HG13 | 1:CJ:228:GLY:H | 1.78 | 0.47 |
| 1:CK:191:LEU:CD2 | 1:CK:191:LEU:N | 2.75 | 0.47 |
| 1:CK:234:ARG:HG2 | 1:CK:280:GLU:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CP:250:TRP:HZ3 | 1:CP:272:TYR:CE1 | 2.25 | 0.47 |
| 1:AF:189:PHE:HD2 | 1:AF:247:ILE:CD1 | 2.27 | 0.47 |
| 1:AH:201:GLY:HA3 | 1:AH:300:GLN:HG2 | 1.96 | 0.47 |
| 1:AJ:203:THR:HB | 1:AJ:300:GLN:CG | 2.45 | 0.47 |
| 1:AN:79:ARG:HG3 | 1:AN:79:ARG:NH1 | 2.18 | 0.47 |
| 1:AQ:393:HIS:CG | 1:AQ:496:PHE:HB3 | 2.49 | 0.47 |
| 1:BI:272:TYR:N | 1:BI:272:TYR:CD1 | 2.83 | 0.47 |
| 1:BT:256:ASN:HD22 | 1:BT:302:ASP:HA | 1.79 | 0.47 |
| 1:CC:191:LEU:CD2 | 1:CC:191:LEU:N | 2.74 | 0.47 |
| 1:CF:454:ASN:HD21 | 1:CF:456:ALA:HB3 | 1.78 | 0.47 |
| 1:CK:237:VAL:HG23 | 1:CK:279:PHE:CD2 | 2.49 | 0.47 |
| 1:CM:30:SER:O | 1:CM:33:LYS:HB2 | 2.14 | 0.47 |
| 1:CO:203:THR:HB | 1:CO:300:GLN:HG3 | 1.96 | 0.47 |
| 1:CP:30:SER:O | 1:CP:33:LYS:HB2 | 2.14 | 0.47 |
| 1:CT:454:ASN:HD21 | 1:CT:456:ALA:HB3 | 1.79 | 0.47 |
| 1:AA:11:PRO:HG2 | 1:AA:18:ARG:HD2 | 1.96 | 0.47 |
| 1:AD:58:ALA:HB2 | 1:AD:102:GLY:HA3 | 1.96 | 0.47 |
| 1:AF:239:ILE:HD12 | 1:AF:275:GLU:HA | 1.96 | 0.47 |
| 1:AG:55:ARG:HD3 | 1:CG:272:TYR:CE2 | 2.49 | 0.47 |
| 1:AM:234:ARG:HG2 | 1:AM:280:GLU:HG2 | 1.96 | 0.47 |
| 1:AM:252:VAL:HG22 | 1:AM:253:SER:N | 2.29 | 0.47 |
| 1:AO:189:PHE:HD2 | 1:AO:247:ILE:HD11 | 1.79 | 0.47 |
| 1:AR:189:PHE:CE1 | 1:AR:198:ARG:HG2 | 2.49 | 0.47 |
| 1:BB:404:LEU:HD22 | 1:BB:486:VAL:HG22 | 1.95 | 0.47 |
| 1:BD:189:PHE:HE2 | 1:BD:249:LEU:HD21 | 1.79 | 0.47 |
| 1:BO:170:PHE:HD1 | 1:BO:389:MET:HE2 | 1.78 | 0.47 |
| 1:BS:232:THR:HB | 1:BS:334:VAL:HG23 | 1.96 | 0.47 |
| 1:BT:55:ARG:HD3 | 1:CA:272:TYR:CE2 | 2.49 | 0.47 |
| 1:CC:379:VAL:HG11 | 1:CC:381:MET:HE1 | 1.96 | 0.47 |
| 1:CI:393:HIS:CG | 1:CI:496:PHE:HB3 | 2.50 | 0.47 |
| 1:CO:272:TYR:CD2 | 1:CR:55:ARG:CZ | 2.97 | 0.47 |
| 1:AA:272:TYR:N | 1:AA:272:TYR:CD1 | 2.82 | 0.47 |
| 1:AD:272:TYR:N | 1:AD:272:TYR:CD1 | 2.82 | 0.47 |
| 1:AE:189:PHE:CE2 | 1:AE:249:LEU:HD21 | 2.43 | 0.47 |
| 1:AN:189:PHE:HD2 | 1:AN:247:ILE:CD1 | 2.27 | 0.47 |
| 1:AS:58:ALA:HB2 | 1:AS:102:GLY:HA3 | 1.95 | 0.47 |
| 1:AS:191:LEU:HD23 | 1:AS:191:LEU:N | 2.21 | 0.47 |
| 1:BF:189:PHE:HD2 | 1:BF:247:ILE:CD1 | 2.28 | 0.47 |
| 1:CB:11:PRO:HG2 | 1:CB:18:ARG:HD2 | 1.96 | 0.47 |
| 1:CH:162:PHE:CD2 | 1:CH:163:LEU:HD13 | 2.49 | 0.47 |
| 1:CI:61:PHE:CD2 | 1:CI:243:ILE:HD11 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CJ:162:PHE:CD2 | 1:CJ:163:LEU:HD13 | 2.49 | 0.47 |
| 1:CJ:237:VAL:HG23 | 1:CJ:279:PHE:CD2 | 2.49 | 0.47 |
| 1:CJ:250:TRP:CE3 | 1:CJ:272:TYR:CD1 | 3.03 | 0.47 |
| 1:CO:30:SER:O | 1:CO:33:LYS:HB2 | 2.15 | 0.47 |
| 1:AB:55:ARG:NE | 1:BB:272:TYR:HE2 | 2.10 | 0.47 |
| 1:AD:30:SER:O | 1:AD:33:LYS:HB2 | 2.13 | 0.47 |
| 1:AH:284:ARG:CG | 1:AH:284:ARG:NH1 | 2.70 | 0.47 |
| 1:AL:170:PHE:HD1 | 1:AL:389:MET:CE | 2.28 | 0.47 |
| 1:BD:239:ILE:HG12 | 1:BD:326:ILE:CD1 | 2.45 | 0.47 |
| 1:BJ:170:PHE:HD1 | 1:BJ:389:MET:HE2 | 1.80 | 0.47 |
| 1:BL:14:CYS:H | 1:BL:138:ASN:HD21 | 1.62 | 0.47 |
| 1:BL:232:THR:HB | 1:BL:334:VAL:CG2 | 2.45 | 0.47 |
| 1:BN:14:CYS:HB3 | 1:BN:64:LEU:HD21 | 1.97 | 0.47 |
| 1:BQ:79:ARG:HH11 | 1:BQ:79:ARG:HG3 | 1.79 | 0.47 |
| 1:BR:232:THR:HB | 1:BR:334:VAL:HG23 | 1.96 | 0.47 |
| 1:BT:232:THR:HB | 1:BT:334:VAL:CG2 | 2.44 | 0.47 |
| 1:CD:272:TYR:N | 1:CD:272:TYR:CD1 | 2.82 | 0.47 |
| 1:CD:454:ASN:HD21 | 1:CD:456:ALA:HB3 | 1.79 | 0.47 |
| 1:CJ:250:TRP:HZ3 | 1:CJ:272:TYR:CE1 | 2.25 | 0.47 |
| 1:CK:191:LEU:HD23 | 1:CK:191:LEU:N | 2.19 | 0.47 |
| 1:CS:191:LEU:CD2 | 1:CS:191:LEU:N | 2.77 | 0.47 |
| 1:AD:74:ASN:ND2 | 1:AD:77:THR:OG1 | 2.48 | 0.47 |
| 1:AF:189:PHE:HD2 | 1:AF:247:ILE:HD11 | 1.80 | 0.47 |
| 1:AG:162:PHE:CD2 | 1:AG:163:LEU:HD13 | 2.48 | 0.47 |
| 1:AH:18:ARG:HG2 | 1:AH:20:LEU:HD23 | 1.96 | 0.47 |
| 1:AI:272:TYR:N | 1:AI:272:TYR:CD1 | 2.83 | 0.47 |
| 1:AK:189:PHE:HE1 | 1:AK:198:ARG:CG | 2.21 | 0.47 |
| 1:AK:203:THR:HB | 1:AK:300:GLN:HG3 | 1.97 | 0.47 |
| 1:AM:239:ILE:HD12 | 1:AM:275:GLU:HA | 1.97 | 0.47 |
| 1:AN:25:ILE:HG23 | 1:AN:152:LEU:HD11 | 1.96 | 0.47 |
| 1:AN:440:ALA:HB3 | 1:AO:444:LEU:HD13 | 1.97 | 0.47 |
| 1:AO:272:TYR:N | 1:AO:272:TYR:CD1 | 2.81 | 0.47 |
| 1:AQ:162:PHE:CD2 | 1:AQ:163:LEU:HD13 | 2.50 | 0.47 |
| 1:BB:189:PHE:HD2 | 1:BB:247:ILE:HD11 | 1.79 | 0.47 |
| 1:BD:162:PHE:CD2 | 1:BD:163:LEU:HD13 | 2.50 | 0.47 |
| 1:BD:379:VAL:HG11 | 1:BD:381:MET:HE1 | 1.97 | 0.47 |
| 1:BD:404:LEU:HD22 | 1:BD:486:VAL:HG22 | 1.96 | 0.47 |
| 1:BF:55:ARG:CZ | 1:CH:272:TYR:CE2 | 2.97 | 0.47 |
| 1:BF:393:HIS:CG | 1:BF:496:PHE:HB3 | 2.50 | 0.47 |
| 1:BG:239:ILE:HG12 | 1:BG:326:ILE:CD1 | 2.45 | 0.47 |
| 1:BH:256:ASN:HD22 | 1:BH:302:ASP:HA | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:252:VAL:HG22 | 1:BI:253:SER:N | 2.30 | 0.47 |
| 1:BI:393:HIS:CG | 1:BI:496:PHE:HB3 | 2.50 | 0.47 |
| 1:BK:58:ALA:HB2 | 1:BK:102:GLY:HA3 | 1.95 | 0.47 |
| 1:BK:442:GLN:HE21 | 1:BL:412:PHE:HB2 | 1.80 | 0.47 |
| 1:BP:272:TYR:CD1 | 1:BP:272:TYR:N | 2.83 | 0.47 |
| 1:BQ:10:ILE:HG21 | 1:BQ:146:TRP:CZ2 | 2.50 | 0.47 |
| 1:BQ:189:PHE:HD2 | 1:BQ:247:ILE:HD11 | 1.79 | 0.47 |
| 1:BR:170:PHE:HD1 | 1:BR:389:MET:CE | 2.27 | 0.47 |
| 1:BT:379:VAL:HG11 | 1:BT:381:MET:HE1 | 1.96 | 0.47 |
| 1:CB:162:PHE:CD2 | 1:CB:163:LEU:HD13 | 2.50 | 0.47 |
| 1:CB:189:PHE:HD2 | 1:CB:247:ILE:CD1 | 2.27 | 0.47 |
| 1:CB:239:ILE:HD12 | 1:CB:275:GLU:HA | 1.97 | 0.47 |
| 1:CC:250:TRP:HE3 | 1:CC:272:TYR:CD1 | 2.33 | 0.47 |
| 1:CC:272:TYR:CD1 | 1:CC:272:TYR:N | 2.78 | 0.47 |
| 1:CD:239:ILE:HG12 | 1:CD:326:ILE:CD1 | 2.45 | 0.47 |
| 1:CE:250:TRP:HZ3 | 1:CE:272:TYR:CE1 | 2.29 | 0.47 |
| 1:CE:393:HIS:CG | 1:CE:496:PHE:HB3 | 2.49 | 0.47 |
| 1:CG:58:ALA:HB2 | 1:CG:102:GLY:HA3 | 1.97 | 0.47 |
| 1:CH:379:VAL:HG11 | 1:CH:381:MET:HE1 | 1.97 | 0.47 |
| 1:CI:61:PHE:CE2 | 1:CI:243:ILE:HD11 | 2.50 | 0.47 |
| 1:CJ:398:GLY:HA3 | 1:CJ:494:PHE:CD2 | 2.49 | 0.47 |
| 1:CL:170:PHE:HD1 | 1:CL:389:MET:CE | 2.28 | 0.47 |
| 1:CL:239:ILE:HG12 | 1:CL:326:ILE:CD1 | 2.45 | 0.47 |
| 1:CM:393:HIS:CG | 1:CM:496:PHE:HB3 | 2.50 | 0.47 |
| 1:CN:58:ALA:HB2 | 1:CN:102:GLY:HA3 | 1.96 | 0.47 |
| 1:CO:25:ILE:HG23 | 1:CO:152:LEU:HD11 | 1.97 | 0.47 |
| 1:CO:234:ARG:HG2 | 1:CO:280:GLU:HG2 | 1.97 | 0.47 |
| 1:CP:189:PHE:HE2 | 1:CP:249:LEU:HD21 | 1.80 | 0.47 |
| 1:CR:182:LEU:HG | 1:CR:330:ILE:HB | 1.97 | 0.47 |
| 1:CS:189:PHE:HD2 | 1:CS:247:ILE:HD11 | 1.80 | 0.47 |
| 1:AA:191:LEU:CD2 | 1:AA:191:LEU:N | 2.74 | 0.47 |
| 1:AB:226:VAL:HG13 | 1:AB:228:GLY:H | 1.80 | 0.47 |
| 1:AE:55:ARG:CZ | 1:CP:272:TYR:CD2 | 2.98 | 0.47 |
| 1:AG:61:PHE:CD2 | 1:AG:243:ILE:HD11 | 2.50 | 0.47 |
| 1:AG:226:VAL:HG13 | 1:AG:228:GLY:H | 1.80 | 0.47 |
| 1:AK:162:PHE:CD2 | 1:AK:163:LEU:HD13 | 2.49 | 0.47 |
| 1:AM:189:PHE:CE2 | 1:AM:249:LEU:HD21 | 2.45 | 0.47 |
| 1:AP:55:ARG:NE | 1:BM:272:TYR:HE2 | 2.10 | 0.47 |
| 1:AP:398:GLY:HA3 | 1:AP:494:PHE:CD2 | 2.49 | 0.47 |
| 1:AQ:189:PHE:CE2 | 1:AQ:249:LEU:HD21 | 2.49 | 0.47 |
| 1:BC:250:TRP:CE3 | 1:BC:272:TYR:CE1 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BC:393:HIS:CG | 1:BC:496:PHE:HB3 | 2.49 | 0.47 |
| 1:BD:226:VAL:HG13 | 1:BD:228:GLY:H | 1.80 | 0.47 |
| 1:BF:288:HIS:HD2 | 1:BF:337:ASP:OD2 | 1.97 | 0.47 |
| 1:BH:16:ALA:O | 1:BH:17:ASN:HB2 | 2.15 | 0.47 |
| 1:BH:379:VAL:HG11 | 1:BH:381:MET:HE1 | 1.97 | 0.47 |
| 1:BO:454:ASN:HD21 | 1:BO:456:ALA:HB3 | 1.80 | 0.47 |
| 1:CA:454:ASN:HD21 | 1:CA:456:ALA:HB3 | 1.79 | 0.47 |
| 1:CB:203:THR:HB | 1:CB:300:GLN:HG3 | 1.97 | 0.47 |
| 1:CD:442:GLN:HE21 | 1:CE:412:PHE:HB2 | 1.79 | 0.47 |
| 1:CE:232:THR:HB | 1:CE:334:VAL:CG2 | 2.45 | 0.47 |
| 1:CF:189:PHE:CE2 | 1:CF:249:LEU:HD21 | 2.46 | 0.47 |
| 1:CF:237:VAL:HG23 | 1:CF:279:PHE:CD2 | 2.50 | 0.47 |
| 1:CH:454:ASN:HD21 | 1:CH:456:ALA:HB3 | 1.79 | 0.47 |
| 1:CK:263:ASN:O | 1:CK:267:LYS:HG3 | 2.15 | 0.47 |
| 1:CM:232:THR:HB | 1:CM:334:VAL:CG2 | 2.45 | 0.47 |
| 1:CN:75:ARG:NH2 | 1:CN:391:ALA:O | 2.47 | 0.47 |
| 1:CN:239:ILE:HD12 | 1:CN:275:GLU:HA | 1.97 | 0.47 |
| 1:CO:379:VAL:HG11 | 1:CO:381:MET:HE1 | 1.95 | 0.47 |
| 1:CP:232:THR:HB | 1:CP:334:VAL:CG2 | 2.45 | 0.47 |
| 1:CQ:189:PHE:CE2 | 1:CQ:249:LEU:HD21 | 2.50 | 0.47 |
| 1:AD:237:VAL:HG23 | 1:AD:279:PHE:CD2 | 2.50 | 0.47 |
| 1:AE:55:ARG:CZ | 1:CP:272:TYR:CE2 | 2.97 | 0.47 |
| 1:AF:189:PHE:CE2 | 1:AF:249:LEU:HD21 | 2.42 | 0.47 |
| 1:AF:454:ASN:HD21 | 1:AF:456:ALA:HB3 | 1.80 | 0.47 |
| 1:AG:189:PHE:CE1 | 1:AG:198:ARG:HG2 | 2.50 | 0.47 |
| 1:AH:191:LEU:CD2 | 1:AH:191:LEU:N | 2.77 | 0.47 |
| 1:AJ:189:PHE:HE1 | 1:AJ:198:ARG:HG2 | 1.74 | 0.47 |
| 1:AM:239:ILE:HG12 | 1:AM:326:ILE:CD1 | 2.44 | 0.47 |
| 1:AN:18:ARG:HG3 | 1:AN:19:TYR:N | 2.30 | 0.47 |
| 1:AN:454:ASN:HD21 | 1:AN:456:ALA:HB3 | 1.80 | 0.47 |
| 1:AP:203:THR:HB | 1:AP:300:GLN:HG3 | 1.97 | 0.47 |
| 1:AQ:30:SER:O | 1:AQ:33:LYS:HB2 | 2.15 | 0.47 |
| 1:AS:170:PHE:HD1 | 1:AS:389:MET:HE2 | 1.79 | 0.47 |
| 1:BA:272:TYR:N | 1:BA:272:TYR:HD1 | 2.12 | 0.47 |
| 1:BG:43:ALA:HB1 | 1:BG:158:GLU:HA | 1.97 | 0.47 |
| 1:BG:162:PHE:CD2 | 1:BG:163:LEU:HD13 | 2.50 | 0.47 |
| 1:BH:162:PHE:CD2 | 1:BH:163:LEU:HD13 | 2.50 | 0.47 |
| 1:BL:393:HIS:CG | 1:BL:496:PHE:HB3 | 2.50 | 0.47 |
| 1:BM:189:PHE:HD2 | 1:BM:247:ILE:CD1 | 2.28 | 0.47 |
| 1:BS:67:VAL:HG23 | 1:BS:135:LEU:HB2 | 1.95 | 0.47 |
| 1:CE:75:ARG:NH2 | 1:CE:391:ALA:O | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CH:189:PHE:CE1 | 1:CH:198:ARG:HG2 | 2.49 | 0.47 |
| 1:CJ:393:HIS:CG | 1:CJ:496:PHE:HB3 | 2.50 | 0.47 |
| 1:CL:226:VAL:HG13 | 1:CL:228:GLY:H | 1.79 | 0.47 |
| 1:CP:170:PHE:HD1 | 1:CP:389:MET:HE2 | 1.80 | 0.47 |
| 1:CP:191:LEU:HD23 | 1:CP:191:LEU:N | 2.17 | 0.47 |
| 1:CS:379:VAL:HG11 | 1:CS:381:MET:HE1 | 1.96 | 0.47 |
| 1:AB:55:ARG:CZ | 1:BB:272:TYR:CD2 | 2.97 | 0.47 |
| 1:AE:75:ARG:NH2 | 1:AE:391:ALA:O | 2.47 | 0.47 |
| 1:AF:79:ARG:CG | 1:AF:79:ARG:NH1 | 2.72 | 0.47 |
| 1:AF:191:LEU:CD2 | 1:AF:191:LEU:N | 2.78 | 0.47 |
| 1:AI:234:ARG:HG2 | 1:AI:280:GLU:HG2 | 1.97 | 0.47 |
| 1:AJ:232:THR:HB | 1:AJ:334:VAL:HG23 | 1.97 | 0.47 |
| 1:AJ:454:ASN:ND2 | 1:AJ:456:ALA:H | 2.09 | 0.47 |
| 1:AN:189:PHE:HD2 | 1:AN:247:ILE:HD11 | 1.80 | 0.47 |
| 1:AP:79:ARG:HH11 | 1:AP:79:ARG:CG | 2.27 | 0.47 |
| 1:AS:393:HIS:CG | 1:AS:496:PHE:HB3 | 2.50 | 0.47 |
| 1:BB:25:ILE:HG23 | 1:BB:152:LEU:HD11 | 1.97 | 0.47 |
| 1:BD:16:ALA:O | 1:BD:17:ASN:HB2 | 2.14 | 0.47 |
| 1:BE:30:SER:O | 1:BE:33:LYS:HB2 | 2.15 | 0.47 |
| 1:BF:58:ALA:HB2 | 1:BF:102:GLY:HA3 | 1.97 | 0.47 |
| 1:BK:379:VAL:HG11 | 1:BK:381:MET:HE1 | 1.97 | 0.47 |
| 1:BL:237:VAL:HG23 | 1:BL:279:PHE:CD2 | 2.50 | 0.47 |
| 1:BM:189:PHE:HD2 | 1:BM:247:ILE:HD11 | 1.80 | 0.47 |
| 1:BP:73:TYR:CZ | 1:BP:394:GLY:HA3 | 2.51 | 0.47 |
| 1:BQ:239:ILE:HD12 | 1:BQ:275:GLU:HA | 1.97 | 0.47 |
| 1:CB:252:VAL:HG22 | 1:CB:253:SER:N | 2.30 | 0.47 |
| 1:CE:79:ARG:HH11 | 1:CE:79:ARG:CG | 2.28 | 0.47 |
| 1:CG:22:THR:OG1 | 1:CG:131:HIS:CD2 | 2.61 | 0.47 |
| 1:CI:162:PHE:CD2 | 1:CI:163:LEU:HD13 | 2.49 | 0.47 |
| 1:CJ:454:ASN:HD21 | 1:CJ:456:ALA:HB3 | 1.80 | 0.47 |
| 1:CK:30:SER:O | 1:CK:33:LYS:HB2 | 2.15 | 0.47 |
| 1:CM:162:PHE:CD2 | 1:CM:163:LEU:HD13 | 2.50 | 0.47 |
| 1:CN:189:PHE:CE2 | 1:CN:249:LEU:HD21 | 2.45 | 0.47 |
| 1:AB:239:ILE:HD12 | 1:AB:275:GLU:HA | 1.96 | 0.46 |
| 1:AQ:454:ASN:ND2 | 1:AQ:456:ALA:H | 2.10 | 0.46 |
| 1:AT:263:ASN:O | 1:AT:267:LYS:HG3 | 2.15 | 0.46 |
| 1:BA:393:HIS:CG | 1:BA:496:PHE:HB3 | 2.50 | 0.46 |
| 1:BC:188:PHE:C | 1:BC:189:PHE:HD1 | 2.17 | 0.46 |
| 1:BD:189:PHE:CE2 | 1:BD:249:LEU:HD21 | 2.50 | 0.46 |
| 1:BF:171:ASP:HA | 1:BF:172:PRO:HD3 | 1.79 | 0.46 |
| 1:BG:25:ILE:HG23 | 1:BG:152:LEU:HD11 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:232:THR:HB | 1:BG:334:VAL:CG2 | 2.45 | 0.46 |
| 1:BL:232:THR:HB | 1:BL:334:VAL:HG23 | 1.97 | 0.46 |
| 1:CA:234:ARG:HG2 | 1:CA:280:GLU:HG2 | 1.97 | 0.46 |
| 1:CA:398:GLY:HA3 | 1:CA:494:PHE:CD2 | 2.49 | 0.46 |
| 1:CC:442:GLN:HE21 | 1:CD:412:PHE:HB2 | 1.80 | 0.46 |
| 1:CE:189:PHE:HD2 | 1:CE:247:ILE:CD1 | 2.27 | 0.46 |
| 1:CG:263:ASN:O | 1:CG:267:LYS:HG3 | 2.15 | 0.46 |
| 1:CG:272:TYR:N | 1:CG:272:TYR:HD1 | 2.13 | 0.46 |
| 1:CI:55:ARG:HD3 | 1:CR:272:TYR:CD2 | 2.50 | 0.46 |
| 1:CL:162:PHE:CD2 | 1:CL:163:LEU:HD13 | 2.51 | 0.46 |
| 1:CN:171:ASP:HA | 1:CN:172:PRO:HD3 | 1.78 | 0.46 |
| 1:CO:272:TYR:N | 1:CO:272:TYR:HD1 | 2.13 | 0.46 |
| 1:AD:226:VAL:HG13 | 1:AD:228:GLY:H | 1.80 | 0.46 |
| 1:AH:272:TYR:HD2 | 1:CF:55:ARG:HD3 | 1.80 | 0.46 |
| 1:AK:272:TYR:N | 1:AK:272:TYR:HD1 | 2.13 | 0.46 |
| 1:AL:189:PHE:CE2 | 1:AL:249:LEU:HD21 | 2.50 | 0.46 |
| 1:AN:55:ARG:HD3 | 1:AS:272:TYR:HD2 | 1.77 | 0.46 |
| 1:AO:239:ILE:HD12 | 1:AO:275:GLU:HA | 1.97 | 0.46 |
| 1:BF:404:LEU:HD22 | 1:BF:486:VAL:HG22 | 1.97 | 0.46 |
| 1:BH:30:SER:O | 1:BH:33:LYS:HB2 | 2.14 | 0.46 |
| 1:BJ:189:PHE:CE2 | 1:BJ:249:LEU:HD21 | 2.47 | 0.46 |
| 1:BM:454:ASN:HD21 | 1:BM:456:ALA:HB3 | 1.80 | 0.46 |
| 1:BO:404:LEU:HD22 | 1:BO:486:VAL:HG22 | 1.96 | 0.46 |
| 1:BQ:232:THR:HB | 1:BQ:334:VAL:HG23 | 1.96 | 0.46 |
| 1:BR:226:VAL:HG13 | 1:BR:228:GLY:H | 1.80 | 0.46 |
| 1:CB:404:LEU:HD22 | 1:CB:486:VAL:HG22 | 1.96 | 0.46 |
| 1:CE:234:ARG:HG2 | 1:CE:280:GLU:HG2 | 1.97 | 0.46 |
| 1:CM:379:VAL:HG11 | 1:CM:381:MET:HE1 | 1.97 | 0.46 |
| 1:CN:232:THR:HB | 1:CN:334:VAL:CG2 | 2.46 | 0.46 |
| 1:CR:284:ARG:CG | 1:CR:284:ARG:NH1 | 2.76 | 0.46 |
| 1:CT:189:PHE:CE2 | 1:CT:249:LEU:HD21 | 2.50 | 0.46 |
| 1:AA:393:HIS:CG | 1:AA:496:PHE:HB3 | 2.51 | 0.46 |
| 1:AB:263:ASN:O | 1:AB:267:LYS:HG3 | 2.16 | 0.46 |
| 1:AD:189:PHE:HD2 | 1:AD:247:ILE:HD11 | 1.79 | 0.46 |
| 1:AE:162:PHE:CD2 | 1:AE:163:LEU:HD13 | 2.49 | 0.46 |
| 1:AE:203:THR:CB | 1:AE:300:GLN:HG3 | 2.43 | 0.46 |
| 1:AG:30:SER:O | 1:AG:33:LYS:HB2 | 2.14 | 0.46 |
| 1:AH:170:PHE:HD1 | 1:AH:389:MET:CE | 2.27 | 0.46 |
| 1:AH:379:VAL:HG11 | 1:AH:381:MET:HE1 | 1.97 | 0.46 |
| 1:AH:454:ASN:ND2 | 1:AH:456:ALA:H | 2.08 | 0.46 |
| 1:AI:55:ARG:HD3 | 1:AR:272:TYR:CD2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:234:ARG:HG2 | 1:AK:280:GLU:HG2 | 1.98 | 0.46 |
| 1:AM:232:THR:HB | 1:AM:334:VAL:CG2 | 2.45 | 0.46 |
| 1:AN:239:ILE:HD12 | 1:AN:275:GLU:HA | 1.97 | 0.46 |
| 1:AO:454:ASN:HD21 | 1:AO:456:ALA:HB3 | 1.80 | 0.46 |
| 1:AP:263:ASN:O | 1:AP:267:LYS:HG3 | 2.15 | 0.46 |
| 1:AR:423:LYS:HE2 | 1:AR:449:GLU:O | 2.15 | 0.46 |
| 1:AT:454:ASN:HD21 | 1:AT:456:ALA:HB3 | 1.80 | 0.46 |
| 1:BE:170:PHE:HD1 | 1:BE:389:MET:CE | 2.28 | 0.46 |
| 1:BE:454:ASN:HD21 | 1:BE:456:ALA:HB3 | 1.79 | 0.46 |
| 1:BH:170:PHE:HD1 | 1:BH:389:MET:HE2 | 1.80 | 0.46 |
| 1:BN:30:SER:O | 1:BN:33:LYS:HB2 | 2.15 | 0.46 |
| 1:BQ:272:TYR:HD2 | 1:CL:55:ARG:HD3 | 1.81 | 0.46 |
| 1:BR:232:THR:HB | 1:BR:334:VAL:CG2 | 2.45 | 0.46 |
| 1:BR:454:ASN:HD21 | 1:BR:456:ALA:HB3 | 1.80 | 0.46 |
| 1:BT:239:ILE:HD12 | 1:BT:275:GLU:HA | 1.96 | 0.46 |
| 1:CA:189:PHE:HD2 | 1:CA:247:ILE:HD11 | 1.80 | 0.46 |
| 1:CJ:263:ASN:O | 1:CJ:267:LYS:HG3 | 2.16 | 0.46 |
| 1:CL:14:CYS:H | 1:CL:138:ASN:ND2 | 2.12 | 0.46 |
| 1:CM:226:VAL:HG13 | 1:CM:228:GLY:H | 1.80 | 0.46 |
| 1:CT:30:SER:O | 1:CT:33:LYS:HB2 | 2.16 | 0.46 |
| 1:AA:162:PHE:CD2 | 1:AA:163:LEU:HD13 | 2.51 | 0.46 |
| 1:AB:232:THR:HB | 1:AB:334:VAL:HG23 | 1.98 | 0.46 |
| 1:AB:454:ASN:ND2 | 1:AB:456:ALA:H | 2.10 | 0.46 |
| 1:AG:55:ARG:HD3 | 1:CG:272:TYR:CD2 | 2.50 | 0.46 |
| 1:AJ:237:VAL:HG23 | 1:AJ:279:PHE:CD2 | 2.50 | 0.46 |
| 1:AK:239:ILE:HG12 | 1:AK:326:ILE:CD1 | 2.46 | 0.46 |
| 1:AK:263:ASN:O | 1:AK:267:LYS:HG3 | 2.15 | 0.46 |
| 1:AO:239:ILE:HG23 | 1:AO:324:LEU:HD21 | 1.96 | 0.46 |
| 1:AR:191:LEU:CD2 | 1:AR:191:LEU:N | 2.73 | 0.46 |
| 1:AS:226:VAL:HG13 | 1:AS:228:GLY:H | 1.80 | 0.46 |
| 1:BB:423:LYS:HE2 | 1:BB:449:GLU:O | 2.16 | 0.46 |
| 1:BC:30:SER:O | 1:BC:33:LYS:HB2 | 2.15 | 0.46 |
| 1:BD:189:PHE:HE1 | 1:BD:198:ARG:CG | 2.27 | 0.46 |
| 1:BH:239:ILE:HD12 | 1:BH:275:GLU:HA | 1.96 | 0.46 |
| 1:BI:74:ASN:ND2 | 1:BI:77:THR:OG1 | 2.48 | 0.46 |
| 1:BO:170:PHE:HD1 | 1:BO:389:MET:CE | 2.28 | 0.46 |
| 1:BS:232:THR:HB | 1:BS:334:VAL:CG2 | 2.46 | 0.46 |
| 1:BS:393:HIS:CG | 1:BS:496:PHE:HB3 | 2.50 | 0.46 |
| 1:CD:20:LEU:HB2 | 1:CD:132:PHE:O | 2.16 | 0.46 |
| 1:CF:234:ARG:HG2 | 1:CF:280:GLU:HG2 | 1.98 | 0.46 |
| 1:CI:10:ILE:HG21 | 1:CI:146:TRP:CZ2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CM:263:ASN:O | 1:CM:267:LYS:HG3 | 2.15 | 0.46 |
| 1:CS:58:ALA:HB2 | 1:CS:102:GLY:HA3 | 1.97 | 0.46 |
| 1:CS:454:ASN:HD21 | 1:CS:456:ALA:HB3 | 1.81 | 0.46 |
| 1:CT:454:ASN:ND2 | 1:CT:456:ALA:H | 2.06 | 0.46 |
| 1:AA:189:PHE:CE2 | 1:AA:249:LEU:HD21 | 2.51 | 0.46 |
| 1:AA:239:ILE:HD12 | 1:AA:275:GLU:HA | 1.96 | 0.46 |
| 1:AB:55:ARG:CZ | 1:BB:272:TYR:CE2 | 2.99 | 0.46 |
| 1:AB:171:ASP:HA | 1:AB:172:PRO:HD3 | 1.79 | 0.46 |
| 1:AD:162:PHE:CD2 | 1:AD:163:LEU:HD13 | 2.50 | 0.46 |
| 1:AG:393:HIS:CG | 1:AG:496:PHE:HB3 | 2.51 | 0.46 |
| 1:AL:239:ILE:HD12 | 1:AL:275:GLU:HA | 1.98 | 0.46 |
| 1:AL:442:GLN:HE21 | 1:AM:412:PHE:HB2 | 1.80 | 0.46 |
| 1:AN:393:HIS:CG | 1:AN:496:PHE:HB3 | 2.50 | 0.46 |
| 1:AO:250:TRP:CE3 | 1:AO:272:TYR:CD1 | 3.04 | 0.46 |
| 1:AP:25:ILE:HG23 | 1:AP:152:LEU:HD11 | 1.97 | 0.46 |
| 1:AR:234:ARG:HG2 | 1:AR:280:GLU:HG2 | 1.98 | 0.46 |
| 1:AS:191:LEU:CD2 | 1:AS:191:LEU:N | 2.79 | 0.46 |
| 1:AS:237:VAL:HG23 | 1:AS:279:PHE:CD2 | 2.50 | 0.46 |
| 1:AT:234:ARG:HG2 | 1:AT:280:GLU:HG2 | 1.97 | 0.46 |
| 1:BD:14:CYS:H | 1:BD:138:ASN:ND2 | 2.14 | 0.46 |
| 1:BE:75:ARG:NH2 | 1:BE:391:ALA:O | 2.49 | 0.46 |
| 1:BL:67:VAL:HG23 | 1:BL:135:LEU:HB2 | 1.98 | 0.46 |
| 1:BM:272:TYR:N | 1:BM:272:TYR:HD1 | 2.14 | 0.46 |
| 1:BN:58:ALA:HB2 | 1:BN:102:GLY:HA3 | 1.96 | 0.46 |
| 1:BR:191:LEU:CD2 | 1:BR:191:LEU:N | 2.77 | 0.46 |
| 1:BT:393:HIS:CG | 1:BT:496:PHE:HB3 | 2.51 | 0.46 |
| 1:CC:300:GLN:HE21 | 1:CC:300:GLN:HB2 | 1.59 | 0.46 |
| 1:CI:272:TYR:N | 1:CI:272:TYR:HD1 | 2.14 | 0.46 |
| 1:CO:189:PHE:HE2 | 1:CO:249:LEU:HD21 | 1.78 | 0.46 |
| 1:CP:58:ALA:HB2 | 1:CP:102:GLY:HA3 | 1.98 | 0.46 |
| 1:CQ:191:LEU:HD23 | 1:CQ:191:LEU:N | 2.17 | 0.46 |
| 1:CT:14:CYS:HB3 | 1:CT:64:LEU:HD21 | 1.97 | 0.46 |
| 1:AC:43:ALA:HB1 | 1:AC:158:GLU:HA | 1.98 | 0.46 |
| 1:AC:73:TYR:O | 1:AC:75:ARG:HG2 | 2.16 | 0.46 |
| 1:AE:239:ILE:HG12 | 1:AE:326:ILE:CD1 | 2.45 | 0.46 |
| 1:AI:18:ARG:HG3 | 1:AI:19:TYR:O | 2.16 | 0.46 |
| 1:AM:189:PHE:CE1 | 1:AM:198:ARG:HG2 | 2.50 | 0.46 |
| 1:AO:393:HIS:CG | 1:AO:496:PHE:HB3 | 2.51 | 0.46 |
| 1:AS:189:PHE:HE2 | 1:AS:249:LEU:HD21 | 1.80 | 0.46 |
| 1:BC:263:ASN:O | 1:BC:267:LYS:HG3 | 2.16 | 0.46 |
| 1:BH:15:GLN:HE21 | 1:BH:15:GLN:CA | 2.09 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BK:30:SER:O | 1:BK:33:LYS:HB2 | 2.15 | 0.46 |
| 1:BK:232:THR:HB | 1:BK:334:VAL:HG23 | 1.97 | 0.46 |
| 1:BL:9:TYR:CE2 | 1:BL:145:ASP:HB3 | 2.50 | 0.46 |
| 1:BL:30:SER:O | 1:BL:33:LYS:HB2 | 2.16 | 0.46 |
| 1:BL:454:ASN:HD21 | 1:BL:456:ALA:HB3 | 1.80 | 0.46 |
| 1:BP:287:TYR:HA | 1:BT:162:PHE:CD1 | 2.50 | 0.46 |
| 1:CA:226:VAL:HG13 | 1:CA:228:GLY:H | 1.79 | 0.46 |
| 1:CD:30:SER:O | 1:CD:33:LYS:HB2 | 2.15 | 0.46 |
| 1:CE:14:CYS:H | 1:CE:138:ASN:ND2 | 2.11 | 0.46 |
| 1:CE:197:LEU:HD13 | 1:CE:309:TYR:CZ | 2.51 | 0.46 |
| 1:CK:272:TYR:CD1 | 1:CK:272:TYR:N | 2.84 | 0.46 |
| 1:CL:272:TYR:N | 1:CL:272:TYR:CD1 | 2.84 | 0.46 |
| 1:CO:170:PHE:HD1 | 1:CO:389:MET:CE | 2.29 | 0.46 |
| 1:CP:393:HIS:CG | 1:CP:496:PHE:HB3 | 2.51 | 0.46 |
| 1:CQ:30:SER:O | 1:CQ:33:LYS:HB2 | 2.16 | 0.46 |
| 1:CR:207:VAL:HA | 1:CR:208:PRO:HD3 | 1.84 | 0.46 |
| 1:AE:189:PHE:HD2 | 1:AE:247:ILE:CD1 | 2.28 | 0.46 |
| 1:AH:182:LEU:HG | 1:AH:330:ILE:HB | 1.98 | 0.46 |
| 1:AI:189:PHE:HD2 | 1:AI:247:ILE:CD1 | 2.28 | 0.46 |
| 1:AR:237:VAL:HG23 | 1:AR:279:PHE:CD2 | 2.51 | 0.46 |
| 1:AS:30:SER:O | 1:AS:33:LYS:HB2 | 2.16 | 0.46 |
| 1:AS:170:PHE:HD1 | 1:AS:389:MET:CE | 2.28 | 0.46 |
| 1:AT:239:ILE:HD12 | 1:AT:275:GLU:HA | 1.98 | 0.46 |
| 1:BA:79:ARG:CG | 1:BA:79:ARG:NH1 | 2.71 | 0.46 |
| 1:BE:300:GLN:HE21 | 1:BE:300:GLN:HB2 | 1.48 | 0.46 |
| 1:BH:234:ARG:HG2 | 1:BH:280:GLU:HG2 | 1.97 | 0.46 |
| 1:BI:189:PHE:HD2 | 1:BI:247:ILE:CD1 | 2.29 | 0.46 |
| 1:BM:234:ARG:HG2 | 1:BM:280:GLU:HG2 | 1.97 | 0.46 |
| 1:BM:379:VAL:HG11 | 1:BM:381:MET:HE1 | 1.97 | 0.46 |
| 1:BN:440:ALA:CB | 1:BO:444:LEU:HD13 | 2.45 | 0.46 |
| 1:BO:11:PRO:HG2 | 1:BO:18:ARG:CD | 2.46 | 0.46 |
| 1:BO:191:LEU:CD2 | 1:BO:191:LEU:N | 2.73 | 0.46 |
| 1:BO:234:ARG:HG2 | 1:BO:280:GLU:HG2 | 1.97 | 0.46 |
| 1:BP:189:PHE:HD2 | 1:BP:247:ILE:HD11 | 1.80 | 0.46 |
| 1:BP:454:ASN:HD21 | 1:BP:456:ALA:HB3 | 1.81 | 0.46 |
| 1:BS:440:ALA:HB3 | 1:BT:444:LEU:HD13 | 1.98 | 0.46 |
| 1:BT:237:VAL:HG23 | 1:BT:279:PHE:CD2 | 2.51 | 0.46 |
| 1:CD:272:TYR:CD2 | 1:CS:55:ARG:CZ | 2.98 | 0.46 |
| 1:CE:61:PHE:CD2 | 1:CE:243:ILE:HD11 | 2.50 | 0.46 |
| 1:CG:454:ASN:HD21 | 1:CG:456:ALA:HB3 | 1.81 | 0.46 |
| 1:CI:67:VAL:HG23 | 1:CI:135:LEU:HB2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CL:189:PHE:HE2 | 1:CL:249:LEU:HD21 | 1.81 | 0.46 |
| 1:CN:189:PHE:CE1 | 1:CN:198:ARG:HG2 | 2.51 | 0.46 |
| 1:CO:79:ARG:CG | 1:CO:79:ARG:NH1 | 2.79 | 0.46 |
| 1:CP:43:ALA:HB1 | 1:CP:158:GLU:HA | 1.97 | 0.46 |
| 1:CR:263:ASN:O | 1:CR:267:LYS:HG3 | 2.16 | 0.46 |
| 1:AC:237:VAL:HG23 | 1:AC:279:PHE:CD2 | 2.50 | 0.46 |
| 1:AH:393:HIS:CG | 1:AH:496:PHE:HB3 | 2.50 | 0.46 |
| 1:AI:189:PHE:CE1 | 1:AI:198:ARG:HG2 | 2.51 | 0.46 |
| 1:AI:454:ASN:HD21 | 1:AI:456:ALA:HB3 | 1.80 | 0.46 |
| 1:AJ:234:ARG:HG2 | 1:AJ:280:GLU:HG2 | 1.98 | 0.46 |
| 1:AM:14:CYS:H | 1:AM:138:ASN:HD21 | 1.64 | 0.46 |
| 1:AN:237:VAL:HG23 | 1:AN:279:PHE:CD2 | 2.51 | 0.46 |
| 1:AQ:74:ASN:ND2 | 1:AQ:77:THR:OG1 | 2.49 | 0.46 |
| 1:AT:189:PHE:HE2 | 1:AT:249:LEU:HD21 | 1.79 | 0.46 |
| 1:BA:22:THR:OG1 | 1:BA:131:HIS:CD2 | 2.61 | 0.46 |
| 1:BC:18:ARG:HG3 | 1:BC:19:TYR:N | 2.31 | 0.46 |
| 1:BN:182:LEU:HG | 1:BN:330:ILE:HB | 1.97 | 0.46 |
| 1:BO:189:PHE:HE2 | 1:BO:249:LEU:HD21 | 1.79 | 0.46 |
| 1:BO:252:VAL:HG22 | 1:BO:253:SER:N | 2.31 | 0.46 |
| 1:BP:272:TYR:CD2 | 1:CE:55:ARG:HD3 | 2.51 | 0.46 |
| 1:BT:18:ARG:HG3 | 1:BT:19:TYR:N | 2.31 | 0.46 |
| 1:BT:43:ALA:HB1 | 1:BT:158:GLU:HA | 1.97 | 0.46 |
| 1:CI:454:ASN:HD21 | 1:CI:456:ALA:HB3 | 1.81 | 0.46 |
| 1:CK:226:VAL:HG13 | 1:CK:228:GLY:H | 1.81 | 0.46 |
| 1:CL:404:LEU:N | 1:CL:404:LEU:HD23 | 2.31 | 0.46 |
| 1:CP:14:CYS:H | 1:CP:138:ASN:HD21 | 1.62 | 0.46 |
| 1:CP:440:ALA:CB | 1:CQ:444:LEU:HD13 | 2.46 | 0.46 |
| 1:CQ:58:ALA:HB2 | 1:CQ:102:GLY:HA3 | 1.98 | 0.46 |
| 1:CQ:393:HIS:CG | 1:CQ:496:PHE:HB3 | 2.51 | 0.46 |
| 1:CR:189:PHE:CE2 | 1:CR:249:LEU:HD21 | 2.45 | 0.46 |
| 1:CS:324:LEU:HD23 | 1:CS:324:LEU:C | 2.36 | 0.46 |
| 1:AA:55:ARG:NH1 | 1:CC:272:TYR:CD2 | 2.84 | 0.46 |
| 1:AF:232:THR:HB | 1:AF:334:VAL:CG2 | 2.46 | 0.46 |
| 1:AF:272:TYR:N | 1:AF:272:TYR:CD1 | 2.84 | 0.46 |
| 1:AF:442:GLN:HE21 | 1:AG:412:PHE:HB2 | 1.80 | 0.46 |
| 1:AI:18:ARG:NH1 | 1:AI:18:ARG:HB2 | 2.31 | 0.46 |
| 1:AJ:58:ALA:HB2 | 1:AJ:102:GLY:HA3 | 1.97 | 0.46 |
| 1:AL:393:HIS:CG | 1:AL:496:PHE:HB3 | 2.50 | 0.46 |
| 1:AN:272:TYR:N | 1:AN:272:TYR:CD1 | 2.83 | 0.46 |
| 1:AP:379:VAL:HG11 | 1:AP:381:MET:HE1 | 1.98 | 0.46 |
| 1:AS:263:ASN:O | 1:AS:267:LYS:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BA:162:PHE:CD2 | 1:BA:163:LEU:HD13 | 2.50 | 0.46 |
| 1:BA:237:VAL:HG23 | 1:BA:279:PHE:CD2 | 2.51 | 0.46 |
| 1:BA:442:GLN:HE21 | 1:BB:412:PHE:HB2 | 1.79 | 0.46 |
| 1:BE:272:TYR:N | 1:BE:272:TYR:CD1 | 2.84 | 0.46 |
| 1:BG:18:ARG:HG2 | 1:BG:20:LEU:HD23 | 1.98 | 0.46 |
| 1:BG:393:HIS:CG | 1:BG:496:PHE:HB3 | 2.51 | 0.46 |
| 1:BH:272:TYR:N | 1:BH:272:TYR:CD1 | 2.83 | 0.46 |
| 1:BJ:232:THR:HB | 1:BJ:334:VAL:HG23 | 1.98 | 0.46 |
| 1:BJ:272:TYR:CE2 | 1:BQ:55:ARG:HD3 | 2.51 | 0.46 |
| 1:BL:25:ILE:HG23 | 1:BL:152:LEU:HD11 | 1.98 | 0.46 |
| 1:CA:232:THR:HB | 1:CA:334:VAL:CG2 | 2.46 | 0.46 |
| 1:CB:58:ALA:HB2 | 1:CB:102:GLY:HA3 | 1.96 | 0.46 |
| 1:CD:14:CYS:H | 1:CD:138:ASN:ND2 | 2.13 | 0.46 |
| 1:CF:232:THR:HB | 1:CF:334:VAL:HG23 | 1.97 | 0.46 |
| 1:CH:189:PHE:CE2 | 1:CH:249:LEU:HD21 | 2.45 | 0.46 |
| 1:CK:379:VAL:HG11 | 1:CK:381:MET:HE1 | 1.98 | 0.46 |
| 1:CL:234:ARG:HG2 | 1:CL:280:GLU:HG2 | 1.97 | 0.46 |
| 1:CP:239:ILE:HD12 | 1:CP:275:GLU:HA | 1.98 | 0.46 |
| 1:CQ:25:ILE:HG23 | 1:CQ:152:LEU:HD11 | 1.98 | 0.46 |
| 1:CT:18:ARG:HG3 | 1:CT:19:TYR:N | 2.30 | 0.46 |
| 1:CT:171:ASP:HA | 1:CT:172:PRO:HD3 | 1.79 | 0.46 |
| 1:CT:272:TYR:N | 1:CT:272:TYR:HD1 | 2.14 | 0.46 |
| 1:AC:189:PHE:HE2 | 1:AC:249:LEU:CD2 | 2.28 | 0.46 |
| 1:AE:272:TYR:CD1 | 1:AE:272:TYR:N | 2.84 | 0.46 |
| 1:AE:454:ASN:HD21 | 1:AE:456:ALA:HB3 | 1.80 | 0.46 |
| 1:AK:442:GLN:HE21 | 1:AL:412:PHE:HB2 | 1.81 | 0.46 |
| 1:AL:440:ALA:HB3 | 1:AM:444:LEU:HD13 | 1.98 | 0.46 |
| 1:AN:162:PHE:CD2 | 1:AN:163:LEU:HD13 | 2.51 | 0.46 |
| 1:AN:272:TYR:N | 1:AN:272:TYR:HD1 | 2.14 | 0.46 |
| 1:BA:371:ASP:OD1 | 1:BA:381:MET:HG2 | 2.16 | 0.46 |
| 1:BB:79:ARG:HH11 | 1:BB:79:ARG:CG | 2.26 | 0.46 |
| 1:BB:414:LYS:HA | 1:BC:411:GLU:HB3 | 1.97 | 0.46 |
| 1:BC:189:PHE:HD2 | 1:BC:247:ILE:HD11 | 1.80 | 0.46 |
| 1:BH:55:ARG:HD3 | 1:BK:272:TYR:HD2 | 1.78 | 0.46 |
| 1:BI:16:ALA:O | 1:BI:17:ASN:HB2 | 2.16 | 0.46 |
| 1:BL:191:LEU:CD2 | 1:BL:191:LEU:N | 2.76 | 0.46 |
| 1:BS:16:ALA:O | 1:BS:17:ASN:HB2 | 2.16 | 0.46 |
| 1:CE:318:SER:HA | 1:CE:319:GLY:HA2 | 1.79 | 0.46 |
| 1:CF:263:ASN:O | 1:CF:267:LYS:HG3 | 2.16 | 0.46 |
| 1:CH:30:SER:O | 1:CH:33:LYS:HB2 | 2.16 | 0.46 |
| 1:CI:171:ASP:HA | 1:CI:172:PRO:HD3 | 1.78 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CK:79:ARG:HH11 | 1:CK:79:ARG:HG3 | 1.80 | 0.46 |
| 1:CR:162:PHE:CD2 | 1:CR:163:LEU:HD13 | 2.51 | 0.46 |
| 1:CR:393:HIS:CG | 1:CR:496:PHE:HB3 | 2.51 | 0.46 |
| 1:AB:61:PHE:CE2 | 1:AB:243:ILE:HD11 | 2.50 | 0.45 |
| 1:AE:30:SER:O | 1:AE:33:LYS:HB2 | 2.16 | 0.45 |
| 1:AE:170:PHE:HD1 | 1:AE:389:MET:CE | 2.29 | 0.45 |
| 1:AE:189:PHE:HD2 | 1:AE:247:ILE:HD11 | 1.80 | 0.45 |
| 1:AE:232:THR:HB | 1:AE:334:VAL:HG23 | 1.99 | 0.45 |
| 1:AJ:43:ALA:HB1 | 1:AJ:158:GLU:HA | 1.98 | 0.45 |
| 1:AL:263:ASN:O | 1:AL:267:LYS:HG3 | 2.17 | 0.45 |
| 1:AM:30:SER:O | 1:AM:33:LYS:HB2 | 2.16 | 0.45 |
| 1:AR:170:PHE:HD1 | 1:AR:389:MET:CE | 2.29 | 0.45 |
| 1:AS:207:VAL:HA | 1:AS:208:PRO:HD3 | 1.83 | 0.45 |
| 1:BB:237:VAL:HG23 | 1:BB:279:PHE:CD2 | 2.51 | 0.45 |
| 1:BC:237:VAL:HG23 | 1:BC:279:PHE:CD2 | 2.49 | 0.45 |
| 1:BD:237:VAL:HG23 | 1:BD:279:PHE:CD2 | 2.51 | 0.45 |
| 1:BE:189:PHE:CE2 | 1:BE:249:LEU:HD21 | 2.47 | 0.45 |
| 1:BI:25:ILE:HG23 | 1:BI:152:LEU:HD11 | 1.98 | 0.45 |
| 1:BJ:189:PHE:HD2 | 1:BJ:247:ILE:HD11 | 1.80 | 0.45 |
| 1:BN:255:TRP:CE3 | 1:BN:285:SER:HB2 | 2.51 | 0.45 |
| 1:BN:393:HIS:CG | 1:BN:496:PHE:HB3 | 2.51 | 0.45 |
| 1:BP:237:VAL:HG23 | 1:BP:279:PHE:CD2 | 2.51 | 0.45 |
| 1:BP:250:TRP:CZ3 | 1:BP:272:TYR:CD1 | 3.05 | 0.45 |
| 1:BR:250:TRP:HZ3 | 1:BR:272:TYR:CE1 | 2.27 | 0.45 |
| 1:BS:30:SER:O | 1:BS:33:LYS:HB2 | 2.16 | 0.45 |
| 1:CB:239:ILE:HG12 | 1:CB:326:ILE:CD1 | 2.46 | 0.45 |
| 1:CD:203:THR:HB | 1:CD:300:GLN:HG3 | 1.98 | 0.45 |
| 1:CG:232:THR:HB | 1:CG:334:VAL:HG23 | 1.97 | 0.45 |
| 1:CH:371:ASP:OD1 | 1:CH:381:MET:HG2 | 2.16 | 0.45 |
| 1:CK:189:PHE:HD2 | 1:CK:247:ILE:HD11 | 1.80 | 0.45 |
| 1:CN:232:THR:HB | 1:CN:334:VAL:HG23 | 1.99 | 0.45 |
| 1:CO:272:TYR:N | 1:CO:272:TYR:CD1 | 2.84 | 0.45 |
| 1:CP:237:VAL:HG23 | 1:CP:279:PHE:CD2 | 2.51 | 0.45 |
| 1:CQ:75:ARG:NH2 | 1:CQ:391:ALA:O | 2.48 | 0.45 |
| 1:CS:263:ASN:O | 1:CS:267:LYS:HG3 | 2.17 | 0.45 |
| 1:AB:189:PHE:CE2 | 1:AB:249:LEU:HD21 | 2.46 | 0.45 |
| 1:AC:393:HIS:CG | 1:AC:496:PHE:HB3 | 2.51 | 0.45 |
| 1:AF:284:ARG:CG | 1:AF:284:ARG:NH1 | 2.70 | 0.45 |
| 1:AH:272:TYR:N | 1:AH:272:TYR:CD1 | 2.85 | 0.45 |
| 1:AI:79:ARG:HG3 | 1:AI:79:ARG:NH1 | 2.18 | 0.45 |
| 1:AM:454:ASN:HD21 | 1:AM:456:ALA:HB3 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:61:PHE:CD2 | 1:AP:243:ILE:HD11 | 2.51 | 0.45 |
| 1:AS:189:PHE:CE2 | 1:AS:249:LEU:HD21 | 2.51 | 0.45 |
| 1:AT:395:LEU:HB2 | 1:AT:497:TYR:HB2 | 1.98 | 0.45 |
| 1:BC:22:THR:OG1 | 1:BC:131:HIS:CD2 | 2.59 | 0.45 |
| 1:BE:234:ARG:HG2 | 1:BE:280:GLU:HG2 | 1.98 | 0.45 |
| 1:BG:442:GLN:HE21 | 1:BH:412:PHE:HB2 | 1.82 | 0.45 |
| 1:BL:252:VAL:HG22 | 1:BL:253:SER:N | 2.31 | 0.45 |
| 1:BM:30:SER:O | 1:BM:33:LYS:HB2 | 2.15 | 0.45 |
| 1:CC:170:PHE:HD1 | 1:CC:389:MET:CE | 2.30 | 0.45 |
| 1:CC:188:PHE:C | 1:CC:189:PHE:HD1 | 2.19 | 0.45 |
| 1:CE:454:ASN:ND2 | 1:CE:456:ALA:H | 2.11 | 0.45 |
| 1:CG:234:ARG:HG2 | 1:CG:280:GLU:HG2 | 1.97 | 0.45 |
| 1:CH:226:VAL:HG13 | 1:CH:228:GLY:H | 1.82 | 0.45 |
| 1:CJ:189:PHE:CE1 | 1:CJ:198:ARG:HG2 | 2.52 | 0.45 |
| 1:CO:191:LEU:CD2 | 1:CO:191:LEU:N | 2.76 | 0.45 |
| 1:CQ:171:ASP:HA | 1:CQ:172:PRO:HD3 | 1.78 | 0.45 |
| 1:CT:226:VAL:HG13 | 1:CT:228:GLY:H | 1.81 | 0.45 |
| 1:AD:189:PHE:CE2 | 1:AD:249:LEU:HD21 | 2.51 | 0.45 |
| 1:AG:170:PHE:HD1 | 1:AG:389:MET:CE | 2.29 | 0.45 |
| 1:AJ:379:VAL:HG11 | 1:AJ:381:MET:HE1 | 1.99 | 0.45 |
| 1:AJ:454:ASN:HD21 | 1:AJ:456:ALA:HB3 | 1.81 | 0.45 |
| 1:AK:182:LEU:HG | 1:AK:330:ILE:HB | 1.98 | 0.45 |
| 1:AQ:379:VAL:HG11 | 1:AQ:381:MET:HE1 | 1.98 | 0.45 |
| 1:AT:404:LEU:HD22 | 1:AT:486:VAL:HG22 | 1.97 | 0.45 |
| 1:BB:318:SER:HA | 1:BB:319:GLY:HA2 | 1.78 | 0.45 |
| 1:BB:393:HIS:CG | 1:BB:496:PHE:HB3 | 2.51 | 0.45 |
| 1:BE:25:ILE:HG23 | 1:BE:152:LEU:HD11 | 1.98 | 0.45 |
| 1:BF:202:LEU:HB2 | 1:BF:304:SER:O | 2.17 | 0.45 |
| 1:BK:189:PHE:CE2 | 1:BK:249:LEU:HD21 | 2.51 | 0.45 |
| 1:BM:252:VAL:HG22 | 1:BM:253:SER:N | 2.31 | 0.45 |
| 1:BQ:263:ASN:O | 1:BQ:267:LYS:HG3 | 2.17 | 0.45 |
| 1:BR:14:CYS:H | 1:BR:138:ASN:HD21 | 1.65 | 0.45 |
| 1:CB:79:ARG:HG3 | 1:CB:79:ARG:NH1 | 2.30 | 0.45 |
| 1:CE:189:PHE:HD2 | 1:CE:247:ILE:HD11 | 1.81 | 0.45 |
| 1:CH:237:VAL:HG23 | 1:CH:279:PHE:CD2 | 2.51 | 0.45 |
| 1:CI:43:ALA:HB1 | 1:CI:158:GLU:HA | 1.97 | 0.45 |
| 1:CI:170:PHE:HD1 | 1:CI:389:MET:CE | 2.29 | 0.45 |
| 1:CJ:20:LEU:HB2 | 1:CJ:132:PHE:O | 2.16 | 0.45 |
| 1:CO:252:VAL:HG22 | 1:CO:253:SER:N | 2.32 | 0.45 |
| 1:CS:423:LYS:HE2 | 1:CS:449:GLU:O | 2.17 | 0.45 |
| 1:CS:442:GLN:HE21 | 1:CT:412:PHE:HB2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CT:239:ILE:HG12 | 1:CT:326:ILE:CD1 | 2.45 | 0.45 |
| 1:AA:189:PHE:HD2 | 1:AA:247:ILE:HD11 | 1.81 | 0.45 |
| 1:AE:239:ILE:HD12 | 1:AE:275:GLU:HA | 1.98 | 0.45 |
| 1:AG:171:ASP:HA | 1:AG:172:PRO:HD3 | 1.80 | 0.45 |
| 1:AG:189:PHE:HD2 | 1:AG:247:ILE:HD11 | 1.81 | 0.45 |
| 1:AI:284:ARG:CG | 1:AI:284:ARG:NH1 | 2.70 | 0.45 |
| 1:AK:226:VAL:HG13 | 1:AK:228:GLY:H | 1.81 | 0.45 |
| 1:AK:393:HIS:CG | 1:AK:496:PHE:HB3 | 2.52 | 0.45 |
| 1:AL:25:ILE:HG23 | 1:AL:152:LEU:HD11 | 1.97 | 0.45 |
| 1:AM:170:PHE:HD1 | 1:AM:389:MET:HE2 | 1.81 | 0.45 |
| 1:AM:272:TYR:N | 1:AM:272:TYR:CD1 | 2.85 | 0.45 |
| 1:AN:234:ARG:HG2 | 1:AN:280:GLU:HG2 | 1.99 | 0.45 |
| 1:AS:25:ILE:HG23 | 1:AS:152:LEU:HD11 | 1.98 | 0.45 |
| 1:BB:163:LEU:HD12 | 1:BB:163:LEU:HA | 1.83 | 0.45 |
| 1:BE:189:PHE:HD2 | 1:BE:247:ILE:CD1 | 2.30 | 0.45 |
| 1:BE:237:VAL:HG23 | 1:BE:279:PHE:CD2 | 2.51 | 0.45 |
| 1:BF:25:ILE:HG23 | 1:BF:152:LEU:HD11 | 1.99 | 0.45 |
| 1:BF:454:ASN:ND2 | 1:BF:456:ALA:H | 2.05 | 0.45 |
| 1:BG:189:PHE:HD2 | 1:BG:247:ILE:HD11 | 1.82 | 0.45 |
| 1:BH:189:PHE:CE2 | 1:BH:249:LEU:HD21 | 2.44 | 0.45 |
| 1:BJ:263:ASN:O | 1:BJ:267:LYS:HG3 | 2.16 | 0.45 |
| 1:BL:162:PHE:CD2 | 1:BL:163:LEU:HD13 | 2.51 | 0.45 |
| 1:BL:239:ILE:HD12 | 1:BL:275:GLU:HA | 1.97 | 0.45 |
| 1:BO:15:GLN:HE21 | 1:BO:15:GLN:CA | 2.22 | 0.45 |
| 1:BO:162:PHE:CD2 | 1:BO:163:LEU:HD13 | 2.51 | 0.45 |
| 1:BO:250:TRP:CZ3 | 1:BO:272:TYR:CD1 | 3.04 | 0.45 |
| 1:BQ:232:THR:HB | 1:BQ:334:VAL:CG2 | 2.46 | 0.45 |
| 1:BT:12:LYS:HB3 | 1:BT:144:ALA:C | 2.37 | 0.45 |
| 1:CA:442:GLN:HE21 | 1:CB:412:PHE:HB2 | 1.81 | 0.45 |
| 1:CB:191:LEU:CD2 | 1:CB:191:LEU:N | 2.74 | 0.45 |
| 1:CC:252:VAL:HG22 | 1:CC:253:SER:N | 2.31 | 0.45 |
| 1:CE:170:PHE:HD1 | 1:CE:389:MET:CE | 2.29 | 0.45 |
| 1:CJ:234:ARG:HG2 | 1:CJ:280:GLU:HG2 | 1.98 | 0.45 |
| 1:CJ:239:ILE:HD12 | 1:CJ:275:GLU:HA | 1.98 | 0.45 |
| 1:CK:58:ALA:HB2 | 1:CK:102:GLY:HA3 | 1.99 | 0.45 |
| 1:CK:423:LYS:HE2 | 1:CK:449:GLU:O | 2.16 | 0.45 |
| 1:CL:237:VAL:HG23 | 1:CL:279:PHE:CD2 | 2.52 | 0.45 |
| 1:CL:324:LEU:HD23 | 1:CL:324:LEU:C | 2.37 | 0.45 |
| 1:CP:170:PHE:HD1 | 1:CP:389:MET:CE | 2.30 | 0.45 |
| 1:AB:379:VAL:HG11 | 1:AB:381:MET:HE1 | 1.98 | 0.45 |
| 1:AC:189:PHE:HD2 | 1:AC:247:ILE:HD11 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AC:272:TYR:HE2 | 1:BA:55:ARG:NE | 2.10 | 0.45 |
| 1:AC:272:TYR:N | 1:AC:272:TYR:CD1 | 2.85 | 0.45 |
| 1:AE:284:ARG:CG | 1:AE:284:ARG:NH1 | 2.72 | 0.45 |
| 1:AL:162:PHE:CD2 | 1:AL:163:LEU:HD13 | 2.51 | 0.45 |
| 1:AL:234:ARG:HG2 | 1:AL:280:GLU:HG2 | 1.99 | 0.45 |
| 1:AM:232:THR:HB | 1:AM:334:VAL:HG23 | 1.98 | 0.45 |
| 1:AO:189:PHE:HE2 | 1:AO:249:LEU:HD21 | 1.82 | 0.45 |
| 1:AO:234:ARG:HG2 | 1:AO:280:GLU:HG2 | 1.99 | 0.45 |
| 1:AP:189:PHE:CE1 | 1:AP:198:ARG:CG | 2.99 | 0.45 |
| 1:AP:272:TYR:N | 1:AP:272:TYR:HD1 | 2.15 | 0.45 |
| 1:AR:393:HIS:CG | 1:AR:496:PHE:HB3 | 2.52 | 0.45 |
| 1:AS:442:GLN:HE21 | 1:AT:412:PHE:HB2 | 1.81 | 0.45 |
| 1:BE:226:VAL:HG13 | 1:BE:228:GLY:H | 1.81 | 0.45 |
| 1:BE:454:ASN:ND2 | 1:BE:456:ALA:H | 2.08 | 0.45 |
| 1:BL:191:LEU:HD23 | 1:BL:191:LEU:N | 2.21 | 0.45 |
| 1:BL:404:LEU:HD22 | 1:BL:486:VAL:HG22 | 1.99 | 0.45 |
| 1:BL:440:ALA:HB3 | 1:BM:444:LEU:HD13 | 1.98 | 0.45 |
| 1:BP:226:VAL:HG13 | 1:BP:228:GLY:H | 1.82 | 0.45 |
| 1:BR:30:SER:O | 1:BR:33:LYS:HB2 | 2.15 | 0.45 |
| 1:CA:191:LEU:CD2 | 1:CA:191:LEU:N | 2.74 | 0.45 |
| 1:CB:170:PHE:HD1 | 1:CB:389:MET:CE | 2.28 | 0.45 |
| 1:CI:189:PHE:HD2 | 1:CI:247:ILE:HD11 | 1.81 | 0.45 |
| 1:CJ:79:ARG:HH11 | 1:CJ:79:ARG:CG | 2.29 | 0.45 |
| 1:CN:398:GLY:HA3 | 1:CN:494:PHE:CD2 | 2.52 | 0.45 |
| 1:CO:226:VAL:HG13 | 1:CO:228:GLY:H | 1.81 | 0.45 |
| 1:CT:170:PHE:HD1 | 1:CT:389:MET:CE | 2.30 | 0.45 |
| 1:AA:237:VAL:HG23 | 1:AA:279:PHE:CD2 | 2.51 | 0.45 |
| 1:AC:404:LEU:HD22 | 1:AC:486:VAL:HG22 | 1.99 | 0.45 |
| 1:AF:393:HIS:CG | 1:AF:496:PHE:HB3 | 2.52 | 0.45 |
| 1:AI:272:TYR:N | 1:AI:272:TYR:HD1 | 2.15 | 0.45 |
| 1:AJ:162:PHE:CD2 | 1:AJ:163:LEU:HD13 | 2.52 | 0.45 |
| 1:AT:79:ARG:HH11 | 1:AT:79:ARG:CG | 2.29 | 0.45 |
| 1:AT:226:VAL:HG13 | 1:AT:228:GLY:H | 1.81 | 0.45 |
| 1:BA:239:ILE:HD12 | 1:BA:275:GLU:HA | 1.98 | 0.45 |
| 1:BD:393:HIS:CG | 1:BD:496:PHE:HB3 | 2.52 | 0.45 |
| 1:BE:232:THR:HB | 1:BE:334:VAL:CG2 | 2.47 | 0.45 |
| 1:BF:14:CYS:H | 1:BF:138:ASN:ND2 | 2.14 | 0.45 |
| 1:BG:189:PHE:CE1 | 1:BG:198:ARG:HG2 | 2.51 | 0.45 |
| 1:BK:234:ARG:HG2 | 1:BK:280:GLU:HG2 | 1.99 | 0.45 |
| 1:BL:74:ASN:ND2 | 1:BL:77:THR:OG1 | 2.50 | 0.45 |
| 1:BM:75:ARG:NH2 | 1:BM:391:ALA:O | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BN:191:LEU:CD2 | 1:BN:191:LEU:N | 2.77 | 0.45 |
| 1:BO:263:ASN:O | 1:BO:267:LYS:HG3 | 2.17 | 0.45 |
| 1:BP:79:ARG:HG3 | 1:BP:79:ARG:NH1 | 2.26 | 0.45 |
| 1:BP:189:PHE:CE2 | 1:BP:249:LEU:HD21 | 2.52 | 0.45 |
| 1:BP:288:HIS:HD2 | 1:BP:337:ASP:OD2 | 2.00 | 0.45 |
| 1:BQ:237:VAL:HG23 | 1:BQ:279:PHE:CD2 | 2.52 | 0.45 |
| 1:CE:263:ASN:O | 1:CE:267:LYS:HG3 | 2.16 | 0.45 |
| 1:CF:272:TYR:N | 1:CF:272:TYR:CD1 | 2.85 | 0.45 |
| 1:CK:162:PHE:CD2 | 1:CK:163:LEU:HD13 | 2.51 | 0.45 |
| 1:CM:77:THR:O | 1:CM:81:THR:HG23 | 2.16 | 0.45 |
| 1:CO:207:VAL:HA | 1:CO:208:PRO:HD3 | 1.83 | 0.45 |
| 1:CP:18:ARG:HH11 | 1:CP:18:ARG:HG3 | 1.82 | 0.45 |
| 1:AD:191:LEU:HD23 | 1:AD:191:LEU:N | 2.18 | 0.45 |
| 1:AF:75:ARG:NH2 | 1:AF:391:ALA:O | 2.49 | 0.45 |
| 1:AH:232:THR:HB | 1:AH:334:VAL:HG23 | 1.99 | 0.45 |
| 1:AI:207:VAL:HA | 1:AI:208:PRO:HD3 | 1.84 | 0.45 |
| 1:AL:14:CYS:HB3 | 1:AL:64:LEU:HD21 | 1.98 | 0.45 |
| 1:AP:18:ARG:CG | 1:AP:18:ARG:HH11 | 2.29 | 0.45 |
| 1:BA:234:ARG:HG2 | 1:BA:280:GLU:HG2 | 1.97 | 0.45 |
| 1:BG:263:ASN:O | 1:BG:267:LYS:HG3 | 2.17 | 0.45 |
| 1:BH:25:ILE:HG23 | 1:BH:152:LEU:HD11 | 1.98 | 0.45 |
| 1:BH:423:LYS:HE2 | 1:BH:449:GLU:O | 2.16 | 0.45 |
| 1:BK:232:THR:HB | 1:BK:334:VAL:CG2 | 2.47 | 0.45 |
| 1:BK:393:HIS:CG | 1:BK:496:PHE:HB3 | 2.52 | 0.45 |
| 1:BO:239:ILE:HD12 | 1:BO:275:GLU:HA | 1.99 | 0.45 |
| 1:BP:55:ARG:NE | 1:CM:272:TYR:HE2 | 2.10 | 0.45 |
| 1:BQ:272:TYR:N | 1:BQ:272:TYR:CD1 | 2.84 | 0.45 |
| 1:BR:272:TYR:N | 1:BR:272:TYR:CD1 | 2.85 | 0.45 |
| 1:CF:393:HIS:CG | 1:CF:496:PHE:HB3 | 2.52 | 0.45 |
| 1:CH:74:ASN:ND2 | 1:CH:77:THR:OG1 | 2.50 | 0.45 |
| 1:CJ:232:THR:HB | 1:CJ:334:VAL:HG23 | 1.99 | 0.45 |
| 1:CK:25:ILE:HG23 | 1:CK:152:LEU:HD11 | 1.99 | 0.45 |
| 1:CM:234:ARG:HG2 | 1:CM:280:GLU:HG2 | 1.99 | 0.45 |
| 1:CP:379:VAL:HG11 | 1:CP:381:MET:HE1 | 1.98 | 0.45 |
| 1:CQ:170:PHE:HD1 | 1:CQ:389:MET:HE2 | 1.81 | 0.45 |
| 1:AB:393:HIS:CG | 1:AB:496:PHE:HB3 | 2.51 | 0.45 |
| 1:AD:234:ARG:HG2 | 1:AD:280:GLU:HG2 | 1.98 | 0.45 |
| 1:AG:234:ARG:HG2 | 1:AG:280:GLU:HG2 | 1.98 | 0.45 |
| 1:AM:43:ALA:HB1 | 1:AM:158:GLU:HA | 1.99 | 0.45 |
| 1:AN:263:ASN:O | 1:AN:267:LYS:HG3 | 2.17 | 0.45 |
| 1:AP:318:SER:HA | 1:AP:319:GLY:HA2 | 1.76 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:454:ASN:ND2 | 1:AS:456:ALA:H | 2.09 | 0.45 |
| 1:BE:393:HIS:CG | 1:BE:496:PHE:HB3 | 2.51 | 0.45 |
| 1:BF:239:ILE:HD12 | 1:BF:275:GLU:HA | 1.99 | 0.45 |
| 1:BI:239:ILE:HD12 | 1:BI:275:GLU:HA | 1.98 | 0.45 |
| 1:BP:171:ASP:HA | 1:BP:172:PRO:HD3 | 1.79 | 0.45 |
| 1:BQ:170:PHE:HD1 | 1:BQ:389:MET:CE | 2.30 | 0.45 |
| 1:BS:170:PHE:HD1 | 1:BS:389:MET:HE2 | 1.82 | 0.45 |
| 1:BT:171:ASP:HA | 1:BT:172:PRO:HD3 | 1.81 | 0.45 |
| 1:BT:191:LEU:CD2 | 1:BT:191:LEU:N | 2.74 | 0.45 |
| 1:CC:18:ARG:HG3 | 1:CC:19:TYR:N | 2.30 | 0.45 |
| 1:CE:423:LYS:HE2 | 1:CE:449:GLU:O | 2.17 | 0.45 |
| 1:CH:10:ILE:HA | 1:CH:11:PRO:HD3 | 1.86 | 0.45 |
| 1:CH:442:GLN:HE21 | 1:CI:412:PHE:HB2 | 1.81 | 0.45 |
| 1:CJ:207:VAL:HA | 1:CJ:208:PRO:HD3 | 1.83 | 0.45 |
| 1:CP:440:ALA:HB3 | 1:CQ:444:LEU:HD13 | 1.97 | 0.45 |
| 1:AD:55:ARG:CZ | 1:AN:272:TYR:CD2 | 3.00 | 0.45 |
| 1:AD:203:THR:HB | 1:AD:300:GLN:HG3 | 1.99 | 0.45 |
| 1:AH:232:THR:HB | 1:AH:334:VAL:CG2 | 2.47 | 0.45 |
| 1:AH:239:ILE:HG12 | 1:AH:326:ILE:CD1 | 2.46 | 0.45 |
| 1:AI:250:TRP:HZ3 | 1:AI:272:TYR:CE1 | 2.31 | 0.45 |
| 1:AK:55:ARG:HD3 | 1:CF:272:TYR:HD2 | 1.81 | 0.45 |
| 1:AQ:191:LEU:CD2 | 1:AQ:191:LEU:N | 2.75 | 0.45 |
| 1:BB:425:VAL:HG11 | 1:BC:342:SER:HB2 | 1.98 | 0.45 |
| 1:BC:440:ALA:CB | 1:BD:444:LEU:HD13 | 2.47 | 0.45 |
| 1:BJ:75:ARG:NH2 | 1:BJ:391:ALA:O | 2.49 | 0.45 |
| 1:BL:442:GLN:HE21 | 1:BM:412:PHE:HB2 | 1.81 | 0.45 |
| 1:BR:237:VAL:HG23 | 1:BR:279:PHE:CD2 | 2.52 | 0.45 |
| 1:CI:14:CYS:H | 1:CI:138:ASN:ND2 | 2.15 | 0.45 |
| 1:CJ:22:THR:OG1 | 1:CJ:131:HIS:CD2 | 2.60 | 0.45 |
| 1:CJ:284:ARG:CG | 1:CJ:284:ARG:NH1 | 2.74 | 0.45 |
| 1:CK:393:HIS:CG | 1:CK:496:PHE:HB3 | 2.52 | 0.45 |
| 1:CL:191:LEU:HD23 | 1:CL:191:LEU:N | 2.19 | 0.45 |
| 1:CQ:43:ALA:HB1 | 1:CQ:158:GLU:HA | 1.99 | 0.45 |
| 1:CS:162:PHE:CD2 | 1:CS:163:LEU:HD13 | 2.52 | 0.45 |
| 1:AB:74:ASN:ND2 | 1:AB:77:THR:OG1 | 2.50 | 0.45 |
| 1:AF:263:ASN:O | 1:AF:267:LYS:HG3 | 2.17 | 0.45 |
| 1:AG:371:ASP:OD1 | 1:AG:381:MET:HG2 | 2.17 | 0.45 |
| 1:AG:423:LYS:HE2 | 1:AG:449:GLU:O | 2.17 | 0.45 |
| 1:AH:237:VAL:HG23 | 1:AH:279:PHE:CD2 | 2.52 | 0.45 |
| 1:AJ:381:MET:HE2 | 1:AJ:381:MET:HB2 | 1.82 | 0.45 |
| 1:AK:232:THR:HB | 1:AK:334:VAL:HG23 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:170:PHE:HD1 | 1:AP:389:MET:CE | 2.30 | 0.45 |
| 1:AS:188:PHE:C | 1:AS:189:PHE:HD1 | 2.20 | 0.45 |
| 1:BC:239:ILE:HD12 | 1:BC:275:GLU:HA | 1.98 | 0.45 |
| 1:BG:272:TYR:N | 1:BG:272:TYR:HD1 | 2.14 | 0.45 |
| 1:BH:10:ILE:HD13 | 1:BH:20:LEU:HD13 | 1.99 | 0.45 |
| 1:BJ:232:THR:HB | 1:BJ:334:VAL:CG2 | 2.47 | 0.45 |
| 1:BJ:250:TRP:CZ3 | 1:BJ:272:TYR:CD1 | 3.04 | 0.45 |
| 1:BL:58:ALA:HB2 | 1:BL:102:GLY:HA3 | 1.98 | 0.45 |
| 1:BP:182:LEU:HG | 1:BP:330:ILE:HB | 1.99 | 0.45 |
| 1:BQ:203:THR:HB | 1:BQ:300:GLN:HG3 | 1.99 | 0.45 |
| 1:BR:189:PHE:HD2 | 1:BR:247:ILE:HD11 | 1.81 | 0.45 |
| 1:CA:162:PHE:CD2 | 1:CA:163:LEU:HD13 | 2.51 | 0.45 |
| 1:CA:272:TYR:N | 1:CA:272:TYR:CD1 | 2.85 | 0.45 |
| 1:CA:393:HIS:CG | 1:CA:496:PHE:HB3 | 2.52 | 0.45 |
| 1:CB:170:PHE:HD1 | 1:CB:389:MET:HE2 | 1.82 | 0.45 |
| 1:CB:324:LEU:HD23 | 1:CB:324:LEU:C | 2.38 | 0.45 |
| 1:CB:371:ASP:OD1 | 1:CB:381:MET:HG2 | 2.16 | 0.45 |
| 1:CE:162:PHE:CD2 | 1:CE:163:LEU:HD13 | 2.52 | 0.45 |
| 1:CK:189:PHE:HE1 | 1:CK:198:ARG:CG | 2.27 | 0.45 |
| 1:CO:170:PHE:HD1 | 1:CO:389:MET:HE2 | 1.81 | 0.45 |
| 1:CR:191:LEU:HD23 | 1:CR:191:LEU:N | 2.19 | 0.45 |
| 1:CR:234:ARG:HG2 | 1:CR:280:GLU:HG2 | 1.97 | 0.45 |
| 1:CS:171:ASP:HA | 1:CS:172:PRO:HD3 | 1.78 | 0.45 |
| 1:CT:207:VAL:HA | 1:CT:208:PRO:HD3 | 1.84 | 0.45 |
| 1:AA:272:TYR:N | 1:AA:272:TYR:HD1 | 2.15 | 0.44 |
| 1:AF:234:ARG:HG2 | 1:AF:280:GLU:HG2 | 1.99 | 0.44 |
| 1:AF:324:LEU:C | 1:AF:324:LEU:HD23 | 2.36 | 0.44 |
| 1:AH:234:ARG:HG2 | 1:AH:280:GLU:HG2 | 1.98 | 0.44 |
| 1:AH:239:ILE:HD12 | 1:AH:275:GLU:HA | 1.98 | 0.44 |
| 1:AI:393:HIS:CG | 1:AI:496:PHE:HB3 | 2.52 | 0.44 |
| 1:AJ:393:HIS:CG | 1:AJ:496:PHE:HB3 | 2.51 | 0.44 |
| 1:AS:14:CYS:H | 1:AS:138:ASN:HD21 | 1.64 | 0.44 |
| 1:AT:189:PHE:CE2 | 1:AT:249:LEU:HD21 | 2.52 | 0.44 |
| 1:BA:404:LEU:HD22 | 1:BA:486:VAL:HG22 | 1.98 | 0.44 |
| 1:BD:272:TYR:CE2 | 1:BS:55:ARG:CZ | 2.99 | 0.44 |
| 1:BF:203:THR:HB | 1:BF:300:GLN:HG3 | 1.99 | 0.44 |
| 1:BG:79:ARG:HG3 | 1:BG:79:ARG:NH1 | 2.30 | 0.44 |
| 1:BI:170:PHE:HD1 | 1:BI:389:MET:CE | 2.30 | 0.44 |
| 1:BI:234:ARG:HG2 | 1:BI:280:GLU:HG2 | 1.98 | 0.44 |
| 1:BK:272:TYR:N | 1:BK:272:TYR:CD1 | 2.85 | 0.44 |
| 1:BN:234:ARG:HG2 | 1:BN:280:GLU:HG2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BR:189:PHE:HD2 | 1:BR:247:ILE:CD1 | 2.30 | 0.44 |
| 1:BT:423:LYS:HE2 | 1:BT:449:GLU:O | 2.16 | 0.44 |
| 1:CA:454:ASN:ND2 | 1:CA:456:ALA:H | 2.08 | 0.44 |
| 1:CC:232:THR:HB | 1:CC:334:VAL:HG23 | 1.99 | 0.44 |
| 1:CD:16:ALA:O | 1:CD:17:ASN:HB2 | 2.17 | 0.44 |
| 1:CF:189:PHE:HD2 | 1:CF:247:ILE:HD11 | 1.81 | 0.44 |
| 1:CH:201:GLY:HA3 | 1:CH:300:GLN:HG2 | 1.98 | 0.44 |
| 1:CH:263:ASN:O | 1:CH:267:LYS:HG3 | 2.17 | 0.44 |
| 1:CJ:189:PHE:CE2 | 1:CJ:249:LEU:HD21 | 2.47 | 0.44 |
| 1:CL:30:SER:O | 1:CL:33:LYS:HB2 | 2.17 | 0.44 |
| 1:CP:232:THR:HB | 1:CP:334:VAL:HG23 | 1.98 | 0.44 |
| 1:CP:454:ASN:ND2 | 1:CP:456:ALA:H | 2.13 | 0.44 |
| 1:CQ:272:TYR:N | 1:CQ:272:TYR:CD1 | 2.83 | 0.44 |
| 1:CR:14:CYS:H | 1:CR:138:ASN:ND2 | 2.15 | 0.44 |
| 1:AG:379:VAL:HG11 | 1:AG:381:MET:HE1 | 1.99 | 0.44 |
| 1:AH:252:VAL:HG22 | 1:AH:253:SER:N | 2.32 | 0.44 |
| 1:AJ:239:ILE:HG12 | 1:AJ:326:ILE:CD1 | 2.48 | 0.44 |
| 1:AP:272:TYR:CD2 | 1:BE:55:ARG:CZ | 3.00 | 0.44 |
| 1:AP:393:HIS:CG | 1:AP:496:PHE:HB3 | 2.51 | 0.44 |
| 1:AR:25:ILE:HG23 | 1:AR:152:LEU:HD11 | 1.99 | 0.44 |
| 1:BQ:272:TYR:N | 1:BQ:272:TYR:HD1 | 2.15 | 0.44 |
| 1:BS:237:VAL:HG23 | 1:BS:279:PHE:CD2 | 2.52 | 0.44 |
| 1:CA:189:PHE:HE2 | 1:CA:249:LEU:HD21 | 1.82 | 0.44 |
| 1:CC:454:ASN:HD21 | 1:CC:456:ALA:HB3 | 1.83 | 0.44 |
| 1:CE:272:TYR:CE2 | 1:CM:55:ARG:CZ | 3.00 | 0.44 |
| 1:CF:238:HIS:HE1 | 1:CF:329:GLN:OE1 | 2.00 | 0.44 |
| 1:CJ:232:THR:HB | 1:CJ:334:VAL:CG2 | 2.47 | 0.44 |
| 1:CL:393:HIS:CG | 1:CL:496:PHE:HB3 | 2.52 | 0.44 |
| 1:CM:171:ASP:HA | 1:CM:172:PRO:HD3 | 1.79 | 0.44 |
| 1:CO:58:ALA:HB2 | 1:CO:102:GLY:HA3 | 1.99 | 0.44 |
| 1:CO:454:ASN:HD21 | 1:CO:456:ALA:HB3 | 1.82 | 0.44 |
| 1:CQ:162:PHE:CD2 | 1:CQ:163:LEU:HD13 | 2.52 | 0.44 |
| 1:AA:263:ASN:O | 1:AA:267:LYS:HG3 | 2.17 | 0.44 |
| 1:AG:252:VAL:HG22 | 1:AG:253:SER:N | 2.33 | 0.44 |
| 1:AJ:232:THR:HB | 1:AJ:334:VAL:CG2 | 2.47 | 0.44 |
| 1:AL:203:THR:HB | 1:AL:300:GLN:HG3 | 1.98 | 0.44 |
| 1:AP:18:ARG:HH11 | 1:AP:18:ARG:HG3 | 1.81 | 0.44 |
| 1:AQ:252:VAL:HG22 | 1:AQ:253:SER:N | 2.32 | 0.44 |
| 1:AR:10:ILE:HG21 | 1:AR:146:TRP:CE2 | 2.52 | 0.44 |
| 1:AS:454:ASN:HD21 | 1:AS:456:ALA:HB3 | 1.82 | 0.44 |
| 1:BF:272:TYR:N | 1:BF:272:TYR:CD1 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:237:VAL:HG23 | 1:BJ:279:PHE:CD2 | 2.51 | 0.44 |
| 1:BM:232:THR:HB | 1:BM:334:VAL:CG2 | 2.47 | 0.44 |
| 1:BM:232:THR:HB | 1:BM:334:VAL:HG23 | 2.00 | 0.44 |
| 1:BM:263:ASN:O | 1:BM:267:LYS:HG3 | 2.17 | 0.44 |
| 1:BN:28:MET:HE2 | 1:BN:152:LEU:HG | 1.98 | 0.44 |
| 1:BQ:189:PHE:CE2 | 1:BQ:249:LEU:HD21 | 2.52 | 0.44 |
| 1:BS:191:LEU:CD2 | 1:BS:191:LEU:N | 2.75 | 0.44 |
| 1:CB:272:TYR:N | 1:CB:272:TYR:CD1 | 2.85 | 0.44 |
| 1:CC:250:TRP:CZ3 | 1:CC:272:TYR:CD1 | 3.03 | 0.44 |
| 1:CG:393:HIS:CG | 1:CG:496:PHE:HB3 | 2.52 | 0.44 |
| 1:CJ:300:GLN:HE21 | 1:CJ:300:GLN:HB2 | 1.59 | 0.44 |
| 1:CT:79:ARG:HH11 | 1:CT:79:ARG:HG3 | 1.83 | 0.44 |
| 1:AC:226:VAL:HG13 | 1:AC:228:GLY:H | 1.83 | 0.44 |
| 1:AC:423:LYS:HE2 | 1:AC:449:GLU:O | 2.17 | 0.44 |
| 1:AE:170:PHE:HD1 | 1:AE:389:MET:HE2 | 1.82 | 0.44 |
| 1:AF:170:PHE:HD1 | 1:AF:389:MET:CE | 2.30 | 0.44 |
| 1:AF:404:LEU:HD22 | 1:AF:486:VAL:HG22 | 2.00 | 0.44 |
| 1:AJ:75:ARG:NH2 | 1:AJ:391:ALA:O | 2.47 | 0.44 |
| 1:AN:191:LEU:CD2 | 1:AN:191:LEU:N | 2.77 | 0.44 |
| 1:AN:379:VAL:HG11 | 1:AN:381:MET:HE1 | 1.99 | 0.44 |
| 1:AP:272:TYR:N | 1:AP:272:TYR:CD1 | 2.85 | 0.44 |
| 1:AQ:226:VAL:HG13 | 1:AQ:228:GLY:H | 1.83 | 0.44 |
| 1:AR:61:PHE:CD2 | 1:AR:243:ILE:HD11 | 2.52 | 0.44 |
| 1:AS:404:LEU:HD22 | 1:AS:486:VAL:HG22 | 1.98 | 0.44 |
| 1:BC:272:TYR:N | 1:BC:272:TYR:CD1 | 2.85 | 0.44 |
| 1:BD:423:LYS:HE2 | 1:BD:449:GLU:O | 2.18 | 0.44 |
| 1:BE:191:LEU:CD2 | 1:BE:191:LEU:N | 2.74 | 0.44 |
| 1:BH:393:HIS:CG | 1:BH:496:PHE:HB3 | 2.51 | 0.44 |
| 1:BN:162:PHE:CD2 | 1:BN:163:LEU:HD13 | 2.52 | 0.44 |
| 1:CC:234:ARG:HG2 | 1:CC:280:GLU:HG2 | 1.99 | 0.44 |
| 1:CD:234:ARG:HG2 | 1:CD:280:GLU:HG2 | 1.99 | 0.44 |
| 1:CI:191:LEU:HD23 | 1:CI:191:LEU:N | 2.17 | 0.44 |
| 1:CJ:318:SER:HA | 1:CJ:319:GLY:HA2 | 1.81 | 0.44 |
| 1:CM:395:LEU:HB2 | 1:CM:497:TYR:HB2 | 1.99 | 0.44 |
| 1:CP:189:PHE:CE2 | 1:CP:249:LEU:HD21 | 2.53 | 0.44 |
| 1:CQ:189:PHE:HD2 | 1:CQ:247:ILE:HD11 | 1.81 | 0.44 |
| 1:CR:232:THR:HB | 1:CR:334:VAL:HG23 | 1.99 | 0.44 |
| 1:AA:43:ALA:HB1 | 1:AA:158:GLU:HA | 2.00 | 0.44 |
| 1:AE:232:THR:HB | 1:AE:334:VAL:CG2 | 2.48 | 0.44 |
| 1:AE:404:LEU:HD22 | 1:AE:486:VAL:HG22 | 1.98 | 0.44 |
| 1:AG:263:ASN:O | 1:AG:267:LYS:HG3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AI:25:ILE:HG23 | 1:AI:152:LEU:HD11 | 1.98 | 0.44 |
| 1:AM:423:LYS:HE2 | 1:AM:449:GLU:O | 2.18 | 0.44 |
| 1:AN:170:PHE:HD1 | 1:AN:389:MET:CE | 2.30 | 0.44 |
| 1:AQ:272:TYR:N | 1:AQ:272:TYR:CD1 | 2.85 | 0.44 |
| 1:AS:182:LEU:C | 1:AS:182:LEU:HD12 | 2.37 | 0.44 |
| 1:AT:232:THR:HB | 1:AT:334:VAL:HG23 | 1.98 | 0.44 |
| 1:BC:61:PHE:CD2 | 1:BC:243:ILE:HD11 | 2.53 | 0.44 |
| 1:BC:162:PHE:CD2 | 1:BC:163:LEU:HD13 | 2.52 | 0.44 |
| 1:BC:454:ASN:HD21 | 1:BC:456:ALA:HB3 | 1.82 | 0.44 |
| 1:BF:423:LYS:HE2 | 1:BF:449:GLU:O | 2.17 | 0.44 |
| 1:BG:404:LEU:HD23 | 1:BG:404:LEU:N | 2.32 | 0.44 |
| 1:BM:18:ARG:HG2 | 1:BM:20:LEU:HD23 | 2.00 | 0.44 |
| 1:BM:74:ASN:ND2 | 1:BM:77:THR:OG1 | 2.51 | 0.44 |
| 1:BM:237:VAL:HG23 | 1:BM:279:PHE:CD2 | 2.52 | 0.44 |
| 1:BM:404:LEU:HD22 | 1:BM:486:VAL:HG22 | 2.00 | 0.44 |
| 1:BN:232:THR:HB | 1:BN:334:VAL:CG2 | 2.47 | 0.44 |
| 1:BO:189:PHE:CE2 | 1:BO:249:LEU:HD21 | 2.52 | 0.44 |
| 1:BP:22:THR:OG1 | 1:BP:131:HIS:CD2 | 2.58 | 0.44 |
| 1:BP:379:VAL:HG11 | 1:BP:381:MET:HE1 | 1.99 | 0.44 |
| 1:BS:75:ARG:NH2 | 1:BS:391:ALA:O | 2.50 | 0.44 |
| 1:BS:189:PHE:CE2 | 1:BS:249:LEU:HD21 | 2.53 | 0.44 |
| 1:CA:188:PHE:C | 1:CA:189:PHE:HD1 | 2.21 | 0.44 |
| 1:CD:232:THR:HB | 1:CD:334:VAL:CG2 | 2.48 | 0.44 |
| 1:CD:237:VAL:HG23 | 1:CD:279:PHE:CD2 | 2.53 | 0.44 |
| 1:CE:43:ALA:HB1 | 1:CE:158:GLU:HA | 2.00 | 0.44 |
| 1:CF:404:LEU:HD22 | 1:CF:486:VAL:HG22 | 1.98 | 0.44 |
| 1:CG:232:THR:HB | 1:CG:334:VAL:CG2 | 2.48 | 0.44 |
| 1:CL:171:ASP:HA | 1:CL:172:PRO:HD3 | 1.80 | 0.44 |
| 1:CN:15:GLN:OE1 | 1:CN:15:GLN:HA | 2.17 | 0.44 |
| 1:CN:423:LYS:HE2 | 1:CN:449:GLU:O | 2.17 | 0.44 |
| 1:CQ:189:PHE:HE1 | 1:CQ:198:ARG:CG | 2.29 | 0.44 |
| 1:CT:162:PHE:CD2 | 1:CT:163:LEU:HD13 | 2.53 | 0.44 |
| 1:AB:189:PHE:HD2 | 1:AB:247:ILE:HD11 | 1.83 | 0.44 |
| 1:AC:188:PHE:C | 1:AC:189:PHE:HD1 | 2.20 | 0.44 |
| 1:AC:442:GLN:HE21 | 1:AD:412:PHE:HB2 | 1.83 | 0.44 |
| 1:AE:55:ARG:HD3 | 1:CP:272:TYR:HD2 | 1.79 | 0.44 |
| 1:AE:272:TYR:N | 1:AE:272:TYR:HD1 | 2.15 | 0.44 |
| 1:AH:35:VAL:O | 1:AH:39:LYS:HG3 | 2.18 | 0.44 |
| 1:AI:16:ALA:O | 1:AI:17:ASN:HB2 | 2.17 | 0.44 |
| 1:AJ:189:PHE:HD2 | 1:AJ:247:ILE:HD11 | 1.82 | 0.44 |
| 1:AK:30:SER:O | 1:AK:33:LYS:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AL:237:VAL:HG23 | 1:AL:279:PHE:CD2 | 2.52 | 0.44 |
| 1:AO:237:VAL:HG23 | 1:AO:279:PHE:CD2 | 2.53 | 0.44 |
| 1:AO:284:ARG:CG | 1:AO:284:ARG:NH1 | 2.71 | 0.44 |
| 1:BA:263:ASN:O | 1:BA:267:LYS:HG3 | 2.17 | 0.44 |
| 1:BB:232:THR:HB | 1:BB:334:VAL:CG2 | 2.47 | 0.44 |
| 1:BB:371:ASP:OD1 | 1:BB:381:MET:HG2 | 2.17 | 0.44 |
| 1:BD:454:ASN:HD21 | 1:BD:456:ALA:HB3 | 1.82 | 0.44 |
| 1:BE:16:ALA:O | 1:BE:17:ASN:CB | 2.64 | 0.44 |
| 1:BE:404:LEU:HD22 | 1:BE:486:VAL:HG22 | 2.00 | 0.44 |
| 1:BF:11:PRO:HG2 | 1:BF:18:ARG:CD | 2.48 | 0.44 |
| 1:BF:318:SER:HA | 1:BF:319:GLY:HA2 | 1.84 | 0.44 |
| 1:BG:234:ARG:HG2 | 1:BG:280:GLU:HG2 | 1.99 | 0.44 |
| 1:BH:404:LEU:HD22 | 1:BH:486:VAL:HG22 | 1.99 | 0.44 |
| 1:BK:239:ILE:HD12 | 1:BK:275:GLU:HA | 2.00 | 0.44 |
| 1:BK:318:SER:HA | 1:BK:319:GLY:HA2 | 1.80 | 0.44 |
| 1:BK:404:LEU:HD22 | 1:BK:486:VAL:HG22 | 1.99 | 0.44 |
| 1:BO:14:CYS:H | 1:BO:138:ASN:ND2 | 2.14 | 0.44 |
| 1:BP:324:LEU:HA | 1:BP:325:PRO:HD3 | 1.84 | 0.44 |
| 1:BQ:234:ARG:HG2 | 1:BQ:280:GLU:HG2 | 2.00 | 0.44 |
| 1:BT:58:ALA:HB2 | 1:BT:102:GLY:HA3 | 2.00 | 0.44 |
| 1:CA:444:LEU:HD13 | 1:CE:440:ALA:CB | 2.48 | 0.44 |
| 1:CC:43:ALA:HB1 | 1:CC:158:GLU:HA | 1.99 | 0.44 |
| 1:CD:239:ILE:HD12 | 1:CD:275:GLU:HA | 1.99 | 0.44 |
| 1:CG:379:VAL:HG11 | 1:CG:381:MET:HE1 | 1.99 | 0.44 |
| 1:CH:232:THR:HB | 1:CH:334:VAL:HG23 | 1.99 | 0.44 |
| 1:CI:300:GLN:HE21 | 1:CI:300:GLN:HB2 | 1.70 | 0.44 |
| 1:CK:272:TYR:N | 1:CK:272:TYR:HD1 | 2.16 | 0.44 |
| 1:CM:189:PHE:CE2 | 1:CM:249:LEU:HD21 | 2.45 | 0.44 |
| 1:CM:232:THR:HB | 1:CM:334:VAL:HG23 | 2.00 | 0.44 |
| 1:CM:241:ALA:HB1 | 1:CM:242:PRO:HD2 | 1.99 | 0.44 |
| 1:CP:67:VAL:HG23 | 1:CP:135:LEU:HB2 | 1.98 | 0.44 |
| 1:AA:18:ARG:HG3 | 1:AA:19:TYR:N | 2.32 | 0.44 |
| 1:AD:171:ASP:HA | 1:AD:172:PRO:HD3 | 1.79 | 0.44 |
| 1:AD:232:THR:HB | 1:AD:334:VAL:HG23 | 2.00 | 0.44 |
| 1:AE:237:VAL:HG23 | 1:AE:279:PHE:CD2 | 2.52 | 0.44 |
| 1:AH:272:TYR:N | 1:AH:272:TYR:HD1 | 2.16 | 0.44 |
| 1:AH:404:LEU:HD22 | 1:AH:486:VAL:HG22 | 2.00 | 0.44 |
| 1:AJ:226:VAL:HG13 | 1:AJ:228:GLY:H | 1.82 | 0.44 |
| 1:AS:250:TRP:CZ3 | 1:AS:272:TYR:CD1 | 3.05 | 0.44 |
| 1:BA:300:GLN:HE21 | 1:BA:300:GLN:HB2 | 1.55 | 0.44 |
| 1:BF:189:PHE:HD2 | 1:BF:247:ILE:HD11 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BF:252:VAL:HG22 | 1:BF:253:SER:N | 2.33 | 0.44 |
| 1:BJ:189:PHE:HD2 | 1:BJ:247:ILE:CD1 | 2.30 | 0.44 |
| 1:BM:239:ILE:HD12 | 1:BM:275:GLU:HA | 1.99 | 0.44 |
| 1:BP:289:ARG:NH1 | 1:BP:337:ASP:OD1 | 2.51 | 0.44 |
| 1:BP:300:GLN:HE21 | 1:BP:300:GLN:HB2 | 1.58 | 0.44 |
| 1:BQ:423:LYS:HE2 | 1:BQ:449:GLU:O | 2.18 | 0.44 |
| 1:BS:440:ALA:CB | 1:BT:444:LEU:HD13 | 2.48 | 0.44 |
| 1:BT:226:VAL:HG13 | 1:BT:228:GLY:H | 1.83 | 0.44 |
| 1:CA:58:ALA:HB2 | 1:CA:102:GLY:HA3 | 2.00 | 0.44 |
| 1:CA:237:VAL:HG23 | 1:CA:279:PHE:CD2 | 2.53 | 0.44 |
| 1:CD:171:ASP:HA | 1:CD:172:PRO:HD3 | 1.79 | 0.44 |
| 1:CD:272:TYR:HD2 | 1:CS:55:ARG:HD3 | 1.77 | 0.44 |
| 1:CD:404:LEU:HD22 | 1:CD:486:VAL:HG22 | 2.00 | 0.44 |
| 1:CM:207:VAL:HA | 1:CM:208:PRO:HD3 | 1.85 | 0.44 |
| 1:CN:263:ASN:O | 1:CN:267:LYS:HG3 | 2.18 | 0.44 |
| 1:CQ:237:VAL:HG23 | 1:CQ:279:PHE:CD2 | 2.52 | 0.44 |
| 1:CQ:239:ILE:HD12 | 1:CQ:275:GLU:HA | 1.99 | 0.44 |
| 1:CQ:252:VAL:HG22 | 1:CQ:253:SER:N | 2.33 | 0.44 |
| 1:CR:77:THR:O | 1:CR:81:THR:HG23 | 2.17 | 0.44 |
| 1:CT:191:LEU:CD2 | 1:CT:191:LEU:N | 2.76 | 0.44 |
| 1:CT:393:HIS:CG | 1:CT:496:PHE:HB3 | 2.51 | 0.44 |
| 1:AB:404:LEU:HD22 | 1:AB:486:VAL:HG22 | 2.00 | 0.44 |
| 1:AG:404:LEU:HD22 | 1:AG:486:VAL:HG22 | 1.98 | 0.44 |
| 1:AI:237:VAL:HG23 | 1:AI:279:PHE:CD2 | 2.52 | 0.44 |
| 1:AJ:25:ILE:HG23 | 1:AJ:152:LEU:HD11 | 1.99 | 0.44 |
| 1:AK:191:LEU:CD2 | 1:AK:191:LEU:N | 2.74 | 0.44 |
| 1:AL:170:PHE:HD1 | 1:AL:389:MET:HE2 | 1.83 | 0.44 |
| 1:AL:324:LEU:C | 1:AL:324:LEU:HD23 | 2.38 | 0.44 |
| 1:AP:272:TYR:CE2 | 1:BE:55:ARG:CZ | 3.00 | 0.44 |
| 1:AS:423:LYS:HE2 | 1:AS:449:GLU:O | 2.18 | 0.44 |
| 1:AT:272:TYR:N | 1:AT:272:TYR:CD1 | 2.83 | 0.44 |
| 1:AT:272:TYR:N | 1:AT:272:TYR:HD1 | 2.14 | 0.44 |
| 1:BH:252:VAL:HG22 | 1:BH:253:SER:N | 2.33 | 0.44 |
| 1:BI:272:TYR:N | 1:BI:272:TYR:HD1 | 2.16 | 0.44 |
| 1:BK:162:PHE:CD2 | 1:BK:163:LEU:HD13 | 2.53 | 0.44 |
| 1:BM:423:LYS:HE2 | 1:BM:449:GLU:O | 2.17 | 0.44 |
| 1:BO:10:ILE:HA | 1:BO:11:PRO:HD3 | 1.86 | 0.44 |
| 1:BQ:250:TRP:HZ3 | 1:BQ:272:TYR:CE1 | 2.27 | 0.44 |
| 1:BS:263:ASN:O | 1:BS:267:LYS:HG3 | 2.18 | 0.44 |
| 1:BT:25:ILE:HG23 | 1:BT:152:LEU:HD11 | 1.99 | 0.44 |
| 1:CD:162:PHE:CD2 | 1:CD:163:LEU:HD13 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CD:379:VAL:HG11 | 1:CD:381:MET:HE1 | 1.99 | 0.44 |
| 1:CH:423:LYS:HE2 | 1:CH:449:GLU:O | 2.18 | 0.44 |
| 1:CN:170:PHE:HD1 | 1:CN:389:MET:HE2 | 1.82 | 0.44 |
| 1:CP:442:GLN:HE21 | 1:CQ:412:PHE:HB2 | 1.81 | 0.44 |
| 1:CR:272:TYR:N | 1:CR:272:TYR:CD1 | 2.86 | 0.44 |
| 1:CS:207:VAL:HA | 1:CS:208:PRO:HD3 | 1.83 | 0.44 |
| 1:CS:393:HIS:CG | 1:CS:496:PHE:HB3 | 2.53 | 0.44 |
| 1:CT:237:VAL:HG23 | 1:CT:279:PHE:CD2 | 2.53 | 0.44 |
| 1:AA:14:CYS:H | 1:AA:138:ASN:ND2 | 2.12 | 0.44 |
| 1:AC:18:ARG:HG2 | 1:AC:20:LEU:HD23 | 1.98 | 0.44 |
| 1:AC:189:PHE:HE1 | 1:AC:198:ARG:CG | 2.27 | 0.44 |
| 1:AC:272:TYR:N | 1:AC:272:TYR:HD1 | 2.16 | 0.44 |
| 1:AD:207:VAL:HA | 1:AD:208:PRO:HD3 | 1.83 | 0.44 |
| 1:AG:272:TYR:HE2 | 1:BG:55:ARG:NE | 2.13 | 0.44 |
| 1:AI:232:THR:HB | 1:AI:334:VAL:HG23 | 1.98 | 0.44 |
| 1:AJ:108:ILE:HG23 | 1:AJ:113:LEU:HD12 | 2.00 | 0.44 |
| 1:AM:442:GLN:HE21 | 1:AN:412:PHE:HB2 | 1.83 | 0.44 |
| 1:BG:239:ILE:HD12 | 1:BG:275:GLU:HA | 1.99 | 0.44 |
| 1:BI:203:THR:HB | 1:BI:300:GLN:HG3 | 2.00 | 0.44 |
| 1:BJ:182:LEU:HG | 1:BJ:330:ILE:HB | 1.99 | 0.44 |
| 1:BM:189:PHE:CE2 | 1:BM:249:LEU:HD21 | 2.42 | 0.44 |
| 1:BP:74:ASN:ND2 | 1:BP:77:THR:OG1 | 2.50 | 0.44 |
| 1:BQ:36:GLN:HE22 | 1:BQ:156:LEU:H | 1.63 | 0.44 |
| 1:BR:79:ARG:CG | 1:BR:79:ARG:NH1 | 2.77 | 0.44 |
| 1:BR:203:THR:HB | 1:BR:300:GLN:HG3 | 1.99 | 0.44 |
| 1:BR:440:ALA:CB | 1:BS:444:LEU:HD13 | 2.48 | 0.44 |
| 1:CA:170:PHE:HD1 | 1:CA:389:MET:HE2 | 1.82 | 0.44 |
| 1:CA:232:THR:HB | 1:CA:334:VAL:HG23 | 1.99 | 0.44 |
| 1:CC:25:ILE:HG23 | 1:CC:152:LEU:HD11 | 1.99 | 0.44 |
| 1:CD:272:TYR:CE2 | 1:CS:55:ARG:CZ | 3.01 | 0.44 |
| 1:CE:239:ILE:HD12 | 1:CE:275:GLU:HA | 2.00 | 0.44 |
| 1:CE:252:VAL:HG22 | 1:CE:253:SER:N | 2.33 | 0.44 |
| 1:CI:379:VAL:HG11 | 1:CI:381:MET:HE1 | 1.98 | 0.44 |
| 1:CJ:404:LEU:HD22 | 1:CJ:486:VAL:HG22 | 1.99 | 0.44 |
| 1:CO:74:ASN:ND2 | 1:CO:77:THR:OG1 | 2.51 | 0.44 |
| 1:AA:170:PHE:HD1 | 1:AA:389:MET:CE | 2.31 | 0.43 |
| 1:AA:423:LYS:HE2 | 1:AA:449:GLU:O | 2.18 | 0.43 |
| 1:AB:454:ASN:HD21 | 1:AB:456:ALA:HB3 | 1.82 | 0.43 |
| 1:AC:75:ARG:NH2 | 1:AC:391:ALA:O | 2.51 | 0.43 |
| 1:AD:379:VAL:HG12 | 1:AD:381:MET:HE2 | 2.00 | 0.43 |
| 1:AE:393:HIS:CG | 1:AE:496:PHE:HB3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AF:423:LYS:HE2 | 1:AF:449:GLU:O | 2.18 | 0.43 |
| 1:AH:324:LEU:HD23 | 1:AH:324:LEU:C | 2.38 | 0.43 |
| 1:AH:423:LYS:HE2 | 1:AH:449:GLU:O | 2.18 | 0.43 |
| 1:AK:379:VAL:HG11 | 1:AK:381:MET:HE1 | 2.00 | 0.43 |
| 1:AO:300:GLN:HE21 | 1:AO:300:GLN:HB2 | 1.64 | 0.43 |
| 1:AP:189:PHE:HD2 | 1:AP:247:ILE:HD11 | 1.83 | 0.43 |
| 1:AQ:108:ILE:HG23 | 1:AQ:113:LEU:HD12 | 2.00 | 0.43 |
| 1:AT:239:ILE:HG12 | 1:AT:326:ILE:CD1 | 2.48 | 0.43 |
| 1:AT:393:HIS:CG | 1:AT:496:PHE:HB3 | 2.52 | 0.43 |
| 1:BG:15:GLN:HA | 1:BG:15:GLN:NE2 | 2.30 | 0.43 |
| 1:BH:171:ASP:HA | 1:BH:172:PRO:HD3 | 1.78 | 0.43 |
| 1:BL:423:LYS:HE2 | 1:BL:449:GLU:O | 2.18 | 0.43 |
| 1:BO:61:PHE:CE2 | 1:BO:243:ILE:HD11 | 2.53 | 0.43 |
| 1:BP:272:TYR:CD2 | 1:CE:55:ARG:NH1 | 2.86 | 0.43 |
| 1:BQ:393:HIS:CG | 1:BQ:496:PHE:HB3 | 2.53 | 0.43 |
| 1:BR:170:PHE:HD1 | 1:BR:389:MET:HE2 | 1.83 | 0.43 |
| 1:BT:454:ASN:HD21 | 1:BT:456:ALA:HB3 | 1.82 | 0.43 |
| 1:CF:239:ILE:HD12 | 1:CF:275:GLU:HA | 1.99 | 0.43 |
| 1:CF:371:ASP:OD1 | 1:CF:381:MET:HG2 | 2.17 | 0.43 |
| 1:CG:11:PRO:HG2 | 1:CG:18:ARG:HD2 | 2.00 | 0.43 |
| 1:CG:237:VAL:HG23 | 1:CG:279:PHE:CD2 | 2.53 | 0.43 |
| 1:CH:272:TYR:N | 1:CH:272:TYR:CD1 | 2.86 | 0.43 |
| 1:CH:393:HIS:CG | 1:CH:496:PHE:HB3 | 2.53 | 0.43 |
| 1:CK:442:GLN:HE21 | 1:CL:412:PHE:HB2 | 1.82 | 0.43 |
| 1:CM:318:SER:HA | 1:CM:319:GLY:HA2 | 1.77 | 0.43 |
| 1:CP:226:VAL:HG13 | 1:CP:228:GLY:H | 1.82 | 0.43 |
| 1:AA:79:ARG:HH11 | 1:AA:79:ARG:HG3 | 1.82 | 0.43 |
| 1:AB:43:ALA:HB1 | 1:AB:158:GLU:HA | 2.00 | 0.43 |
| 1:AI:232:THR:HB | 1:AI:334:VAL:CG2 | 2.48 | 0.43 |
| 1:AL:272:TYR:N | 1:AL:272:TYR:CD1 | 2.86 | 0.43 |
| 1:AM:189:PHE:HD2 | 1:AM:247:ILE:CD1 | 2.30 | 0.43 |
| 1:BC:18:ARG:NH1 | 1:BC:18:ARG:HB2 | 2.34 | 0.43 |
| 1:BE:11:PRO:HG2 | 1:BE:18:ARG:CD | 2.48 | 0.43 |
| 1:BH:11:PRO:HG2 | 1:BH:18:ARG:HD2 | 1.99 | 0.43 |
| 1:BH:189:PHE:HD2 | 1:BH:247:ILE:HD11 | 1.83 | 0.43 |
| 1:BH:442:GLN:NE2 | 1:BI:412:PHE:HB2 | 2.33 | 0.43 |
| 1:BI:11:PRO:HG2 | 1:BI:18:ARG:HD2 | 2.00 | 0.43 |
| 1:BK:252:VAL:HG22 | 1:BK:253:SER:N | 2.33 | 0.43 |
| 1:BL:418:SER:HB3 | 1:BM:407:SER:HB3 | 2.00 | 0.43 |
| 1:BM:58:ALA:HB2 | 1:BM:102:GLY:HA3 | 1.99 | 0.43 |
| 1:BO:237:VAL:HG23 | 1:BO:279:PHE:CD2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BO:272:TYR:CD2 | 1:BR:55:ARG:NH1 | 2.86 | 0.43 |
| 1:BP:404:LEU:HD22 | 1:BP:486:VAL:HG22 | 2.00 | 0.43 |
| 1:CD:189:PHE:HE2 | 1:CD:249:LEU:CD2 | 2.31 | 0.43 |
| 1:CF:412:PHE:HB2 | 1:CJ:442:GLN:HE21 | 1.83 | 0.43 |
| 1:CH:252:VAL:HG22 | 1:CH:253:SER:N | 2.33 | 0.43 |
| 1:CI:239:ILE:HG12 | 1:CI:326:ILE:CD1 | 2.48 | 0.43 |
| 1:CL:188:PHE:C | 1:CL:189:PHE:HD1 | 2.22 | 0.43 |
| 1:CL:423:LYS:HE2 | 1:CL:449:GLU:O | 2.18 | 0.43 |
| 1:CM:22:THR:OG1 | 1:CM:131:HIS:CD2 | 2.63 | 0.43 |
| 1:CS:237:VAL:HG23 | 1:CS:279:PHE:CD2 | 2.53 | 0.43 |
| 1:AC:234:ARG:HG2 | 1:AC:280:GLU:HG2 | 1.99 | 0.43 |
| 1:AE:379:VAL:HG11 | 1:AE:381:MET:HE1 | 1.99 | 0.43 |
| 1:AG:237:VAL:HG23 | 1:AG:279:PHE:CD2 | 2.54 | 0.43 |
| 1:AK:61:PHE:CD2 | 1:AK:243:ILE:HD11 | 2.54 | 0.43 |
| 1:AO:189:PHE:CE2 | 1:AO:249:LEU:HD21 | 2.53 | 0.43 |
| 1:AO:318:SER:HA | 1:AO:319:GLY:HA2 | 1.79 | 0.43 |
| 1:AR:189:PHE:HE1 | 1:AR:198:ARG:HG2 | 1.78 | 0.43 |
| 1:AR:252:VAL:HG22 | 1:AR:253:SER:N | 2.33 | 0.43 |
| 1:AS:318:SER:HA | 1:AS:319:GLY:HA2 | 1.79 | 0.43 |
| 1:BA:73:TYR:CE2 | 1:BA:394:GLY:HA3 | 2.54 | 0.43 |
| 1:BA:379:VAL:HG11 | 1:BA:381:MET:HE1 | 2.01 | 0.43 |
| 1:BB:263:ASN:O | 1:BB:267:LYS:HG3 | 2.18 | 0.43 |
| 1:BD:234:ARG:HG2 | 1:BD:280:GLU:HG2 | 1.99 | 0.43 |
| 1:BH:226:VAL:HG13 | 1:BH:228:GLY:H | 1.82 | 0.43 |
| 1:BM:393:HIS:CG | 1:BM:496:PHE:HB3 | 2.53 | 0.43 |
| 1:BT:232:THR:HB | 1:BT:334:VAL:HG23 | 2.00 | 0.43 |
| 1:CC:423:LYS:HE2 | 1:CC:449:GLU:O | 2.18 | 0.43 |
| 1:CD:189:PHE:HD2 | 1:CD:247:ILE:HD11 | 1.83 | 0.43 |
| 1:CH:232:THR:HB | 1:CH:334:VAL:CG2 | 2.49 | 0.43 |
| 1:CI:237:VAL:HG23 | 1:CI:279:PHE:CD2 | 2.53 | 0.43 |
| 1:CI:263:ASN:O | 1:CI:267:LYS:HG3 | 2.18 | 0.43 |
| 1:CO:182:LEU:C | 1:CO:182:LEU:HD12 | 2.38 | 0.43 |
| 1:CO:239:ILE:HG23 | 1:CO:324:LEU:HD21 | 2.01 | 0.43 |
| 1:CO:404:LEU:N | 1:CO:404:LEU:HD23 | 2.32 | 0.43 |
| 1:CQ:272:TYR:N | 1:CQ:272:TYR:HD1 | 2.15 | 0.43 |
| 1:CT:423:LYS:HE2 | 1:CT:449:GLU:O | 2.18 | 0.43 |
| 1:AC:232:THR:HB | 1:AC:334:VAL:CG2 | 2.49 | 0.43 |
| 1:AC:440:ALA:HB3 | 1:AD:444:LEU:HD13 | 1.99 | 0.43 |
| 1:AD:11:PRO:HG2 | 1:AD:18:ARG:CD | 2.48 | 0.43 |
| 1:AD:79:ARG:CG | 1:AD:79:ARG:NH1 | 2.81 | 0.43 |
| 1:AE:255:TRP:CE3 | 1:AE:285:SER:HB2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AF:272:TYR:N | 1:AF:272:TYR:HD1 | 2.16 | 0.43 |
| 1:AG:10:ILE:HA | 1:AG:11:PRO:HD3 | 1.81 | 0.43 |
| 1:AG:201:GLY:HA3 | 1:AG:300:GLN:HG2 | 1.99 | 0.43 |
| 1:AI:55:ARG:NE | 1:AR:272:TYR:HE2 | 2.16 | 0.43 |
| 1:AI:404:LEU:HD22 | 1:AI:486:VAL:HG22 | 1.99 | 0.43 |
| 1:AJ:272:TYR:N | 1:AJ:272:TYR:CD1 | 2.86 | 0.43 |
| 1:AK:404:LEU:HD22 | 1:AK:486:VAL:HG22 | 2.00 | 0.43 |
| 1:AK:423:LYS:HE2 | 1:AK:449:GLU:O | 2.18 | 0.43 |
| 1:AP:162:PHE:CD2 | 1:AP:163:LEU:HD13 | 2.53 | 0.43 |
| 1:AP:171:ASP:HA | 1:AP:172:PRO:HD3 | 1.79 | 0.43 |
| 1:AS:74:ASN:ND2 | 1:AS:77:THR:OG1 | 2.52 | 0.43 |
| 1:AT:232:THR:HB | 1:AT:334:VAL:CG2 | 2.48 | 0.43 |
| 1:BB:189:PHE:HE1 | 1:BB:198:ARG:HG2 | 1.76 | 0.43 |
| 1:BC:234:ARG:HG2 | 1:BC:280:GLU:HG2 | 2.00 | 0.43 |
| 1:BI:163:LEU:HD12 | 1:BI:163:LEU:HA | 1.87 | 0.43 |
| 1:BI:207:VAL:HA | 1:BI:208:PRO:HD3 | 1.84 | 0.43 |
| 1:BJ:423:LYS:HE2 | 1:BJ:449:GLU:O | 2.18 | 0.43 |
| 1:BK:170:PHE:HD1 | 1:BK:389:MET:HE2 | 1.83 | 0.43 |
| 1:BK:300:GLN:HE21 | 1:BK:300:GLN:HB2 | 1.60 | 0.43 |
| 1:BL:171:ASP:HA | 1:BL:172:PRO:HD3 | 1.76 | 0.43 |
| 1:BM:171:ASP:HA | 1:BM:172:PRO:HD3 | 1.79 | 0.43 |
| 1:BN:272:TYR:N | 1:BN:272:TYR:CD1 | 2.86 | 0.43 |
| 1:BN:404:LEU:HD22 | 1:BN:486:VAL:HG22 | 2.01 | 0.43 |
| 1:BO:393:HIS:CG | 1:BO:496:PHE:HB3 | 2.52 | 0.43 |
| 1:CA:79:ARG:HG3 | 1:CA:79:ARG:NH1 | 2.29 | 0.43 |
| 1:CA:423:LYS:HE2 | 1:CA:449:GLU:O | 2.19 | 0.43 |
| 1:CC:393:HIS:CG | 1:CC:496:PHE:HB3 | 2.52 | 0.43 |
| 1:CD:226:VAL:HG13 | 1:CD:228:GLY:H | 1.82 | 0.43 |
| 1:CG:423:LYS:HE2 | 1:CG:449:GLU:O | 2.17 | 0.43 |
| 1:CH:404:LEU:HD22 | 1:CH:486:VAL:HG22 | 1.99 | 0.43 |
| 1:CI:324:LEU:HD23 | 1:CI:324:LEU:C | 2.38 | 0.43 |
| 1:CK:188:PHE:C | 1:CK:189:PHE:HD1 | 2.21 | 0.43 |
| 1:CK:252:VAL:HG22 | 1:CK:253:SER:N | 2.33 | 0.43 |
| 1:CO:232:THR:HB | 1:CO:334:VAL:CG2 | 2.49 | 0.43 |
| 1:CS:189:PHE:CE2 | 1:CS:249:LEU:HD21 | 2.53 | 0.43 |
| 1:AD:55:ARG:HD3 | 1:AN:272:TYR:HD2 | 1.78 | 0.43 |
| 1:AD:393:HIS:CG | 1:AD:496:PHE:HB3 | 2.52 | 0.43 |
| 1:AJ:263:ASN:O | 1:AJ:267:LYS:HG3 | 2.18 | 0.43 |
| 1:AK:252:VAL:HG22 | 1:AK:253:SER:N | 2.33 | 0.43 |
| 1:AM:25:ILE:HG23 | 1:AM:152:LEU:HD11 | 2.00 | 0.43 |
| 1:AM:237:VAL:HG23 | 1:AM:279:PHE:CD2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AM:379:VAL:HG11 | 1:AM:381:MET:HE1 | 2.00 | 0.43 |
| 1:AR:250:TRP:HZ3 | 1:AR:272:TYR:HE1 | 1.61 | 0.43 |
| 1:BB:55:ARG:HD3 | 1:CB:272:TYR:HD2 | 1.81 | 0.43 |
| 1:BB:239:ILE:HD12 | 1:BB:275:GLU:HA | 2.00 | 0.43 |
| 1:BC:11:PRO:HG2 | 1:BC:18:ARG:HD2 | 2.00 | 0.43 |
| 1:BC:272:TYR:CE2 | 1:CA:55:ARG:CZ | 3.00 | 0.43 |
| 1:BE:232:THR:HB | 1:BE:334:VAL:HG23 | 1.99 | 0.43 |
| 1:BE:379:VAL:HG11 | 1:BE:381:MET:HE1 | 1.99 | 0.43 |
| 1:BG:232:THR:HB | 1:BG:334:VAL:HG23 | 2.00 | 0.43 |
| 1:BH:55:ARG:NE | 1:BK:272:TYR:HE2 | 2.12 | 0.43 |
| 1:BL:238:HIS:HE1 | 1:BL:329:GLN:OE1 | 2.01 | 0.43 |
| 1:BM:16:ALA:O | 1:BM:17:ASN:CB | 2.65 | 0.43 |
| 1:BN:108:ILE:HG23 | 1:BN:113:LEU:HD12 | 2.00 | 0.43 |
| 1:BN:189:PHE:CE2 | 1:BN:249:LEU:HD21 | 2.48 | 0.43 |
| 1:BO:61:PHE:CD2 | 1:BO:243:ILE:HD11 | 2.53 | 0.43 |
| 1:BP:239:ILE:HD12 | 1:BP:275:GLU:HA | 2.00 | 0.43 |
| 1:BP:442:GLN:HE21 | 1:BQ:412:PHE:HB2 | 1.82 | 0.43 |
| 1:BQ:324:LEU:HD23 | 1:BQ:324:LEU:C | 2.39 | 0.43 |
| 1:BT:371:ASP:OD1 | 1:BT:381:MET:HG2 | 2.19 | 0.43 |
| 1:CA:189:PHE:CE2 | 1:CA:249:LEU:HD21 | 2.53 | 0.43 |
| 1:CI:55:ARG:CZ | 1:CR:272:TYR:CD2 | 3.02 | 0.43 |
| 1:CJ:189:PHE:HD2 | 1:CJ:247:ILE:HD11 | 1.83 | 0.43 |
| 1:CL:58:ALA:HB2 | 1:CL:102:GLY:HA3 | 2.00 | 0.43 |
| 1:CO:188:PHE:C | 1:CO:189:PHE:HD1 | 2.22 | 0.43 |
| 1:CS:239:ILE:HD12 | 1:CS:275:GLU:HA | 1.99 | 0.43 |
| 1:AC:232:THR:HB | 1:AC:334:VAL:HG23 | 2.00 | 0.43 |
| 1:AC:252:VAL:HG22 | 1:AC:253:SER:N | 2.33 | 0.43 |
| 1:AC:300:GLN:HE21 | 1:AC:300:GLN:HB2 | 1.53 | 0.43 |
| 1:AK:232:THR:HB | 1:AK:334:VAL:CG2 | 2.49 | 0.43 |
| 1:AM:170:PHE:HD1 | 1:AM:389:MET:CE | 2.32 | 0.43 |
| 1:AM:454:ASN:HD22 | 1:AM:454:ASN:C | 2.22 | 0.43 |
| 1:AO:191:LEU:HD23 | 1:AO:191:LEU:N | 2.16 | 0.43 |
| 1:AO:263:ASN:O | 1:AO:267:LYS:HG3 | 2.17 | 0.43 |
| 1:AR:77:THR:O | 1:AR:81:THR:HG23 | 2.18 | 0.43 |
| 1:BC:423:LYS:HE2 | 1:BC:449:GLU:O | 2.19 | 0.43 |
| 1:BG:379:VAL:HG12 | 1:BG:381:MET:HE2 | 2.01 | 0.43 |
| 1:BI:202:LEU:HD23 | 1:BI:202:LEU:HA | 1.87 | 0.43 |
| 1:BJ:239:ILE:HD12 | 1:BJ:275:GLU:HA | 2.00 | 0.43 |
| 1:BL:170:PHE:HD1 | 1:BL:389:MET:HE2 | 1.83 | 0.43 |
| 1:BO:22:THR:OG1 | 1:BO:131:HIS:CD2 | 2.65 | 0.43 |
| 1:BO:175:PHE:CD2 | 1:BO:175:PHE:O | 2.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BP:201:GLY:HA3 | 1:BP:300:GLN:HG2 | 1.99 | 0.43 |
| 1:BP:232:THR:HB | 1:BP:334:VAL:CG2 | 2.47 | 0.43 |
| 1:BR:163:LEU:HD12 | 1:BR:163:LEU:HA | 1.87 | 0.43 |
| 1:CA:234:ARG:CG | 1:CA:280:GLU:HG2 | 2.49 | 0.43 |
| 1:CB:237:VAL:HG23 | 1:CB:279:PHE:CD2 | 2.53 | 0.43 |
| 1:CC:189:PHE:HD2 | 1:CC:247:ILE:HD11 | 1.83 | 0.43 |
| 1:CD:202:LEU:HD23 | 1:CD:202:LEU:HA | 1.89 | 0.43 |
| 1:CE:237:VAL:HG23 | 1:CE:279:PHE:CD2 | 2.54 | 0.43 |
| 1:CF:284:ARG:CG | 1:CF:284:ARG:NH1 | 2.74 | 0.43 |
| 1:CI:30:SER:O | 1:CI:33:LYS:HB2 | 2.18 | 0.43 |
| 1:CI:234:ARG:HG2 | 1:CI:280:GLU:HG2 | 1.99 | 0.43 |
| 1:CN:239:ILE:HG12 | 1:CN:326:ILE:CD1 | 2.47 | 0.43 |
| 1:CP:454:ASN:HD21 | 1:CP:456:ALA:HB3 | 1.84 | 0.43 |
| 1:CT:239:ILE:HD12 | 1:CT:275:GLU:HA | 2.01 | 0.43 |
| 1:AB:272:TYR:HE2 | 1:CB:55:ARG:NE | 2.06 | 0.43 |
| 1:AC:170:PHE:HD1 | 1:AC:389:MET:CE | 2.31 | 0.43 |
| 1:AE:234:ARG:HG2 | 1:AE:280:GLU:HG2 | 1.99 | 0.43 |
| 1:AK:189:PHE:HE2 | 1:AK:249:LEU:HD21 | 1.84 | 0.43 |
| 1:AM:10:ILE:HG21 | 1:AM:146:TRP:CZ2 | 2.54 | 0.43 |
| 1:AN:14:CYS:H | 1:AN:138:ASN:ND2 | 2.17 | 0.43 |
| 1:AP:442:GLN:NE2 | 1:AQ:412:PHE:HB2 | 2.34 | 0.43 |
| 1:AT:170:PHE:HD1 | 1:AT:389:MET:HE2 | 1.84 | 0.43 |
| 1:AT:237:VAL:HG23 | 1:AT:279:PHE:CD2 | 2.54 | 0.43 |
| 1:BB:418:SER:HB3 | 1:BC:407:SER:HB3 | 2.00 | 0.43 |
| 1:BC:55:ARG:HD3 | 1:BT:272:TYR:HD2 | 1.84 | 0.43 |
| 1:BD:58:ALA:HB2 | 1:BD:102:GLY:HA3 | 1.99 | 0.43 |
| 1:BE:272:TYR:N | 1:BE:272:TYR:HD1 | 2.16 | 0.43 |
| 1:BG:74:ASN:ND2 | 1:BG:77:THR:OG1 | 2.51 | 0.43 |
| 1:BG:272:TYR:HD2 | 1:CG:55:ARG:HD3 | 1.78 | 0.43 |
| 1:BI:234:ARG:CG | 1:BI:280:GLU:HG2 | 2.49 | 0.43 |
| 1:BL:226:VAL:HG13 | 1:BL:228:GLY:H | 1.83 | 0.43 |
| 1:CB:272:TYR:N | 1:CB:272:TYR:HD1 | 2.16 | 0.43 |
| 1:CE:371:ASP:OD1 | 1:CE:381:MET:HG2 | 2.18 | 0.43 |
| 1:CF:418:SER:HB3 | 1:CG:407:SER:HB3 | 2.01 | 0.43 |
| 1:CG:252:VAL:HG22 | 1:CG:253:SER:N | 2.34 | 0.43 |
| 1:CK:108:ILE:HG23 | 1:CK:113:LEU:HD12 | 2.01 | 0.43 |
| 1:CR:285:SER:HA | 1:CR:286:PRO:HD3 | 1.91 | 0.43 |
| 1:AC:272:TYR:CD2 | 1:BA:55:ARG:CZ | 3.01 | 0.43 |
| 1:AD:5:ARG:HD3 | 1:AN:263:ASN:HD22 | 1.84 | 0.43 |
| 1:AK:237:VAL:HG23 | 1:AK:279:PHE:CD2 | 2.54 | 0.43 |
| 1:AM:189:PHE:HD2 | 1:AM:247:ILE:HD11 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AM:202:LEU:HD23 | 1:AM:202:LEU:HA | 1.86 | 0.43 |
| 1:AN:318:SER:HA | 1:AN:319:GLY:HA2 | 1.78 | 0.43 |
| 1:AP:188:PHE:C | 1:AP:189:PHE:HD1 | 2.22 | 0.43 |
| 1:AQ:371:ASP:OD1 | 1:AQ:381:MET:HG2 | 2.18 | 0.43 |
| 1:BE:171:ASP:HA | 1:BE:172:PRO:HD3 | 1.78 | 0.43 |
| 1:BK:171:ASP:HA | 1:BK:172:PRO:HD3 | 1.81 | 0.43 |
| 1:BM:442:GLN:HE21 | 1:BN:412:PHE:HB2 | 1.83 | 0.43 |
| 1:BP:170:PHE:HD1 | 1:BP:389:MET:CE | 2.32 | 0.43 |
| 1:BP:232:THR:HB | 1:BP:334:VAL:HG23 | 2.01 | 0.43 |
| 1:BP:234:ARG:HG2 | 1:BP:280:GLU:HG2 | 2.00 | 0.43 |
| 1:BS:11:PRO:HG2 | 1:BS:18:ARG:HD2 | 2.01 | 0.43 |
| 1:BS:239:ILE:HD12 | 1:BS:275:GLU:HA | 2.01 | 0.43 |
| 1:BT:272:TYR:N | 1:BT:272:TYR:CD1 | 2.86 | 0.43 |
| 1:CC:33:LYS:HB2 | 1:CC:33:LYS:HE2 | 1.94 | 0.43 |
| 1:CC:55:ARG:CZ | 1:CT:272:TYR:CE2 | 3.01 | 0.43 |
| 1:CF:324:LEU:HD23 | 1:CF:324:LEU:C | 2.39 | 0.43 |
| 1:CJ:191:LEU:CD2 | 1:CJ:191:LEU:N | 2.78 | 0.43 |
| 1:CK:232:THR:HB | 1:CK:334:VAL:CG2 | 2.49 | 0.43 |
| 1:CO:189:PHE:CE2 | 1:CO:249:LEU:HD21 | 2.53 | 0.43 |
| 1:CO:239:ILE:HD12 | 1:CO:275:GLU:HA | 2.00 | 0.43 |
| 1:CO:263:ASN:O | 1:CO:267:LYS:HG3 | 2.19 | 0.43 |
| 1:AA:10:ILE:HG21 | 1:AA:146:TRP:CZ2 | 2.54 | 0.43 |
| 1:AB:371:ASP:OD1 | 1:AB:381:MET:HG2 | 2.19 | 0.43 |
| 1:AG:232:THR:HB | 1:AG:334:VAL:HG23 | 2.01 | 0.43 |
| 1:AK:239:ILE:HD12 | 1:AK:275:GLU:HA | 2.00 | 0.43 |
| 1:AL:379:VAL:HG11 | 1:AL:381:MET:HE1 | 2.00 | 0.43 |
| 1:AL:454:ASN:HD21 | 1:AL:456:ALA:HB3 | 1.84 | 0.43 |
| 1:AM:182:LEU:C | 1:AM:182:LEU:HD12 | 2.39 | 0.43 |
| 1:AN:238:HIS:HE1 | 1:AN:329:GLN:OE1 | 2.00 | 0.43 |
| 1:AN:423:LYS:HE2 | 1:AN:449:GLU:O | 2.19 | 0.43 |
| 1:AP:423:LYS:HE2 | 1:AP:449:GLU:O | 2.19 | 0.43 |
| 1:AQ:237:VAL:HG23 | 1:AQ:279:PHE:CD2 | 2.54 | 0.43 |
| 1:BC:108:ILE:HG23 | 1:BC:113:LEU:HD12 | 2.00 | 0.43 |
| 1:BC:182:LEU:HG | 1:BC:330:ILE:HB | 1.99 | 0.43 |
| 1:BE:263:ASN:O | 1:BE:267:LYS:HG3 | 2.18 | 0.43 |
| 1:BH:272:TYR:N | 1:BH:272:TYR:HD1 | 2.15 | 0.43 |
| 1:BI:272:TYR:CE2 | 1:BO:55:ARG:CZ | 3.02 | 0.43 |
| 1:BR:395:LEU:HB2 | 1:BR:497:TYR:HB2 | 2.01 | 0.43 |
| 1:CA:263:ASN:O | 1:CA:267:LYS:HG3 | 2.18 | 0.43 |
| 1:CI:239:ILE:HD12 | 1:CI:275:GLU:HA | 2.00 | 0.43 |
| 1:CM:79:ARG:HH11 | 1:CM:79:ARG:CG | 2.31 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CR:232:THR:HB | 1:CR:334:VAL:CG2 | 2.49 | 0.43 |
| 1:AA:232:THR:HB | 1:AA:334:VAL:HG23 | 2.01 | 0.43 |
| 1:AB:55:ARG:HD3 | 1:BB:272:TYR:HD2 | 1.81 | 0.43 |
| 1:AB:202:LEU:HB2 | 1:AB:304:SER:O | 2.19 | 0.43 |
| 1:AB:272:TYR:CD2 | 1:CB:55:ARG:CZ | 3.01 | 0.43 |
| 1:AC:25:ILE:HG23 | 1:AC:152:LEU:HD11 | 2.01 | 0.43 |
| 1:AF:444:LEU:HD13 | 1:AJ:440:ALA:CB | 2.49 | 0.43 |
| 1:AI:272:TYR:HD2 | 1:AO:55:ARG:HD3 | 1.83 | 0.43 |
| 1:AK:454:ASN:HD21 | 1:AK:456:ALA:HB3 | 1.83 | 0.43 |
| 1:AO:58:ALA:HB2 | 1:AO:102:GLY:HA3 | 2.01 | 0.43 |
| 1:AP:33:LYS:O | 1:AP:33:LYS:CG | 2.58 | 0.43 |
| 1:AQ:404:LEU:N | 1:AQ:404:LEU:HD23 | 2.34 | 0.43 |
| 1:AS:440:ALA:HB3 | 1:AT:444:LEU:HD13 | 2.01 | 0.43 |
| 1:AT:318:SER:HA | 1:AT:319:GLY:HA2 | 1.78 | 0.43 |
| 1:BB:234:ARG:CG | 1:BB:280:GLU:HG2 | 2.48 | 0.43 |
| 1:BC:170:PHE:HD1 | 1:BC:389:MET:HE2 | 1.84 | 0.43 |
| 1:BD:263:ASN:O | 1:BD:267:LYS:HG3 | 2.19 | 0.43 |
| 1:BT:314:PRO:HB3 | 1:BT:324:LEU:HD13 | 2.00 | 0.43 |
| 1:CA:239:ILE:HD12 | 1:CA:275:GLU:HA | 2.00 | 0.43 |
| 1:CA:272:TYR:N | 1:CA:272:TYR:HD1 | 2.17 | 0.43 |
| 1:CB:442:GLN:HE21 | 1:CC:412:PHE:HB2 | 1.84 | 0.43 |
| 1:CC:237:VAL:HG23 | 1:CC:279:PHE:CD2 | 2.54 | 0.43 |
| 1:CF:43:ALA:HB1 | 1:CF:158:GLU:HA | 2.01 | 0.43 |
| 1:CL:10:ILE:HA | 1:CL:11:PRO:HD3 | 1.88 | 0.43 |
| 1:CR:300:GLN:HE21 | 1:CR:300:GLN:HB2 | 1.71 | 0.43 |
| 1:CS:170:PHE:HD1 | 1:CS:389:MET:CE | 2.31 | 0.43 |
| 1:AA:8:ILE:HG22 | 1:AA:10:ILE:CD1 | 2.49 | 0.42 |
| 1:AB:79:ARG:CG | 1:AB:79:ARG:NH1 | 2.82 | 0.42 |
| 1:AC:272:TYR:HD2 | 1:BA:55:ARG:HD3 | 1.82 | 0.42 |
| 1:AD:232:THR:HB | 1:AD:334:VAL:CG2 | 2.49 | 0.42 |
| 1:AK:324:LEU:HD23 | 1:AK:324:LEU:C | 2.40 | 0.42 |
| 1:AN:22:THR:OG1 | 1:AN:131:HIS:CD2 | 2.63 | 0.42 |
| 1:AN:300:GLN:HE21 | 1:AN:300:GLN:HB2 | 1.60 | 0.42 |
| 1:AR:74:ASN:ND2 | 1:AR:77:THR:OG1 | 2.52 | 0.42 |
| 1:AR:300:GLN:HE21 | 1:AR:300:GLN:HB2 | 1.54 | 0.42 |
| 1:AT:25:ILE:HG23 | 1:AT:152:LEU:HD11 | 2.01 | 0.42 |
| 1:BA:252:VAL:HG22 | 1:BA:253:SER:N | 2.34 | 0.42 |
| 1:BB:14:CYS:H | 1:BB:138:ASN:ND2 | 2.12 | 0.42 |
| 1:BC:170:PHE:HD1 | 1:BC:389:MET:CE | 2.32 | 0.42 |
| 1:BC:239:ILE:HG23 | 1:BC:324:LEU:HD21 | 2.00 | 0.42 |
| 1:BF:226:VAL:HG13 | 1:BF:228:GLY:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BF:237:VAL:HG23 | 1:BF:279:PHE:CD2 | 2.54 | 0.42 |
| 1:BG:189:PHE:HD2 | 1:BG:247:ILE:CD1 | 2.31 | 0.42 |
| 1:BI:404:LEU:N | 1:BI:404:LEU:HD23 | 2.33 | 0.42 |
| 1:BJ:10:ILE:CD1 | 1:BJ:20:LEU:HD13 | 2.49 | 0.42 |
| 1:BJ:25:ILE:HG23 | 1:BJ:152:LEU:HD11 | 2.01 | 0.42 |
| 1:BN:232:THR:HB | 1:BN:334:VAL:HG23 | 2.00 | 0.42 |
| 1:CA:18:ARG:HG3 | 1:CA:19:TYR:N | 2.32 | 0.42 |
| 1:CB:393:HIS:CG | 1:CB:496:PHE:HB3 | 2.53 | 0.42 |
| 1:CD:43:ALA:HB1 | 1:CD:158:GLU:HA | 2.00 | 0.42 |
| 1:CD:250:TRP:CE3 | 1:CD:272:TYR:CD1 | 3.07 | 0.42 |
| 1:CI:299:SER:OG | 1:CI:301:ARG:HG2 | 2.18 | 0.42 |
| 1:CI:442:GLN:HE21 | 1:CJ:412:PHE:HB2 | 1.83 | 0.42 |
| 1:CL:189:PHE:CE2 | 1:CL:249:LEU:HD21 | 2.54 | 0.42 |
| 1:CM:442:GLN:HE21 | 1:CN:412:PHE:HB2 | 1.84 | 0.42 |
| 1:CN:237:VAL:HG23 | 1:CN:279:PHE:CD2 | 2.54 | 0.42 |
| 1:CP:234:ARG:HG2 | 1:CP:280:GLU:HG2 | 1.99 | 0.42 |
| 1:CR:226:VAL:HG13 | 1:CR:228:GLY:H | 1.83 | 0.42 |
| 1:AA:454:ASN:HD21 | 1:AA:456:ALA:HB3 | 1.84 | 0.42 |
| 1:AB:232:THR:HB | 1:AB:334:VAL:CG2 | 2.49 | 0.42 |
| 1:AB:404:LEU:N | 1:AB:404:LEU:HD23 | 2.34 | 0.42 |
| 1:AC:440:ALA:CB | 1:AD:444:LEU:HD13 | 2.49 | 0.42 |
| 1:AI:239:ILE:HD12 | 1:AI:275:GLU:HA | 2.01 | 0.42 |
| 1:AI:423:LYS:HE2 | 1:AI:449:GLU:O | 2.18 | 0.42 |
| 1:AL:232:THR:HB | 1:AL:334:VAL:HG23 | 2.01 | 0.42 |
| 1:AL:272:TYR:CE2 | 1:CJ:55:ARG:CZ | 3.02 | 0.42 |
| 1:AQ:162:PHE:CD1 | 1:AR:287:TYR:HA | 2.54 | 0.42 |
| 1:AR:324:LEU:HA | 1:AR:325:PRO:HD3 | 1.85 | 0.42 |
| 1:AT:30:SER:O | 1:AT:33:LYS:HB2 | 2.19 | 0.42 |
| 1:BC:55:ARG:CZ | 1:BT:272:TYR:CD2 | 3.02 | 0.42 |
| 1:BD:188:PHE:C | 1:BD:189:PHE:HD1 | 2.23 | 0.42 |
| 1:BE:189:PHE:HD2 | 1:BE:247:ILE:HD11 | 1.83 | 0.42 |
| 1:BF:79:ARG:HH11 | 1:BF:79:ARG:CG | 2.19 | 0.42 |
| 1:BI:318:SER:HA | 1:BI:319:GLY:HA2 | 1.78 | 0.42 |
| 1:BK:25:ILE:HG23 | 1:BK:152:LEU:HD11 | 2.01 | 0.42 |
| 1:BO:11:PRO:HG2 | 1:BO:18:ARG:HD2 | 2.01 | 0.42 |
| 1:BS:395:LEU:HB2 | 1:BS:497:TYR:HB2 | 2.00 | 0.42 |
| 1:CC:239:ILE:HD12 | 1:CC:275:GLU:HA | 2.01 | 0.42 |
| 1:CE:20:LEU:HB2 | 1:CE:132:PHE:O | 2.19 | 0.42 |
| 1:CI:79:ARG:HH11 | 1:CI:79:ARG:CG | 2.33 | 0.42 |
| 1:CJ:163:LEU:HD12 | 1:CJ:163:LEU:HA | 1.85 | 0.42 |
| 1:CJ:324:LEU:C | 1:CJ:324:LEU:HD23 | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CK:444:LEU:HD13 | 1:CO:440:ALA:HB3 | 2.01 | 0.42 |
| 1:CL:79:ARG:HH11 | 1:CL:79:ARG:CG | 2.28 | 0.42 |
| 1:CM:423:LYS:HE2 | 1:CM:449:GLU:O | 2.19 | 0.42 |
| 1:CN:234:ARG:HG2 | 1:CN:280:GLU:HG2 | 2.01 | 0.42 |
| 1:CQ:395:LEU:HB2 | 1:CQ:497:TYR:HB2 | 2.01 | 0.42 |
| 1:CQ:423:LYS:HE2 | 1:CQ:449:GLU:O | 2.19 | 0.42 |
| 1:AB:250:TRP:HZ3 | 1:AB:272:TYR:HE1 | 1.61 | 0.42 |
| 1:AD:239:ILE:HD12 | 1:AD:275:GLU:HA | 2.01 | 0.42 |
| 1:AG:239:ILE:HG12 | 1:AG:326:ILE:CD1 | 2.50 | 0.42 |
| 1:AH:14:CYS:H | 1:AH:138:ASN:ND2 | 2.16 | 0.42 |
| 1:AK:170:PHE:HD1 | 1:AK:389:MET:HE2 | 1.83 | 0.42 |
| 1:AL:423:LYS:HE2 | 1:AL:449:GLU:O | 2.19 | 0.42 |
| 1:AN:30:SER:O | 1:AN:33:LYS:HB2 | 2.19 | 0.42 |
| 1:AO:401:ASP:O | 1:AO:488:CYS:HA | 2.19 | 0.42 |
| 1:AO:423:LYS:HE2 | 1:AO:449:GLU:O | 2.18 | 0.42 |
| 1:AP:239:ILE:HD12 | 1:AP:275:GLU:HA | 2.00 | 0.42 |
| 1:AP:255:TRP:CE3 | 1:AP:285:SER:HB2 | 2.54 | 0.42 |
| 1:AP:440:ALA:HB3 | 1:AQ:444:LEU:HD13 | 2.01 | 0.42 |
| 1:AT:252:VAL:HG22 | 1:AT:253:SER:N | 2.35 | 0.42 |
| 1:BA:18:ARG:HG3 | 1:BA:19:TYR:N | 2.34 | 0.42 |
| 1:BA:226:VAL:HG13 | 1:BA:228:GLY:H | 1.84 | 0.42 |
| 1:BB:203:THR:HB | 1:BB:300:GLN:HG3 | 2.01 | 0.42 |
| 1:BG:237:VAL:HG23 | 1:BG:279:PHE:CD2 | 2.54 | 0.42 |
| 1:BK:226:VAL:HG13 | 1:BK:228:GLY:H | 1.83 | 0.42 |
| 1:BK:423:LYS:HE2 | 1:BK:449:GLU:O | 2.20 | 0.42 |
| 1:BM:182:LEU:HD12 | 1:BM:182:LEU:C | 2.39 | 0.42 |
| 1:BP:393:HIS:CG | 1:BP:496:PHE:HB3 | 2.54 | 0.42 |
| 1:BQ:300:GLN:HE21 | 1:BQ:300:GLN:HB2 | 1.60 | 0.42 |
| 1:BR:234:ARG:HG2 | 1:BR:280:GLU:HG2 | 2.01 | 0.42 |
| 1:CB:189:PHE:HD2 | 1:CB:247:ILE:HD11 | 1.83 | 0.42 |
| 1:CF:25:ILE:HG23 | 1:CF:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CG:324:LEU:C | 1:CG:324:LEU:HD23 | 2.40 | 0.42 |
| 1:CI:55:ARG:CZ | 1:CR:272:TYR:CE2 | 3.02 | 0.42 |
| 1:CL:272:TYR:N | 1:CL:272:TYR:HD1 | 2.16 | 0.42 |
| 1:CL:440:ALA:CB | 1:CM:444:LEU:HD13 | 2.49 | 0.42 |
| 1:CP:256:ASN:HD22 | 1:CP:302:ASP:HA | 1.84 | 0.42 |
| 1:CP:404:LEU:HD22 | 1:CP:486:VAL:HG22 | 1.99 | 0.42 |
| 1:CQ:175:PHE:CD2 | 1:CQ:175:PHE:O | 2.73 | 0.42 |
| 1:CR:239:ILE:HG12 | 1:CR:326:ILE:CD1 | 2.48 | 0.42 |
| 1:AF:185:PRO:HA | 1:AF:186:PRO:HD3 | 1.90 | 0.42 |
| 1:AG:442:GLN:HE21 | 1:AH:412:PHE:HB2 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:14:CYS:HB3 | 1:AK:64:LEU:HD21 | 2.01 | 0.42 |
| 1:AM:318:SER:HA | 1:AM:319:GLY:HA2 | 1.80 | 0.42 |
| 1:AQ:263:ASN:O | 1:AQ:267:LYS:HG3 | 2.19 | 0.42 |
| 1:AQ:318:SER:HA | 1:AQ:319:GLY:HA2 | 1.80 | 0.42 |
| 1:BD:371:ASP:OD1 | 1:BD:381:MET:HG2 | 2.20 | 0.42 |
| 1:BF:232:THR:HB | 1:BF:334:VAL:HG23 | 2.00 | 0.42 |
| 1:BF:442:GLN:HE21 | 1:BG:412:PHE:HB2 | 1.84 | 0.42 |
| 1:BJ:371:ASP:OD1 | 1:BJ:381:MET:HG2 | 2.19 | 0.42 |
| 1:BN:423:LYS:HE2 | 1:BN:449:GLU:O | 2.19 | 0.42 |
| 1:BO:171:ASP:HA | 1:BO:172:PRO:HD3 | 1.79 | 0.42 |
| 1:BO:423:LYS:HE2 | 1:BO:449:GLU:O | 2.19 | 0.42 |
| 1:BP:324:LEU:C | 1:BP:324:LEU:HD23 | 2.40 | 0.42 |
| 1:BR:25:ILE:HG23 | 1:BR:152:LEU:HD11 | 2.00 | 0.42 |
| 1:CB:189:PHE:CE2 | 1:CB:249:LEU:HD21 | 2.49 | 0.42 |
| 1:CB:207:VAL:HA | 1:CB:208:PRO:HD3 | 1.82 | 0.42 |
| 1:CH:25:ILE:HG23 | 1:CH:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CH:207:VAL:HA | 1:CH:208:PRO:HD3 | 1.84 | 0.42 |
| 1:CH:318:SER:HA | 1:CH:319:GLY:HA2 | 1.76 | 0.42 |
| 1:CL:442:GLN:HE21 | 1:CM:412:PHE:HB2 | 1.85 | 0.42 |
| 1:CN:272:TYR:CD1 | 1:CN:272:TYR:N | 2.87 | 0.42 |
| 1:CN:404:LEU:HD22 | 1:CN:486:VAL:HG22 | 2.00 | 0.42 |
| 1:CP:324:LEU:HD23 | 1:CP:324:LEU:C | 2.40 | 0.42 |
| 1:AA:239:ILE:HG23 | 1:AA:324:LEU:HD21 | 2.01 | 0.42 |
| 1:AA:379:VAL:HG11 | 1:AA:381:MET:HE1 | 2.02 | 0.42 |
| 1:AA:404:LEU:HD22 | 1:AA:486:VAL:HG22 | 2.00 | 0.42 |
| 1:AG:234:ARG:CG | 1:AG:280:GLU:HG2 | 2.49 | 0.42 |
| 1:AI:404:LEU:N | 1:AI:404:LEU:HD23 | 2.34 | 0.42 |
| 1:AL:395:LEU:HB2 | 1:AL:497:TYR:HB2 | 2.01 | 0.42 |
| 1:AM:324:LEU:HD23 | 1:AM:324:LEU:C | 2.40 | 0.42 |
| 1:AO:252:VAL:HG22 | 1:AO:253:SER:N | 2.33 | 0.42 |
| 1:BA:207:VAL:HA | 1:BA:208:PRO:HD3 | 1.86 | 0.42 |
| 1:BB:191:LEU:CD2 | 1:BB:191:LEU:N | 2.73 | 0.42 |
| 1:BF:272:TYR:N | 1:BF:272:TYR:HD1 | 2.17 | 0.42 |
| 1:BI:170:PHE:HD1 | 1:BI:389:MET:HE2 | 1.84 | 0.42 |
| 1:BI:232:THR:HB | 1:BI:334:VAL:CG2 | 2.49 | 0.42 |
| 1:BI:237:VAL:HG23 | 1:BI:279:PHE:CD2 | 2.54 | 0.42 |
| 1:BK:272:TYR:N | 1:BK:272:TYR:HD1 | 2.17 | 0.42 |
| 1:BK:437:HIS:CE1 | 1:BL:405:GLN:NE2 | 2.88 | 0.42 |
| 1:BL:239:ILE:HG23 | 1:BL:324:LEU:HD21 | 2.01 | 0.42 |
| 1:BP:55:ARG:CZ | 1:CM:272:TYR:CE2 | 3.03 | 0.42 |
| 1:BQ:454:ASN:HD21 | 1:BQ:456:ALA:HB3 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BR:404:LEU:HD22 | 1:BR:486:VAL:HG22 | 2.01 | 0.42 |
| 1:BS:340:LEU:HD23 | 1:BS:340:LEU:HA | 1.88 | 0.42 |
| 1:BT:182:LEU:C | 1:BT:182:LEU:HD12 | 2.39 | 0.42 |
| 1:BT:252:VAL:HG22 | 1:BT:253:SER:N | 2.33 | 0.42 |
| 1:CB:234:ARG:HG2 | 1:CB:280:GLU:HG2 | 2.00 | 0.42 |
| 1:CD:25:ILE:HG23 | 1:CD:152:LEU:HD11 | 2.00 | 0.42 |
| 1:CH:79:ARG:NH1 | 1:CH:79:ARG:CG | 2.77 | 0.42 |
| 1:CH:234:ARG:HG2 | 1:CH:280:GLU:HG2 | 2.00 | 0.42 |
| 1:CK:171:ASP:HA | 1:CK:172:PRO:HD3 | 1.79 | 0.42 |
| 1:CL:22:THR:OG1 | 1:CL:131:HIS:CD2 | 2.63 | 0.42 |
| 1:CR:14:CYS:HB3 | 1:CR:64:LEU:HD21 | 2.01 | 0.42 |
| 1:CT:234:ARG:HG2 | 1:CT:280:GLU:HG2 | 2.02 | 0.42 |
| 1:AC:74:ASN:ND2 | 1:AC:77:THR:OG1 | 2.53 | 0.42 |
| 1:AD:442:GLN:NE2 | 1:AE:412:PHE:HB2 | 2.34 | 0.42 |
| 1:AE:263:ASN:O | 1:AE:267:LYS:HG3 | 2.19 | 0.42 |
| 1:AF:55:ARG:CZ | 1:BH:272:TYR:CE2 | 3.02 | 0.42 |
| 1:AJ:61:PHE:CD2 | 1:AJ:243:ILE:HD11 | 2.55 | 0.42 |
| 1:AK:55:ARG:CZ | 1:CF:272:TYR:CE2 | 3.02 | 0.42 |
| 1:AN:418:SER:HB3 | 1:AO:407:SER:HB3 | 2.01 | 0.42 |
| 1:AP:285:SER:HA | 1:AP:286:PRO:HD3 | 1.91 | 0.42 |
| 1:AQ:234:ARG:CG | 1:AQ:280:GLU:HG2 | 2.49 | 0.42 |
| 1:AR:182:LEU:HG | 1:AR:330:ILE:HB | 2.02 | 0.42 |
| 1:AT:79:ARG:HG3 | 1:AT:79:ARG:NH1 | 2.31 | 0.42 |
| 1:BA:189:PHE:HD2 | 1:BA:247:ILE:CD1 | 2.33 | 0.42 |
| 1:BA:324:LEU:HD23 | 1:BA:324:LEU:C | 2.39 | 0.42 |
| 1:BC:232:THR:HB | 1:BC:334:VAL:HG23 | 2.02 | 0.42 |
| 1:BC:430:MET:CE | 1:BD:296:ALA:HA | 2.49 | 0.42 |
| 1:BG:423:LYS:HE2 | 1:BG:449:GLU:O | 2.18 | 0.42 |
| 1:BH:14:CYS:H | 1:BH:138:ASN:ND2 | 2.14 | 0.42 |
| 1:BH:237:VAL:HG23 | 1:BH:279:PHE:CD2 | 2.54 | 0.42 |
| 1:BI:171:ASP:HA | 1:BI:172:PRO:HD3 | 1.79 | 0.42 |
| 1:BM:203:THR:CB | 1:BM:300:GLN:HG3 | 2.49 | 0.42 |
| 1:BM:381:MET:HE2 | 1:BM:381:MET:HB2 | 1.84 | 0.42 |
| 1:BO:182:LEU:HG | 1:BO:330:ILE:HB | 2.02 | 0.42 |
| 1:BS:423:LYS:HE2 | 1:BS:449:GLU:O | 2.20 | 0.42 |
| 1:BT:14:CYS:H | 1:BT:138:ASN:ND2 | 2.14 | 0.42 |
| 1:CC:18:ARG:HG2 | 1:CC:20:LEU:HD23 | 2.01 | 0.42 |
| 1:CF:20:LEU:HB2 | 1:CF:132:PHE:O | 2.19 | 0.42 |
| 1:CH:272:TYR:N | 1:CH:272:TYR:HD1 | 2.17 | 0.42 |
| 1:CJ:25:ILE:HG23 | 1:CJ:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CL:191:LEU:CD2 | 1:CL:191:LEU:N | 2.75 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CM:418:SER:HB3 | 1:CN:407:SER:HB3 | 2.01 | 0.42 |
| 1:CN:379:VAL:HG11 | 1:CN:381:MET:HE1 | 2.02 | 0.42 |
| 1:CQ:442:GLN:HE21 | 1:CR:412:PHE:HB2 | 1.84 | 0.42 |
| 1:AI:442:GLN:HE21 | 1:AJ:412:PHE:HB2 | 1.84 | 0.42 |
| 1:AK:10:ILE:HA | 1:AK:11:PRO:HD3 | 1.88 | 0.42 |
| 1:AM:440:ALA:HB3 | 1:AN:444:LEU:HD13 | 2.00 | 0.42 |
| 1:AN:252:VAL:HG22 | 1:AN:253:SER:N | 2.34 | 0.42 |
| 1:AR:55:ARG:HG2 | 1:AR:55:ARG:HH11 | 1.83 | 0.42 |
| 1:BA:33:LYS:O | 1:BA:33:LYS:CG | 2.59 | 0.42 |
| 1:BA:191:LEU:CD2 | 1:BA:191:LEU:N | 2.77 | 0.42 |
| 1:BB:226:VAL:HG13 | 1:BB:228:GLY:H | 1.84 | 0.42 |
| 1:BE:182:LEU:C | 1:BE:182:LEU:HD12 | 2.40 | 0.42 |
| 1:BF:300:GLN:HE21 | 1:BF:300:GLN:HB2 | 1.58 | 0.42 |
| 1:BI:182:LEU:C | 1:BI:182:LEU:HD12 | 2.40 | 0.42 |
| 1:BJ:162:PHE:CD2 | 1:BJ:163:LEU:HD13 | 2.55 | 0.42 |
| 1:BJ:201:GLY:HA3 | 1:BJ:300:GLN:HG2 | 2.00 | 0.42 |
| 1:BK:263:ASN:O | 1:BK:267:LYS:HG3 | 2.20 | 0.42 |
| 1:BL:272:TYR:CD1 | 1:BL:272:TYR:N | 2.85 | 0.42 |
| 1:BO:250:TRP:HE3 | 1:BO:272:TYR:CD1 | 2.37 | 0.42 |
| 1:CB:226:VAL:HG13 | 1:CB:228:GLY:H | 1.84 | 0.42 |
| 1:CD:440:ALA:CB | 1:CE:444:LEU:HD13 | 2.50 | 0.42 |
| 1:CG:418:SER:HB3 | 1:CH:407:SER:HB3 | 2.02 | 0.42 |
| 1:CJ:379:VAL:HG11 | 1:CJ:381:MET:HE1 | 2.02 | 0.42 |
| 1:CJ:404:LEU:N | 1:CJ:404:LEU:HD23 | 2.35 | 0.42 |
| 1:CM:182:LEU:C | 1:CM:182:LEU:HD12 | 2.40 | 0.42 |
| 1:CM:252:VAL:HG22 | 1:CM:253:SER:N | 2.35 | 0.42 |
| 1:CR:324:LEU:C | 1:CR:324:LEU:HD23 | 2.40 | 0.42 |
| 1:AC:18:ARG:HG3 | 1:AC:19:TYR:N | 2.34 | 0.42 |
| 1:AC:256:ASN:HD22 | 1:AC:302:ASP:HA | 1.85 | 0.42 |
| 1:AD:423:LYS:HE2 | 1:AD:449:GLU:O | 2.19 | 0.42 |
| 1:AE:252:VAL:HG22 | 1:AE:253:SER:N | 2.35 | 0.42 |
| 1:AF:43:ALA:HB1 | 1:AF:158:GLU:HA | 2.02 | 0.42 |
| 1:AF:232:THR:HB | 1:AF:334:VAL:HG23 | 2.01 | 0.42 |
| 1:AF:412:PHE:HB2 | 1:AJ:442:GLN:NE2 | 2.35 | 0.42 |
| 1:AJ:234:ARG:CG | 1:AJ:280:GLU:HG2 | 2.50 | 0.42 |
| 1:AL:239:ILE:HG12 | 1:AL:326:ILE:CD1 | 2.50 | 0.42 |
| 1:AO:10:ILE:HA | 1:AO:11:PRO:HD3 | 1.90 | 0.42 |
| 1:AQ:423:LYS:HE2 | 1:AQ:449:GLU:O | 2.20 | 0.42 |
| 1:AT:163:LEU:HD12 | 1:AT:163:LEU:HA | 1.84 | 0.42 |
| 1:AT:207:VAL:HA | 1:AT:208:PRO:HD3 | 1.85 | 0.42 |
| 1:BB:232:THR:HB | 1:BB:334:VAL:HG23 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BB:238:HIS:HE1 | 1:BB:329:GLN:OE1 | 2.02 | 0.42 |
| 1:BC:18:ARG:HG2 | 1:BC:20:LEU:HD23 | 2.01 | 0.42 |
| 1:BC:318:SER:HA | 1:BC:319:GLY:HA2 | 1.78 | 0.42 |
| 1:BF:15:GLN:HA | 1:BF:15:GLN:HE21 | 1.84 | 0.42 |
| 1:BF:75:ARG:NH2 | 1:BF:391:ALA:O | 2.49 | 0.42 |
| 1:BK:340:LEU:HD23 | 1:BK:340:LEU:HA | 1.89 | 0.42 |
| 1:BR:28:MET:CE | 1:BR:152:LEU:HG | 2.50 | 0.42 |
| 1:BR:182:LEU:HG | 1:BR:330:ILE:HB | 2.01 | 0.42 |
| 1:BR:272:TYR:N | 1:BR:272:TYR:HD1 | 2.18 | 0.42 |
| 1:BR:371:ASP:OD1 | 1:BR:381:MET:HG2 | 2.20 | 0.42 |
| 1:BS:239:ILE:HG23 | 1:BS:324:LEU:HD21 | 2.02 | 0.42 |
| 1:CA:379:VAL:HG11 | 1:CA:381:MET:HE1 | 2.00 | 0.42 |
| 1:CB:182:LEU:C | 1:CB:182:LEU:HD12 | 2.40 | 0.42 |
| 1:CC:226:VAL:HG13 | 1:CC:228:GLY:H | 1.85 | 0.42 |
| 1:CE:189:PHE:CE1 | 1:CE:198:ARG:HG2 | 2.53 | 0.42 |
| 1:CI:232:THR:HB | 1:CI:334:VAL:CG2 | 2.50 | 0.42 |
| 1:CO:33:LYS:HB2 | 1:CO:33:LYS:HE2 | 1.96 | 0.42 |
| 1:CO:234:ARG:CG | 1:CO:280:GLU:HG2 | 2.50 | 0.42 |
| 1:CO:250:TRP:CE3 | 1:CO:272:TYR:CD1 | 3.07 | 0.42 |
| 1:CP:423:LYS:HE2 | 1:CP:449:GLU:O | 2.20 | 0.42 |
| 1:AA:232:THR:HB | 1:AA:334:VAL:CG2 | 2.50 | 0.42 |
| 1:AE:197:LEU:HD21 | 1:AE:258:THR:HG21 | 2.02 | 0.42 |
| 1:AH:55:ARG:CZ | 1:AK:272:TYR:CE2 | 3.03 | 0.42 |
| 1:AH:58:ALA:HB2 | 1:AH:102:GLY:HA3 | 2.02 | 0.42 |
| 1:AK:55:ARG:CZ | 1:CF:272:TYR:CD2 | 3.02 | 0.42 |
| 1:AN:207:VAL:HA | 1:AN:208:PRO:HD3 | 1.83 | 0.42 |
| 1:AN:285:SER:HA | 1:AN:286:PRO:HD3 | 1.93 | 0.42 |
| 1:AQ:79:ARG:HG3 | 1:AQ:79:ARG:NH1 | 2.32 | 0.42 |
| 1:AQ:182:LEU:HD12 | 1:AQ:182:LEU:C | 2.40 | 0.42 |
| 1:AT:16:ALA:O | 1:AT:17:ASN:HB2 | 2.20 | 0.42 |
| 1:AT:55:ARG:HD3 | 1:BA:272:TYR:HD2 | 1.80 | 0.42 |
| 1:BI:324:LEU:HD23 | 1:BI:324:LEU:C | 2.40 | 0.42 |
| 1:BJ:163:LEU:HD12 | 1:BJ:163:LEU:HA | 1.84 | 0.42 |
| 1:BJ:189:PHE:CE1 | 1:BJ:198:ARG:HG2 | 2.55 | 0.42 |
| 1:BK:170:PHE:HD1 | 1:BK:389:MET:CE | 2.32 | 0.42 |
| 1:BO:234:ARG:CG | 1:BO:280:GLU:HG2 | 2.50 | 0.42 |
| 1:BT:272:TYR:N | 1:BT:272:TYR:HD1 | 2.18 | 0.42 |
| 1:BT:324:LEU:HA | 1:BT:325:PRO:HD3 | 1.88 | 0.42 |
| 1:CB:318:SER:HA | 1:CB:319:GLY:HA2 | 1.76 | 0.42 |
| 1:CD:423:LYS:HE2 | 1:CD:449:GLU:O | 2.19 | 0.42 |
| 1:CN:393:HIS:CG | 1:CN:496:PHE:HB3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CP:25:ILE:HG23 | 1:CP:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CQ:162:PHE:CD1 | 1:CR:287:TYR:HA | 2.55 | 0.42 |
| 1:CS:203:THR:CB | 1:CS:300:GLN:HG3 | 2.49 | 0.42 |
| 1:AA:185:PRO:HA | 1:AA:186:PRO:HD3 | 1.93 | 0.42 |
| 1:AE:272:TYR:CD2 | 1:AM:55:ARG:CZ | 3.03 | 0.42 |
| 1:AG:324:LEU:HA | 1:AG:325:PRO:HD3 | 1.89 | 0.42 |
| 1:AH:191:LEU:HD23 | 1:AH:191:LEU:N | 2.22 | 0.42 |
| 1:AM:263:ASN:O | 1:AM:267:LYS:HG3 | 2.20 | 0.42 |
| 1:AO:188:PHE:C | 1:AO:189:PHE:HD1 | 2.23 | 0.42 |
| 1:AP:189:PHE:HE2 | 1:AP:249:LEU:CD2 | 2.33 | 0.42 |
| 1:AP:237:VAL:HG23 | 1:AP:279:PHE:CD2 | 2.55 | 0.42 |
| 1:AT:18:ARG:HG3 | 1:AT:19:TYR:N | 2.35 | 0.42 |
| 1:BA:163:LEU:HD21 | 1:BA:458:ALA:HB2 | 2.01 | 0.42 |
| 1:BD:324:LEU:HD23 | 1:BD:324:LEU:C | 2.40 | 0.42 |
| 1:BG:175:PHE:CD2 | 1:BG:175:PHE:O | 2.73 | 0.42 |
| 1:BH:202:LEU:HD23 | 1:BH:202:LEU:HA | 1.85 | 0.42 |
| 1:BH:318:SER:HA | 1:BH:319:GLY:HA2 | 1.78 | 0.42 |
| 1:BL:234:ARG:HG2 | 1:BL:280:GLU:HG2 | 2.00 | 0.42 |
| 1:BL:300:GLN:HE21 | 1:BL:300:GLN:HB2 | 1.58 | 0.42 |
| 1:BN:25:ILE:HG23 | 1:BN:152:LEU:HD11 | 2.01 | 0.42 |
| 1:BO:25:ILE:HG23 | 1:BO:152:LEU:HD11 | 2.02 | 0.42 |
| 1:BQ:371:ASP:OD1 | 1:BQ:381:MET:HG2 | 2.20 | 0.42 |
| 1:BS:272:TYR:N | 1:BS:272:TYR:CD1 | 2.88 | 0.42 |
| 1:CB:423:LYS:HE2 | 1:CB:449:GLU:O | 2.20 | 0.42 |
| 1:CC:263:ASN:O | 1:CC:267:LYS:HG3 | 2.19 | 0.42 |
| 1:CD:232:THR:HB | 1:CD:334:VAL:HG23 | 2.02 | 0.42 |
| 1:CD:250:TRP:CZ3 | 1:CD:272:TYR:CD1 | 3.08 | 0.42 |
| 1:CE:25:ILE:HG23 | 1:CE:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CE:234:ARG:CG | 1:CE:280:GLU:HG2 | 2.50 | 0.42 |
| 1:CE:256:ASN:HD22 | 1:CE:302:ASP:HA | 1.84 | 0.42 |
| 1:CF:226:VAL:HG13 | 1:CF:228:GLY:H | 1.85 | 0.42 |
| 1:CI:25:ILE:HG23 | 1:CI:152:LEU:HD11 | 2.01 | 0.42 |
| 1:CI:324:LEU:HA | 1:CI:325:PRO:HD3 | 1.88 | 0.42 |
| 1:CO:237:VAL:HG23 | 1:CO:279:PHE:CD2 | 2.55 | 0.42 |
| 1:CO:250:TRP:CZ3 | 1:CO:272:TYR:CD1 | 3.08 | 0.42 |
| 1:CS:14:CYS:H | 1:CS:138:ASN:ND2 | 2.17 | 0.42 |
| 1:CS:226:VAL:HG13 | 1:CS:228:GLY:H | 1.85 | 0.42 |
| 1:CS:252:VAL:HG22 | 1:CS:253:SER:N | 2.35 | 0.42 |
| 1:AB:170:PHE:HD1 | 1:AB:389:MET:CE | 2.33 | 0.41 |
| 1:AC:263:ASN:O | 1:AC:267:LYS:HG3 | 2.20 | 0.41 |
| 1:AC:404:LEU:N | 1:AC:404:LEU:HD23 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AD:10:ILE:CD1 | 1:AD:20:LEU:HD13 | 2.49 | 0.41 |
| 1:AD:55:ARG:CZ | 1:AN:272:TYR:CE2 | 3.02 | 0.41 |
| 1:AE:272:TYR:HD2 | 1:AM:55:ARG:HD3 | 1.82 | 0.41 |
| 1:AF:371:ASP:OD1 | 1:AF:381:MET:HG2 | 2.20 | 0.41 |
| 1:AI:189:PHE:HD2 | 1:AI:247:ILE:HD11 | 1.85 | 0.41 |
| 1:AJ:48:PRO:HG2 | 1:AJ:50:PHE:CZ | 2.55 | 0.41 |
| 1:AJ:55:ARG:CZ | 1:BL:272:TYR:CE2 | 3.02 | 0.41 |
| 1:AL:55:ARG:CZ | 1:CQ:272:TYR:CD2 | 3.03 | 0.41 |
| 1:AL:381:MET:HE2 | 1:AL:381:MET:HB2 | 1.88 | 0.41 |
| 1:AN:226:VAL:HG13 | 1:AN:228:GLY:H | 1.85 | 0.41 |
| 1:AP:191:LEU:HD23 | 1:AP:191:LEU:N | 2.15 | 0.41 |
| 1:AQ:272:TYR:CD2 | 1:BL:55:ARG:CD | 3.02 | 0.41 |
| 1:AT:300:GLN:HE21 | 1:AT:300:GLN:HB2 | 1.55 | 0.41 |
| 1:BD:25:ILE:HG23 | 1:BD:152:LEU:HD11 | 2.02 | 0.41 |
| 1:BE:175:PHE:CD2 | 1:BE:175:PHE:O | 2.73 | 0.41 |
| 1:BE:252:VAL:HG22 | 1:BE:253:SER:N | 2.36 | 0.41 |
| 1:BG:324:LEU:HD23 | 1:BG:324:LEU:C | 2.40 | 0.41 |
| 1:BH:55:ARG:CZ | 1:BK:272:TYR:CD2 | 3.03 | 0.41 |
| 1:BI:20:LEU:HB2 | 1:BI:132:PHE:O | 2.20 | 0.41 |
| 1:BM:255:TRP:CE3 | 1:BM:285:SER:HB2 | 2.55 | 0.41 |
| 1:CB:379:VAL:HG11 | 1:CB:381:MET:HE1 | 2.02 | 0.41 |
| 1:CC:55:ARG:CZ | 1:CT:272:TYR:CD2 | 3.03 | 0.41 |
| 1:CC:189:PHE:HE2 | 1:CC:249:LEU:HD21 | 1.85 | 0.41 |
| 1:CD:48:PRO:HG2 | 1:CD:50:PHE:CZ | 2.55 | 0.41 |
| 1:CD:79:ARG:HG3 | 1:CD:79:ARG:NH1 | 2.14 | 0.41 |
| 1:CL:232:THR:HB | 1:CL:334:VAL:HG23 | 2.01 | 0.41 |
| 1:CM:58:ALA:HB2 | 1:CM:102:GLY:HA3 | 2.02 | 0.41 |
| 1:CQ:234:ARG:HG2 | 1:CQ:280:GLU:HG2 | 2.02 | 0.41 |
| 1:AF:74:ASN:ND2 | 1:AF:77:THR:OG1 | 2.53 | 0.41 |
| 1:AF:440:ALA:HB3 | 1:AG:444:LEU:HD13 | 2.02 | 0.41 |
| 1:AG:207:VAL:HA | 1:AG:208:PRO:HD3 | 1.81 | 0.41 |
| 1:AK:61:PHE:CE2 | 1:AK:243:ILE:HD11 | 2.54 | 0.41 |
| 1:AM:272:TYR:N | 1:AM:272:TYR:HD1 | 2.18 | 0.41 |
| 1:AN:55:ARG:NE | 1:AS:272:TYR:CD2 | 2.88 | 0.41 |
| 1:AN:77:THR:O | 1:AN:81:THR:HG23 | 2.20 | 0.41 |
| 1:AN:379:VAL:HG12 | 1:AN:381:MET:HE2 | 2.02 | 0.41 |
| 1:AP:234:ARG:HG2 | 1:AP:280:GLU:HG2 | 2.01 | 0.41 |
| 1:AQ:58:ALA:HB2 | 1:AQ:102:GLY:HA3 | 2.02 | 0.41 |
| 1:AR:318:SER:HA | 1:AR:319:GLY:HA2 | 1.75 | 0.41 |
| 1:BB:16:ALA:O | 1:BB:17:ASN:CB | 2.64 | 0.41 |
| 1:BB:170:PHE:HD1 | 1:BB:389:MET:CE | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BB:252:VAL:HG22 | 1:BB:253:SER:N | 2.35 | 0.41 |
| 1:BG:379:VAL:HG11 | 1:BG:381:MET:HE1 | 2.01 | 0.41 |
| 1:BK:191:LEU:CD2 | 1:BK:191:LEU:N | 2.76 | 0.41 |
| 1:BK:440:ALA:HB3 | 1:BL:444:LEU:HD13 | 2.02 | 0.41 |
| 1:BO:226:VAL:HG13 | 1:BO:228:GLY:H | 1.85 | 0.41 |
| 1:CA:19:TYR:CZ | 1:CA:81:THR:HG22 | 2.55 | 0.41 |
| 1:CB:14:CYS:H | 1:CB:138:ASN:ND2 | 2.18 | 0.41 |
| 1:CC:16:ALA:O | 1:CC:17:ASN:HB2 | 2.20 | 0.41 |
| 1:CD:252:VAL:HG22 | 1:CD:253:SER:N | 2.35 | 0.41 |
| 1:CD:371:ASP:OD1 | 1:CD:381:MET:HG2 | 2.20 | 0.41 |
| 1:CJ:379:VAL:HG12 | 1:CJ:381:MET:HE2 | 2.02 | 0.41 |
| 1:CK:189:PHE:CE2 | 1:CK:249:LEU:HD21 | 2.55 | 0.41 |
| 1:CN:14:CYS:HB3 | 1:CN:64:LEU:HD21 | 2.01 | 0.41 |
| 1:AA:238:HIS:HE1 | 1:AA:329:GLN:OE1 | 2.03 | 0.41 |
| 1:AB:300:GLN:HE21 | 1:AB:300:GLN:HB2 | 1.46 | 0.41 |
| 1:AC:185:PRO:HA | 1:AC:186:PRO:HD3 | 1.93 | 0.41 |
| 1:AF:207:VAL:HA | 1:AF:208:PRO:HD3 | 1.86 | 0.41 |
| 1:AG:36:GLN:HE22 | 1:AG:156:LEU:H | 1.66 | 0.41 |
| 1:AK:188:PHE:C | 1:AK:189:PHE:HD1 | 2.24 | 0.41 |
| 1:AL:232:THR:HB | 1:AL:334:VAL:CG2 | 2.50 | 0.41 |
| 1:BA:423:LYS:HE2 | 1:BA:449:GLU:O | 2.20 | 0.41 |
| 1:BC:372:PHE:H | 1:BC:381:MET:HE1 | 1.85 | 0.41 |
| 1:BE:324:LEU:HA | 1:BE:325:PRO:HD3 | 1.87 | 0.41 |
| 1:BF:189:PHE:CE2 | 1:BF:249:LEU:HD21 | 2.49 | 0.41 |
| 1:BP:272:TYR:CE2 | 1:CE:55:ARG:HD3 | 2.55 | 0.41 |
| 1:BQ:379:VAL:HG11 | 1:BQ:381:MET:HE1 | 2.02 | 0.41 |
| 1:BS:182:LEU:C | 1:BS:182:LEU:HD12 | 2.41 | 0.41 |
| 1:BT:285:SER:HA | 1:BT:286:PRO:HD3 | 1.92 | 0.41 |
| 1:CC:232:THR:HB | 1:CC:334:VAL:CG2 | 2.49 | 0.41 |
| 1:CF:272:TYR:N | 1:CF:272:TYR:HD1 | 2.16 | 0.41 |
| 1:CG:202:LEU:HD23 | 1:CG:202:LEU:HA | 1.93 | 0.41 |
| 1:CG:404:LEU:HD22 | 1:CG:486:VAL:HG22 | 2.02 | 0.41 |
| 1:CH:182:LEU:C | 1:CH:182:LEU:HD12 | 2.40 | 0.41 |
| 1:CI:189:PHE:CE1 | 1:CI:198:ARG:HG2 | 2.55 | 0.41 |
| 1:CI:379:VAL:HG12 | 1:CI:381:MET:HE2 | 2.01 | 0.41 |
| 1:CJ:171:ASP:HA | 1:CJ:172:PRO:HD3 | 1.78 | 0.41 |
| 1:CL:239:ILE:HD12 | 1:CL:275:GLU:HA | 2.01 | 0.41 |
| 1:CM:237:VAL:HG23 | 1:CM:279:PHE:CD2 | 2.55 | 0.41 |
| 1:CN:55:ARG:CZ | 1:CS:272:TYR:CE2 | 3.03 | 0.41 |
| 1:CP:188:PHE:C | 1:CP:189:PHE:HD1 | 2.24 | 0.41 |
| 1:CT:318:SER:HA | 1:CT:319:GLY:HA2 | 1.78 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AD:324:LEU:C | 1:AD:324:LEU:HD23 | 2.41 | 0.41 |
| 1:AF:22:THR:OG1 | 1:AF:131:HIS:CD2 | 2.60 | 0.41 |
| 1:AG:14:CYS:H | 1:AG:138:ASN:ND2 | 2.15 | 0.41 |
| 1:AH:234:ARG:CG | 1:AH:280:GLU:HG2 | 2.50 | 0.41 |
| 1:AK:47:MET:HG2 | 1:AK:117:ALA:HB2 | 2.03 | 0.41 |
| 1:AK:189:PHE:CE2 | 1:AK:249:LEU:HD21 | 2.55 | 0.41 |
| 1:AL:404:LEU:N | 1:AL:404:LEU:HD23 | 2.34 | 0.41 |
| 1:AM:440:ALA:CB | 1:AN:444:LEU:HD13 | 2.50 | 0.41 |
| 1:AO:372:PHE:H | 1:AO:381:MET:HE1 | 1.85 | 0.41 |
| 1:AP:14:CYS:H | 1:AP:138:ASN:ND2 | 2.18 | 0.41 |
| 1:AQ:272:TYR:N | 1:AQ:272:TYR:HD1 | 2.17 | 0.41 |
| 1:AS:22:THR:OG1 | 1:AS:131:HIS:CD2 | 2.63 | 0.41 |
| 1:BF:55:ARG:CZ | 1:CH:272:TYR:CD2 | 3.04 | 0.41 |
| 1:BH:22:THR:OG1 | 1:BH:131:HIS:CD2 | 2.64 | 0.41 |
| 1:BH:55:ARG:CZ | 1:BK:272:TYR:CE2 | 3.04 | 0.41 |
| 1:BS:300:GLN:HE21 | 1:BS:300:GLN:HB2 | 1.57 | 0.41 |
| 1:BS:379:VAL:HG11 | 1:BS:381:MET:HE1 | 2.02 | 0.41 |
| 1:CD:163:LEU:HD12 | 1:CD:163:LEU:HA | 1.85 | 0.41 |
| 1:CE:207:VAL:HA | 1:CE:208:PRO:HD3 | 1.83 | 0.41 |
| 1:CE:272:TYR:CD2 | 1:CM:55:ARG:CZ | 3.03 | 0.41 |
| 1:CF:207:VAL:HA | 1:CF:208:PRO:HD3 | 1.83 | 0.41 |
| 1:CF:239:ILE:HG23 | 1:CF:324:LEU:HD21 | 2.02 | 0.41 |
| 1:CG:175:PHE:CD2 | 1:CG:175:PHE:O | 2.74 | 0.41 |
| 1:CG:239:ILE:HG23 | 1:CG:324:LEU:HD21 | 2.02 | 0.41 |
| 1:CJ:423:LYS:HE2 | 1:CJ:449:GLU:O | 2.20 | 0.41 |
| 1:CL:379:VAL:HG11 | 1:CL:381:MET:HE1 | 2.01 | 0.41 |
| 1:CT:182:LEU:HG | 1:CT:330:ILE:HB | 2.02 | 0.41 |
| 1:AA:202:LEU:HD23 | 1:AA:202:LEU:HA | 1.91 | 0.41 |
| 1:AE:300:GLN:HE21 | 1:AE:300:GLN:HB2 | 1.72 | 0.41 |
| 1:AG:25:ILE:HG23 | 1:AG:152:LEU:HD11 | 2.03 | 0.41 |
| 1:AG:285:SER:HA | 1:AG:286:PRO:HD3 | 1.94 | 0.41 |
| 1:AH:163:LEU:HD12 | 1:AH:163:LEU:HA | 1.90 | 0.41 |
| 1:AK:52:ILE:HD11 | 1:AK:108:ILE:HD12 | 2.03 | 0.41 |
| 1:AK:202:LEU:HB2 | 1:AK:304:SER:O | 2.21 | 0.41 |
| 1:AN:20:LEU:HB2 | 1:AN:132:PHE:O | 2.21 | 0.41 |
| 1:AO:79:ARG:NH1 | 1:AO:79:ARG:CG | 2.84 | 0.41 |
| 1:AO:250:TRP:CZ3 | 1:AO:272:TYR:CD1 | 3.06 | 0.41 |
| 1:AR:43:ALA:HB1 | 1:AR:158:GLU:HA | 2.02 | 0.41 |
| 1:AS:239:ILE:HD12 | 1:AS:275:GLU:HA | 2.02 | 0.41 |
| 1:AS:252:VAL:HG22 | 1:AS:253:SER:N | 2.35 | 0.41 |
| 1:AT:379:VAL:CG1 | 1:AT:381:MET:CE | 2.98 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BD:239:ILE:HD12 | 1:BD:275:GLU:HA | 2.02 | 0.41 |
| 1:BD:442:GLN:HE21 | 1:BE:412:PHE:HB2 | 1.86 | 0.41 |
| 1:BG:170:PHE:HD1 | 1:BG:389:MET:CE | 2.33 | 0.41 |
| 1:BL:170:PHE:HD1 | 1:BL:389:MET:CE | 2.33 | 0.41 |
| 1:BO:379:VAL:HG11 | 1:BO:381:MET:HE1 | 2.01 | 0.41 |
| 1:BP:412:PHE:HB2 | 1:BT:442:GLN:HE21 | 1.86 | 0.41 |
| 1:BR:252:VAL:HG22 | 1:BR:253:SER:N | 2.36 | 0.41 |
| 1:BT:234:ARG:CG | 1:BT:280:GLU:HG2 | 2.50 | 0.41 |
| 1:CA:412:PHE:HB2 | 1:CE:442:GLN:HE21 | 1.85 | 0.41 |
| 1:CE:163:LEU:HD12 | 1:CE:163:LEU:HA | 1.88 | 0.41 |
| 1:CE:171:ASP:HA | 1:CE:172:PRO:HD3 | 1.80 | 0.41 |
| 1:CF:252:VAL:HG22 | 1:CF:253:SER:N | 2.36 | 0.41 |
| 1:CF:423:LYS:HE2 | 1:CF:449:GLU:O | 2.19 | 0.41 |
| 1:CI:232:THR:HB | 1:CI:334:VAL:HG23 | 2.03 | 0.41 |
| 1:CM:20:LEU:HB2 | 1:CM:132:PHE:O | 2.21 | 0.41 |
| 1:CP:28:MET:CE | 1:CP:152:LEU:HG | 2.51 | 0.41 |
| 1:CP:250:TRP:CE3 | 1:CP:272:TYR:CD1 | 3.08 | 0.41 |
| 1:CP:252:VAL:HG22 | 1:CP:253:SER:N | 2.35 | 0.41 |
| 1:CP:255:TRP:CG | 1:CP:286:PRO:HD3 | 2.56 | 0.41 |
| 1:CQ:318:SER:HA | 1:CQ:319:GLY:HA2 | 1.76 | 0.41 |
| 1:CS:232:THR:HB | 1:CS:334:VAL:CG2 | 2.51 | 0.41 |
| 1:CT:324:LEU:HD23 | 1:CT:324:LEU:C | 2.41 | 0.41 |
| 1:CT:324:LEU:HA | 1:CT:325:PRO:HD3 | 1.87 | 0.41 |
| 1:AA:171:ASP:HA | 1:AA:172:PRO:HD3 | 1.83 | 0.41 |
| 1:AE:324:LEU:HD23 | 1:AE:324:LEU:C | 2.41 | 0.41 |
| 1:AE:371:ASP:OD1 | 1:AE:381:MET:HG2 | 2.20 | 0.41 |
| 1:AG:182:LEU:HG | 1:AG:330:ILE:HB | 2.03 | 0.41 |
| 1:AH:28:MET:HE2 | 1:AH:152:LEU:HG | 2.03 | 0.41 |
| 1:AH:55:ARG:NE | 1:AK:272:TYR:HE2 | 2.14 | 0.41 |
| 1:AI:61:PHE:CD2 | 1:AI:243:ILE:HD11 | 2.55 | 0.41 |
| 1:AI:182:LEU:C | 1:AI:182:LEU:HD12 | 2.41 | 0.41 |
| 1:AI:285:SER:HA | 1:AI:286:PRO:HD3 | 1.93 | 0.41 |
| 1:AO:202:LEU:HB2 | 1:AO:304:SER:O | 2.21 | 0.41 |
| 1:AR:239:ILE:HD12 | 1:AR:275:GLU:HA | 2.02 | 0.41 |
| 1:AS:11:PRO:HG2 | 1:AS:18:ARG:CD | 2.51 | 0.41 |
| 1:AS:182:LEU:HG | 1:AS:330:ILE:HB | 2.03 | 0.41 |
| 1:BB:300:GLN:HE21 | 1:BB:300:GLN:HB2 | 1.67 | 0.41 |
| 1:BE:201:GLY:HA3 | 1:BE:300:GLN:HG2 | 2.02 | 0.41 |
| 1:BF:108:ILE:HG23 | 1:BF:113:LEU:HD12 | 2.02 | 0.41 |
| 1:BH:163:LEU:HD12 | 1:BH:163:LEU:HA | 1.85 | 0.41 |
| 1:BI:263:ASN:O | 1:BI:267:LYS:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:425:VAL:HG11 | 1:BJ:342:SER:HB2 | 2.01 | 0.41 |
| 1:BL:52:ILE:HG12 | 1:BL:152:LEU:CD2 | 2.51 | 0.41 |
| 1:BM:170:PHE:HD1 | 1:BM:389:MET:HE2 | 1.85 | 0.41 |
| 1:BN:171:ASP:HA | 1:BN:172:PRO:HD3 | 1.79 | 0.41 |
| 1:BN:189:PHE:HD2 | 1:BN:247:ILE:HD11 | 1.86 | 0.41 |
| 1:BN:300:GLN:HE21 | 1:BN:300:GLN:HB2 | 1.53 | 0.41 |
| 1:BQ:226:VAL:HG13 | 1:BQ:228:GLY:H | 1.86 | 0.41 |
| 1:BR:255:TRP:CE3 | 1:BR:285:SER:HB2 | 2.56 | 0.41 |
| 1:BS:234:ARG:HG2 | 1:BS:280:GLU:HG2 | 2.03 | 0.41 |
| 1:CB:79:ARG:HH11 | 1:CB:79:ARG:CG | 2.27 | 0.41 |
| 1:CC:22:THR:OG1 | 1:CC:131:HIS:CD2 | 2.66 | 0.41 |
| 1:CC:171:ASP:HA | 1:CC:172:PRO:HD3 | 1.79 | 0.41 |
| 1:CD:175:PHE:CD2 | 1:CD:175:PHE:O | 2.74 | 0.41 |
| 1:CG:454:ASN:ND2 | 1:CG:456:ALA:H | 2.08 | 0.41 |
| 1:CH:28:MET:HE2 | 1:CH:152:LEU:HG | 2.02 | 0.41 |
| 1:CI:318:SER:HA | 1:CI:319:GLY:HA2 | 1.78 | 0.41 |
| 1:CL:440:ALA:HB3 | 1:CM:444:LEU:HD13 | 2.02 | 0.41 |
| 1:CN:162:PHE:CD2 | 1:CN:163:LEU:HD13 | 2.55 | 0.41 |
| 1:CN:226:VAL:HG13 | 1:CN:228:GLY:H | 1.85 | 0.41 |
| 1:CO:232:THR:HB | 1:CO:334:VAL:HG23 | 2.02 | 0.41 |
| 1:CQ:182:LEU:C | 1:CQ:182:LEU:HD12 | 2.41 | 0.41 |
| 1:CQ:404:LEU:HD22 | 1:CQ:486:VAL:HG22 | 2.03 | 0.41 |
| 1:CR:272:TYR:N | 1:CR:272:TYR:HD1 | 2.18 | 0.41 |
| 1:AA:272:TYR:CE2 | 1:CT:55:ARG:CZ | 3.04 | 0.41 |
| 1:AC:189:PHE:CE2 | 1:AC:249:LEU:HD21 | 2.56 | 0.41 |
| 1:AE:74:ASN:ND2 | 1:AE:77:THR:OG1 | 2.53 | 0.41 |
| 1:AF:324:LEU:HA | 1:AF:325:PRO:HD3 | 1.85 | 0.41 |
| 1:AI:170:PHE:HB2 | 1:AI:496:PHE:HE1 | 1.86 | 0.41 |
| 1:AI:454:ASN:ND2 | 1:AI:456:ALA:H | 2.12 | 0.41 |
| 1:AK:340:LEU:HD23 | 1:AK:340:LEU:HA | 1.89 | 0.41 |
| 1:AL:202:LEU:HD23 | 1:AL:202:LEU:HA | 1.86 | 0.41 |
| 1:AO:170:PHE:HD1 | 1:AO:389:MET:CE | 2.33 | 0.41 |
| 1:AP:232:THR:HB | 1:AP:334:VAL:CG2 | 2.51 | 0.41 |
| 1:AQ:170:PHE:HB2 | 1:AQ:496:PHE:HE1 | 1.85 | 0.41 |
| 1:AQ:188:PHE:C | 1:AQ:189:PHE:HD1 | 2.24 | 0.41 |
| 1:AR:226:VAL:HG13 | 1:AR:228:GLY:H | 1.85 | 0.41 |
| 1:AT:28:MET:CE | 1:AT:152:LEU:HG | 2.51 | 0.41 |
| 1:BD:33:LYS:HB2 | 1:BD:33:LYS:HE2 | 1.96 | 0.41 |
| 1:BG:454:ASN:HD21 | 1:BG:456:ALA:HB3 | 1.84 | 0.41 |
| 1:BK:14:CYS:H | 1:BK:138:ASN:ND2 | 2.15 | 0.41 |
| 1:BN:203:THR:HB | 1:BN:300:GLN:OE1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BO:73:TYR:CE2 | 1:BO:394:GLY:HA3 | 2.56 | 0.41 |
| 1:BO:324:LEU:HD23 | 1:BO:324:LEU:C | 2.41 | 0.41 |
| 1:BP:25:ILE:HG23 | 1:BP:152:LEU:HD11 | 2.01 | 0.41 |
| 1:BQ:404:LEU:N | 1:BQ:404:LEU:HD23 | 2.36 | 0.41 |
| 1:BS:108:ILE:HG23 | 1:BS:113:LEU:HD12 | 2.02 | 0.41 |
| 1:BS:252:VAL:HG22 | 1:BS:253:SER:N | 2.36 | 0.41 |
| 1:CD:263:ASN:O | 1:CD:267:LYS:HG3 | 2.21 | 0.41 |
| 1:CD:272:TYR:CD2 | 1:CS:55:ARG:CD | 3.02 | 0.41 |
| 1:CE:404:LEU:HD22 | 1:CE:486:VAL:HG22 | 2.03 | 0.41 |
| 1:CF:14:CYS:H | 1:CF:138:ASN:ND2 | 2.18 | 0.41 |
| 1:CJ:272:TYR:HD2 | 1:CQ:55:ARG:HD3 | 1.85 | 0.41 |
| 1:CK:9:TYR:HE1 | 1:CK:147:GLN:NE2 | 2.17 | 0.41 |
| 1:CK:10:ILE:HG21 | 1:CK:146:TRP:CZ2 | 2.56 | 0.41 |
| 1:CK:12:LYS:HB3 | 1:CK:144:ALA:C | 2.41 | 0.41 |
| 1:CK:300:GLN:HE21 | 1:CK:300:GLN:HB2 | 1.58 | 0.41 |
| 1:CK:395:LEU:HB2 | 1:CK:497:TYR:HB2 | 2.02 | 0.41 |
| 1:CM:239:ILE:HG23 | 1:CM:324:LEU:HD21 | 2.02 | 0.41 |
| 1:CO:454:ASN:ND2 | 1:CO:456:ALA:H | 2.09 | 0.41 |
| 1:CP:33:LYS:HB2 | 1:CP:33:LYS:HE2 | 1.93 | 0.41 |
| 1:CP:171:ASP:HA | 1:CP:172:PRO:HD3 | 1.76 | 0.41 |
| 1:CP:263:ASN:O | 1:CP:267:LYS:HG3 | 2.20 | 0.41 |
| 1:CR:108:ILE:HG23 | 1:CR:113:LEU:HD12 | 2.03 | 0.41 |
| 1:CS:324:LEU:HA | 1:CS:325:PRO:HD3 | 1.84 | 0.41 |
| 1:CS:401:ASP:O | 1:CS:488:CYS:HA | 2.21 | 0.41 |
| 1:AA:61:PHE:CD2 | 1:AA:243:ILE:HD11 | 2.56 | 0.41 |
| 1:AA:182:LEU:HG | 1:AA:330:ILE:HB | 2.02 | 0.41 |
| 1:AB:237:VAL:HG23 | 1:AB:279:PHE:CD2 | 2.55 | 0.41 |
| 1:AE:423:LYS:HE2 | 1:AE:449:GLU:O | 2.21 | 0.41 |
| 1:AF:241:ALA:HB1 | 1:AF:242:PRO:HD2 | 2.02 | 0.41 |
| 1:AG:182:LEU:C | 1:AG:182:LEU:HD12 | 2.40 | 0.41 |
| 1:AL:188:PHE:C | 1:AL:189:PHE:HD1 | 2.24 | 0.41 |
| 1:AQ:33:LYS:HB2 | 1:AQ:33:LYS:HE2 | 1.95 | 0.41 |
| 1:AT:28:MET:HE2 | 1:AT:152:LEU:HG | 2.02 | 0.41 |
| 1:BE:404:LEU:N | 1:BE:404:LEU:HD23 | 2.36 | 0.41 |
| 1:BF:232:THR:HB | 1:BF:334:VAL:CG2 | 2.50 | 0.41 |
| 1:BF:324:LEU:C | 1:BF:324:LEU:HD23 | 2.41 | 0.41 |
| 1:BF:475:LEU:HB3 | 1:BF:478:ALA:HB2 | 2.03 | 0.41 |
| 1:BG:11:PRO:HG2 | 1:BG:18:ARG:CD | 2.49 | 0.41 |
| 1:BG:185:PRO:HA | 1:BG:186:PRO:HD3 | 1.92 | 0.41 |
| 1:BG:202:LEU:HD23 | 1:BG:202:LEU:HA | 1.93 | 0.41 |
| 1:BI:442:GLN:HE21 | 1:BJ:412:PHE:HB2 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BJ:340:LEU:HD23 | 1:BJ:340:LEU:HA | 1.90 | 0.41 |
| 1:BJ:372:PHE:H | 1:BJ:381:MET:HE1 | 1.85 | 0.41 |
| 1:BN:182:LEU:C | 1:BN:182:LEU:HD12 | 2.41 | 0.41 |
| 1:BO:47:MET:HG2 | 1:BO:117:ALA:HB2 | 2.03 | 0.41 |
| 1:BO:185:PRO:HA | 1:BO:186:PRO:HD3 | 1.95 | 0.41 |
| 1:BP:185:PRO:HA | 1:BP:186:PRO:HD3 | 1.95 | 0.41 |
| 1:BQ:272:TYR:CE2 | 1:CL:55:ARG:CZ | 3.04 | 0.41 |
| 1:BR:170:PHE:HB2 | 1:BR:496:PHE:HE1 | 1.86 | 0.41 |
| 1:BR:324:LEU:HD23 | 1:BR:324:LEU:C | 2.41 | 0.41 |
| 1:BS:243:ILE:N | 1:BS:243:ILE:HD12 | 2.36 | 0.41 |
| 1:CF:379:VAL:CG1 | 1:CF:381:MET:CE | 2.98 | 0.41 |
| 1:CH:14:CYS:H | 1:CH:138:ASN:ND2 | 2.18 | 0.41 |
| 1:CJ:252:VAL:HG22 | 1:CJ:253:SER:N | 2.35 | 0.41 |
| 1:CK:232:THR:HB | 1:CK:334:VAL:HG23 | 2.02 | 0.41 |
| 1:CK:407:SER:HB3 | 1:CO:418:SER:HB3 | 2.02 | 0.41 |
| 1:CL:207:VAL:HA | 1:CL:208:PRO:HD3 | 1.85 | 0.41 |
| 1:CM:189:PHE:HD2 | 1:CM:247:ILE:HD11 | 1.84 | 0.41 |
| 1:CP:318:SER:HA | 1:CP:319:GLY:HA2 | 1.75 | 0.41 |
| 1:AA:11:PRO:HG2 | 1:AA:18:ARG:CD | 2.51 | 0.41 |
| 1:AA:108:ILE:HG23 | 1:AA:113:LEU:HD12 | 2.02 | 0.41 |
| 1:AA:203:THR:HB | 1:AA:300:GLN:HG3 | 2.01 | 0.41 |
| 1:AA:234:ARG:HG2 | 1:AA:280:GLU:HG2 | 2.01 | 0.41 |
| 1:AB:372:PHE:H | 1:AB:381:MET:HE1 | 1.86 | 0.41 |
| 1:AC:14:CYS:H | 1:AC:138:ASN:HD21 | 1.68 | 0.41 |
| 1:AC:55:ARG:CZ | 1:AT:272:TYR:CE2 | 3.03 | 0.41 |
| 1:AC:324:LEU:HA | 1:AC:325:PRO:HD3 | 1.86 | 0.41 |
| 1:AC:454:ASN:ND2 | 1:AC:456:ALA:HB3 | 2.36 | 0.41 |
| 1:AD:25:ILE:HG23 | 1:AD:152:LEU:HD11 | 2.03 | 0.41 |
| 1:AD:108:ILE:HG23 | 1:AD:113:LEU:HD12 | 2.03 | 0.41 |
| 1:AF:182:LEU:C | 1:AF:182:LEU:HD12 | 2.42 | 0.41 |
| 1:AF:182:LEU:HG | 1:AF:330:ILE:HB | 2.02 | 0.41 |
| 1:AH:256:ASN:HD22 | 1:AH:302:ASP:HA | 1.86 | 0.41 |
| 1:AH:263:ASN:O | 1:AH:267:LYS:HG3 | 2.21 | 0.41 |
| 1:AI:252:VAL:HG22 | 1:AI:253:SER:N | 2.36 | 0.41 |
| 1:AL:10:ILE:H | 1:AL:10:ILE:HG12 | 1.76 | 0.41 |
| 1:AL:43:ALA:HB1 | 1:AL:158:GLU:HA | 2.03 | 0.41 |
| 1:AL:207:VAL:HA | 1:AL:208:PRO:HD3 | 1.83 | 0.41 |
| 1:AL:252:VAL:HG22 | 1:AL:253:SER:N | 2.36 | 0.41 |
| 1:AM:185:PRO:HA | 1:AM:186:PRO:HD3 | 1.91 | 0.41 |
| 1:AO:171:ASP:HA | 1:AO:172:PRO:HD3 | 1.81 | 0.41 |
| 1:AO:185:PRO:HA | 1:AO:186:PRO:HD3 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AP:252:VAL:HG22 | 1:AP:253:SER:N | 2.36 | 0.41 |
| 1:AP:340:LEU:HD23 | 1:AP:340:LEU:HA | 1.91 | 0.41 |
| 1:AP:412:PHE:HB2 | 1:AT:442:GLN:HE21 | 1.85 | 0.41 |
| 1:AR:371:ASP:OD1 | 1:AR:381:MET:HG2 | 2.21 | 0.41 |
| 1:AR:440:ALA:CB | 1:AS:444:LEU:HD13 | 2.50 | 0.41 |
| 1:AR:440:ALA:HB3 | 1:AS:444:LEU:HD13 | 2.03 | 0.41 |
| 1:AS:77:THR:O | 1:AS:81:THR:HG23 | 2.21 | 0.41 |
| 1:AS:372:PHE:H | 1:AS:381:MET:HE1 | 1.86 | 0.41 |
| 1:AT:371:ASP:OD1 | 1:AT:381:MET:HG2 | 2.21 | 0.41 |
| 1:BC:379:VAL:HG11 | 1:BC:381:MET:HE1 | 2.02 | 0.41 |
| 1:BF:79:ARG:CG | 1:BF:79:ARG:NH1 | 2.80 | 0.41 |
| 1:BG:25:ILE:HD12 | 1:BG:128:PRO:HB2 | 2.03 | 0.41 |
| 1:BI:22:THR:OG1 | 1:BI:131:HIS:CD2 | 2.63 | 0.41 |
| 1:BI:55:ARG:HD3 | 1:BR:272:TYR:HD2 | 1.81 | 0.41 |
| 1:BJ:324:LEU:HA | 1:BJ:325:PRO:HD3 | 1.84 | 0.41 |
| 1:BL:189:PHE:HE2 | 1:BL:249:LEU:HD21 | 1.86 | 0.41 |
| 1:BL:272:TYR:N | 1:BL:272:TYR:HD1 | 2.19 | 0.41 |
| 1:BN:207:VAL:HA | 1:BN:208:PRO:HD3 | 1.83 | 0.41 |
| 1:BO:371:ASP:OD1 | 1:BO:381:MET:HG2 | 2.21 | 0.41 |
| 1:BP:250:TRP:HE3 | 1:BP:272:TYR:CD1 | 2.39 | 0.41 |
| 1:BR:28:MET:HE2 | 1:BR:152:LEU:HG | 2.03 | 0.41 |
| 1:BR:58:ALA:HB2 | 1:BR:102:GLY:HA3 | 2.03 | 0.41 |
| 1:BR:423:LYS:HE2 | 1:BR:449:GLU:O | 2.21 | 0.41 |
| 1:BT:20:LEU:HD11 | 1:BT:66:TRP:CD1 | 2.56 | 0.41 |
| 1:BT:263:ASN:O | 1:BT:267:LYS:HG3 | 2.20 | 0.41 |
| 1:CA:324:LEU:C | 1:CA:324:LEU:HD23 | 2.41 | 0.41 |
| 1:CD:126:GLU:HG3 | 1:CD:127:SER:H | 1.86 | 0.41 |
| 1:CF:475:LEU:HB3 | 1:CF:478:ALA:HB2 | 2.02 | 0.41 |
| 1:CG:48:PRO:HG2 | 1:CG:50:PHE:CZ | 2.56 | 0.41 |
| 1:CG:395:LEU:HB2 | 1:CG:497:TYR:HB2 | 2.02 | 0.41 |
| 1:CI:55:ARG:HD3 | 1:CR:272:TYR:CE2 | 2.55 | 0.41 |
| 1:CI:170:PHE:HD1 | 1:CI:389:MET:HE2 | 1.86 | 0.41 |
| 1:CI:252:VAL:HG22 | 1:CI:253:SER:N | 2.36 | 0.41 |
| 1:CI:443:LYS:HD3 | 1:CI:443:LYS:HA | 1.93 | 0.41 |
| 1:CJ:372:PHE:H | 1:CJ:381:MET:HE1 | 1.85 | 0.41 |
| 1:CM:108:ILE:HG23 | 1:CM:113:LEU:HD12 | 2.02 | 0.41 |
| 1:CM:170:PHE:HD1 | 1:CM:389:MET:CE | 2.34 | 0.41 |
| 1:CM:201:GLY:HA3 | 1:CM:300:GLN:HG2 | 2.02 | 0.41 |
| 1:CM:256:ASN:HD22 | 1:CM:302:ASP:HA | 1.86 | 0.41 |
| 1:CM:440:ALA:HB3 | 1:CN:444:LEU:HD13 | 2.03 | 0.41 |
| 1:CN:318:SER:HA | 1:CN:319:GLY:HA2 | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CN:340:LEU:HA | 1:CN:340:LEU:HD23 | 1.88 | 0.41 |
| 1:CN:404:LEU:N | 1:CN:404:LEU:HD23 | 2.35 | 0.41 |
| 1:CO:9:TYR:HE1 | 1:CO:147:GLN:HE21 | 1.69 | 0.41 |
| 1:CO:43:ALA:HB1 | 1:CO:158:GLU:HA | 2.03 | 0.41 |
| 1:CR:189:PHE:HD2 | 1:CR:247:ILE:HD11 | 1.86 | 0.41 |
| 1:CR:440:ALA:CB | 1:CS:444:LEU:HD13 | 2.51 | 0.41 |
| 1:AA:444:LEU:HD13 | 1:AE:440:ALA:CB | 2.51 | 0.41 |
| 1:AD:285:SER:HA | 1:AD:286:PRO:HD3 | 1.92 | 0.41 |
| 1:AD:371:ASP:OD1 | 1:AD:381:MET:HG2 | 2.20 | 0.41 |
| 1:AE:36:GLN:HE22 | 1:AE:156:LEU:H | 1.69 | 0.41 |
| 1:AL:28:MET:CE | 1:AL:152:LEU:HG | 2.51 | 0.41 |
| 1:AL:250:TRP:HZ3 | 1:AL:272:TYR:HE1 | 1.64 | 0.41 |
| 1:AL:442:GLN:NE2 | 1:AM:412:PHE:HB2 | 2.35 | 0.41 |
| 1:AM:33:LYS:HB2 | 1:AM:33:LYS:HE2 | 1.95 | 0.41 |
| 1:AN:175:PHE:O | 1:AN:175:PHE:CD2 | 2.74 | 0.41 |
| 1:AT:324:LEU:C | 1:AT:324:LEU:HD23 | 2.40 | 0.41 |
| 1:BA:37:TYR:O | 1:BA:40:TRP:HB3 | 2.21 | 0.41 |
| 1:BE:285:SER:HA | 1:BE:286:PRO:HD3 | 1.93 | 0.41 |
| 1:BF:263:ASN:O | 1:BF:267:LYS:HG3 | 2.21 | 0.41 |
| 1:BK:239:ILE:HG23 | 1:BK:324:LEU:HD21 | 2.02 | 0.41 |
| 1:BL:371:ASP:OD1 | 1:BL:381:MET:HG2 | 2.21 | 0.41 |
| 1:BO:25:ILE:HD12 | 1:BO:128:PRO:HB2 | 2.01 | 0.41 |
| 1:BO:401:ASP:O | 1:BO:488:CYS:HA | 2.22 | 0.41 |
| 1:BP:207:VAL:HA | 1:BP:208:PRO:HD3 | 1.83 | 0.41 |
| 1:BR:239:ILE:HG12 | 1:BR:326:ILE:CD1 | 2.50 | 0.41 |
| 1:BR:379:VAL:HG11 | 1:BR:381:MET:HE1 | 2.02 | 0.41 |
| 1:BR:379:VAL:HG12 | 1:BR:381:MET:HE2 | 2.03 | 0.41 |
| 1:BT:20:LEU:HB2 | 1:BT:132:PHE:O | 2.21 | 0.41 |
| 1:CA:182:LEU:HG | 1:CA:330:ILE:HB | 2.03 | 0.41 |
| 1:CA:252:VAL:HG22 | 1:CA:253:SER:N | 2.36 | 0.41 |
| 1:CA:444:LEU:HD13 | 1:CE:440:ALA:HB3 | 2.02 | 0.41 |
| 1:CD:324:LEU:C | 1:CD:324:LEU:HD23 | 2.40 | 0.41 |
| 1:CF:48:PRO:HG2 | 1:CF:50:PHE:CZ | 2.56 | 0.41 |
| 1:CF:162:PHE:CD1 | 1:CG:287:TYR:HA | 2.56 | 0.41 |
| 1:CF:324:LEU:HA | 1:CF:325:PRO:HD3 | 1.85 | 0.41 |
| 1:CI:20:LEU:HB2 | 1:CI:132:PHE:O | 2.21 | 0.41 |
| 1:CK:175:PHE:CD2 | 1:CK:175:PHE:O | 2.74 | 0.41 |
| 1:CK:412:PHE:HB2 | 1:CO:442:GLN:NE2 | 2.35 | 0.41 |
| 1:CM:163:LEU:HD12 | 1:CM:163:LEU:HA | 1.87 | 0.41 |
| 1:CQ:182:LEU:HG | 1:CQ:330:ILE:HB | 2.03 | 0.41 |
| 1:AB:18:ARG:HB2 | 1:AB:18:ARG:NH1 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AB:175:PHE:O | 1:AB:175:PHE:CD2 | 2.75 | 0.40 |
| 1:AC:234:ARG:CG | 1:AC:280:GLU:HG2 | 2.51 | 0.40 |
| 1:AG:239:ILE:HD12 | 1:AG:275:GLU:HA | 2.04 | 0.40 |
| 1:AH:10:ILE:HA | 1:AH:11:PRO:HD3 | 1.95 | 0.40 |
| 1:AH:182:LEU:C | 1:AH:182:LEU:HD12 | 2.41 | 0.40 |
| 1:AI:171:ASP:HA | 1:AI:172:PRO:HD3 | 1.77 | 0.40 |
| 1:AI:379:VAL:CG1 | 1:AI:381:MET:CE | 2.99 | 0.40 |
| 1:AM:393:HIS:CG | 1:AM:496:PHE:HB3 | 2.56 | 0.40 |
| 1:AN:241:ALA:HB1 | 1:AN:242:PRO:HD2 | 2.03 | 0.40 |
| 1:AO:74:ASN:ND2 | 1:AO:77:THR:OG1 | 2.55 | 0.40 |
| 1:AO:203:THR:HB | 1:AO:300:GLN:CG | 2.49 | 0.40 |
| 1:AP:75:ARG:NH2 | 1:AP:391:ALA:O | 2.53 | 0.40 |
| 1:AR:379:VAL:CG1 | 1:AR:381:MET:CE | 2.99 | 0.40 |
| 1:BF:379:VAL:CG1 | 1:BF:381:MET:CE | 2.99 | 0.40 |
| 1:BG:108:ILE:HG23 | 1:BG:113:LEU:HD12 | 2.04 | 0.40 |
| 1:BG:434:GLY:O | 1:BH:349:VAL:HG23 | 2.21 | 0.40 |
| 1:BH:18:ARG:HG2 | 1:BH:20:LEU:HD23 | 2.03 | 0.40 |
| 1:BH:207:VAL:HA | 1:BH:208:PRO:HD3 | 1.81 | 0.40 |
| 1:BH:234:ARG:CG | 1:BH:280:GLU:HG2 | 2.51 | 0.40 |
| 1:BK:237:VAL:HG23 | 1:BK:279:PHE:CD2 | 2.55 | 0.40 |
| 1:BK:442:GLN:NE2 | 1:BL:412:PHE:HB2 | 2.36 | 0.40 |
| 1:BM:170:PHE:HB2 | 1:BM:496:PHE:HE1 | 1.86 | 0.40 |
| 1:BQ:272:TYR:CD2 | 1:CL:55:ARG:CZ | 3.04 | 0.40 |
| 1:BS:379:VAL:HG12 | 1:BS:381:MET:HE2 | 2.03 | 0.40 |
| 1:CA:203:THR:HB | 1:CA:300:GLN:HG3 | 2.03 | 0.40 |
| 1:CA:340:LEU:HA | 1:CA:340:LEU:HD23 | 1.88 | 0.40 |
| 1:CB:10:ILE:HA | 1:CB:11:PRO:HD3 | 1.94 | 0.40 |
| 1:CC:189:PHE:CE2 | 1:CC:249:LEU:HD21 | 2.56 | 0.40 |
| 1:CE:340:LEU:HA | 1:CE:340:LEU:HD23 | 1.88 | 0.40 |
| 1:CF:318:SER:HA | 1:CF:319:GLY:HA2 | 1.76 | 0.40 |
| 1:CG:33:LYS:HB2 | 1:CG:33:LYS:HE2 | 1.93 | 0.40 |
| 1:CG:163:LEU:HD12 | 1:CG:163:LEU:HA | 1.89 | 0.40 |
| 1:CG:207:VAL:HA | 1:CG:208:PRO:HD3 | 1.82 | 0.40 |
| 1:CG:442:GLN:HE21 | 1:CH:412:PHE:HB2 | 1.86 | 0.40 |
| 1:CI:272:TYR:CE2 | 1:CO:55:ARG:CZ | 3.04 | 0.40 |
| 1:CL:202:LEU:HD23 | 1:CL:202:LEU:HA | 1.93 | 0.40 |
| 1:CQ:170:PHE:HB2 | 1:CQ:496:PHE:HE1 | 1.85 | 0.40 |
| 1:CQ:203:THR:HB | 1:CQ:300:GLN:HG3 | 2.03 | 0.40 |
| 1:CT:252:VAL:HG22 | 1:CT:253:SER:N | 2.35 | 0.40 |
| 1:AB:423:LYS:HE2 | 1:AB:449:GLU:O | 2.20 | 0.40 |
| 1:AD:43:ALA:HB1 | 1:AD:158:GLU:HA | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AD:234:ARG:CG | 1:AD:280:GLU:HG2 | 2.50 | 0.40 |
| 1:AD:379:VAL:CG1 | 1:AD:381:MET:HE2 | 2.51 | 0.40 |
| 1:AI:371:ASP:OD1 | 1:AI:381:MET:HG2 | 2.21 | 0.40 |
| 1:AJ:423:LYS:HE2 | 1:AJ:449:GLU:O | 2.20 | 0.40 |
| 1:AP:222:LEU:O | 1:AP:225:CYS:HB2 | 2.21 | 0.40 |
| 1:BB:324:LEU:C | 1:BB:324:LEU:HD23 | 2.42 | 0.40 |
| 1:BB:340:LEU:HA | 1:BB:340:LEU:HD23 | 1.89 | 0.40 |
| 1:BF:175:PHE:O | 1:BF:175:PHE:CD2 | 2.75 | 0.40 |
| 1:BF:182:LEU:HG | 1:BF:330:ILE:HB | 2.02 | 0.40 |
| 1:BG:284:ARG:CG | 1:BG:284:ARG:NH1 | 2.71 | 0.40 |
| 1:BI:238:HIS:HE1 | 1:BI:329:GLN:OE1 | 2.04 | 0.40 |
| 1:BI:423:LYS:HE2 | 1:BI:449:GLU:O | 2.21 | 0.40 |
| 1:BJ:324:LEU:HD23 | 1:BJ:324:LEU:C | 2.42 | 0.40 |
| 1:BK:201:GLY:HA3 | 1:BK:300:GLN:HG2 | 2.03 | 0.40 |
| 1:BL:318:SER:HA | 1:BL:319:GLY:HA2 | 1.77 | 0.40 |
| 1:BQ:108:ILE:HG23 | 1:BQ:113:LEU:HD12 | 2.03 | 0.40 |
| 1:BS:43:ALA:HB1 | 1:BS:158:GLU:HA | 2.03 | 0.40 |
| 1:CA:243:ILE:N | 1:CA:243:ILE:HD12 | 2.37 | 0.40 |
| 1:CG:371:ASP:OD1 | 1:CG:381:MET:HG2 | 2.21 | 0.40 |
| 1:CH:55:ARG:CZ | 1:CK:272:TYR:CD2 | 3.05 | 0.40 |
| 1:CH:182:LEU:HG | 1:CH:330:ILE:HB | 2.02 | 0.40 |
| 1:CI:75:ARG:NH2 | 1:CI:391:ALA:O | 2.53 | 0.40 |
| 1:CI:234:ARG:CG | 1:CI:280:GLU:HG2 | 2.51 | 0.40 |
| 1:CI:255:TRP:CE3 | 1:CI:285:SER:HB2 | 2.56 | 0.40 |
| 1:CJ:170:PHE:HD1 | 1:CJ:389:MET:HE2 | 1.86 | 0.40 |
| 1:CL:232:THR:HB | 1:CL:334:VAL:CG2 | 2.50 | 0.40 |
| 1:CM:14:CYS:H | 1:CM:138:ASN:ND2 | 2.18 | 0.40 |
| 1:CM:404:LEU:N | 1:CM:404:LEU:HD23 | 2.36 | 0.40 |
| 1:CO:175:PHE:CD2 | 1:CO:175:PHE:O | 2.75 | 0.40 |
| 1:CS:43:ALA:HB1 | 1:CS:158:GLU:HA | 2.02 | 0.40 |
| 1:CS:404:LEU:HD22 | 1:CS:486:VAL:HG22 | 2.04 | 0.40 |
| 1:AA:36:GLN:HE22 | 1:AA:156:LEU:H | 1.67 | 0.40 |
| 1:AA:342:SER:HB2 | 1:AE:425:VAL:HG11 | 2.02 | 0.40 |
| 1:AB:73:TYR:CE2 | 1:AB:394:GLY:HA3 | 2.57 | 0.40 |
| 1:AD:182:LEU:C | 1:AD:182:LEU:HD12 | 2.42 | 0.40 |
| 1:AD:272:TYR:CE2 | 1:AS:55:ARG:CZ | 3.04 | 0.40 |
| 1:AF:440:ALA:CB | 1:AG:444:LEU:HD13 | 2.52 | 0.40 |
| 1:AH:272:TYR:CD2 | 1:CF:55:ARG:CZ | 3.05 | 0.40 |
| 1:AI:202:LEU:HD23 | 1:AI:202:LEU:HA | 1.87 | 0.40 |
| 1:AJ:22:THR:OG1 | 1:AJ:131:HIS:CD2 | 2.66 | 0.40 |
| 1:AS:440:ALA:CB | 1:AT:444:LEU:HD13 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AT:20:LEU:HB2 | 1:AT:132:PHE:O | 2.21 | 0.40 |
| 1:BA:11:PRO:HG2 | 1:BA:18:ARG:CD | 2.51 | 0.40 |
| 1:BB:33:LYS:HB2 | 1:BB:33:LYS:HE2 | 1.95 | 0.40 |
| 1:BB:182:LEU:HD12 | 1:BB:182:LEU:C | 2.42 | 0.40 |
| 1:BC:207:VAL:HA | 1:BC:208:PRO:HD3 | 1.84 | 0.40 |
| 1:BC:232:THR:HB | 1:BC:334:VAL:CG2 | 2.52 | 0.40 |
| 1:BD:272:TYR:HD2 | 1:BS:55:ARG:HD3 | 1.85 | 0.40 |
| 1:BE:423:LYS:HE2 | 1:BE:449:GLU:O | 2.20 | 0.40 |
| 1:BF:18:ARG:HG3 | 1:BF:19:TYR:N | 2.36 | 0.40 |
| 1:BG:238:HIS:HE1 | 1:BG:329:GLN:OE1 | 2.03 | 0.40 |
| 1:BG:256:ASN:HD22 | 1:BG:302:ASP:HA | 1.87 | 0.40 |
| 1:BH:15:GLN:NE2 | 1:BH:15:GLN:CA | 2.81 | 0.40 |
| 1:BH:335:ARG:N | 1:BH:336:PRO:HD3 | 2.36 | 0.40 |
| 1:BM:234:ARG:CG | 1:BM:280:GLU:HG2 | 2.52 | 0.40 |
| 1:BN:371:ASP:OD1 | 1:BN:381:MET:HG2 | 2.21 | 0.40 |
| 1:BP:73:TYR:CE2 | 1:BP:394:GLY:HA3 | 2.56 | 0.40 |
| 1:BP:182:LEU:HD12 | 1:BP:182:LEU:C | 2.42 | 0.40 |
| 1:BQ:395:LEU:HB2 | 1:BQ:497:TYR:HB2 | 2.03 | 0.40 |
| 1:BS:37:TYR:O | 1:BS:40:TRP:HB3 | 2.21 | 0.40 |
| 1:BS:285:SER:HA | 1:BS:286:PRO:HD3 | 1.95 | 0.40 |
| 1:CB:256:ASN:HD22 | 1:CB:302:ASP:HA | 1.85 | 0.40 |
| 1:CD:55:ARG:CZ | 1:CN:272:TYR:CE2 | 3.03 | 0.40 |
| 1:CI:423:LYS:HE2 | 1:CI:449:GLU:O | 2.21 | 0.40 |
| 1:CK:289:ARG:HH11 | 1:CK:289:ARG:HD3 | 1.76 | 0.40 |
| 1:CL:43:ALA:HB1 | 1:CL:158:GLU:HA | 2.02 | 0.40 |
| 1:CM:340:LEU:HD23 | 1:CM:340:LEU:HA | 1.92 | 0.40 |
| 1:CN:272:TYR:N | 1:CN:272:TYR:HD1 | 2.18 | 0.40 |
| 1:CO:108:ILE:HG23 | 1:CO:113:LEU:HD12 | 2.02 | 0.40 |
| 1:CO:255:TRP:CE3 | 1:CO:285:SER:HB2 | 2.57 | 0.40 |
| 1:CO:423:LYS:HE2 | 1:CO:449:GLU:O | 2.21 | 0.40 |
| 1:CQ:335:ARG:N | 1:CQ:336:PRO:HD3 | 2.36 | 0.40 |
| 1:CQ:404:LEU:HD23 | 1:CQ:404:LEU:N | 2.37 | 0.40 |
| 1:AA:272:TYR:CD2 | 1:CT:55:ARG:CZ | 3.05 | 0.40 |
| 1:AA:340:LEU:HD23 | 1:AA:340:LEU:HA | 1.92 | 0.40 |
| 1:AC:272:TYR:CE2 | 1:BA:55:ARG:CZ | 3.04 | 0.40 |
| 1:AC:324:LEU:C | 1:AC:324:LEU:HD23 | 2.42 | 0.40 |
| 1:AF:52:ILE:HG12 | 1:AF:152:LEU:CD2 | 2.51 | 0.40 |
| 1:AF:55:ARG:HD3 | 1:BH:272:TYR:HD2 | 1.84 | 0.40 |
| 1:AF:55:ARG:CZ | 1:BH:272:TYR:CD2 | 3.05 | 0.40 |
| 1:AF:189:PHE:CE1 | 1:AF:198:ARG:HG2 | 2.55 | 0.40 |
| 1:AK:170:PHE:HB2 | 1:AK:496:PHE:HE1 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AK:171:ASP:HA | 1:AK:172:PRO:HD3 | 1.79 | 0.40 |
| 1:AN:308:PHE:CZ | 1:AN:328:VAL:HG21 | 2.56 | 0.40 |
| 1:AO:207:VAL:HA | 1:AO:208:PRO:HD3 | 1.86 | 0.40 |
| 1:AP:33:LYS:HB2 | 1:AP:33:LYS:HE2 | 1.97 | 0.40 |
| 1:AP:61:PHE:CE2 | 1:AP:243:ILE:HD11 | 2.57 | 0.40 |
| 1:AP:440:ALA:CB | 1:AQ:444:LEU:HD13 | 2.51 | 0.40 |
| 1:AR:33:LYS:HB2 | 1:AR:33:LYS:HE2 | 1.97 | 0.40 |
| 1:AT:10:ILE:HG21 | 1:AT:146:TRP:CZ2 | 2.57 | 0.40 |
| 1:AT:55:ARG:CZ | 1:BA:272:TYR:CE2 | 3.05 | 0.40 |
| 1:AT:379:VAL:HG12 | 1:AT:381:MET:HE2 | 2.03 | 0.40 |
| 1:BA:10:ILE:HA | 1:BA:11:PRO:HD3 | 1.89 | 0.40 |
| 1:BA:73:TYR:CZ | 1:BA:394:GLY:HA3 | 2.55 | 0.40 |
| 1:BA:379:VAL:HG12 | 1:BA:381:MET:HE2 | 2.03 | 0.40 |
| 1:BB:250:TRP:HZ3 | 1:BB:272:TYR:HE1 | 1.63 | 0.40 |
| 1:BC:55:ARG:CZ | 1:BT:272:TYR:CE2 | 3.04 | 0.40 |
| 1:BC:201:GLY:HA3 | 1:BC:300:GLN:HG2 | 2.03 | 0.40 |
| 1:BD:55:ARG:CZ | 1:BN:272:TYR:CE2 | 3.04 | 0.40 |
| 1:BD:175:PHE:CD2 | 1:BD:175:PHE:O | 2.74 | 0.40 |
| 1:BD:232:THR:HB | 1:BD:334:VAL:CG2 | 2.51 | 0.40 |
| 1:BD:318:SER:HA | 1:BD:319:GLY:HA2 | 1.81 | 0.40 |
| 1:BE:33:LYS:HB2 | 1:BE:33:LYS:HE2 | 1.97 | 0.40 |
| 1:BF:20:LEU:HB2 | 1:BF:132:PHE:O | 2.22 | 0.40 |
| 1:BF:30:SER:HA | 1:BF:37:TYR:CD1 | 2.57 | 0.40 |
| 1:BF:440:ALA:CB | 1:BG:444:LEU:HD13 | 2.51 | 0.40 |
| 1:BG:33:LYS:HB2 | 1:BG:33:LYS:HE2 | 1.98 | 0.40 |
| 1:BG:234:ARG:CG | 1:BG:280:GLU:HG2 | 2.52 | 0.40 |
| 1:BG:395:LEU:HB2 | 1:BG:497:TYR:HB2 | 2.03 | 0.40 |
| 1:BJ:234:ARG:HG2 | 1:BJ:280:GLU:HG2 | 2.03 | 0.40 |
| 1:BJ:335:ARG:N | 1:BJ:336:PRO:HD3 | 2.37 | 0.40 |
| 1:BJ:379:VAL:HG11 | 1:BJ:381:MET:HE1 | 2.03 | 0.40 |
| 1:BL:182:LEU:HD12 | 1:BL:182:LEU:C | 2.42 | 0.40 |
| 1:BL:379:VAL:HG11 | 1:BL:381:MET:HE1 | 2.03 | 0.40 |
| 1:BO:182:LEU:HD12 | 1:BO:182:LEU:C | 2.42 | 0.40 |
| 1:BQ:285:SER:HA | 1:BQ:286:PRO:HD3 | 1.93 | 0.40 |
| 1:BR:454:ASN:HD22 | 1:BR:454:ASN:C | 2.25 | 0.40 |
| 1:BS:28:MET:CE | 1:BS:152:LEU:HG | 2.52 | 0.40 |
| 1:BS:207:VAL:HA | 1:BS:208:PRO:HD3 | 1.85 | 0.40 |
| 1:BS:226:VAL:HG13 | 1:BS:228:GLY:H | 1.87 | 0.40 |
| 1:CH:55:ARG:CZ | 1:CK:272:TYR:CE2 | 3.04 | 0.40 |
| 1:CH:171:ASP:HA | 1:CH:172:PRO:HD3 | 1.79 | 0.40 |
| 1:CN:33:LYS:HB2 | 1:CN:33:LYS:HE2 | 1.96 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CO:241:ALA:HB1 | 1:CO:242:PRO:HD2 | 2.03 | 0.40 |
| 1:CO:324:LEU:C | 1:CO:324:LEU:HD23 | 2.42 | 0.40 |
| 1:CR:252:VAL:HG22 | 1:CR:253:SER:N | 2.36 | 0.40 |
| 1:CR:442:GLN:HE21 | 1:CS:412:PHE:HB2 | 1.86 | 0.40 |
| 1:CS:33:LYS:HB2 | 1:CS:33:LYS:HE2 | 1.95 | 0.40 |
| 1:CS:234:ARG:CG | 1:CS:280:GLU:HG2 | 2.51 | 0.40 |
| 1:AB:318:SER:HA | 1:AB:319:GLY:HA2 | 1.78 | 0.40 |
| 1:AC:418:SER:HB3 | 1:AD:407:SER:HB3 | 2.04 | 0.40 |
| 1:AD:324:LEU:HA | 1:AD:325:PRO:HD3 | 1.86 | 0.40 |
| 1:AD:372:PHE:H | 1:AD:381:MET:HE1 | 1.87 | 0.40 |
| 1:AE:324:LEU:HA | 1:AE:325:PRO:HD3 | 1.84 | 0.40 |
| 1:AI:79:ARG:CG | 1:AI:79:ARG:NH1 | 2.80 | 0.40 |
| 1:AI:189:PHE:CE2 | 1:AI:249:LEU:HD21 | 2.45 | 0.40 |
| 1:AJ:284:ARG:CG | 1:AJ:284:ARG:NH1 | 2.75 | 0.40 |
| 1:AN:33:LYS:HB2 | 1:AN:33:LYS:HE2 | 1.93 | 0.40 |
| 1:AN:55:ARG:CD | 1:AS:272:TYR:CD2 | 2.98 | 0.40 |
| 1:AN:108:ILE:HG23 | 1:AN:113:LEU:HD12 | 2.03 | 0.40 |
| 1:AQ:77:THR:O | 1:AQ:81:THR:HG23 | 2.20 | 0.40 |
| 1:AQ:272:TYR:CD2 | 1:BL:55:ARG:CZ | 3.04 | 0.40 |
| 1:AR:236:ARG:HA | 1:AR:278:SER:HA | 2.04 | 0.40 |
| 1:AS:234:ARG:CG | 1:AS:280:GLU:HG2 | 2.51 | 0.40 |
| 1:AS:418:SER:HB3 | 1:AT:407:SER:HB3 | 2.02 | 0.40 |
| 1:AT:243:ILE:N | 1:AT:243:ILE:HD12 | 2.37 | 0.40 |
| 1:BA:412:PHE:HB2 | 1:BE:442:GLN:HE21 | 1.86 | 0.40 |
| 1:BB:171:ASP:HA | 1:BB:172:PRO:HD3 | 1.80 | 0.40 |
| 1:BD:454:ASN:ND2 | 1:BD:456:ALA:H | 2.14 | 0.40 |
| 1:BE:324:LEU:C | 1:BE:324:LEU:HD23 | 2.42 | 0.40 |
| 1:BG:454:ASN:ND2 | 1:BG:456:ALA:H | 2.11 | 0.40 |
| 1:BI:33:LYS:HB2 | 1:BI:33:LYS:HE2 | 1.97 | 0.40 |
| 1:BI:185:PRO:HA | 1:BI:186:PRO:HD3 | 1.93 | 0.40 |
| 1:BI:299:SER:O | 1:BI:302:ASP:HB2 | 2.22 | 0.40 |
| 1:BI:418:SER:HB3 | 1:BJ:407:SER:HB3 | 2.02 | 0.40 |
| 1:BJ:55:ARG:CZ | 1:CL:272:TYR:CE2 | 3.05 | 0.40 |
| 1:BL:22:THR:OG1 | 1:BL:131:HIS:CD2 | 2.63 | 0.40 |
| 1:BM:318:SER:HA | 1:BM:319:GLY:HA2 | 1.78 | 0.40 |
| 1:BN:272:TYR:N | 1:BN:272:TYR:HD1 | 2.18 | 0.40 |
| 1:BP:252:VAL:HG22 | 1:BP:253:SER:N | 2.36 | 0.40 |
| 1:BR:393:HIS:CG | 1:BR:496:PHE:HB3 | 2.57 | 0.40 |
| 1:BS:188:PHE:C | 1:BS:189:PHE:HD1 | 2.25 | 0.40 |
| 1:BT:241:ALA:HB1 | 1:BT:242:PRO:HD2 | 2.03 | 0.40 |
| 1:CE:126:GLU:HG3 | 1:CE:127:SER:H | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CF:163:LEU:HD12 | 1:CF:163:LEU:HA | 1.87 | 0.40 |
| 1:CG:372:PHE:H | 1:CG:381:MET:HE1 | 1.85 | 0.40 |
| 1:CJ:250:TRP:CZ3 | 1:CJ:272:TYR:CD1 | 3.08 | 0.40 |
| 1:CT:25:ILE:HG23 | 1:CT:152:LEU:HD11 | 2.03 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | AA | 502/504 (100%) | 478 (95%) | 23 (5%) | 1 (0%) | 47 | 82 |
| 1 | AB | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AC | 502/504 (100%) | 480 (96%) | 20 (4%) | 2 (0%) | 34 | 72 |
| 1 | AD | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | AE | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | AF | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | AG | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 34 | 72 |
| 1 | AH | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 34 | 72 |
| 1 | AI | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AJ | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | AK | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AL | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AM | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | AN | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | AO | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AP | 502/504 (100%) | 483 (96%) | 19 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | AQ | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | AR | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 47 | 82 |
| 1 | AS | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | AT | 502/504 (100%) | 484 (96%) | 17 (3%) | 1 (0%) | 47 | 82 |
| 1 | BA | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | BB | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 34 | 72 |
| 1 | BC | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BD | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | BE | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BF | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 34 | 72 |
| 1 | BG | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | BH | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 47 | 82 |
| 1 | BI | 502/504 (100%) | 479 (95%) | 22 (4%) | 1 (0%) | 47 | 82 |
| 1 | BJ | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BK | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 47 | 82 |
| 1 | BL | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | BM | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | BN | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BO | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | BP | 502/504 (100%) | 479 (95%) | 21 (4%) | 2 (0%) | 34 | 72 |
| 1 | BQ | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BR | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BS | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | BT | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | CA | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | CB | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | CC | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | CD | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | CE | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 47 | 82 |
| 1 | CF | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | CG | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | CH | 502/504 (100%) | 481 (96%) | 21 (4%) | 0 | 100 | 100 |
| 1 | CI | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | CJ | 502/504 (100%) | 484 (96%) | 17 (3%) | 1 (0%) | 47 | 82 |
| 1 | CK | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 82 |
| 1 | CL | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | CM | 502/504 (100%) | 480 (96%) | 20 (4%) | 2 (0%) | 34 | 72 |
| 1 | CN | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | CO | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | CP | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 47 | 82 |
| 1 | CQ | 502/504 (100%) | 482 (96%) | 18 (4%) | 2 (0%) | 34 | 72 |
| 1 | CR | 502/504 (100%) | 478 (95%) | 22 (4%) | 2 (0%) | 34 | 72 |
| 1 | CS | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 47 | 82 |
| 1 | CT | 502/504 (100%) | 479 (95%) | 22 (4%) | 1 (0%) | 47 | 82 |
| All | All | 30120/30240 (100%) | 28870 (96%) | 1187 (4%) | 63 (0%) | 47 | 82 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BP | 82 | ALA |
| 1 | CR | 82 | ALA |
| 1 | BM | 17 | ASN |
| 1 | AC | 78 | SER |
| 1 | BB | 17 | ASN |
| 1 | BD | 17 | ASN |
| 1 | BF | 78 | SER |
| 1 | CM | 17 | ASN |
| 1 | AH | 17 | ASN |
| 1 | BA | 498 | GLY |
| 1 | CQ | 17 | ASN |
| 1 | AG | 17 | ASN |
| 1 | AN | 498 | GLY |
| 1 | AT | 498 | GLY |
| 1 | BG | 498 | GLY |
| 1 | BP | 498 | GLY |
| 1 | BT | 498 | GLY |
| 1 | CF | 498 | GLY |
| 1 | CG | 498 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CT | 498 | GLY |
| 1 | AE | 498 | GLY |
| 1 | AQ | 498 | GLY |
| 1 | BF | 498 | GLY |
| 1 | BK | 498 | GLY |
| 1 | BL | 498 | GLY |
| 1 | CK | 498 | GLY |
| 1 | CL | 498 | GLY |
| 1 | CM | 498 | GLY |
| 1 | CR | 498 | GLY |
| 1 | AA | 498 | GLY |
| 1 | AG | 498 | GLY |
| 1 | AK | 498 | GLY |
| 1 | AM | 498 | GLY |
| 1 | BC | 498 | GLY |
| 1 | BE | 498 | GLY |
| 1 | BJ | 498 | GLY |
| 1 | BN | 498 | GLY |
| 1 | BO | 498 | GLY |
| 1 | CD | 498 | GLY |
| 1 | CO | 498 | GLY |
| 1 | AJ | 498 | GLY |
| 1 | AS | 498 | GLY |
| 1 | BH | 498 | GLY |
| 1 | BR | 498 | GLY |
| 1 | BS | 498 | GLY |
| 1 | CB | 498 | GLY |
| 1 | CE | 498 | GLY |
| 1 | CP | 498 | GLY |
| 1 | CS | 498 | GLY |
| 1 | AH | 498 | GLY |
| 1 | AI | 498 | GLY |
| 1 | AO | 498 | GLY |
| 1 | AR | 498 | GLY |
| 1 | BB | 498 | GLY |
| 1 | CA | 498 | GLY |
| 1 | CJ | 498 | GLY |
| 1 | CQ | 498 | GLY |
| 1 | AB | 498 | GLY |
| 1 | AC | 498 | GLY |
| 1 | AL | 498 | GLY |
| 1 | BI | 498 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BQ | 498 | GLY |
| 1 | CC | 498 | GLY |

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | AA | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | AB | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | AC | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | AD | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | AE | 430/430 (100%) | 409 (95%) | 21 (5%) | 25 | 61 |
| 1 | AF | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | AG | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | AH | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | AI | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | AJ | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | AK | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | AL | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | AM | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | AN | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | AO | 430/430 (100%) | 408 (95%) | 22 (5%) | 24 | 60 |
| 1 | AP | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | AQ | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | AR | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | AS | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | AT | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | BA | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BB | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | BC | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BD | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BE | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BF | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | BG | 430/430 (100%) | 408 (95%) | 22 (5%) | 24 | 60 |
| 1 | BH | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | BI | 430/430 (100%) | 408 (95%) | 22 (5%) | 24 | 60 |
| 1 | BJ | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | BK | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | BL | 430/430 (100%) | 403 (94%) | 27 (6%) | 18 | 51 |
| 1 | BM | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | BN | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | BO | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BP | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BQ | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | BR | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | BS | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | BT | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CA | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | CB | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CC | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | CD | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CE | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CF | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CG | 430/430 (100%) | 408 (95%) | 22 (5%) | 24 | 60 |
| 1 | CH | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | CI | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CJ | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | CK | 430/430 (100%) | 406 (94%) | 24 (6%) | 21 | 56 |
| 1 | CL | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | CM | 430/430 (100%) | 403 (94%) | 27 (6%) | 18 | 51 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | CN | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | CO | 430/430 (100%) | 408 (95%) | 22 (5%) | 24 | 60 |
| 1 | CP | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | CQ | 430/430 (100%) | 404 (94%) | 26 (6%) | 19 | 53 |
| 1 | CR | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| 1 | CS | 430/430 (100%) | 407 (95%) | 23 (5%) | 22 | 58 |
| 1 | CT | 430/430 (100%) | 405 (94%) | 25 (6%) | 20 | 55 |
| All | All | 25800/25800 (100%) | 24352 (94%) | 1448 (6%) | 21 | 56 |

All (1448) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AA | 105 | SER |
| 1 | AA | 129 | ARG |
| 1 | AA | 160 | THR |
| 1 | AA | 161 | SER |
| 1 | AA | 163 | LEU |
| 1 | AA | 167 | THR |
| 1 | AA | 182 | LEU |
| 1 | AA | 191 | LEU |
| 1 | AA | 199 | SER |
| 1 | AA | 226 | VAL |
| 1 | AA | 229 | MET |
| 1 | AA | 243 | ILE |
| 1 | AA | 260 | MET |
| 1 | AA | 272 | TYR |
| 1 | AA | 284 | ARG |
| 1 | AA | 289 | ARG |
| 1 | AA | 301 | ARG |
| 1 | AA | 378 | ARG |
| 1 | AA | 384 | ASN |
| 1 | AA | 449 | GLU |
| 1 | AA | 454 | ASN |
| 1 | AA | 475 | LEU |
| 1 | AA | 504 | VAL |
| 1 | AB | 79 | ARG |
| 1 | AB | 105 | SER |
| 1 | AB | 129 | ARG |
| 1 | AB | 160 | THR |
| 1 | AB | 161 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AB | 163 | LEU |
| 1 | AB | 167 | THR |
| 1 | AB | 182 | LEU |
| 1 | AB | 191 | LEU |
| 1 | AB | 199 | SER |
| 1 | AB | 226 | VAL |
| 1 | AB | 243 | ILE |
| 1 | AB | 260 | MET |
| 1 | AB | 272 | TYR |
| 1 | AB | 284 | ARG |
| 1 | AB | 289 | ARG |
| 1 | AB | 299 | SER |
| 1 | AB | 300 | GLN |
| 1 | AB | 301 | ARG |
| 1 | AB | 336 | PRO |
| 1 | AB | 378 | ARG |
| 1 | AB | 384 | ASN |
| 1 | AB | 449 | GLU |
| 1 | AB | 454 | ASN |
| 1 | AB | 475 | LEU |
| 1 | AB | 504 | VAL |
| 1 | AC | 18 | ARG |
| 1 | AC | 105 | SER |
| 1 | AC | 129 | ARG |
| 1 | AC | 160 | THR |
| 1 | AC | 161 | SER |
| 1 | AC | 163 | LEU |
| 1 | AC | 167 | THR |
| 1 | AC | 182 | LEU |
| 1 | AC | 191 | LEU |
| 1 | AC | 199 | SER |
| 1 | AC | 226 | VAL |
| 1 | AC | 243 | ILE |
| 1 | AC | 260 | MET |
| 1 | AC | 272 | TYR |
| 1 | AC | 284 | ARG |
| 1 | AC | 289 | ARG |
| 1 | AC | 300 | GLN |
| 1 | AC | 301 | ARG |
| 1 | AC | 378 | ARG |
| 1 | AC | 384 | ASN |
| 1 | AC | 449 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AC | 454 | ASN |
| 1 | AC | 475 | LEU |
| 1 | AC | 504 | VAL |
| 1 | AD | 15 | GLN |
| 1 | AD | 57 | PRO |
| 1 | AD | 79 | ARG |
| 1 | AD | 105 | SER |
| 1 | AD | 129 | ARG |
| 1 | AD | 160 | THR |
| 1 | AD | 161 | SER |
| 1 | AD | 163 | LEU |
| 1 | AD | 167 | THR |
| 1 | AD | 182 | LEU |
| 1 | AD | 191 | LEU |
| 1 | AD | 199 | SER |
| 1 | AD | 226 | VAL |
| 1 | AD | 229 | MET |
| 1 | AD | 243 | ILE |
| 1 | AD | 260 | MET |
| 1 | AD | 272 | TYR |
| 1 | AD | 284 | ARG |
| 1 | AD | 289 | ARG |
| 1 | AD | 301 | ARG |
| 1 | AD | 378 | ARG |
| 1 | AD | 384 | ASN |
| 1 | AD | 449 | GLU |
| 1 | AD | 454 | ASN |
| 1 | AD | 475 | LEU |
| 1 | AD | 504 | VAL |
| 1 | AE | 10 | ILE |
| 1 | AE | 105 | SER |
| 1 | AE | 160 | THR |
| 1 | AE | 161 | SER |
| 1 | AE | 163 | LEU |
| 1 | AE | 167 | THR |
| 1 | AE | 191 | LEU |
| 1 | AE | 199 | SER |
| 1 | AE | 226 | VAL |
| 1 | AE | 243 | ILE |
| 1 | AE | 260 | MET |
| 1 | AE | 272 | TYR |
| 1 | AE | 284 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AE | 289 | ARG |
| 1 | AE | 301 | ARG |
| 1 | AE | 378 | ARG |
| 1 | AE | 384 | ASN |
| 1 | AE | 449 | GLU |
| 1 | AE | 454 | ASN |
| 1 | AE | 475 | LEU |
| 1 | AE | 504 | VAL |
| 1 | AF | 79 | ARG |
| 1 | AF | 105 | SER |
| 1 | AF | 129 | ARG |
| 1 | AF | 160 | THR |
| 1 | AF | 161 | SER |
| 1 | AF | 163 | LEU |
| 1 | AF | 167 | THR |
| 1 | AF | 182 | LEU |
| 1 | AF | 191 | LEU |
| 1 | AF | 199 | SER |
| 1 | AF | 226 | VAL |
| 1 | AF | 243 | ILE |
| 1 | AF | 260 | MET |
| 1 | AF | 272 | TYR |
| 1 | AF | 284 | ARG |
| 1 | AF | 289 | ARG |
| 1 | AF | 301 | ARG |
| 1 | AF | 378 | ARG |
| 1 | AF | 384 | ASN |
| 1 | AF | 449 | GLU |
| 1 | AF | 454 | ASN |
| 1 | AF | 475 | LEU |
| 1 | AF | 504 | VAL |
| 1 | AG | 10 | ILE |
| 1 | AG | 79 | ARG |
| 1 | AG | 105 | SER |
| 1 | AG | 129 | ARG |
| 1 | AG | 160 | THR |
| 1 | AG | 161 | SER |
| 1 | AG | 163 | LEU |
| 1 | AG | 167 | THR |
| 1 | AG | 182 | LEU |
| 1 | AG | 191 | LEU |
| 1 | AG | 199 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AG | 226 | VAL |
| 1 | AG | 243 | ILE |
| 1 | AG | 260 | MET |
| 1 | AG | 272 | TYR |
| 1 | AG | 284 | ARG |
| 1 | AG | 289 | ARG |
| 1 | AG | 300 | GLN |
| 1 | AG | 301 | ARG |
| 1 | AG | 378 | ARG |
| 1 | AG | 384 | ASN |
| 1 | AG | 449 | GLU |
| 1 | AG | 454 | ASN |
| 1 | AG | 475 | LEU |
| 1 | AG | 504 | VAL |
| 1 | AH | 15 | GLN |
| 1 | AH | 18 | ARG |
| 1 | AH | 105 | SER |
| 1 | AH | 129 | ARG |
| 1 | AH | 160 | THR |
| 1 | AH | 161 | SER |
| 1 | AH | 163 | LEU |
| 1 | AH | 167 | THR |
| 1 | AH | 182 | LEU |
| 1 | AH | 191 | LEU |
| 1 | AH | 199 | SER |
| 1 | AH | 226 | VAL |
| 1 | AH | 243 | ILE |
| 1 | AH | 260 | MET |
| 1 | AH | 272 | TYR |
| 1 | AH | 284 | ARG |
| 1 | AH | 289 | ARG |
| 1 | AH | 300 | GLN |
| 1 | AH | 378 | ARG |
| 1 | AH | 384 | ASN |
| 1 | AH | 449 | GLU |
| 1 | AH | 454 | ASN |
| 1 | AH | 475 | LEU |
| 1 | AH | 504 | VAL |
| 1 | AI | 18 | ARG |
| 1 | AI | 79 | ARG |
| 1 | AI | 105 | SER |
| 1 | AI | 129 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AI | 160 | THR |
| 1 | AI | 161 | SER |
| 1 | AI | 163 | LEU |
| 1 | AI | 167 | THR |
| 1 | AI | 182 | LEU |
| 1 | AI | 191 | LEU |
| 1 | AI | 199 | SER |
| 1 | AI | 226 | VAL |
| 1 | AI | 229 | MET |
| 1 | AI | 243 | ILE |
| 1 | AI | 260 | MET |
| 1 | AI | 272 | TYR |
| 1 | AI | 284 | ARG |
| 1 | AI | 289 | ARG |
| 1 | AI | 300 | GLN |
| 1 | AI | 301 | ARG |
| 1 | AI | 378 | ARG |
| 1 | AI | 384 | ASN |
| 1 | AI | 449 | GLU |
| 1 | AI | 454 | ASN |
| 1 | AI | 475 | LEU |
| 1 | AI | 504 | VAL |
| 1 | AJ | 18 | ARG |
| 1 | AJ | 105 | SER |
| 1 | AJ | 129 | ARG |
| 1 | AJ | 160 | THR |
| 1 | AJ | 161 | SER |
| 1 | AJ | 163 | LEU |
| 1 | AJ | 167 | THR |
| 1 | AJ | 182 | LEU |
| 1 | AJ | 191 | LEU |
| 1 | AJ | 199 | SER |
| 1 | AJ | 226 | VAL |
| 1 | AJ | 229 | MET |
| 1 | AJ | 243 | ILE |
| 1 | AJ | 260 | MET |
| 1 | AJ | 272 | TYR |
| 1 | AJ | 284 | ARG |
| 1 | AJ | 289 | ARG |
| 1 | AJ | 301 | ARG |
| 1 | AJ | 378 | ARG |
| 1 | AJ | 384 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AJ | 449 | GLU |
| 1 | AJ | 454 | ASN |
| 1 | AJ | 475 | LEU |
| 1 | AJ | 504 | VAL |
| 1 | AK | 18 | ARG |
| 1 | AK | 105 | SER |
| 1 | AK | 129 | ARG |
| 1 | AK | 160 | THR |
| 1 | AK | 161 | SER |
| 1 | AK | 163 | LEU |
| 1 | AK | 167 | THR |
| 1 | AK | 182 | LEU |
| 1 | AK | 191 | LEU |
| 1 | AK | 199 | SER |
| 1 | AK | 226 | VAL |
| 1 | AK | 229 | MET |
| 1 | AK | 243 | ILE |
| 1 | AK | 260 | MET |
| 1 | AK | 272 | TYR |
| 1 | AK | 284 | ARG |
| 1 | AK | 289 | ARG |
| 1 | AK | 300 | GLN |
| 1 | AK | 301 | ARG |
| 1 | AK | 336 | PRO |
| 1 | AK | 378 | ARG |
| 1 | AK | 384 | ASN |
| 1 | AK | 449 | GLU |
| 1 | AK | 454 | ASN |
| 1 | AK | 475 | LEU |
| 1 | AK | 504 | VAL |
| 1 | AL | 9 | TYR |
| 1 | AL | 10 | ILE |
| 1 | AL | 79 | ARG |
| 1 | AL | 105 | SER |
| 1 | AL | 129 | ARG |
| 1 | AL | 160 | THR |
| 1 | AL | 161 | SER |
| 1 | AL | 163 | LEU |
| 1 | AL | 167 | THR |
| 1 | AL | 182 | LEU |
| 1 | AL | 191 | LEU |
| 1 | AL | 199 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AL | 226 | VAL |
| 1 | AL | 243 | ILE |
| 1 | AL | 260 | MET |
| 1 | AL | 272 | TYR |
| 1 | AL | 284 | ARG |
| 1 | AL | 289 | ARG |
| 1 | AL | 299 | SER |
| 1 | AL | 301 | ARG |
| 1 | AL | 378 | ARG |
| 1 | AL | 384 | ASN |
| 1 | AL | 449 | GLU |
| 1 | AL | 454 | ASN |
| 1 | AL | 475 | LEU |
| 1 | AL | 504 | VAL |
| 1 | AM | 11 | PRO |
| 1 | AM | 105 | SER |
| 1 | AM | 129 | ARG |
| 1 | AM | 160 | THR |
| 1 | AM | 161 | SER |
| 1 | AM | 163 | LEU |
| 1 | AM | 167 | THR |
| 1 | AM | 182 | LEU |
| 1 | AM | 191 | LEU |
| 1 | AM | 199 | SER |
| 1 | AM | 226 | VAL |
| 1 | AM | 243 | ILE |
| 1 | AM | 260 | MET |
| 1 | AM | 272 | TYR |
| 1 | AM | 284 | ARG |
| 1 | AM | 289 | ARG |
| 1 | AM | 301 | ARG |
| 1 | AM | 378 | ARG |
| 1 | AM | 384 | ASN |
| 1 | AM | 449 | GLU |
| 1 | AM | 454 | ASN |
| 1 | AM | 475 | LEU |
| 1 | AM | 504 | VAL |
| 1 | AN | 10 | ILE |
| 1 | AN | 79 | ARG |
| 1 | AN | 105 | SER |
| 1 | AN | 129 | ARG |
| 1 | AN | 160 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AN | 161 | SER |
| 1 | AN | 163 | LEU |
| 1 | AN | 167 | THR |
| 1 | AN | 182 | LEU |
| 1 | AN | 191 | LEU |
| 1 | AN | 199 | SER |
| 1 | AN | 226 | VAL |
| 1 | AN | 243 | ILE |
| 1 | AN | 260 | MET |
| 1 | AN | 272 | TYR |
| 1 | AN | 284 | ARG |
| 1 | AN | 289 | ARG |
| 1 | AN | 301 | ARG |
| 1 | AN | 378 | ARG |
| 1 | AN | 384 | ASN |
| 1 | AN | 449 | GLU |
| 1 | AN | 454 | ASN |
| 1 | AN | 475 | LEU |
| 1 | AN | 504 | VAL |
| 1 | AO | 105 | SER |
| 1 | AO | 129 | ARG |
| 1 | AO | 160 | THR |
| 1 | AO | 161 | SER |
| 1 | AO | 163 | LEU |
| 1 | AO | 167 | THR |
| 1 | AO | 182 | LEU |
| 1 | AO | 191 | LEU |
| 1 | AO | 199 | SER |
| 1 | AO | 226 | VAL |
| 1 | AO | 243 | ILE |
| 1 | AO | 260 | MET |
| 1 | AO | 272 | TYR |
| 1 | AO | 284 | ARG |
| 1 | AO | 289 | ARG |
| 1 | AO | 301 | ARG |
| 1 | AO | 378 | ARG |
| 1 | AO | 384 | ASN |
| 1 | AO | 449 | GLU |
| 1 | AO | 454 | ASN |
| 1 | AO | 475 | LEU |
| 1 | AO | 504 | VAL |
| 1 | AP | 79 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AP | 105 | SER |
| 1 | AP | 129 | ARG |
| 1 | AP | 160 | THR |
| 1 | AP | 161 | SER |
| 1 | AP | 163 | LEU |
| 1 | AP | 167 | THR |
| 1 | AP | 182 | LEU |
| 1 | AP | 191 | LEU |
| 1 | AP | 199 | SER |
| 1 | AP | 226 | VAL |
| 1 | AP | 243 | ILE |
| 1 | AP | 260 | MET |
| 1 | AP | 272 | TYR |
| 1 | AP | 284 | ARG |
| 1 | AP | 289 | ARG |
| 1 | AP | 301 | ARG |
| 1 | AP | 378 | ARG |
| 1 | AP | 384 | ASN |
| 1 | AP | 449 | GLU |
| 1 | AP | 454 | ASN |
| 1 | AP | 475 | LEU |
| 1 | AP | 504 | VAL |
| 1 | AQ | 10 | ILE |
| 1 | AQ | 105 | SER |
| 1 | AQ | 129 | ARG |
| 1 | AQ | 160 | THR |
| 1 | AQ | 161 | SER |
| 1 | AQ | 163 | LEU |
| 1 | AQ | 167 | THR |
| 1 | AQ | 182 | LEU |
| 1 | AQ | 191 | LEU |
| 1 | AQ | 199 | SER |
| 1 | AQ | 226 | VAL |
| 1 | AQ | 243 | ILE |
| 1 | AQ | 260 | MET |
| 1 | AQ | 272 | TYR |
| 1 | AQ | 284 | ARG |
| 1 | AQ | 285 | SER |
| 1 | AQ | 289 | ARG |
| 1 | AQ | 301 | ARG |
| 1 | AQ | 336 | PRO |
| 1 | AQ | 378 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AQ | 384 | ASN |
| 1 | AQ | 449 | GLU |
| 1 | AQ | 454 | ASN |
| 1 | AQ | 475 | LEU |
| 1 | AQ | 504 | VAL |
| 1 | AR | 75 | ARG |
| 1 | AR | 105 | SER |
| 1 | AR | 129 | ARG |
| 1 | AR | 160 | THR |
| 1 | AR | 161 | SER |
| 1 | AR | 163 | LEU |
| 1 | AR | 167 | THR |
| 1 | AR | 182 | LEU |
| 1 | AR | 191 | LEU |
| 1 | AR | 199 | SER |
| 1 | AR | 226 | VAL |
| 1 | AR | 243 | ILE |
| 1 | AR | 260 | MET |
| 1 | AR | 272 | TYR |
| 1 | AR | 284 | ARG |
| 1 | AR | 289 | ARG |
| 1 | AR | 300 | GLN |
| 1 | AR | 301 | ARG |
| 1 | AR | 378 | ARG |
| 1 | AR | 384 | ASN |
| 1 | AR | 449 | GLU |
| 1 | AR | 454 | ASN |
| 1 | AR | 475 | LEU |
| 1 | AR | 504 | VAL |
| 1 | AS | 10 | ILE |
| 1 | AS | 105 | SER |
| 1 | AS | 129 | ARG |
| 1 | AS | 160 | THR |
| 1 | AS | 161 | SER |
| 1 | AS | 163 | LEU |
| 1 | AS | 167 | THR |
| 1 | AS | 182 | LEU |
| 1 | AS | 191 | LEU |
| 1 | AS | 199 | SER |
| 1 | AS | 226 | VAL |
| 1 | AS | 229 | MET |
| 1 | AS | 243 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 260 | MET |
| 1 | AS | 272 | TYR |
| 1 | AS | 284 | ARG |
| 1 | AS | 289 | ARG |
| 1 | AS | 301 | ARG |
| 1 | AS | 305 | SER |
| 1 | AS | 378 | ARG |
| 1 | AS | 384 | ASN |
| 1 | AS | 449 | GLU |
| 1 | AS | 454 | ASN |
| 1 | AS | 475 | LEU |
| 1 | AS | 504 | VAL |
| 1 | AT | 105 | SER |
| 1 | AT | 129 | ARG |
| 1 | AT | 160 | THR |
| 1 | AT | 161 | SER |
| 1 | AT | 163 | LEU |
| 1 | AT | 167 | THR |
| 1 | AT | 182 | LEU |
| 1 | AT | 191 | LEU |
| 1 | AT | 199 | SER |
| 1 | AT | 226 | VAL |
| 1 | AT | 229 | MET |
| 1 | AT | 243 | ILE |
| 1 | AT | 260 | MET |
| 1 | AT | 272 | TYR |
| 1 | AT | 284 | ARG |
| 1 | AT | 289 | ARG |
| 1 | AT | 300 | GLN |
| 1 | AT | 301 | ARG |
| 1 | AT | 378 | ARG |
| 1 | AT | 384 | ASN |
| 1 | AT | 449 | GLU |
| 1 | AT | 454 | ASN |
| 1 | AT | 475 | LEU |
| 1 | AT | 504 | VAL |
| 1 | BA | 79 | ARG |
| 1 | BA | 105 | SER |
| 1 | BA | 129 | ARG |
| 1 | BA | 160 | THR |
| 1 | BA | 161 | SER |
| 1 | BA | 163 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BA | 167 | THR |
| 1 | BA | 182 | LEU |
| 1 | BA | 191 | LEU |
| 1 | BA | 199 | SER |
| 1 | BA | 226 | VAL |
| 1 | BA | 243 | ILE |
| 1 | BA | 260 | MET |
| 1 | BA | 272 | TYR |
| 1 | BA | 284 | ARG |
| 1 | BA | 289 | ARG |
| 1 | BA | 301 | ARG |
| 1 | BA | 378 | ARG |
| 1 | BA | 384 | ASN |
| 1 | BA | 449 | GLU |
| 1 | BA | 454 | ASN |
| 1 | BA | 475 | LEU |
| 1 | BA | 504 | VAL |
| 1 | BB | 79 | ARG |
| 1 | BB | 105 | SER |
| 1 | BB | 129 | ARG |
| 1 | BB | 160 | THR |
| 1 | BB | 161 | SER |
| 1 | BB | 163 | LEU |
| 1 | BB | 167 | THR |
| 1 | BB | 182 | LEU |
| 1 | BB | 191 | LEU |
| 1 | BB | 199 | SER |
| 1 | BB | 226 | VAL |
| 1 | BB | 243 | ILE |
| 1 | BB | 260 | MET |
| 1 | BB | 272 | TYR |
| 1 | BB | 284 | ARG |
| 1 | BB | 289 | ARG |
| 1 | BB | 300 | GLN |
| 1 | BB | 301 | ARG |
| 1 | BB | 336 | PRO |
| 1 | BB | 378 | ARG |
| 1 | BB | 384 | ASN |
| 1 | BB | 449 | GLU |
| 1 | BB | 454 | ASN |
| 1 | BB | 475 | LEU |
| 1 | BB | 504 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BC | 18 | ARG |
| 1 | BC | 105 | SER |
| 1 | BC | 129 | ARG |
| 1 | BC | 160 | THR |
| 1 | BC | 161 | SER |
| 1 | BC | 163 | LEU |
| 1 | BC | 167 | THR |
| 1 | BC | 182 | LEU |
| 1 | BC | 191 | LEU |
| 1 | BC | 199 | SER |
| 1 | BC | 226 | VAL |
| 1 | BC | 243 | ILE |
| 1 | BC | 260 | MET |
| 1 | BC | 272 | TYR |
| 1 | BC | 284 | ARG |
| 1 | BC | 289 | ARG |
| 1 | BC | 301 | ARG |
| 1 | BC | 378 | ARG |
| 1 | BC | 384 | ASN |
| 1 | BC | 449 | GLU |
| 1 | BC | 454 | ASN |
| 1 | BC | 475 | LEU |
| 1 | BC | 504 | VAL |
| 1 | BD | 105 | SER |
| 1 | BD | 129 | ARG |
| 1 | BD | 160 | THR |
| 1 | BD | 161 | SER |
| 1 | BD | 163 | LEU |
| 1 | BD | 167 | THR |
| 1 | BD | 182 | LEU |
| 1 | BD | 191 | LEU |
| 1 | BD | 199 | SER |
| 1 | BD | 226 | VAL |
| 1 | BD | 243 | ILE |
| 1 | BD | 260 | MET |
| 1 | BD | 272 | TYR |
| 1 | BD | 284 | ARG |
| 1 | BD | 289 | ARG |
| 1 | BD | 300 | GLN |
| 1 | BD | 301 | ARG |
| 1 | BD | 378 | ARG |
| 1 | BD | 384 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BD | 449 | GLU |
| 1 | BD | 454 | ASN |
| 1 | BD | 475 | LEU |
| 1 | BD | 504 | VAL |
| 1 | BE | 105 | SER |
| 1 | BE | 129 | ARG |
| 1 | BE | 160 | THR |
| 1 | BE | 161 | SER |
| 1 | BE | 163 | LEU |
| 1 | BE | 167 | THR |
| 1 | BE | 182 | LEU |
| 1 | BE | 191 | LEU |
| 1 | BE | 199 | SER |
| 1 | BE | 226 | VAL |
| 1 | BE | 243 | ILE |
| 1 | BE | 260 | MET |
| 1 | BE | 272 | TYR |
| 1 | BE | 284 | ARG |
| 1 | BE | 289 | ARG |
| 1 | BE | 300 | GLN |
| 1 | BE | 301 | ARG |
| 1 | BE | 378 | ARG |
| 1 | BE | 384 | ASN |
| 1 | BE | 449 | GLU |
| 1 | BE | 454 | ASN |
| 1 | BE | 475 | LEU |
| 1 | BE | 504 | VAL |
| 1 | BF | 10 | ILE |
| 1 | BF | 18 | ARG |
| 1 | BF | 79 | ARG |
| 1 | BF | 105 | SER |
| 1 | BF | 129 | ARG |
| 1 | BF | 160 | THR |
| 1 | BF | 161 | SER |
| 1 | BF | 163 | LEU |
| 1 | BF | 167 | THR |
| 1 | BF | 182 | LEU |
| 1 | BF | 191 | LEU |
| 1 | BF | 199 | SER |
| 1 | BF | 226 | VAL |
| 1 | BF | 243 | ILE |
| 1 | BF | 260 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BF | 272 | TYR |
| 1 | BF | 284 | ARG |
| 1 | BF | 289 | ARG |
| 1 | BF | 299 | SER |
| 1 | BF | 301 | ARG |
| 1 | BF | 378 | ARG |
| 1 | BF | 384 | ASN |
| 1 | BF | 449 | GLU |
| 1 | BF | 454 | ASN |
| 1 | BF | 475 | LEU |
| 1 | BF | 504 | VAL |
| 1 | BG | 105 | SER |
| 1 | BG | 129 | ARG |
| 1 | BG | 160 | THR |
| 1 | BG | 161 | SER |
| 1 | BG | 163 | LEU |
| 1 | BG | 167 | THR |
| 1 | BG | 182 | LEU |
| 1 | BG | 191 | LEU |
| 1 | BG | 199 | SER |
| 1 | BG | 226 | VAL |
| 1 | BG | 229 | MET |
| 1 | BG | 243 | ILE |
| 1 | BG | 260 | MET |
| 1 | BG | 272 | TYR |
| 1 | BG | 284 | ARG |
| 1 | BG | 289 | ARG |
| 1 | BG | 301 | ARG |
| 1 | BG | 378 | ARG |
| 1 | BG | 384 | ASN |
| 1 | BG | 454 | ASN |
| 1 | BG | 475 | LEU |
| 1 | BG | 504 | VAL |
| 1 | BH | 15 | GLN |
| 1 | BH | 18 | ARG |
| 1 | BH | 105 | SER |
| 1 | BH | 129 | ARG |
| 1 | BH | 160 | THR |
| 1 | BH | 161 | SER |
| 1 | BH | 163 | LEU |
| 1 | BH | 167 | THR |
| 1 | BH | 182 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BH | 191 | LEU |
| 1 | BH | 199 | SER |
| 1 | BH | 226 | VAL |
| 1 | BH | 229 | MET |
| 1 | BH | 243 | ILE |
| 1 | BH | 260 | MET |
| 1 | BH | 272 | TYR |
| 1 | BH | 284 | ARG |
| 1 | BH | 289 | ARG |
| 1 | BH | 301 | ARG |
| 1 | BH | 305 | SER |
| 1 | BH | 378 | ARG |
| 1 | BH | 384 | ASN |
| 1 | BH | 449 | GLU |
| 1 | BH | 454 | ASN |
| 1 | BH | 475 | LEU |
| 1 | BH | 504 | VAL |
| 1 | BI | 105 | SER |
| 1 | BI | 129 | ARG |
| 1 | BI | 160 | THR |
| 1 | BI | 161 | SER |
| 1 | BI | 163 | LEU |
| 1 | BI | 167 | THR |
| 1 | BI | 182 | LEU |
| 1 | BI | 191 | LEU |
| 1 | BI | 199 | SER |
| 1 | BI | 226 | VAL |
| 1 | BI | 243 | ILE |
| 1 | BI | 260 | MET |
| 1 | BI | 272 | TYR |
| 1 | BI | 284 | ARG |
| 1 | BI | 289 | ARG |
| 1 | BI | 301 | ARG |
| 1 | BI | 378 | ARG |
| 1 | BI | 384 | ASN |
| 1 | BI | 449 | GLU |
| 1 | BI | 454 | ASN |
| 1 | BI | 475 | LEU |
| 1 | BI | 504 | VAL |
| 1 | BJ | 18 | ARG |
| 1 | BJ | 79 | ARG |
| 1 | BJ | 105 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BJ | 129 | ARG |
| 1 | BJ | 160 | THR |
| 1 | BJ | 161 | SER |
| 1 | BJ | 163 | LEU |
| 1 | BJ | 167 | THR |
| 1 | BJ | 182 | LEU |
| 1 | BJ | 191 | LEU |
| 1 | BJ | 199 | SER |
| 1 | BJ | 226 | VAL |
| 1 | BJ | 243 | ILE |
| 1 | BJ | 260 | MET |
| 1 | BJ | 272 | TYR |
| 1 | BJ | 284 | ARG |
| 1 | BJ | 289 | ARG |
| 1 | BJ | 301 | ARG |
| 1 | BJ | 378 | ARG |
| 1 | BJ | 384 | ASN |
| 1 | BJ | 449 | GLU |
| 1 | BJ | 454 | ASN |
| 1 | BJ | 475 | LEU |
| 1 | BJ | 504 | VAL |
| 1 | BK | 18 | ARG |
| 1 | BK | 105 | SER |
| 1 | BK | 129 | ARG |
| 1 | BK | 160 | THR |
| 1 | BK | 161 | SER |
| 1 | BK | 163 | LEU |
| 1 | BK | 167 | THR |
| 1 | BK | 182 | LEU |
| 1 | BK | 191 | LEU |
| 1 | BK | 199 | SER |
| 1 | BK | 226 | VAL |
| 1 | BK | 229 | MET |
| 1 | BK | 243 | ILE |
| 1 | BK | 260 | MET |
| 1 | BK | 272 | TYR |
| 1 | BK | 284 | ARG |
| 1 | BK | 289 | ARG |
| 1 | BK | 299 | SER |
| 1 | BK | 300 | GLN |
| 1 | BK | 301 | ARG |
| 1 | BK | 378 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BK | 384 | ASN |
| 1 | BK | 449 | GLU |
| 1 | BK | 454 | ASN |
| 1 | BK | 475 | LEU |
| 1 | BK | 504 | VAL |
| 1 | BL | 9 | TYR |
| 1 | BL | 79 | ARG |
| 1 | BL | 105 | SER |
| 1 | BL | 129 | ARG |
| 1 | BL | 160 | THR |
| 1 | BL | 161 | SER |
| 1 | BL | 163 | LEU |
| 1 | BL | 167 | THR |
| 1 | BL | 182 | LEU |
| 1 | BL | 191 | LEU |
| 1 | BL | 199 | SER |
| 1 | BL | 226 | VAL |
| 1 | BL | 229 | MET |
| 1 | BL | 243 | ILE |
| 1 | BL | 260 | MET |
| 1 | BL | 272 | TYR |
| 1 | BL | 284 | ARG |
| 1 | BL | 289 | ARG |
| 1 | BL | 299 | SER |
| 1 | BL | 300 | GLN |
| 1 | BL | 301 | ARG |
| 1 | BL | 378 | ARG |
| 1 | BL | 384 | ASN |
| 1 | BL | 449 | GLU |
| 1 | BL | 454 | ASN |
| 1 | BL | 475 | LEU |
| 1 | BL | 504 | VAL |
| 1 | BM | 18 | ARG |
| 1 | BM | 57 | PRO |
| 1 | BM | 79 | ARG |
| 1 | BM | 105 | SER |
| 1 | BM | 129 | ARG |
| 1 | BM | 160 | THR |
| 1 | BM | 161 | SER |
| 1 | BM | 163 | LEU |
| 1 | BM | 167 | THR |
| 1 | BM | 182 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BM | 191 | LEU |
| 1 | BM | 199 | SER |
| 1 | BM | 226 | VAL |
| 1 | BM | 243 | ILE |
| 1 | BM | 260 | MET |
| 1 | BM | 272 | TYR |
| 1 | BM | 284 | ARG |
| 1 | BM | 289 | ARG |
| 1 | BM | 300 | GLN |
| 1 | BM | 301 | ARG |
| 1 | BM | 378 | ARG |
| 1 | BM | 384 | ASN |
| 1 | BM | 449 | GLU |
| 1 | BM | 454 | ASN |
| 1 | BM | 475 | LEU |
| 1 | BM | 504 | VAL |
| 1 | BN | 18 | ARG |
| 1 | BN | 105 | SER |
| 1 | BN | 129 | ARG |
| 1 | BN | 160 | THR |
| 1 | BN | 161 | SER |
| 1 | BN | 163 | LEU |
| 1 | BN | 167 | THR |
| 1 | BN | 182 | LEU |
| 1 | BN | 191 | LEU |
| 1 | BN | 199 | SER |
| 1 | BN | 226 | VAL |
| 1 | BN | 229 | MET |
| 1 | BN | 243 | ILE |
| 1 | BN | 260 | MET |
| 1 | BN | 272 | TYR |
| 1 | BN | 284 | ARG |
| 1 | BN | 285 | SER |
| 1 | BN | 289 | ARG |
| 1 | BN | 301 | ARG |
| 1 | BN | 378 | ARG |
| 1 | BN | 384 | ASN |
| 1 | BN | 449 | GLU |
| 1 | BN | 454 | ASN |
| 1 | BN | 475 | LEU |
| 1 | BN | 504 | VAL |
| 1 | BO | 15 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BO | 105 | SER |
| 1 | BO | 129 | ARG |
| 1 | BO | 160 | THR |
| 1 | BO | 161 | SER |
| 1 | BO | 163 | LEU |
| 1 | BO | 167 | THR |
| 1 | BO | 182 | LEU |
| 1 | BO | 191 | LEU |
| 1 | BO | 199 | SER |
| 1 | BO | 226 | VAL |
| 1 | BO | 243 | ILE |
| 1 | BO | 260 | MET |
| 1 | BO | 284 | ARG |
| 1 | BO | 289 | ARG |
| 1 | BO | 301 | ARG |
| 1 | BO | 336 | PRO |
| 1 | BO | 378 | ARG |
| 1 | BO | 384 | ASN |
| 1 | BO | 449 | GLU |
| 1 | BO | 454 | ASN |
| 1 | BO | 475 | LEU |
| 1 | BO | 504 | VAL |
| 1 | BP | 79 | ARG |
| 1 | BP | 105 | SER |
| 1 | BP | 160 | THR |
| 1 | BP | 161 | SER |
| 1 | BP | 163 | LEU |
| 1 | BP | 167 | THR |
| 1 | BP | 182 | LEU |
| 1 | BP | 191 | LEU |
| 1 | BP | 199 | SER |
| 1 | BP | 226 | VAL |
| 1 | BP | 243 | ILE |
| 1 | BP | 260 | MET |
| 1 | BP | 272 | TYR |
| 1 | BP | 284 | ARG |
| 1 | BP | 289 | ARG |
| 1 | BP | 300 | GLN |
| 1 | BP | 301 | ARG |
| 1 | BP | 378 | ARG |
| 1 | BP | 384 | ASN |
| 1 | BP | 449 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BP | 454 | ASN |
| 1 | BP | 475 | LEU |
| 1 | BP | 504 | VAL |
| 1 | BQ | 18 | ARG |
| 1 | BQ | 105 | SER |
| 1 | BQ | 129 | ARG |
| 1 | BQ | 160 | THR |
| 1 | BQ | 161 | SER |
| 1 | BQ | 163 | LEU |
| 1 | BQ | 167 | THR |
| 1 | BQ | 182 | LEU |
| 1 | BQ | 191 | LEU |
| 1 | BQ | 199 | SER |
| 1 | BQ | 226 | VAL |
| 1 | BQ | 229 | MET |
| 1 | BQ | 243 | ILE |
| 1 | BQ | 260 | MET |
| 1 | BQ | 272 | TYR |
| 1 | BQ | 284 | ARG |
| 1 | BQ | 289 | ARG |
| 1 | BQ | 301 | ARG |
| 1 | BQ | 378 | ARG |
| 1 | BQ | 384 | ASN |
| 1 | BQ | 404 | LEU |
| 1 | BQ | 449 | GLU |
| 1 | BQ | 454 | ASN |
| 1 | BQ | 475 | LEU |
| 1 | BQ | 504 | VAL |
| 1 | BR | 79 | ARG |
| 1 | BR | 105 | SER |
| 1 | BR | 160 | THR |
| 1 | BR | 161 | SER |
| 1 | BR | 163 | LEU |
| 1 | BR | 167 | THR |
| 1 | BR | 182 | LEU |
| 1 | BR | 191 | LEU |
| 1 | BR | 199 | SER |
| 1 | BR | 226 | VAL |
| 1 | BR | 243 | ILE |
| 1 | BR | 260 | MET |
| 1 | BR | 272 | TYR |
| 1 | BR | 284 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BR | 289 | ARG |
| 1 | BR | 299 | SER |
| 1 | BR | 301 | ARG |
| 1 | BR | 378 | ARG |
| 1 | BR | 384 | ASN |
| 1 | BR | 449 | GLU |
| 1 | BR | 454 | ASN |
| 1 | BR | 475 | LEU |
| 1 | BR | 504 | VAL |
| 1 | BS | 79 | ARG |
| 1 | BS | 105 | SER |
| 1 | BS | 129 | ARG |
| 1 | BS | 160 | THR |
| 1 | BS | 161 | SER |
| 1 | BS | 163 | LEU |
| 1 | BS | 167 | THR |
| 1 | BS | 182 | LEU |
| 1 | BS | 191 | LEU |
| 1 | BS | 199 | SER |
| 1 | BS | 226 | VAL |
| 1 | BS | 243 | ILE |
| 1 | BS | 260 | MET |
| 1 | BS | 284 | ARG |
| 1 | BS | 289 | ARG |
| 1 | BS | 299 | SER |
| 1 | BS | 301 | ARG |
| 1 | BS | 336 | PRO |
| 1 | BS | 378 | ARG |
| 1 | BS | 384 | ASN |
| 1 | BS | 449 | GLU |
| 1 | BS | 454 | ASN |
| 1 | BS | 475 | LEU |
| 1 | BS | 504 | VAL |
| 1 | BT | 105 | SER |
| 1 | BT | 129 | ARG |
| 1 | BT | 160 | THR |
| 1 | BT | 161 | SER |
| 1 | BT | 163 | LEU |
| 1 | BT | 167 | THR |
| 1 | BT | 182 | LEU |
| 1 | BT | 191 | LEU |
| 1 | BT | 199 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BT | 226 | VAL |
| 1 | BT | 243 | ILE |
| 1 | BT | 260 | MET |
| 1 | BT | 272 | TYR |
| 1 | BT | 284 | ARG |
| 1 | BT | 289 | ARG |
| 1 | BT | 299 | SER |
| 1 | BT | 300 | GLN |
| 1 | BT | 301 | ARG |
| 1 | BT | 378 | ARG |
| 1 | BT | 384 | ASN |
| 1 | BT | 449 | GLU |
| 1 | BT | 454 | ASN |
| 1 | BT | 475 | LEU |
| 1 | BT | 504 | VAL |
| 1 | CA | 10 | ILE |
| 1 | CA | 18 | ARG |
| 1 | CA | 105 | SER |
| 1 | CA | 129 | ARG |
| 1 | CA | 160 | THR |
| 1 | CA | 161 | SER |
| 1 | CA | 163 | LEU |
| 1 | CA | 167 | THR |
| 1 | CA | 182 | LEU |
| 1 | CA | 191 | LEU |
| 1 | CA | 226 | VAL |
| 1 | CA | 243 | ILE |
| 1 | CA | 260 | MET |
| 1 | CA | 272 | TYR |
| 1 | CA | 284 | ARG |
| 1 | CA | 289 | ARG |
| 1 | CA | 301 | ARG |
| 1 | CA | 378 | ARG |
| 1 | CA | 384 | ASN |
| 1 | CA | 449 | GLU |
| 1 | CA | 454 | ASN |
| 1 | CA | 475 | LEU |
| 1 | CA | 504 | VAL |
| 1 | CB | 18 | ARG |
| 1 | CB | 105 | SER |
| 1 | CB | 129 | ARG |
| 1 | CB | 160 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CB | 161 | SER |
| 1 | CB | 163 | LEU |
| 1 | CB | 167 | THR |
| 1 | CB | 182 | LEU |
| 1 | CB | 191 | LEU |
| 1 | CB | 199 | SER |
| 1 | CB | 226 | VAL |
| 1 | CB | 243 | ILE |
| 1 | CB | 260 | MET |
| 1 | CB | 272 | TYR |
| 1 | CB | 284 | ARG |
| 1 | CB | 289 | ARG |
| 1 | CB | 300 | GLN |
| 1 | CB | 301 | ARG |
| 1 | CB | 378 | ARG |
| 1 | CB | 384 | ASN |
| 1 | CB | 449 | GLU |
| 1 | CB | 454 | ASN |
| 1 | CB | 475 | LEU |
| 1 | CB | 504 | VAL |
| 1 | CC | 105 | SER |
| 1 | CC | 129 | ARG |
| 1 | CC | 160 | THR |
| 1 | CC | 161 | SER |
| 1 | CC | 163 | LEU |
| 1 | CC | 167 | THR |
| 1 | CC | 182 | LEU |
| 1 | CC | 191 | LEU |
| 1 | CC | 199 | SER |
| 1 | CC | 226 | VAL |
| 1 | CC | 243 | ILE |
| 1 | CC | 260 | MET |
| 1 | CC | 272 | TYR |
| 1 | CC | 284 | ARG |
| 1 | CC | 289 | ARG |
| 1 | CC | 300 | GLN |
| 1 | CC | 301 | ARG |
| 1 | CC | 378 | ARG |
| 1 | CC | 384 | ASN |
| 1 | CC | 449 | GLU |
| 1 | CC | 454 | ASN |
| 1 | CC | 475 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CC | 504 | VAL |
| 1 | CD | 79 | ARG |
| 1 | CD | 105 | SER |
| 1 | CD | 129 | ARG |
| 1 | CD | 160 | THR |
| 1 | CD | 161 | SER |
| 1 | CD | 163 | LEU |
| 1 | CD | 167 | THR |
| 1 | CD | 182 | LEU |
| 1 | CD | 191 | LEU |
| 1 | CD | 199 | SER |
| 1 | CD | 226 | VAL |
| 1 | CD | 229 | MET |
| 1 | CD | 243 | ILE |
| 1 | CD | 260 | MET |
| 1 | CD | 272 | TYR |
| 1 | CD | 284 | ARG |
| 1 | CD | 289 | ARG |
| 1 | CD | 301 | ARG |
| 1 | CD | 378 | ARG |
| 1 | CD | 384 | ASN |
| 1 | CD | 449 | GLU |
| 1 | CD | 454 | ASN |
| 1 | CD | 475 | LEU |
| 1 | CD | 504 | VAL |
| 1 | CE | 79 | ARG |
| 1 | CE | 105 | SER |
| 1 | CE | 129 | ARG |
| 1 | CE | 160 | THR |
| 1 | CE | 161 | SER |
| 1 | CE | 163 | LEU |
| 1 | CE | 167 | THR |
| 1 | CE | 182 | LEU |
| 1 | CE | 191 | LEU |
| 1 | CE | 199 | SER |
| 1 | CE | 226 | VAL |
| 1 | CE | 243 | ILE |
| 1 | CE | 260 | MET |
| 1 | CE | 272 | TYR |
| 1 | CE | 284 | ARG |
| 1 | CE | 289 | ARG |
| 1 | CE | 301 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CE | 336 | PRO |
| 1 | CE | 378 | ARG |
| 1 | CE | 384 | ASN |
| 1 | CE | 449 | GLU |
| 1 | CE | 454 | ASN |
| 1 | CE | 475 | LEU |
| 1 | CE | 504 | VAL |
| 1 | CF | 79 | ARG |
| 1 | CF | 105 | SER |
| 1 | CF | 129 | ARG |
| 1 | CF | 160 | THR |
| 1 | CF | 161 | SER |
| 1 | CF | 163 | LEU |
| 1 | CF | 167 | THR |
| 1 | CF | 182 | LEU |
| 1 | CF | 191 | LEU |
| 1 | CF | 199 | SER |
| 1 | CF | 226 | VAL |
| 1 | CF | 243 | ILE |
| 1 | CF | 260 | MET |
| 1 | CF | 272 | TYR |
| 1 | CF | 284 | ARG |
| 1 | CF | 289 | ARG |
| 1 | CF | 300 | GLN |
| 1 | CF | 301 | ARG |
| 1 | CF | 378 | ARG |
| 1 | CF | 384 | ASN |
| 1 | CF | 449 | GLU |
| 1 | CF | 454 | ASN |
| 1 | CF | 475 | LEU |
| 1 | CF | 504 | VAL |
| 1 | CG | 79 | ARG |
| 1 | CG | 105 | SER |
| 1 | CG | 129 | ARG |
| 1 | CG | 160 | THR |
| 1 | CG | 161 | SER |
| 1 | CG | 163 | LEU |
| 1 | CG | 167 | THR |
| 1 | CG | 182 | LEU |
| 1 | CG | 191 | LEU |
| 1 | CG | 199 | SER |
| 1 | CG | 226 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CG | 243 | ILE |
| 1 | CG | 260 | MET |
| 1 | CG | 272 | TYR |
| 1 | CG | 284 | ARG |
| 1 | CG | 289 | ARG |
| 1 | CG | 301 | ARG |
| 1 | CG | 378 | ARG |
| 1 | CG | 384 | ASN |
| 1 | CG | 454 | ASN |
| 1 | CG | 475 | LEU |
| 1 | CG | 504 | VAL |
| 1 | CH | 10 | ILE |
| 1 | CH | 15 | GLN |
| 1 | CH | 105 | SER |
| 1 | CH | 129 | ARG |
| 1 | CH | 160 | THR |
| 1 | CH | 161 | SER |
| 1 | CH | 163 | LEU |
| 1 | CH | 167 | THR |
| 1 | CH | 182 | LEU |
| 1 | CH | 191 | LEU |
| 1 | CH | 199 | SER |
| 1 | CH | 226 | VAL |
| 1 | CH | 229 | MET |
| 1 | CH | 243 | ILE |
| 1 | CH | 260 | MET |
| 1 | CH | 272 | TYR |
| 1 | CH | 284 | ARG |
| 1 | CH | 289 | ARG |
| 1 | CH | 301 | ARG |
| 1 | CH | 378 | ARG |
| 1 | CH | 384 | ASN |
| 1 | CH | 449 | GLU |
| 1 | CH | 454 | ASN |
| 1 | CH | 475 | LEU |
| 1 | CH | 504 | VAL |
| 1 | CI | 79 | ARG |
| 1 | CI | 105 | SER |
| 1 | CI | 129 | ARG |
| 1 | CI | 160 | THR |
| 1 | CI | 161 | SER |
| 1 | CI | 163 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CI | 167 | THR |
| 1 | CI | 182 | LEU |
| 1 | CI | 191 | LEU |
| 1 | CI | 199 | SER |
| 1 | CI | 226 | VAL |
| 1 | CI | 243 | ILE |
| 1 | CI | 260 | MET |
| 1 | CI | 272 | TYR |
| 1 | CI | 284 | ARG |
| 1 | CI | 289 | ARG |
| 1 | CI | 299 | SER |
| 1 | CI | 301 | ARG |
| 1 | CI | 378 | ARG |
| 1 | CI | 384 | ASN |
| 1 | CI | 449 | GLU |
| 1 | CI | 454 | ASN |
| 1 | CI | 475 | LEU |
| 1 | CI | 504 | VAL |
| 1 | CJ | 18 | ARG |
| 1 | CJ | 105 | SER |
| 1 | CJ | 129 | ARG |
| 1 | CJ | 160 | THR |
| 1 | CJ | 161 | SER |
| 1 | CJ | 163 | LEU |
| 1 | CJ | 182 | LEU |
| 1 | CJ | 191 | LEU |
| 1 | CJ | 199 | SER |
| 1 | CJ | 226 | VAL |
| 1 | CJ | 243 | ILE |
| 1 | CJ | 260 | MET |
| 1 | CJ | 272 | TYR |
| 1 | CJ | 284 | ARG |
| 1 | CJ | 289 | ARG |
| 1 | CJ | 300 | GLN |
| 1 | CJ | 301 | ARG |
| 1 | CJ | 378 | ARG |
| 1 | CJ | 384 | ASN |
| 1 | CJ | 449 | GLU |
| 1 | CJ | 454 | ASN |
| 1 | CJ | 475 | LEU |
| 1 | CJ | 504 | VAL |
| 1 | CK | 18 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CK | 77 | THR |
| 1 | CK | 105 | SER |
| 1 | CK | 129 | ARG |
| 1 | CK | 160 | THR |
| 1 | CK | 161 | SER |
| 1 | CK | 163 | LEU |
| 1 | CK | 167 | THR |
| 1 | CK | 182 | LEU |
| 1 | CK | 191 | LEU |
| 1 | CK | 199 | SER |
| 1 | CK | 226 | VAL |
| 1 | CK | 243 | ILE |
| 1 | CK | 260 | MET |
| 1 | CK | 272 | TYR |
| 1 | CK | 284 | ARG |
| 1 | CK | 289 | ARG |
| 1 | CK | 301 | ARG |
| 1 | CK | 378 | ARG |
| 1 | CK | 384 | ASN |
| 1 | CK | 449 | GLU |
| 1 | CK | 454 | ASN |
| 1 | CK | 475 | LEU |
| 1 | CK | 504 | VAL |
| 1 | CL | 9 | TYR |
| 1 | CL | 105 | SER |
| 1 | CL | 129 | ARG |
| 1 | CL | 160 | THR |
| 1 | CL | 161 | SER |
| 1 | CL | 163 | LEU |
| 1 | CL | 167 | THR |
| 1 | CL | 182 | LEU |
| 1 | CL | 191 | LEU |
| 1 | CL | 199 | SER |
| 1 | CL | 226 | VAL |
| 1 | CL | 229 | MET |
| 1 | CL | 243 | ILE |
| 1 | CL | 260 | MET |
| 1 | CL | 272 | TYR |
| 1 | CL | 284 | ARG |
| 1 | CL | 289 | ARG |
| 1 | CL | 299 | SER |
| 1 | CL | 301 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CL | 378 | ARG |
| 1 | CL | 384 | ASN |
| 1 | CL | 449 | GLU |
| 1 | CL | 454 | ASN |
| 1 | CL | 475 | LEU |
| 1 | CL | 504 | VAL |
| 1 | CM | 10 | ILE |
| 1 | CM | 18 | ARG |
| 1 | CM | 57 | PRO |
| 1 | CM | 79 | ARG |
| 1 | CM | 105 | SER |
| 1 | CM | 129 | ARG |
| 1 | CM | 160 | THR |
| 1 | CM | 161 | SER |
| 1 | CM | 163 | LEU |
| 1 | CM | 167 | THR |
| 1 | CM | 182 | LEU |
| 1 | CM | 191 | LEU |
| 1 | CM | 199 | SER |
| 1 | CM | 226 | VAL |
| 1 | CM | 243 | ILE |
| 1 | CM | 260 | MET |
| 1 | CM | 272 | TYR |
| 1 | CM | 284 | ARG |
| 1 | CM | 289 | ARG |
| 1 | CM | 299 | SER |
| 1 | CM | 301 | ARG |
| 1 | CM | 378 | ARG |
| 1 | CM | 384 | ASN |
| 1 | CM | 449 | GLU |
| 1 | CM | 454 | ASN |
| 1 | CM | 475 | LEU |
| 1 | CM | 504 | VAL |
| 1 | CN | 105 | SER |
| 1 | CN | 160 | THR |
| 1 | CN | 161 | SER |
| 1 | CN | 163 | LEU |
| 1 | CN | 167 | THR |
| 1 | CN | 182 | LEU |
| 1 | CN | 191 | LEU |
| 1 | CN | 199 | SER |
| 1 | CN | 226 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CN | 229 | MET |
| 1 | CN | 243 | ILE |
| 1 | CN | 260 | MET |
| 1 | CN | 272 | TYR |
| 1 | CN | 284 | ARG |
| 1 | CN | 289 | ARG |
| 1 | CN | 301 | ARG |
| 1 | CN | 336 | PRO |
| 1 | CN | 378 | ARG |
| 1 | CN | 384 | ASN |
| 1 | CN | 449 | GLU |
| 1 | CN | 454 | ASN |
| 1 | CN | 475 | LEU |
| 1 | CN | 504 | VAL |
| 1 | CO | 57 | PRO |
| 1 | CO | 79 | ARG |
| 1 | CO | 105 | SER |
| 1 | CO | 160 | THR |
| 1 | CO | 161 | SER |
| 1 | CO | 163 | LEU |
| 1 | CO | 167 | THR |
| 1 | CO | 191 | LEU |
| 1 | CO | 199 | SER |
| 1 | CO | 226 | VAL |
| 1 | CO | 243 | ILE |
| 1 | CO | 260 | MET |
| 1 | CO | 272 | TYR |
| 1 | CO | 284 | ARG |
| 1 | CO | 289 | ARG |
| 1 | CO | 301 | ARG |
| 1 | CO | 378 | ARG |
| 1 | CO | 384 | ASN |
| 1 | CO | 449 | GLU |
| 1 | CO | 454 | ASN |
| 1 | CO | 475 | LEU |
| 1 | CO | 504 | VAL |
| 1 | CP | 10 | ILE |
| 1 | CP | 79 | ARG |
| 1 | CP | 105 | SER |
| 1 | CP | 129 | ARG |
| 1 | CP | 160 | THR |
| 1 | CP | 161 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CP | 163 | LEU |
| 1 | CP | 167 | THR |
| 1 | CP | 182 | LEU |
| 1 | CP | 191 | LEU |
| 1 | CP | 199 | SER |
| 1 | CP | 226 | VAL |
| 1 | CP | 243 | ILE |
| 1 | CP | 260 | MET |
| 1 | CP | 272 | TYR |
| 1 | CP | 284 | ARG |
| 1 | CP | 289 | ARG |
| 1 | CP | 300 | GLN |
| 1 | CP | 301 | ARG |
| 1 | CP | 378 | ARG |
| 1 | CP | 384 | ASN |
| 1 | CP | 449 | GLU |
| 1 | CP | 454 | ASN |
| 1 | CP | 475 | LEU |
| 1 | CP | 504 | VAL |
| 1 | CQ | 18 | ARG |
| 1 | CQ | 105 | SER |
| 1 | CQ | 129 | ARG |
| 1 | CQ | 160 | THR |
| 1 | CQ | 161 | SER |
| 1 | CQ | 163 | LEU |
| 1 | CQ | 167 | THR |
| 1 | CQ | 182 | LEU |
| 1 | CQ | 191 | LEU |
| 1 | CQ | 199 | SER |
| 1 | CQ | 226 | VAL |
| 1 | CQ | 229 | MET |
| 1 | CQ | 243 | ILE |
| 1 | CQ | 260 | MET |
| 1 | CQ | 272 | TYR |
| 1 | CQ | 284 | ARG |
| 1 | CQ | 289 | ARG |
| 1 | CQ | 300 | GLN |
| 1 | CQ | 301 | ARG |
| 1 | CQ | 336 | PRO |
| 1 | CQ | 378 | ARG |
| 1 | CQ | 384 | ASN |
| 1 | CQ | 449 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CQ | 454 | ASN |
| 1 | CQ | 475 | LEU |
| 1 | CQ | 504 | VAL |
| 1 | CR | 78 | SER |
| 1 | CR | 79 | ARG |
| 1 | CR | 105 | SER |
| 1 | CR | 160 | THR |
| 1 | CR | 161 | SER |
| 1 | CR | 163 | LEU |
| 1 | CR | 167 | THR |
| 1 | CR | 182 | LEU |
| 1 | CR | 191 | LEU |
| 1 | CR | 199 | SER |
| 1 | CR | 226 | VAL |
| 1 | CR | 229 | MET |
| 1 | CR | 243 | ILE |
| 1 | CR | 260 | MET |
| 1 | CR | 272 | TYR |
| 1 | CR | 284 | ARG |
| 1 | CR | 289 | ARG |
| 1 | CR | 299 | SER |
| 1 | CR | 301 | ARG |
| 1 | CR | 378 | ARG |
| 1 | CR | 384 | ASN |
| 1 | CR | 449 | GLU |
| 1 | CR | 454 | ASN |
| 1 | CR | 475 | LEU |
| 1 | CR | 504 | VAL |
| 1 | CS | 105 | SER |
| 1 | CS | 160 | THR |
| 1 | CS | 161 | SER |
| 1 | CS | 163 | LEU |
| 1 | CS | 167 | THR |
| 1 | CS | 182 | LEU |
| 1 | CS | 191 | LEU |
| 1 | CS | 199 | SER |
| 1 | CS | 226 | VAL |
| 1 | CS | 229 | MET |
| 1 | CS | 243 | ILE |
| 1 | CS | 260 | MET |
| 1 | CS | 272 | TYR |
| 1 | CS | 284 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CS | 289 | ARG |
| 1 | CS | 299 | SER |
| 1 | CS | 301 | ARG |
| 1 | CS | 378 | ARG |
| 1 | CS | 384 | ASN |
| 1 | CS | 449 | GLU |
| 1 | CS | 454 | ASN |
| 1 | CS | 475 | LEU |
| 1 | CS | 504 | VAL |
| 1 | CT | 105 | SER |
| 1 | CT | 129 | ARG |
| 1 | CT | 160 | THR |
| 1 | CT | 161 | SER |
| 1 | CT | 163 | LEU |
| 1 | CT | 167 | THR |
| 1 | CT | 182 | LEU |
| 1 | CT | 191 | LEU |
| 1 | CT | 199 | SER |
| 1 | CT | 226 | VAL |
| 1 | CT | 229 | MET |
| 1 | CT | 243 | ILE |
| 1 | CT | 260 | MET |
| 1 | CT | 272 | TYR |
| 1 | CT | 284 | ARG |
| 1 | CT | 289 | ARG |
| 1 | CT | 299 | SER |
| 1 | CT | 301 | ARG |
| 1 | CT | 336 | PRO |
| 1 | CT | 378 | ARG |
| 1 | CT | 384 | ASN |
| 1 | CT | 449 | GLU |
| 1 | CT | 454 | ASN |
| 1 | CT | 475 | LEU |
| 1 | CT | 504 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (662) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AA | 36 | GLN |
| 1 | AA | 74 | ASN |
| 1 | AA | 131 | HIS |
| 1 | AA | 138 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AA | 238 | HIS |
| 1 | AA | 256 | ASN |
| 1 | AA | 263 | ASN |
| 1 | AA | 288 | HIS |
| 1 | AA | 300 | GLN |
| 1 | AA | 437 | HIS |
| 1 | AA | 454 | ASN |
| 1 | AB | 36 | GLN |
| 1 | AB | 74 | ASN |
| 1 | AB | 131 | HIS |
| 1 | AB | 138 | ASN |
| 1 | AB | 147 | GLN |
| 1 | AB | 238 | HIS |
| 1 | AB | 256 | ASN |
| 1 | AB | 263 | ASN |
| 1 | AB | 288 | HIS |
| 1 | AB | 300 | GLN |
| 1 | AB | 454 | ASN |
| 1 | AC | 36 | GLN |
| 1 | AC | 74 | ASN |
| 1 | AC | 131 | HIS |
| 1 | AC | 138 | ASN |
| 1 | AC | 147 | GLN |
| 1 | AC | 238 | HIS |
| 1 | AC | 256 | ASN |
| 1 | AC | 263 | ASN |
| 1 | AC | 288 | HIS |
| 1 | AC | 300 | GLN |
| 1 | AC | 437 | HIS |
| 1 | AC | 454 | ASN |
| 1 | AD | 36 | GLN |
| 1 | AD | 74 | ASN |
| 1 | AD | 131 | HIS |
| 1 | AD | 138 | ASN |
| 1 | AD | 147 | GLN |
| 1 | AD | 238 | HIS |
| 1 | AD | 256 | ASN |
| 1 | AD | 263 | ASN |
| 1 | AD | 288 | HIS |
| 1 | AD | 454 | ASN |
| 1 | AE | 36 | GLN |
| 1 | AE | 74 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AE | 131 | HIS |
| 1 | AE | 138 | ASN |
| 1 | AE | 147 | GLN |
| 1 | AE | 238 | HIS |
| 1 | AE | 256 | ASN |
| 1 | AE | 263 | ASN |
| 1 | AE | 288 | HIS |
| 1 | AE | 454 | ASN |
| 1 | AF | 15 | GLN |
| 1 | AF | 36 | GLN |
| 1 | AF | 74 | ASN |
| 1 | AF | 131 | HIS |
| 1 | AF | 138 | ASN |
| 1 | AF | 147 | GLN |
| 1 | AF | 238 | HIS |
| 1 | AF | 256 | ASN |
| 1 | AF | 263 | ASN |
| 1 | AF | 288 | HIS |
| 1 | AF | 300 | GLN |
| 1 | AF | 454 | ASN |
| 1 | AG | 15 | GLN |
| 1 | AG | 36 | GLN |
| 1 | AG | 74 | ASN |
| 1 | AG | 131 | HIS |
| 1 | AG | 138 | ASN |
| 1 | AG | 238 | HIS |
| 1 | AG | 256 | ASN |
| 1 | AG | 263 | ASN |
| 1 | AG | 288 | HIS |
| 1 | AG | 300 | GLN |
| 1 | AG | 454 | ASN |
| 1 | AH | 15 | GLN |
| 1 | AH | 36 | GLN |
| 1 | AH | 74 | ASN |
| 1 | AH | 131 | HIS |
| 1 | AH | 138 | ASN |
| 1 | AH | 238 | HIS |
| 1 | AH | 256 | ASN |
| 1 | AH | 263 | ASN |
| 1 | AH | 288 | HIS |
| 1 | AH | 300 | GLN |
| 1 | AH | 454 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AI | 36 | GLN |
| 1 | AI | 74 | ASN |
| 1 | AI | 131 | HIS |
| 1 | AI | 138 | ASN |
| 1 | AI | 238 | HIS |
| 1 | AI | 256 | ASN |
| 1 | AI | 263 | ASN |
| 1 | AI | 288 | HIS |
| 1 | AI | 300 | GLN |
| 1 | AI | 454 | ASN |
| 1 | AJ | 15 | GLN |
| 1 | AJ | 36 | GLN |
| 1 | AJ | 74 | ASN |
| 1 | AJ | 131 | HIS |
| 1 | AJ | 138 | ASN |
| 1 | AJ | 147 | GLN |
| 1 | AJ | 238 | HIS |
| 1 | AJ | 256 | ASN |
| 1 | AJ | 263 | ASN |
| 1 | AJ | 288 | HIS |
| 1 | AJ | 454 | ASN |
| 1 | AK | 36 | GLN |
| 1 | AK | 74 | ASN |
| 1 | AK | 131 | HIS |
| 1 | AK | 138 | ASN |
| 1 | AK | 147 | GLN |
| 1 | AK | 238 | HIS |
| 1 | AK | 256 | ASN |
| 1 | AK | 263 | ASN |
| 1 | AK | 288 | HIS |
| 1 | AK | 300 | GLN |
| 1 | AK | 437 | HIS |
| 1 | AK | 454 | ASN |
| 1 | AL | 36 | GLN |
| 1 | AL | 74 | ASN |
| 1 | AL | 131 | HIS |
| 1 | AL | 138 | ASN |
| 1 | AL | 147 | GLN |
| 1 | AL | 238 | HIS |
| 1 | AL | 256 | ASN |
| 1 | AL | 263 | ASN |
| 1 | AL | 288 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AL | 454 | ASN |
| 1 | AM | 36 | GLN |
| 1 | AM | 74 | ASN |
| 1 | AM | 131 | HIS |
| 1 | AM | 138 | ASN |
| 1 | AM | 238 | HIS |
| 1 | AM | 256 | ASN |
| 1 | AM | 263 | ASN |
| 1 | AM | 288 | HIS |
| 1 | AM | 454 | ASN |
| 1 | AN | 36 | GLN |
| 1 | AN | 74 | ASN |
| 1 | AN | 131 | HIS |
| 1 | AN | 138 | ASN |
| 1 | AN | 147 | GLN |
| 1 | AN | 238 | HIS |
| 1 | AN | 256 | ASN |
| 1 | AN | 263 | ASN |
| 1 | AN | 288 | HIS |
| 1 | AN | 300 | GLN |
| 1 | AN | 454 | ASN |
| 1 | AO | 36 | GLN |
| 1 | AO | 74 | ASN |
| 1 | AO | 131 | HIS |
| 1 | AO | 138 | ASN |
| 1 | AO | 147 | GLN |
| 1 | AO | 238 | HIS |
| 1 | AO | 256 | ASN |
| 1 | AO | 263 | ASN |
| 1 | AO | 288 | HIS |
| 1 | AO | 300 | GLN |
| 1 | AO | 437 | HIS |
| 1 | AO | 454 | ASN |
| 1 | AP | 36 | GLN |
| 1 | AP | 74 | ASN |
| 1 | AP | 131 | HIS |
| 1 | AP | 138 | ASN |
| 1 | AP | 147 | GLN |
| 1 | AP | 238 | HIS |
| 1 | AP | 256 | ASN |
| 1 | AP | 263 | ASN |
| 1 | AP | 288 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AP | 300 | GLN |
| 1 | AP | 437 | HIS |
| 1 | AP | 454 | ASN |
| 1 | AQ | 36 | GLN |
| 1 | AQ | 74 | ASN |
| 1 | AQ | 131 | HIS |
| 1 | AQ | 138 | ASN |
| 1 | AQ | 147 | GLN |
| 1 | AQ | 238 | HIS |
| 1 | AQ | 256 | ASN |
| 1 | AQ | 263 | ASN |
| 1 | AQ | 288 | HIS |
| 1 | AQ | 300 | GLN |
| 1 | AQ | 454 | ASN |
| 1 | AR | 36 | GLN |
| 1 | AR | 74 | ASN |
| 1 | AR | 131 | HIS |
| 1 | AR | 138 | ASN |
| 1 | AR | 147 | GLN |
| 1 | AR | 238 | HIS |
| 1 | AR | 256 | ASN |
| 1 | AR | 263 | ASN |
| 1 | AR | 288 | HIS |
| 1 | AR | 300 | GLN |
| 1 | AR | 454 | ASN |
| 1 | AS | 36 | GLN |
| 1 | AS | 74 | ASN |
| 1 | AS | 131 | HIS |
| 1 | AS | 138 | ASN |
| 1 | AS | 147 | GLN |
| 1 | AS | 238 | HIS |
| 1 | AS | 256 | ASN |
| 1 | AS | 263 | ASN |
| 1 | AS | 288 | HIS |
| 1 | AS | 300 | GLN |
| 1 | AS | 437 | HIS |
| 1 | AS | 454 | ASN |
| 1 | AT | 36 | GLN |
| 1 | AT | 74 | ASN |
| 1 | AT | 131 | HIS |
| 1 | AT | 138 | ASN |
| 1 | AT | 147 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AT | 238 | HIS |
| 1 | AT | 256 | ASN |
| 1 | AT | 263 | ASN |
| 1 | AT | 288 | HIS |
| 1 | AT | 300 | GLN |
| 1 | AT | 454 | ASN |
| 1 | BA | 36 | GLN |
| 1 | BA | 74 | ASN |
| 1 | BA | 131 | HIS |
| 1 | BA | 138 | ASN |
| 1 | BA | 147 | GLN |
| 1 | BA | 238 | HIS |
| 1 | BA | 256 | ASN |
| 1 | BA | 263 | ASN |
| 1 | BA | 288 | HIS |
| 1 | BA | 300 | GLN |
| 1 | BA | 454 | ASN |
| 1 | BB | 36 | GLN |
| 1 | BB | 74 | ASN |
| 1 | BB | 131 | HIS |
| 1 | BB | 138 | ASN |
| 1 | BB | 147 | GLN |
| 1 | BB | 238 | HIS |
| 1 | BB | 256 | ASN |
| 1 | BB | 263 | ASN |
| 1 | BB | 288 | HIS |
| 1 | BB | 300 | GLN |
| 1 | BB | 437 | HIS |
| 1 | BB | 454 | ASN |
| 1 | BC | 36 | GLN |
| 1 | BC | 74 | ASN |
| 1 | BC | 131 | HIS |
| 1 | BC | 138 | ASN |
| 1 | BC | 147 | GLN |
| 1 | BC | 238 | HIS |
| 1 | BC | 256 | ASN |
| 1 | BC | 263 | ASN |
| 1 | BC | 288 | HIS |
| 1 | BC | 300 | GLN |
| 1 | BC | 437 | HIS |
| 1 | BC | 454 | ASN |
| 1 | BD | 36 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BD | 74 | ASN |
| 1 | BD | 131 | HIS |
| 1 | BD | 138 | ASN |
| 1 | BD | 147 | GLN |
| 1 | BD | 238 | HIS |
| 1 | BD | 256 | ASN |
| 1 | BD | 263 | ASN |
| 1 | BD | 288 | HIS |
| 1 | BD | 300 | GLN |
| 1 | BD | 454 | ASN |
| 1 | BE | 36 | GLN |
| 1 | BE | 74 | ASN |
| 1 | BE | 131 | HIS |
| 1 | BE | 138 | ASN |
| 1 | BE | 147 | GLN |
| 1 | BE | 238 | HIS |
| 1 | BE | 256 | ASN |
| 1 | BE | 263 | ASN |
| 1 | BE | 288 | HIS |
| 1 | BE | 300 | GLN |
| 1 | BE | 454 | ASN |
| 1 | BF | 15 | GLN |
| 1 | BF | 36 | GLN |
| 1 | BF | 74 | ASN |
| 1 | BF | 131 | HIS |
| 1 | BF | 138 | ASN |
| 1 | BF | 147 | GLN |
| 1 | BF | 238 | HIS |
| 1 | BF | 256 | ASN |
| 1 | BF | 263 | ASN |
| 1 | BF | 288 | HIS |
| 1 | BF | 300 | GLN |
| 1 | BF | 437 | HIS |
| 1 | BF | 454 | ASN |
| 1 | BG | 15 | GLN |
| 1 | BG | 36 | GLN |
| 1 | BG | 74 | ASN |
| 1 | BG | 131 | HIS |
| 1 | BG | 138 | ASN |
| 1 | BG | 147 | GLN |
| 1 | BG | 238 | HIS |
| 1 | BG | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BG | 263 | ASN |
| 1 | BG | 288 | HIS |
| 1 | BG | 300 | GLN |
| 1 | BG | 454 | ASN |
| 1 | BH | 15 | GLN |
| 1 | BH | 36 | GLN |
| 1 | BH | 74 | ASN |
| 1 | BH | 131 | HIS |
| 1 | BH | 138 | ASN |
| 1 | BH | 147 | GLN |
| 1 | BH | 238 | HIS |
| 1 | BH | 256 | ASN |
| 1 | BH | 263 | ASN |
| 1 | BH | 288 | HIS |
| 1 | BH | 454 | ASN |
| 1 | BI | 36 | GLN |
| 1 | BI | 74 | ASN |
| 1 | BI | 131 | HIS |
| 1 | BI | 138 | ASN |
| 1 | BI | 147 | GLN |
| 1 | BI | 238 | HIS |
| 1 | BI | 256 | ASN |
| 1 | BI | 263 | ASN |
| 1 | BI | 288 | HIS |
| 1 | BI | 300 | GLN |
| 1 | BI | 454 | ASN |
| 1 | BJ | 36 | GLN |
| 1 | BJ | 74 | ASN |
| 1 | BJ | 131 | HIS |
| 1 | BJ | 138 | ASN |
| 1 | BJ | 238 | HIS |
| 1 | BJ | 256 | ASN |
| 1 | BJ | 263 | ASN |
| 1 | BJ | 288 | HIS |
| 1 | BJ | 300 | GLN |
| 1 | BJ | 437 | HIS |
| 1 | BJ | 454 | ASN |
| 1 | BK | 36 | GLN |
| 1 | BK | 74 | ASN |
| 1 | BK | 131 | HIS |
| 1 | BK | 138 | ASN |
| 1 | BK | 147 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BK | 238 | HIS |
| 1 | BK | 256 | ASN |
| 1 | BK | 263 | ASN |
| 1 | BK | 288 | HIS |
| 1 | BK | 454 | ASN |
| 1 | BL | 36 | GLN |
| 1 | BL | 74 | ASN |
| 1 | BL | 131 | HIS |
| 1 | BL | 138 | ASN |
| 1 | BL | 147 | GLN |
| 1 | BL | 238 | HIS |
| 1 | BL | 256 | ASN |
| 1 | BL | 263 | ASN |
| 1 | BL | 288 | HIS |
| 1 | BL | 300 | GLN |
| 1 | BL | 437 | HIS |
| 1 | BL | 454 | ASN |
| 1 | BM | 36 | GLN |
| 1 | BM | 74 | ASN |
| 1 | BM | 131 | HIS |
| 1 | BM | 138 | ASN |
| 1 | BM | 147 | GLN |
| 1 | BM | 238 | HIS |
| 1 | BM | 256 | ASN |
| 1 | BM | 263 | ASN |
| 1 | BM | 288 | HIS |
| 1 | BM | 300 | GLN |
| 1 | BM | 437 | HIS |
| 1 | BM | 454 | ASN |
| 1 | BN | 36 | GLN |
| 1 | BN | 74 | ASN |
| 1 | BN | 131 | HIS |
| 1 | BN | 138 | ASN |
| 1 | BN | 238 | HIS |
| 1 | BN | 256 | ASN |
| 1 | BN | 263 | ASN |
| 1 | BN | 288 | HIS |
| 1 | BN | 454 | ASN |
| 1 | BO | 15 | GLN |
| 1 | BO | 36 | GLN |
| 1 | BO | 74 | ASN |
| 1 | BO | 131 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BO | 138 | ASN |
| 1 | BO | 147 | GLN |
| 1 | BO | 238 | HIS |
| 1 | BO | 256 | ASN |
| 1 | BO | 263 | ASN |
| 1 | BO | 288 | HIS |
| 1 | BO | 300 | GLN |
| 1 | BO | 454 | ASN |
| 1 | BP | 36 | GLN |
| 1 | BP | 74 | ASN |
| 1 | BP | 131 | HIS |
| 1 | BP | 138 | ASN |
| 1 | BP | 147 | GLN |
| 1 | BP | 238 | HIS |
| 1 | BP | 256 | ASN |
| 1 | BP | 263 | ASN |
| 1 | BP | 288 | HIS |
| 1 | BP | 300 | GLN |
| 1 | BP | 437 | HIS |
| 1 | BP | 454 | ASN |
| 1 | BQ | 36 | GLN |
| 1 | BQ | 74 | ASN |
| 1 | BQ | 131 | HIS |
| 1 | BQ | 138 | ASN |
| 1 | BQ | 147 | GLN |
| 1 | BQ | 238 | HIS |
| 1 | BQ | 256 | ASN |
| 1 | BQ | 263 | ASN |
| 1 | BQ | 288 | HIS |
| 1 | BQ | 454 | ASN |
| 1 | BR | 36 | GLN |
| 1 | BR | 74 | ASN |
| 1 | BR | 131 | HIS |
| 1 | BR | 138 | ASN |
| 1 | BR | 147 | GLN |
| 1 | BR | 238 | HIS |
| 1 | BR | 256 | ASN |
| 1 | BR | 263 | ASN |
| 1 | BR | 288 | HIS |
| 1 | BR | 300 | GLN |
| 1 | BR | 437 | HIS |
| 1 | BR | 454 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BS | 36 | GLN |
| 1 | BS | 74 | ASN |
| 1 | BS | 131 | HIS |
| 1 | BS | 138 | ASN |
| 1 | BS | 147 | GLN |
| 1 | BS | 238 | HIS |
| 1 | BS | 256 | ASN |
| 1 | BS | 263 | ASN |
| 1 | BS | 288 | HIS |
| 1 | BS | 300 | GLN |
| 1 | BS | 454 | ASN |
| 1 | BT | 36 | GLN |
| 1 | BT | 74 | ASN |
| 1 | BT | 131 | HIS |
| 1 | BT | 138 | ASN |
| 1 | BT | 147 | GLN |
| 1 | BT | 238 | HIS |
| 1 | BT | 256 | ASN |
| 1 | BT | 263 | ASN |
| 1 | BT | 288 | HIS |
| 1 | BT | 300 | GLN |
| 1 | BT | 454 | ASN |
| 1 | CA | 36 | GLN |
| 1 | CA | 74 | ASN |
| 1 | CA | 131 | HIS |
| 1 | CA | 138 | ASN |
| 1 | CA | 238 | HIS |
| 1 | CA | 256 | ASN |
| 1 | CA | 263 | ASN |
| 1 | CA | 288 | HIS |
| 1 | CA | 454 | ASN |
| 1 | CB | 36 | GLN |
| 1 | CB | 74 | ASN |
| 1 | CB | 131 | HIS |
| 1 | CB | 138 | ASN |
| 1 | CB | 238 | HIS |
| 1 | CB | 256 | ASN |
| 1 | CB | 263 | ASN |
| 1 | CB | 288 | HIS |
| 1 | CB | 300 | GLN |
| 1 | CB | 454 | ASN |
| 1 | CC | 36 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CC | 74 | ASN |
| 1 | CC | 131 | HIS |
| 1 | CC | 147 | GLN |
| 1 | CC | 238 | HIS |
| 1 | CC | 256 | ASN |
| 1 | CC | 263 | ASN |
| 1 | CC | 288 | HIS |
| 1 | CC | 300 | GLN |
| 1 | CC | 454 | ASN |
| 1 | CD | 36 | GLN |
| 1 | CD | 74 | ASN |
| 1 | CD | 131 | HIS |
| 1 | CD | 138 | ASN |
| 1 | CD | 147 | GLN |
| 1 | CD | 238 | HIS |
| 1 | CD | 256 | ASN |
| 1 | CD | 263 | ASN |
| 1 | CD | 288 | HIS |
| 1 | CD | 454 | ASN |
| 1 | CE | 36 | GLN |
| 1 | CE | 74 | ASN |
| 1 | CE | 131 | HIS |
| 1 | CE | 138 | ASN |
| 1 | CE | 147 | GLN |
| 1 | CE | 238 | HIS |
| 1 | CE | 256 | ASN |
| 1 | CE | 263 | ASN |
| 1 | CE | 288 | HIS |
| 1 | CE | 454 | ASN |
| 1 | CF | 36 | GLN |
| 1 | CF | 74 | ASN |
| 1 | CF | 131 | HIS |
| 1 | CF | 138 | ASN |
| 1 | CF | 147 | GLN |
| 1 | CF | 238 | HIS |
| 1 | CF | 256 | ASN |
| 1 | CF | 263 | ASN |
| 1 | CF | 288 | HIS |
| 1 | CF | 300 | GLN |
| 1 | CF | 454 | ASN |
| 1 | CG | 36 | GLN |
| 1 | CG | 74 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CG | 131 | HIS |
| 1 | CG | 138 | ASN |
| 1 | CG | 147 | GLN |
| 1 | CG | 238 | HIS |
| 1 | CG | 256 | ASN |
| 1 | CG | 263 | ASN |
| 1 | CG | 288 | HIS |
| 1 | CG | 300 | GLN |
| 1 | CG | 437 | HIS |
| 1 | CG | 454 | ASN |
| 1 | CH | 15 | GLN |
| 1 | CH | 36 | GLN |
| 1 | CH | 74 | ASN |
| 1 | CH | 131 | HIS |
| 1 | CH | 138 | ASN |
| 1 | CH | 238 | HIS |
| 1 | CH | 256 | ASN |
| 1 | CH | 263 | ASN |
| 1 | CH | 288 | HIS |
| 1 | CH | 437 | HIS |
| 1 | CH | 454 | ASN |
| 1 | CI | 36 | GLN |
| 1 | CI | 74 | ASN |
| 1 | CI | 131 | HIS |
| 1 | CI | 138 | ASN |
| 1 | CI | 147 | GLN |
| 1 | CI | 238 | HIS |
| 1 | CI | 256 | ASN |
| 1 | CI | 263 | ASN |
| 1 | CI | 288 | HIS |
| 1 | CI | 300 | GLN |
| 1 | CI | 437 | HIS |
| 1 | CI | 454 | ASN |
| 1 | CJ | 15 | GLN |
| 1 | CJ | 36 | GLN |
| 1 | CJ | 74 | ASN |
| 1 | CJ | 131 | HIS |
| 1 | CJ | 138 | ASN |
| 1 | CJ | 238 | HIS |
| 1 | CJ | 256 | ASN |
| 1 | CJ | 263 | ASN |
| 1 | CJ | 288 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CJ | 300 | GLN |
| 1 | CJ | 454 | ASN |
| 1 | CK | 36 | GLN |
| 1 | CK | 74 | ASN |
| 1 | CK | 131 | HIS |
| 1 | CK | 138 | ASN |
| 1 | CK | 147 | GLN |
| 1 | CK | 238 | HIS |
| 1 | CK | 256 | ASN |
| 1 | CK | 263 | ASN |
| 1 | CK | 288 | HIS |
| 1 | CK | 454 | ASN |
| 1 | CL | 36 | GLN |
| 1 | CL | 74 | ASN |
| 1 | CL | 131 | HIS |
| 1 | CL | 138 | ASN |
| 1 | CL | 147 | GLN |
| 1 | CL | 238 | HIS |
| 1 | CL | 256 | ASN |
| 1 | CL | 263 | ASN |
| 1 | CL | 288 | HIS |
| 1 | CL | 454 | ASN |
| 1 | CM | 36 | GLN |
| 1 | CM | 74 | ASN |
| 1 | CM | 131 | HIS |
| 1 | CM | 138 | ASN |
| 1 | CM | 147 | GLN |
| 1 | CM | 238 | HIS |
| 1 | CM | 256 | ASN |
| 1 | CM | 263 | ASN |
| 1 | CM | 288 | HIS |
| 1 | CM | 454 | ASN |
| 1 | CN | 36 | GLN |
| 1 | CN | 74 | ASN |
| 1 | CN | 131 | HIS |
| 1 | CN | 138 | ASN |
| 1 | CN | 147 | GLN |
| 1 | CN | 238 | HIS |
| 1 | CN | 256 | ASN |
| 1 | CN | 263 | ASN |
| 1 | CN | 288 | HIS |
| 1 | CN | 300 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CN | 437 | HIS |
| 1 | CN | 454 | ASN |
| 1 | CO | 36 | GLN |
| 1 | CO | 74 | ASN |
| 1 | CO | 131 | HIS |
| 1 | CO | 138 | ASN |
| 1 | CO | 147 | GLN |
| 1 | CO | 238 | HIS |
| 1 | CO | 256 | ASN |
| 1 | CO | 263 | ASN |
| 1 | CO | 288 | HIS |
| 1 | CO | 300 | GLN |
| 1 | CO | 454 | ASN |
| 1 | CP | 36 | GLN |
| 1 | CP | 74 | ASN |
| 1 | CP | 131 | HIS |
| 1 | CP | 138 | ASN |
| 1 | CP | 147 | GLN |
| 1 | CP | 238 | HIS |
| 1 | CP | 256 | ASN |
| 1 | CP | 263 | ASN |
| 1 | CP | 288 | HIS |
| 1 | CP | 300 | GLN |
| 1 | CP | 454 | ASN |
| 1 | CQ | 36 | GLN |
| 1 | CQ | 74 | ASN |
| 1 | CQ | 131 | HIS |
| 1 | CQ | 138 | ASN |
| 1 | CQ | 147 | GLN |
| 1 | CQ | 238 | HIS |
| 1 | CQ | 256 | ASN |
| 1 | CQ | 263 | ASN |
| 1 | CQ | 288 | HIS |
| 1 | CQ | 300 | GLN |
| 1 | CQ | 454 | ASN |
| 1 | CR | 36 | GLN |
| 1 | CR | 74 | ASN |
| 1 | CR | 131 | HIS |
| 1 | CR | 138 | ASN |
| 1 | CR | 147 | GLN |
| 1 | CR | 238 | HIS |
| 1 | CR | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CR | 263 | ASN |
| 1 | CR | 288 | HIS |
| 1 | CR | 300 | GLN |
| 1 | CR | 437 | HIS |
| 1 | CR | 454 | ASN |
| 1 | CS | 36 | GLN |
| 1 | CS | 74 | ASN |
| 1 | CS | 131 | HIS |
| 1 | CS | 138 | ASN |
| 1 | CS | 147 | GLN |
| 1 | CS | 238 | HIS |
| 1 | CS | 256 | ASN |
| 1 | CS | 263 | ASN |
| 1 | CS | 288 | HIS |
| 1 | CS | 437 | HIS |
| 1 | CS | 454 | ASN |
| 1 | CT | 15 | GLN |
| 1 | CT | 36 | GLN |
| 1 | CT | 74 | ASN |
| 1 | CT | 131 | HIS |
| 1 | CT | 138 | ASN |
| 1 | CT | 238 | HIS |
| 1 | CT | 256 | ASN |
| 1 | CT | 263 | ASN |
| 1 | CT | 288 | HIS |
| 1 | CT | 300 | GLN |
| 1 | CT | 437 | HIS |
| 1 | CT | 454 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | AA | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 23, 33, 53, 78 | 0 |
| 1 | AB | 504/504 (100%) | -0.62 | 0 | 100 | 100 | 22, 34, 54, 78 | 0 |
| 1 | AC | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 23, 34, 54, 78 | 0 |
| 1 | AD | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 22, 33, 52, 78 | 0 |
| 1 | AE | 504/504 (100%) | -0.53 | 0 | 100 | 100 | 17, 31, 52, 77 | 0 |
| 1 | AF | 504/504 (100%) | -0.63 | 0 | 100 | 100 | 24, 34, 54, 80 | 0 |
| 1 | AG | 504/504 (100%) | -0.62 | 0 | 100 | 100 | 23, 34, 55, 80 | 0 |
| 1 | AH | 504/504 (100%) | -0.62 | 0 | 100 | 100 | 24, 35, 56, 79 | 0 |
| 1 | AI | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 34, 55, 80 | 0 |
| 1 | AJ | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 22, 34, 54, 80 | 0 |
| 1 | AK | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 34, 54, 79 | 0 |
| 1 | AL | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 23, 33, 54, 77 | 0 |
| 1 | AM | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 21, 32, 52, 77 | 0 |
| 1 | AN | 504/504 (100%) | -0.55 | 0 | 100 | 100 | 22, 33, 54, 78 | 0 |
| 1 | AO | 504/504 (100%) | -0.53 | 0 | 100 | 100 | 21, 33, 54, 80 | 0 |
| 1 | AP | 504/504 (100%) | -0.55 | 0 | 100 | 100 | 19, 32, 53, 79 | 0 |
| 1 | AQ | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 33, 54, 77 | 0 |
| 1 | AR | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 21, 32, 52, 77 | 0 |
| 1 | AS | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 23, 33, 54, 80 | 0 |
| 1 | AT | 504/504 (100%) | -0.55 | 0 | 100 | 100 | 22, 33, 54, 77 | 0 |
| 1 | BA | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 23, 33, 54, 79 | 0 |
| 1 | BB | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 23, 34, 55, 77 | 0 |
| 1 | BC | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 23, 34, 54, 78 | 0 |
| 1 | BD | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 23, 34, 54, 79 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | BE | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 23, 33, 54, 77 | 0 |
| 1 | BF | 504/504 (100%) | -0.54 | 0 | 100 | 100 | 22, 35, 56, 80 | 0 |
| 1 | BG | 504/504 (100%) | -0.62 | 0 | 100 | 100 | 22, 34, 54, 79 | 0 |
| 1 | BH | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 21, 33, 54, 75 | 0 |
| 1 | BI | 504/504 (100%) | -0.53 | 0 | 100 | 100 | 22, 32, 54, 78 | 0 |
| 1 | BJ | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 22, 34, 54, 79 | 0 |
| 1 | BK | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 22, 33, 53, 77 | 0 |
| 1 | BL | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 21, 32, 52, 75 | 0 |
| 1 | BM | 504/504 (100%) | -0.51 | 0 | 100 | 100 | 21, 32, 52, 77 | 0 |
| 1 | BN | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 20, 33, 53, 76 | 0 |
| 1 | BO | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 22, 33, 53, 80 | 0 |
| 1 | BP | 504/504 (100%) | -0.50 | 1 (0%) | 95 | 87 | 21, 32, 53, 76 | 0 |
| 1 | BQ | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 22, 33, 54, 80 | 0 |
| 1 | BR | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 22, 33, 54, 79 | 0 |
| 1 | BS | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 22, 33, 54, 80 | 0 |
| 1 | BT | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 22, 34, 53, 77 | 0 |
| 1 | CA | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 35, 56, 80 | 0 |
| 1 | CB | 504/504 (100%) | -0.64 | 0 | 100 | 100 | 23, 34, 54, 77 | 0 |
| 1 | CC | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 34, 54, 81 | 0 |
| 1 | CD | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 23, 34, 54, 79 | 0 |
| 1 | CE | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 33, 54, 78 | 0 |
| 1 | CF | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 23, 34, 55, 80 | 0 |
| 1 | CG | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 24, 34, 55, 81 | 0 |
| 1 | CH | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 24, 34, 55, 79 | 0 |
| 1 | CI | 504/504 (100%) | -0.59 | 0 | 100 | 100 | 23, 33, 53, 79 | 0 |
| 1 | CJ | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 24, 33, 54, 79 | 0 |
| 1 | CK | 504/504 (100%) | -0.54 | 0 | 100 | 100 | 21, 34, 54, 79 | 0 |
| 1 | CL | 504/504 (100%) | -0.61 | 0 | 100 | 100 | 22, 33, 54, 77 | 0 |
| 1 | CM | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 22, 32, 53, 79 | 0 |
| 1 | CN | 504/504 (100%) | -0.57 | 0 | 100 | 100 | 22, 32, 54, 79 | 0 |
| 1 | CO | 504/504 (100%) | -0.56 | 0 | 100 | 100 | 23, 32, 54, 78 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | CP | 504/504 (100%) | -0.55 | 0 | 100 | 100 | 21, 31, 53, 78 | 0 |
| 1 | CQ | 504/504 (100%) | -0.56 | 0 | 100 | 100 | 21, 32, 53, 79 | 0 |
| 1 | CR | 504/504 (100%) | -0.47 | 1 (0%) | 95 | 87 | 17, 31, 53, 75 | 0 |
| 1 | CS | 504/504 (100%) | -0.58 | 0 | 100 | 100 | 22, 32, 53, 78 | 0 |
| 1 | CT | 504/504 (100%) | -0.60 | 0 | 100 | 100 | 21, 32, 52, 77 | 0 |
| All | All | 30240/30240 (100%) | -0.58 | 2 (0%) | 100 | 100 | 17, 33, 54, 81 | 0 |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | CR | 83 | SER | 2.5 |
| 1 | BP | 83 | SER | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.