# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 08:05 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 3NOG |
| Title | : | Designed ankyrin repeat protein (DARPin) Binders to AcrB: Plasticity of the Interface |
| Authors | : | Monroe, N.; Briand, C.; Gruetter, M.G. |
| Deposited on | : | 2010-06-25 |
| Resolution | : | 3.34 Å(reported) |

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

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

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

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

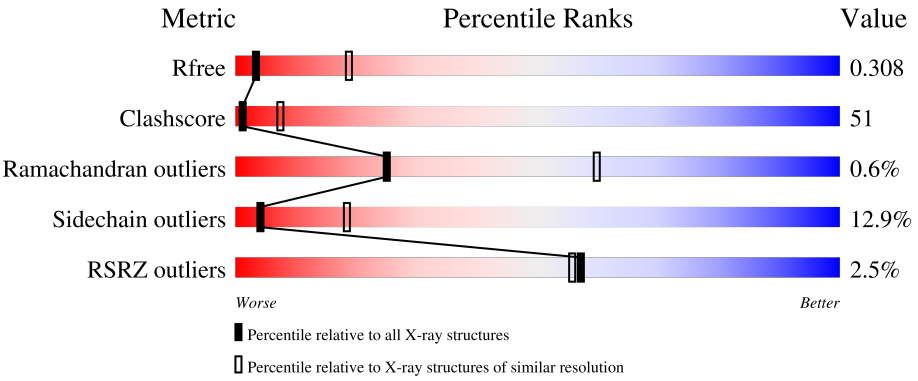
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (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 3.34 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 | 1060 (3.38-3.30) |
| Clashscore | 141614 | 1111 (3.38-3.30) |
| Ramachandran outliers | 138981 | 1090 (3.38-3.30) |
| Sidechain outliers | 138945 | 1089 (3.38-3.30) |
| RSRZ outliers | 127900 | 1028 (3.38-3.30) |

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 | A | 1049 | 50% 40% 7% |
| 1 | B | 1049 | 2% 41% 47% 9% |
| 1 | C | 1049 | 45% 45% 9% |
| 2 | D | 169 | 6% 44% 40% 7% 9% |
| 2 | E | 169 | 23% 48% 37% 11% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 1 | FME | B | 1 | - | - | X | - |
| 1 | FME | C | 1 | - | - | X | - |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24874 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 Acriflavine resistance protein B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1012 | Total | C | N | O | S | 27 | 0 | 0 |
| | | | 7464 | 4806 | 1218 | 1399 | 41 | | | |
| 1 | B | 1028 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7547 | 4853 | 1237 | 1414 | 43 | | | |
| 1 | C | 1040 | Total | C | N | O | S | 20 | 0 | 0 |
| | | | 7736 | 4979 | 1270 | 1444 | 43 | | | |

- Molecule 2 is a protein called Designed ankyrin repeat protein.

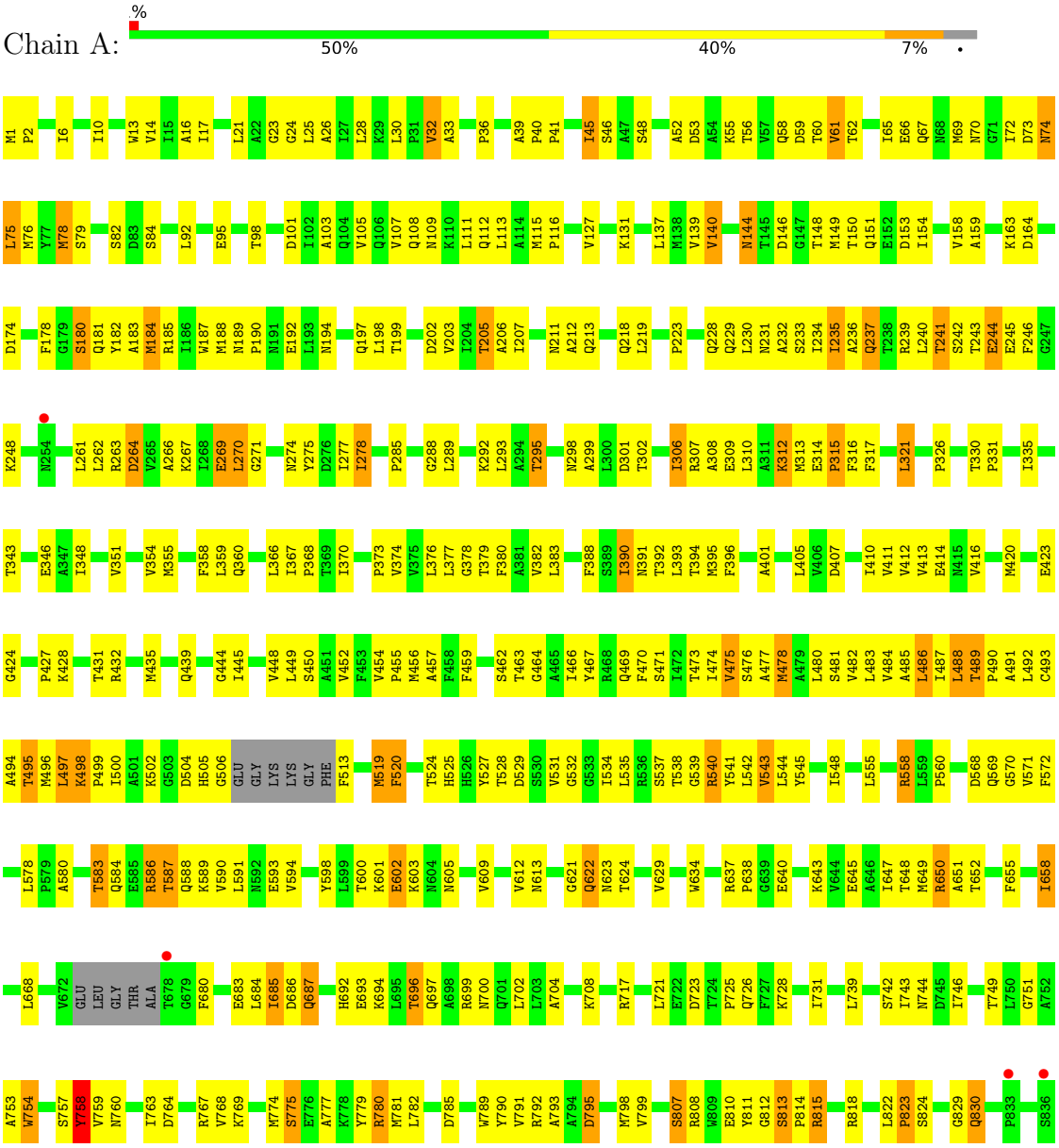
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 154 | Total | C | N | O | S | 4 | 0 | 0 |
| | | | 1097 | 686 | 194 | 216 | 1 | | | |
| 2 | E | 151 | Total | C | N | O | S | 21 | 0 | 0 |
| | | | 1030 | 641 | 185 | 203 | 1 | | | |

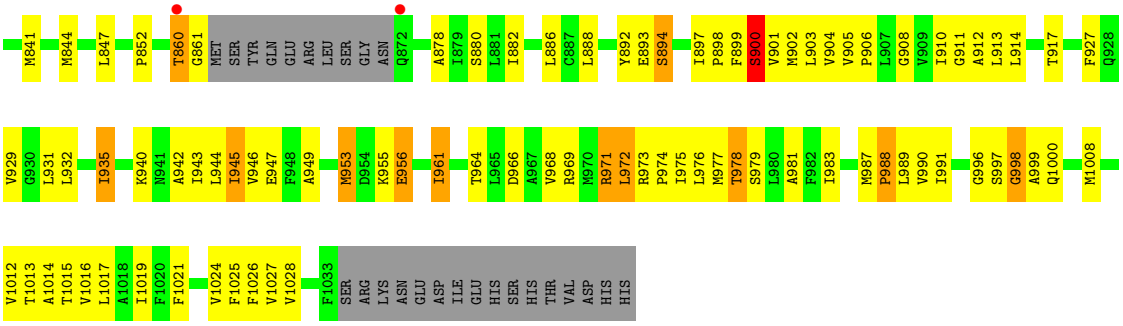
# 3 Residue-property plots (i)

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: Acriflavine resistance protein B

Chain A:



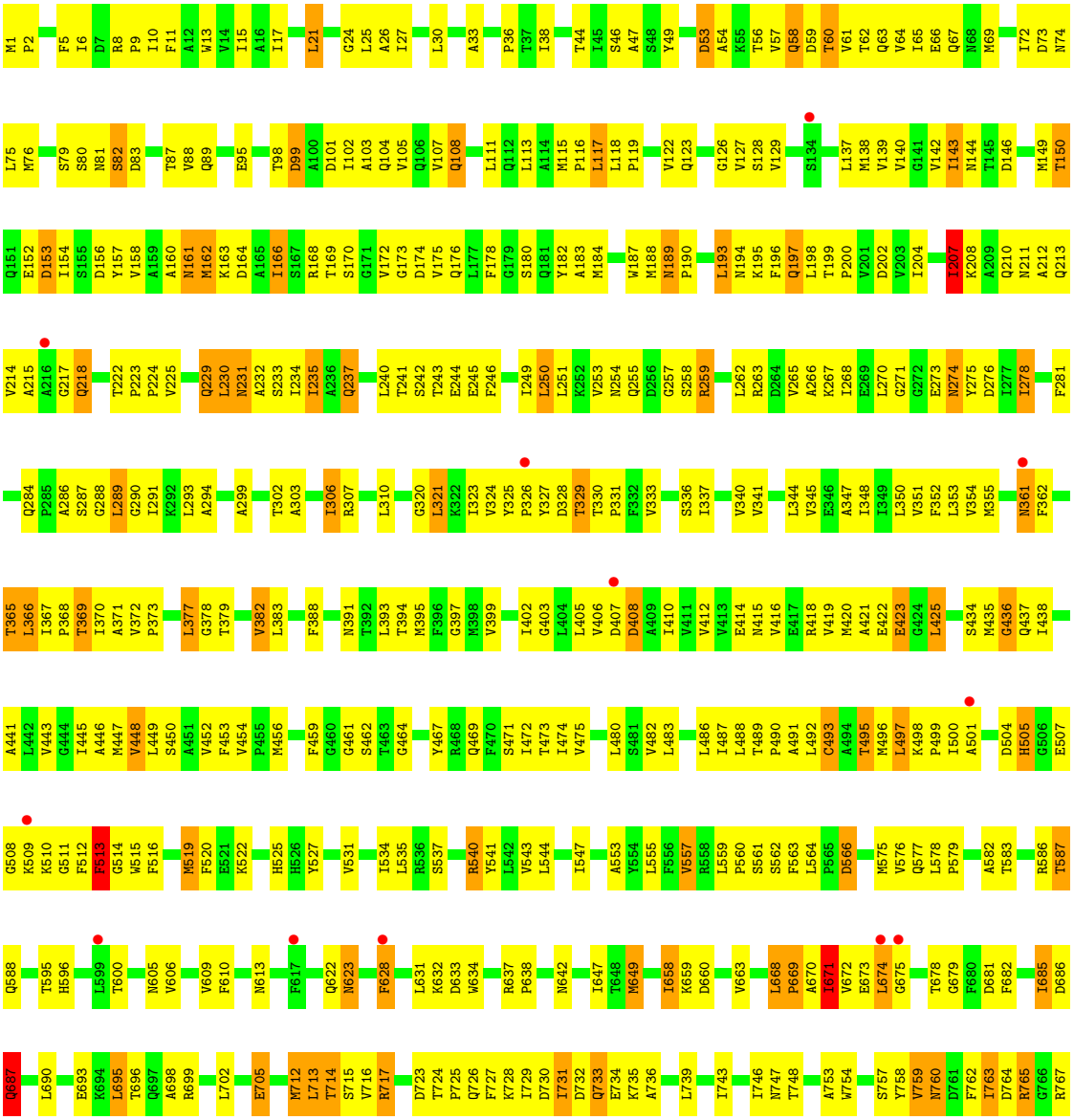


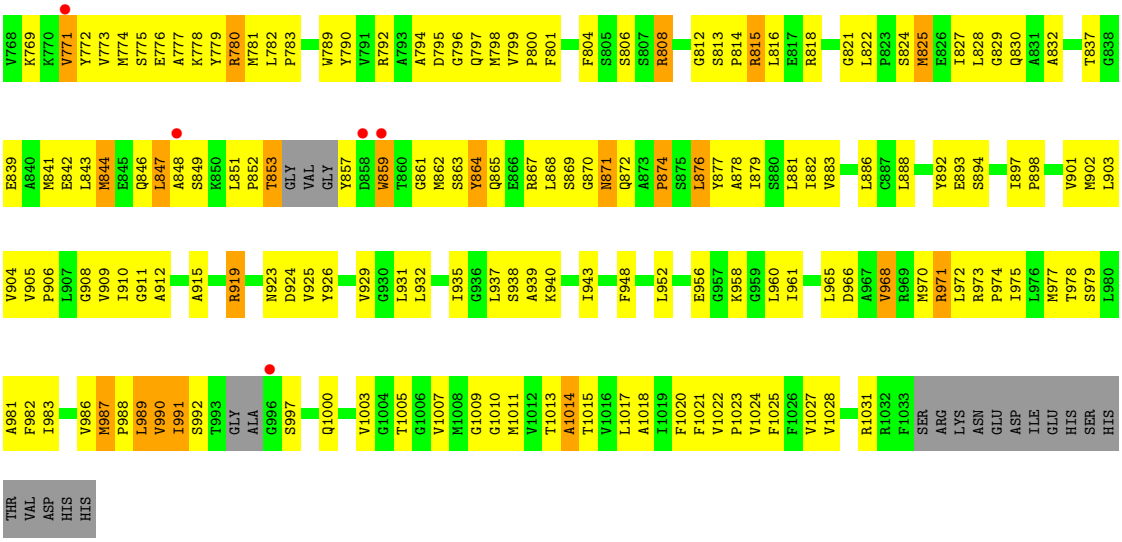




• Molecule 1: Acriflavine resistance protein B

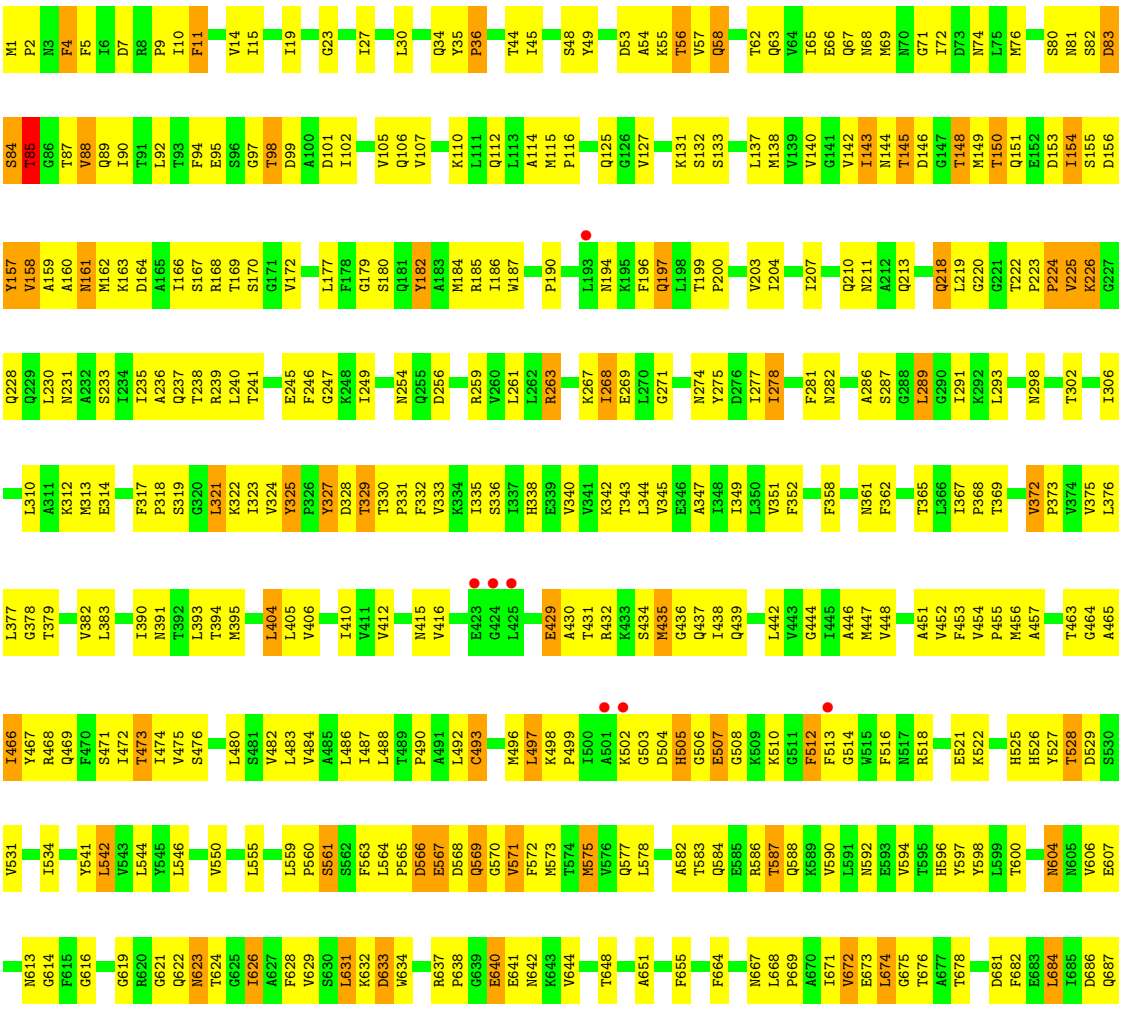
Chain B:

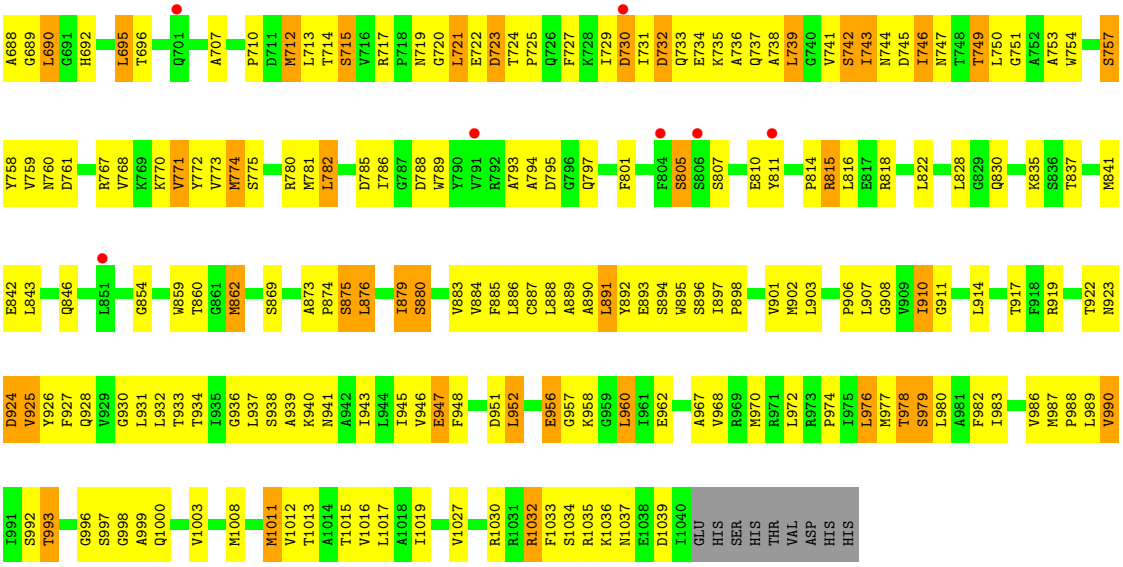





• Molecule 1: Acriflavine resistance protein B

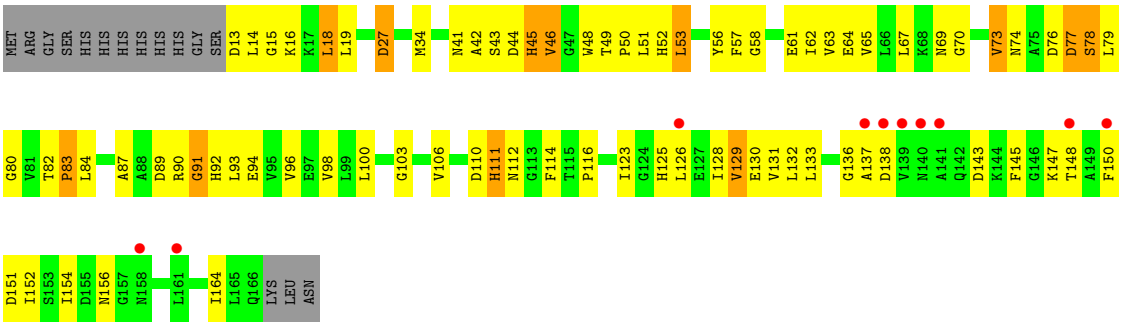
Chain C:



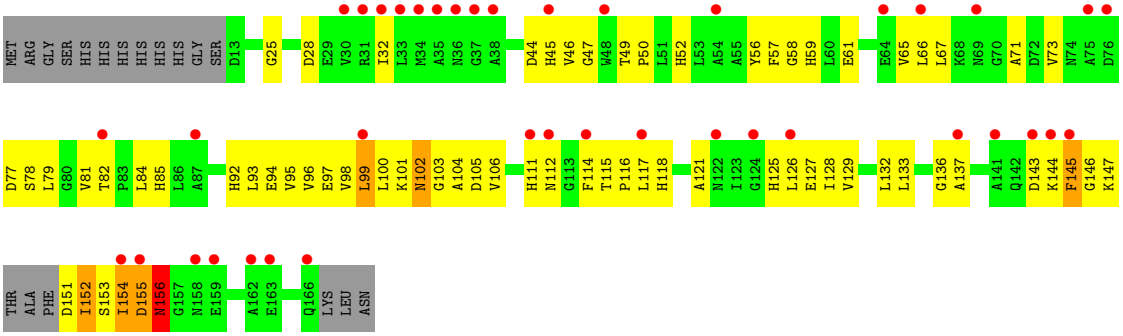
• Molecule 2: Designed ankyrin repeat protein

Chain D:

• Molecule 2: Designed ankyrin repeat protein

Chain E:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 145.40Å 158.00Å 258.60Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 48.78 – 3.34<br>49.15 – 3.34 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.8 (48.78-3.34)<br>99.8 (49.15-3.34) | Depositor<br>EDS |
| $R_{merge}$ | 0.14 | Depositor |
| $R_{sym}$ | 0.14 | Depositor |
| $< I/\sigma(I) >$ [1] | 3.46 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX 1.6.2_432 | Depositor |
| R, $R_{free}$ | 0.257 , 0.307<br>0.252 , 0.308 | Depositor<br>DCC |
| $R_{free}$ test set | 1043 reflections (1.20%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 70.8 | Xtriage |
| Anisotropy | 0.506 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.24 , 49.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.42$, $< L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.86 | EDS |
| Total number of atoms | 24874 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.77 | 2/7591 (0.0%) | 0.74 | 9/10342 (0.1%) |
| 1 | B | 0.77 | 0/7675 | 0.79 | 15/10467 (0.1%) |
| 1 | C | 0.82 | 2/7874 (0.0%) | 0.79 | 12/10720 (0.1%) |
| 2 | D | 0.87 | 0/1115 | 0.89 | 3/1525 (0.2%) |
| 2 | E | 0.40 | 0/1046 | 0.62 | 2/1434 (0.1%) |
| All | All | 0.78 | 4/25301 (0.0%) | 0.77 | 41/34488 (0.1%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 493 | CYS | CB-SG | -5.86 | 1.72 | 1.81 |
| 1 | C | 225 | VAL | CA-CB | -5.37 | 1.43 | 1.54 |
| 1 | A | 475 | VAL | CA-CB | -5.18 | 1.43 | 1.54 |
| 1 | A | 758 | TYR | CD2-CE2 | -5.09 | 1.31 | 1.39 |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D | 138 | ASP | N-CA-C | -8.41 | 88.30 | 111.00 |
| 1 | A | 945 | ILE | CB-CA-C | -7.27 | 97.07 | 111.60 |
| 1 | B | 668 | LEU | C-N-CD | -7.16 | 104.85 | 120.60 |
| 1 | B | 259 | ARG | N-CA-CB | -7.06 | 97.90 | 110.60 |
| 1 | C | 85 | THR | N-CA-C | -6.79 | 92.65 | 111.00 |
| 2 | E | 156 | ASN | N-CA-C | 6.78 | 129.30 | 111.00 |
| 1 | A | 61 | VAL | CB-CA-C | -6.76 | 98.55 | 111.40 |
| 1 | C | 83 | ASP | N-CA-C | 6.75 | 129.21 | 111.00 |
| 1 | C | 1032 | ARG | N-CA-C | -6.61 | 93.16 | 111.00 |
| 2 | D | 42 | ALA | N-CA-C | -6.51 | 93.43 | 111.00 |
| 1 | B | 679 | GLY | N-CA-C | -6.46 | 96.96 | 113.10 |
| 1 | C | 97 | GLY | N-CA-C | -6.40 | 97.10 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 952 | LEU | CA-CB-CG | -6.28 | 100.85 | 115.30 |
| 1 | B | 760 | ASN | CB-CA-C | -6.24 | 97.92 | 110.40 |
| 1 | A | 270 | LEU | N-CA-C | -6.22 | 94.22 | 111.00 |
| 1 | B | 685 | ILE | N-CA-C | 6.14 | 127.58 | 111.00 |
| 1 | C | 925 | VAL | CB-CA-C | -6.04 | 99.92 | 111.40 |
| 1 | C | 327 | TYR | N-CA-C | 6.03 | 127.29 | 111.00 |
| 1 | A | 540 | ARG | N-CA-C | -5.91 | 95.04 | 111.00 |
| 1 | B | 685 | ILE | CB-CA-C | -5.88 | 99.84 | 111.60 |
| 1 | B | 847 | LEU | CA-CB-CG | 5.80 | 128.64 | 115.30 |
| 1 | B | 861 | GLY | N-CA-C | -5.78 | 98.65 | 113.10 |
| 2 | E | 156 | ASN | C-N-CA | 5.76 | 134.40 | 122.30 |
| 1 | B | 514 | GLY | N-CA-C | -5.72 | 98.79 | 113.10 |
| 1 | A | 759 | VAL | N-CA-C | 5.63 | 126.20 | 111.00 |
| 1 | C | 57 | VAL | CB-CA-C | -5.50 | 100.95 | 111.40 |
| 1 | B | 207 | ILE | CB-CA-C | -5.49 | 100.61 | 111.60 |
| 1 | A | 759 | VAL | CB-CA-C | -5.44 | 101.06 | 111.40 |
| 1 | A | 61 | VAL | N-CA-C | 5.35 | 125.44 | 111.00 |
| 1 | B | 505 | HIS | N-CA-C | -5.29 | 96.71 | 111.00 |
| 1 | A | 900 | SER | N-CA-C | -5.26 | 96.79 | 111.00 |
| 1 | B | 687 | GLN | N-CA-C | 5.24 | 125.15 | 111.00 |
| 1 | C | 672 | VAL | N-CA-C | 5.17 | 124.97 | 111.00 |
| 1 | C | 131 | LYS | N-CA-C | -5.16 | 97.06 | 111.00 |
| 1 | B | 671 | ILE | CB-CA-C | -5.15 | 101.31 | 111.60 |
| 2 | D | 91 | GLY | N-CA-C | 5.14 | 125.96 | 113.10 |
| 1 | C | 158 | VAL | CB-CA-C | -5.13 | 101.65 | 111.40 |
| 1 | A | 45 | ILE | CB-CA-C | -5.06 | 101.47 | 111.60 |
| 1 | B | 513 | PHE | N-CA-C | -5.05 | 97.36 | 111.00 |
| 1 | B | 509 | LYS | N-CA-C | -5.02 | 97.45 | 111.00 |
| 1 | C | 746 | ILE | CB-CA-C | -5.01 | 101.58 | 111.60 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 7464 | 0 | 7440 | 661 | 0 |
| 1 | B | 7547 | 0 | 7469 | 863 | 0 |
| 1 | C | 7736 | 0 | 7730 | 828 | 0 |
| 2 | D | 1097 | 0 | 1008 | 142 | 0 |
| 2 | E | 1030 | 0 | 896 | 94 | 0 |
| All | All | 24874 | 0 | 24543 | 2520 | 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 51.

All (2520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:234:ILE:C | 1:A:235:ILE:HD13 | 1.18 | 1.50 |
| 1:C:314:GLU:HA | 1:C:317:PHE:CE1 | 1.48 | 1.48 |
| 1:B:563:PHE:C | 1:B:564:LEU:HD12 | 1.33 | 1.48 |
| 1:B:705:GLU:HG2 | 1:B:847:LEU:CD2 | 1.40 | 1.47 |
| 1:C:689:GLY:C | 1:C:690:LEU:HD23 | 1.36 | 1.39 |
| 1:B:919:ARG:NH1 | 1:B:919:ARG:HB3 | 1.39 | 1.38 |
| 1:A:496:MET:C | 1:A:497:LEU:HD23 | 1.44 | 1.36 |
| 1:B:222:THR:CG2 | 1:C:275:TYR:HB2 | 1.55 | 1.35 |
| 1:A:75:LEU:HD12 | 1:A:76:MET:N | 1.39 | 1.34 |
| 1:A:808:ARG:NH1 | 1:A:808:ARG:HB2 | 1.42 | 1.34 |
| 1:C:671:ILE:CD1 | 1:C:674:LEU:HD11 | 1.59 | 1.33 |
| 1:B:250:LEU:HD23 | 1:B:251:LEU:N | 1.43 | 1.32 |
| 2:D:56:TYR:CE1 | 2:D:90:ARG:HD3 | 1.64 | 1.31 |
| 1:B:270:LEU:HD23 | 1:B:271:GLY:N | 1.46 | 1.30 |
| 1:B:799:VAL:HG13 | 1:B:800:PRO:CD | 1.59 | 1.30 |
| 1:A:482:VAL:O | 1:A:486:LEU:HD21 | 1.28 | 1.30 |
| 1:B:197:GLN:HA | 1:B:798:MET:CE | 1.61 | 1.29 |
| 1:A:721:LEU:CD1 | 1:A:814:PRO:HG3 | 1.62 | 1.29 |
| 1:B:960:LEU:HD23 | 1:B:960:LEU:O | 1.33 | 1.27 |
| 1:C:185:ARG:HH12 | 1:C:774:MET:CE | 1.48 | 1.27 |
| 1:C:879:ILE:O | 1:C:879:ILE:HD12 | 1.35 | 1.26 |
| 1:C:741:VAL:CG1 | 1:C:746:ILE:HD11 | 1.64 | 1.25 |
| 1:A:234:ILE:C | 1:A:235:ILE:CD1 | 2.05 | 1.24 |
| 2:D:56:TYR:CE1 | 2:D:90:ARG:CD | 2.21 | 1.23 |
| 1:B:919:ARG:HH11 | 1:B:919:ARG:CB | 1.51 | 1.23 |
| 2:D:51:LEU:HD23 | 2:D:51:LEU:O | 1.34 | 1.23 |
| 1:C:154:ILE:HD12 | 1:C:154:ILE:C | 1.56 | 1.22 |
| 2:D:56:TYR:HE1 | 2:D:90:ARG:CD | 1.51 | 1.22 |
| 1:B:230:LEU:O | 1:B:230:LEU:HD23 | 1.33 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:197:GLN:CA | 1:B:798:MET:HE3 | 1.70 | 1.21 |
| 1:B:270:LEU:HD23 | 1:B:270:LEU:C | 1.49 | 1.21 |
| 1:C:671:ILE:CG1 | 1:C:674:LEU:HD21 | 1.71 | 1.21 |
| 1:C:750:LEU:HD23 | 1:C:750:LEU:C | 1.59 | 1.21 |
| 1:B:799:VAL:CG1 | 1:B:800:PRO:HD2 | 1.70 | 1.20 |
| 2:E:152:ILE:C | 2:E:152:ILE:HD12 | 1.62 | 1.20 |
| 1:B:562:SER:O | 1:B:924:ASP:HA | 1.39 | 1.19 |
| 1:B:668:LEU:HD12 | 1:B:668:LEU:O | 1.39 | 1.19 |
| 1:B:960:LEU:HD23 | 1:B:960:LEU:C | 1.59 | 1.19 |
| 1:C:750:LEU:HD23 | 1:C:750:LEU:O | 1.34 | 1.19 |
| 2:D:18:LEU:HD23 | 2:D:18:LEU:O | 1.42 | 1.19 |
| 2:D:129:VAL:O | 2:D:133:LEU:HD12 | 1.38 | 1.19 |
| 1:A:488:LEU:HD12 | 1:A:488:LEU:O | 1.40 | 1.19 |
| 1:A:428:LYS:O | 1:A:431:THR:HG22 | 1.39 | 1.19 |
| 1:C:607:GLU:OE2 | 1:C:632:LYS:HG2 | 1.38 | 1.18 |
| 1:C:671:ILE:HD11 | 1:C:674:LEU:CD1 | 1.71 | 1.18 |
| 1:C:154:ILE:HD12 | 1:C:154:ILE:O | 1.37 | 1.18 |
| 2:E:46:VAL:HG13 | 2:E:47:GLY:H | 1.02 | 1.18 |
| 1:C:674:LEU:H | 1:C:674:LEU:CD2 | 1.52 | 1.17 |
| 1:C:314:GLU:HA | 1:C:317:PHE:CD1 | 1.79 | 1.16 |
| 1:B:188:MET:CE | 1:B:773:VAL:HG22 | 1.74 | 1.16 |
| 1:C:688:ALA:HB3 | 1:C:690:LEU:HD21 | 1.20 | 1.16 |
| 1:A:423:GLU:CA | 1:A:502:LYS:HE3 | 1.76 | 1.16 |
| 1:A:486:LEU:H | 1:A:486:LEU:CD2 | 1.52 | 1.16 |
| 1:A:721:LEU:CD1 | 1:A:814:PRO:CG | 2.24 | 1.16 |
| 1:B:254:ASN:HD22 | 1:B:258:SER:HB3 | 1.11 | 1.16 |
| 1:C:960:LEU:O | 1:C:960:LEU:HD13 | 1.43 | 1.16 |
| 1:A:498:LYS:HE3 | 1:A:498:LYS:O | 1.45 | 1.15 |
| 1:B:668:LEU:HD12 | 1:B:668:LEU:C | 1.67 | 1.15 |
| 1:B:989:LEU:HD23 | 1:B:1000:GLN:HG2 | 1.26 | 1.15 |
| 1:A:808:ARG:CB | 1:A:808:ARG:HH11 | 1.61 | 1.14 |
| 1:B:705:GLU:HG2 | 1:B:847:LEU:HD22 | 1.26 | 1.14 |
| 2:D:53:LEU:H | 2:D:53:LEU:CD2 | 1.58 | 1.14 |
| 1:A:478:MET:O | 1:A:482:VAL:HG23 | 1.45 | 1.14 |
| 1:C:575:MET:HG3 | 1:C:575:MET:O | 1.43 | 1.14 |
| 1:B:197:GLN:CA | 1:B:798:MET:CE | 2.22 | 1.13 |
| 1:C:144:ASN:HD22 | 1:C:149:MET:CB | 1.60 | 1.13 |
| 1:A:486:LEU:HD22 | 1:A:486:LEU:N | 1.60 | 1.13 |
| 1:C:879:ILE:HD12 | 1:C:879:ILE:C | 1.62 | 1.13 |
| 1:B:193:LEU:HD23 | 1:B:193:LEU:N | 1.52 | 1.13 |
| 1:B:230:LEU:HD23 | 1:B:230:LEU:C | 1.60 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:674:LEU:HD22 | 1:C:674:LEU:N | 1.59 | 1.13 |
| 1:B:991:ILE:HD12 | 1:B:991:ILE:O | 1.49 | 1.12 |
| 1:B:222:THR:HG21 | 1:C:275:TYR:HB2 | 1.26 | 1.12 |
| 2:D:61:GLU:O | 2:D:65:VAL:HG23 | 1.49 | 1.12 |
| 1:A:931:LEU:O | 1:A:935:ILE:HG22 | 1.50 | 1.11 |
| 1:C:739:LEU:HD13 | 1:C:739:LEU:N | 1.50 | 1.11 |
| 1:B:705:GLU:CG | 1:B:847:LEU:CD2 | 2.28 | 1.11 |
| 1:B:848:ALA:HA | 1:B:851:LEU:CD1 | 1.79 | 1.11 |
| 1:A:360:GLN:HG2 | 1:A:513:PHE:CZ | 1.84 | 1.11 |
| 1:A:486:LEU:N | 1:A:486:LEU:HD13 | 1.59 | 1.11 |
| 1:B:188:MET:HE2 | 1:B:773:VAL:HG22 | 1.11 | 1.11 |
| 2:E:112:ASN:O | 2:E:144:LYS:HG2 | 1.51 | 1.11 |
| 1:C:83:ASP:HB3 | 1:C:85:THR:HG23 | 1.24 | 1.10 |
| 1:B:222:THR:CG2 | 1:C:275:TYR:CB | 2.28 | 1.10 |
| 1:C:879:ILE:HD11 | 1:C:883:VAL:HG23 | 1.30 | 1.10 |
| 1:A:519:MET:SD | 1:A:519:MET:C | 2.30 | 1.10 |
| 1:C:671:ILE:HG13 | 1:C:671:ILE:O | 1.41 | 1.10 |
| 1:C:200:PRO:CD | 1:C:749:THR:HG23 | 1.79 | 1.10 |
| 1:C:447:MET:SD | 1:C:891:LEU:HD21 | 1.91 | 1.09 |
| 1:A:971:ARG:O | 1:A:974:PRO:HD2 | 1.52 | 1.09 |
| 1:B:534:ILE:HG13 | 1:B:541:TYR:CE2 | 1.87 | 1.09 |
| 1:C:741:VAL:HG13 | 1:C:746:ILE:CD1 | 1.81 | 1.09 |
| 1:A:234:ILE:O | 1:A:235:ILE:CD1 | 2.00 | 1.09 |
| 1:B:563:PHE:C | 1:B:564:LEU:CD1 | 2.19 | 1.08 |
| 1:A:971:ARG:HH11 | 1:A:971:ARG:HG3 | 1.06 | 1.08 |
| 1:C:497:LEU:HD23 | 1:C:498:LYS:H | 1.03 | 1.08 |
| 1:C:671:ILE:HD11 | 1:C:674:LEU:HD11 | 1.10 | 1.08 |
| 1:A:721:LEU:HD12 | 1:A:814:PRO:HG3 | 1.31 | 1.08 |
| 1:B:182:TYR:HB3 | 1:B:270:LEU:HD11 | 1.31 | 1.08 |
| 1:C:144:ASN:ND2 | 1:C:149:MET:HB2 | 1.68 | 1.08 |
| 1:C:435:MET:HA | 1:C:435:MET:CE | 1.84 | 1.08 |
| 2:E:152:ILE:HD12 | 2:E:152:ILE:O | 1.53 | 1.08 |
| 1:A:971:ARG:HH11 | 1:A:971:ARG:CG | 1.67 | 1.08 |
| 1:B:871:ASN:HB3 | 1:B:872:GLN:HG2 | 1.35 | 1.07 |
| 1:A:235:ILE:HD13 | 1:A:235:ILE:N | 1.57 | 1.07 |
| 1:A:379:THR:O | 1:A:383:LEU:HD23 | 1.50 | 1.07 |
| 1:C:919:ARG:HH12 | 1:C:990:VAL:HG12 | 1.20 | 1.07 |
| 1:B:649:MET:HA | 1:B:649:MET:CE | 1.82 | 1.07 |
| 1:B:671:ILE:HD13 | 1:B:671:ILE:O | 1.52 | 1.07 |
| 1:A:498:LYS:HD3 | 1:A:498:LYS:H | 1.14 | 1.07 |
| 1:A:808:ARG:HB2 | 1:A:808:ARG:HH11 | 0.91 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:534:ILE:HG13 | 1:B:541:TYR:CZ | 1.89 | 1.07 |
| 1:A:721:LEU:HD12 | 1:A:814:PRO:CG | 1.84 | 1.06 |
| 1:B:717:ARG:HG2 | 1:B:717:ARG:HH11 | 0.95 | 1.06 |
| 1:B:194:ASN:ND2 | 1:B:790:TYR:CG | 2.22 | 1.06 |
| 1:B:658:ILE:CD1 | 1:B:658:ILE:H | 1.67 | 1.06 |
| 1:A:519:MET:SD | 1:A:520:PHE:N | 2.29 | 1.06 |
| 1:B:182:TYR:CB | 1:B:270:LEU:HD11 | 1.84 | 1.06 |
| 1:C:11:PHE:O | 1:C:11:PHE:HD1 | 1.38 | 1.05 |
| 1:C:54:ALA:HB2 | 1:C:814:PRO:O | 1.55 | 1.05 |
| 1:A:411:VAL:HG21 | 1:A:971:ARG:HH21 | 1.09 | 1.05 |
| 1:B:712:MET:O | 1:B:713:LEU:HD12 | 1.56 | 1.05 |
| 1:C:435:MET:HA | 1:C:435:MET:HE3 | 1.05 | 1.05 |
| 2:E:92:HIS:O | 2:E:96:VAL:HG23 | 1.55 | 1.05 |
| 1:C:200:PRO:HD2 | 1:C:749:THR:HG23 | 1.08 | 1.04 |
| 2:D:51:LEU:HD23 | 2:D:51:LEU:C | 1.71 | 1.04 |
| 1:B:207:ILE:HG22 | 1:B:760:ASN:ND2 | 1.72 | 1.04 |
| 2:E:112:ASN:HA | 2:E:144:LYS:HE2 | 1.40 | 1.04 |
| 1:C:570:GLY:O | 1:C:571:VAL:HG12 | 1.55 | 1.04 |
| 1:A:527:TYR:CE1 | 1:A:972:LEU:HD23 | 1.92 | 1.03 |
| 1:C:44:THR:HB | 1:C:132:SER:OG | 1.57 | 1.03 |
| 1:B:874:PRO:HB2 | 1:B:877:TYR:HD2 | 1.22 | 1.03 |
| 1:B:874:PRO:CB | 1:B:877:TYR:HD2 | 1.70 | 1.03 |
| 1:C:497:LEU:CD2 | 1:C:498:LYS:H | 1.69 | 1.03 |
| 1:C:567:GLU:OE1 | 1:C:998:GLY:HA3 | 1.59 | 1.03 |
| 1:A:498:LYS:H | 1:A:498:LYS:CD | 1.64 | 1.03 |
| 1:B:222:THR:HG22 | 1:C:275:TYR:HB2 | 1.39 | 1.03 |
| 1:B:197:GLN:HA | 1:B:798:MET:HE3 | 1.04 | 1.02 |
| 1:C:314:GLU:CA | 1:C:317:PHE:CE1 | 2.43 | 1.02 |
| 1:A:935:ILE:HD12 | 1:A:935:ILE:O | 1.59 | 1.02 |
| 1:B:119:PRO:O | 1:B:123:GLN:HG3 | 1.59 | 1.02 |
| 1:A:240:LEU:HD12 | 1:A:240:LEU:N | 1.68 | 1.02 |
| 1:C:671:ILE:HG13 | 1:C:674:LEU:HD21 | 1.05 | 1.02 |
| 1:A:360:GLN:HG2 | 1:A:513:PHE:HZ | 1.15 | 1.02 |
| 1:B:156:ASP:CB | 1:B:182:TYR:CE2 | 2.43 | 1.02 |
| 1:B:158:VAL:HA | 1:B:162:MET:HG3 | 1.40 | 1.02 |
| 1:B:194:ASN:ND2 | 1:B:790:TYR:CD2 | 2.25 | 1.02 |
| 1:B:250:LEU:HD23 | 1:B:250:LEU:C | 1.76 | 1.02 |
| 2:D:56:TYR:HE1 | 2:D:90:ARG:HD3 | 0.97 | 1.02 |
| 1:B:705:GLU:CG | 1:B:847:LEU:HD22 | 1.88 | 1.01 |
| 1:C:989:LEU:HD22 | 1:C:1000:GLN:HB3 | 1.42 | 1.01 |
| 2:D:56:TYR:CE1 | 2:D:90:ARG:NE | 2.26 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:204:ILE:O | 1:B:208:LYS:HG3 | 1.58 | 1.01 |
| 2:D:53:LEU:H | 2:D:53:LEU:HD23 | 1.18 | 1.01 |
| 2:E:152:ILE:HG13 | 2:E:153:SER:N | 1.73 | 1.01 |
| 1:B:471:SER:O | 1:B:475:VAL:HG12 | 1.61 | 1.01 |
| 1:B:672:VAL:O | 1:B:672:VAL:HG22 | 1.53 | 1.01 |
| 1:C:185:ARG:HH12 | 1:C:774:MET:HE3 | 1.19 | 1.01 |
| 1:C:83:ASP:HB3 | 1:C:85:THR:CG2 | 1.91 | 1.01 |
| 1:C:879:ILE:CD1 | 1:C:883:VAL:HG23 | 1.90 | 1.01 |
| 1:A:73:ASP:HB3 | 1:A:74:ASN:OD1 | 1.60 | 1.00 |
| 1:B:250:LEU:C | 1:B:250:LEU:CD2 | 2.30 | 1.00 |
| 1:C:689:GLY:C | 1:C:690:LEU:CD2 | 2.29 | 1.00 |
| 1:B:712:MET:C | 1:B:713:LEU:CD1 | 2.30 | 1.00 |
| 1:C:497:LEU:HD23 | 1:C:498:LYS:N | 1.74 | 1.00 |
| 1:C:896:SER:OG | 1:C:897:ILE:HD12 | 1.61 | 1.00 |
| 1:C:671:ILE:HG13 | 1:C:674:LEU:CD2 | 1.91 | 1.00 |
| 2:E:93:LEU:CD2 | 2:E:128:ILE:HG12 | 1.92 | 1.00 |
| 1:B:799:VAL:CG1 | 1:B:800:PRO:CD | 2.33 | 1.00 |
| 1:C:434:SER:O | 1:C:438:ILE:HG12 | 1.60 | 1.00 |
| 1:B:164:ASP:O | 1:B:168:ARG:HG3 | 1.62 | 1.00 |
| 1:A:423:GLU:HA | 1:A:502:LYS:HE3 | 1.01 | 0.99 |
| 1:B:960:LEU:C | 1:B:960:LEU:CD2 | 2.30 | 0.99 |
| 1:A:497:LEU:HD23 | 1:A:497:LEU:N | 1.58 | 0.99 |
| 1:B:758:TYR:HB2 | 1:B:772:TYR:CE1 | 1.97 | 0.99 |
| 1:C:568:ASP:OD2 | 1:C:644:VAL:HG13 | 1.61 | 0.99 |
| 1:C:623:ASN:C | 1:C:623:ASN:HD22 | 1.65 | 0.99 |
| 1:C:741:VAL:HG13 | 1:C:746:ILE:HD11 | 1.00 | 0.99 |
| 1:B:270:LEU:C | 1:B:270:LEU:CD2 | 2.29 | 0.99 |
| 1:C:314:GLU:O | 1:C:317:PHE:HD1 | 1.42 | 0.99 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:CB | 2.10 | 0.99 |
| 1:B:726:GLN:HE22 | 1:B:812:GLY:HA3 | 1.25 | 0.99 |
| 1:A:519:MET:HE1 | 1:A:519:MET:O | 1.62 | 0.98 |
| 1:B:222:THR:HG21 | 1:C:275:TYR:CB | 1.90 | 0.98 |
| 1:C:146:ASP:CB | 1:C:148:THR:CG2 | 2.40 | 0.98 |
| 1:C:325:TYR:N | 1:C:325:TYR:CD1 | 2.30 | 0.98 |
| 1:C:721:LEU:HD23 | 1:C:721:LEU:N | 1.77 | 0.98 |
| 1:C:144:ASN:HD22 | 1:C:149:MET:HB2 | 0.84 | 0.98 |
| 1:C:688:ALA:CB | 1:C:690:LEU:HD21 | 1.94 | 0.98 |
| 1:C:200:PRO:HD2 | 1:C:749:THR:CG2 | 1.93 | 0.98 |
| 1:B:658:ILE:HD12 | 1:B:658:ILE:N | 1.78 | 0.98 |
| 1:B:197:GLN:C | 1:B:798:MET:CE | 2.32 | 0.98 |
| 2:D:18:LEU:HD23 | 2:D:18:LEU:C | 1.81 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:736:ALA:O | 1:C:741:VAL:HB | 1.63 | 0.98 |
| 1:B:190:PRO:HG3 | 1:B:789:TRP:CH2 | 1.99 | 0.97 |
| 2:E:100:LEU:HD21 | 2:E:106:VAL:HG12 | 1.47 | 0.97 |
| 1:B:193:LEU:HD23 | 1:B:193:LEU:H | 1.29 | 0.97 |
| 1:B:511:GLY:HA2 | 1:B:513:PHE:O | 1.64 | 0.96 |
| 1:A:527:TYR:CE1 | 1:A:972:LEU:CD2 | 2.48 | 0.96 |
| 1:C:879:ILE:HD11 | 1:C:883:VAL:CG2 | 1.95 | 0.96 |
| 1:B:207:ILE:CG2 | 1:B:760:ASN:ND2 | 2.27 | 0.96 |
| 1:C:673:GLU:H | 1:C:673:GLU:CD | 1.69 | 0.96 |
| 1:A:32:VAL:HG12 | 1:A:390:ILE:HB | 1.47 | 0.96 |
| 1:B:948:PHE:HE2 | 1:B:971:ARG:HE | 1.02 | 0.96 |
| 1:B:61:VAL:O | 1:B:65:ILE:HG13 | 1.66 | 0.96 |
| 1:B:69:MET:CE | 1:B:72:ILE:HD11 | 1.96 | 0.96 |
| 1:C:435:MET:HE3 | 1:C:435:MET:CA | 1.96 | 0.96 |
| 1:C:741:VAL:CG1 | 1:C:746:ILE:CD1 | 2.38 | 0.96 |
| 1:A:411:VAL:CG2 | 1:A:971:ARG:HH21 | 1.79 | 0.95 |
| 1:B:685:ILE:HG22 | 1:B:686:ASP:N | 1.80 | 0.95 |
| 1:C:671:ILE:HD11 | 1:C:674:LEU:CG | 1.95 | 0.95 |
| 1:A:498:LYS:N | 1:A:498:LYS:CE | 2.30 | 0.95 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:HB3 | 1.65 | 0.95 |
| 1:B:459:PHE:HB2 | 1:B:464:GLY:HA2 | 1.48 | 0.95 |
| 1:C:314:GLU:CA | 1:C:317:PHE:HE1 | 1.77 | 0.95 |
| 1:A:527:TYR:O | 1:A:531:VAL:HG23 | 1.64 | 0.95 |
| 1:B:207:ILE:CG2 | 1:B:760:ASN:HD22 | 1.79 | 0.95 |
| 1:B:361:ASN:H | 1:B:361:ASN:HD22 | 1.01 | 0.95 |
| 1:A:423:GLU:HA | 1:A:502:LYS:CE | 1.95 | 0.95 |
| 1:C:671:ILE:CD1 | 1:C:674:LEU:HD21 | 1.96 | 0.95 |
| 1:C:750:LEU:C | 1:C:750:LEU:CD2 | 2.30 | 0.95 |
| 1:C:196:PHE:C | 1:C:197:GLN:HG2 | 1.87 | 0.94 |
| 2:E:46:VAL:HG13 | 2:E:47:GLY:N | 1.82 | 0.94 |
| 2:D:14:LEU:H | 2:D:14:LEU:HD12 | 1.31 | 0.94 |
| 1:C:919:ARG:HG3 | 1:C:919:ARG:O | 1.67 | 0.94 |
| 1:B:649:MET:HA | 1:B:649:MET:HE3 | 1.49 | 0.94 |
| 1:B:717:ARG:HH11 | 1:B:717:ARG:CG | 1.77 | 0.94 |
| 1:B:361:ASN:HD22 | 1:B:361:ASN:N | 1.60 | 0.94 |
| 1:B:799:VAL:HG13 | 1:B:800:PRO:HD2 | 0.96 | 0.94 |
| 1:C:1:FME:N | 1:C:2:PRO:CD | 2.30 | 0.94 |
| 1:C:875:SER:O | 1:C:879:ILE:HG22 | 1.68 | 0.94 |
| 1:C:976:LEU:O | 1:C:980:LEU:HD23 | 1.66 | 0.94 |
| 1:B:685:ILE:CG2 | 1:B:686:ASP:N | 2.29 | 0.94 |
| 1:C:506:GLY:C | 1:C:507:GLU:HG2 | 1.88 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:496:MET:C | 1:A:497:LEU:CD2 | 2.36 | 0.94 |
| 1:A:973:ARG:O | 1:A:977:MET:HG3 | 1.68 | 0.93 |
| 1:C:447:MET:SD | 1:C:891:LEU:CD2 | 2.55 | 0.93 |
| 1:C:960:LEU:HD11 | 1:C:1027:VAL:HG22 | 1.47 | 0.93 |
| 1:A:480:LEU:O | 1:A:484:VAL:HG23 | 1.67 | 0.93 |
| 1:B:196:PHE:HA | 1:B:197:GLN:HE22 | 1.34 | 0.93 |
| 1:C:739:LEU:N | 1:C:739:LEU:CD1 | 2.30 | 0.93 |
| 1:B:102:ILE:CG2 | 1:B:103:ALA:N | 2.32 | 0.93 |
| 1:B:717:ARG:HG2 | 1:B:717:ARG:NH1 | 1.76 | 0.93 |
| 1:C:439:GLN:HA | 1:C:442:LEU:HD12 | 1.49 | 0.93 |
| 1:B:229:GLN:H | 1:B:229:GLN:CD | 1.64 | 0.93 |
| 1:C:4:PHE:O | 1:C:4:PHE:HD2 | 1.49 | 0.93 |
| 1:B:678:THR:HG22 | 1:B:678:THR:O | 1.65 | 0.93 |
| 1:C:690:LEU:HD23 | 1:C:690:LEU:N | 1.84 | 0.93 |
| 1:C:733:GLN:HE22 | 1:C:743:ILE:HG21 | 1.34 | 0.93 |
| 2:E:152:ILE:C | 2:E:152:ILE:CD1 | 2.30 | 0.93 |
| 1:C:185:ARG:NH1 | 1:C:774:MET:CE | 2.32 | 0.92 |
| 1:B:1:FME:CE | 1:B:487:ILE:HD11 | 1.98 | 0.92 |
| 1:B:422:GLU:C | 1:B:423:GLU:HG2 | 1.87 | 0.92 |
| 1:B:705:GLU:HG2 | 1:B:847:LEU:HD23 | 1.47 | 0.92 |
| 1:C:144:ASN:ND2 | 1:C:149:MET:CB | 2.28 | 0.92 |
| 1:B:117:LEU:CD1 | 1:B:117:LEU:N | 2.30 | 0.92 |
| 1:C:896:SER:OG | 1:C:897:ILE:N | 1.98 | 0.92 |
| 1:A:486:LEU:H | 1:A:486:LEU:HD22 | 0.76 | 0.92 |
| 1:B:726:GLN:NE2 | 1:B:812:GLY:HA3 | 1.84 | 0.92 |
| 1:B:352:PHE:HD1 | 1:B:365:THR:HG1 | 0.97 | 0.92 |
| 1:C:68:ASN:HD22 | 1:C:114:ALA:HB2 | 1.35 | 0.92 |
| 1:B:1:FME:HE1 | 1:B:487:ILE:HD11 | 1.52 | 0.92 |
| 1:B:563:PHE:O | 1:B:564:LEU:HG | 1.69 | 0.92 |
| 1:C:327:TYR:HD2 | 1:C:327:TYR:O | 1.53 | 0.92 |
| 1:C:960:LEU:HD13 | 1:C:960:LEU:C | 1.90 | 0.92 |
| 1:B:234:ILE:O | 1:B:235:ILE:CD1 | 2.18 | 0.92 |
| 1:C:200:PRO:CD | 1:C:749:THR:CG2 | 2.46 | 0.92 |
| 1:A:901:VAL:O | 1:A:901:VAL:HG12 | 1.68 | 0.92 |
| 1:B:188:MET:CE | 1:B:773:VAL:CG2 | 2.48 | 0.92 |
| 1:B:117:LEU:N | 1:B:117:LEU:HD13 | 1.84 | 0.91 |
| 1:A:754:TRP:HZ3 | 1:C:219:LEU:HD23 | 1.32 | 0.91 |
| 1:B:240:LEU:HD23 | 1:B:245:GLU:HB3 | 1.48 | 0.91 |
| 1:B:739:LEU:HD13 | 1:B:799:VAL:HG21 | 1.52 | 0.91 |
| 1:A:971:ARG:HG3 | 1:A:971:ARG:NH1 | 1.76 | 0.91 |
| 1:B:765:ARG:HB3 | 1:B:765:ARG:HH11 | 1.34 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:190:PRO:HG3 | 1:B:789:TRP:CZ2 | 2.06 | 0.91 |
| 1:B:712:MET:C | 1:B:713:LEU:HD13 | 1.91 | 0.91 |
| 1:C:146:ASP:CB | 1:C:148:THR:HG23 | 2.01 | 0.91 |
| 1:C:447:MET:CE | 1:C:891:LEU:CD2 | 2.48 | 0.91 |
| 1:A:904:VAL:O | 1:A:904:VAL:HG22 | 1.67 | 0.91 |
| 1:B:563:PHE:O | 1:B:564:LEU:CD1 | 2.17 | 0.91 |
| 1:A:240:LEU:N | 1:A:240:LEU:CD1 | 2.33 | 0.91 |
| 1:B:874:PRO:HG2 | 1:B:874:PRO:O | 1.68 | 0.90 |
| 1:C:185:ARG:NH1 | 1:C:774:MET:HE3 | 1.86 | 0.90 |
| 2:D:53:LEU:CD2 | 2:D:53:LEU:N | 2.30 | 0.90 |
| 2:E:152:ILE:CG1 | 2:E:153:SER:N | 2.33 | 0.90 |
| 1:B:705:GLU:HG2 | 1:B:847:LEU:HD21 | 1.50 | 0.90 |
| 1:C:83:ASP:CB | 1:C:85:THR:HG23 | 2.01 | 0.90 |
| 1:C:879:ILE:C | 1:C:879:ILE:CD1 | 2.38 | 0.90 |
| 1:C:497:LEU:CD2 | 1:C:498:LYS:N | 2.30 | 0.90 |
| 1:C:674:LEU:H | 1:C:674:LEU:HD22 | 0.73 | 0.90 |
| 1:B:361:ASN:H | 1:B:361:ASN:ND2 | 1.66 | 0.90 |
| 1:B:250:LEU:CD2 | 1:B:251:LEU:N | 2.34 | 0.90 |
| 1:B:563:PHE:O | 1:B:564:LEU:CG | 2.19 | 0.90 |
| 1:C:154:ILE:C | 1:C:154:ILE:CD1 | 2.32 | 0.90 |
| 1:B:362:PHE:O | 1:B:365:THR:HG22 | 1.72 | 0.90 |
| 1:A:298:ASN:ND2 | 1:A:301:ASP:H | 1.70 | 0.89 |
| 1:C:268:ILE:HD13 | 1:C:268:ILE:N | 1.85 | 0.89 |
| 1:C:84:SER:HB3 | 1:C:814:PRO:O | 1.72 | 0.89 |
| 1:A:721:LEU:HD11 | 1:A:814:PRO:CG | 2.02 | 0.89 |
| 1:B:193:LEU:N | 1:B:193:LEU:CD2 | 2.30 | 0.89 |
| 1:A:248:LYS:O | 1:A:261:LEU:HD23 | 1.73 | 0.89 |
| 1:B:874:PRO:HB2 | 1:B:877:TYR:CD2 | 2.07 | 0.89 |
| 2:D:125:HIS:ND1 | 2:D:128:ILE:HG13 | 1.88 | 0.89 |
| 1:B:815:ARG:HG2 | 1:B:815:ARG:HH11 | 1.38 | 0.89 |
| 1:A:431:THR:HG23 | 1:A:432:ARG:N | 1.87 | 0.89 |
| 1:B:197:GLN:CA | 1:B:798:MET:HE2 | 2.01 | 0.89 |
| 1:A:431:THR:CG2 | 1:A:432:ARG:N | 2.36 | 0.88 |
| 1:B:69:MET:HE3 | 1:B:72:ILE:HD11 | 1.55 | 0.88 |
| 1:C:54:ALA:CB | 1:C:814:PRO:O | 2.21 | 0.88 |
| 1:C:896:SER:OG | 1:C:897:ILE:CD1 | 2.20 | 0.88 |
| 2:D:18:LEU:C | 2:D:18:LEU:CD2 | 2.40 | 0.88 |
| 2:D:49:THR:O | 2:D:53:LEU:CD2 | 2.20 | 0.88 |
| 1:C:993:THR:HG23 | 1:C:993:THR:O | 1.73 | 0.88 |
| 1:B:150:THR:HG23 | 1:B:153:ASP:OD2 | 1.72 | 0.88 |
| 2:E:94:GLU:O | 2:E:98:VAL:HG23 | 1.73 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:218:GLN:HB2 | 1:A:233:SER:HA | 1.56 | 0.88 |
| 1:C:447:MET:HE1 | 1:C:891:LEU:HD23 | 1.56 | 0.88 |
| 2:E:97:GLU:OE1 | 2:E:97:GLU:HA | 1.71 | 0.88 |
| 1:A:534:ILE:HA | 1:A:541:TYR:HE1 | 1.39 | 0.88 |
| 1:C:291:ILE:HD13 | 1:C:306:ILE:HD13 | 1.52 | 0.88 |
| 1:C:689:GLY:O | 1:C:690:LEU:HD23 | 1.73 | 0.88 |
| 1:A:75:LEU:HD12 | 1:A:76:MET:H | 0.98 | 0.88 |
| 1:A:234:ILE:O | 1:A:235:ILE:HD12 | 1.74 | 0.88 |
| 1:B:712:MET:C | 1:B:713:LEU:HD12 | 1.91 | 0.88 |
| 1:B:169:THR:HG22 | 1:B:172:VAL:HG13 | 1.56 | 0.87 |
| 1:A:67:GLN:HE21 | 1:C:767:ARG:NH1 | 1.72 | 0.87 |
| 1:A:519:MET:SD | 1:A:520:PHE:CA | 2.61 | 0.87 |
| 1:B:564:LEU:HD12 | 1:B:564:LEU:N | 1.89 | 0.87 |
| 1:A:32:VAL:CG1 | 1:A:390:ILE:HB | 2.04 | 0.87 |
| 1:A:758:TYR:CD1 | 1:A:758:TYR:C | 2.46 | 0.87 |
| 1:A:482:VAL:O | 1:A:486:LEU:CD2 | 2.21 | 0.87 |
| 1:A:491:ALA:O | 1:A:495:THR:HG23 | 1.75 | 0.87 |
| 2:D:73:VAL:CG1 | 2:D:74:ASN:N | 2.37 | 0.87 |
| 1:B:705:GLU:CB | 1:B:847:LEU:HD22 | 2.04 | 0.87 |
| 1:C:158:VAL:HG22 | 1:C:162:MET:HE3 | 1.55 | 0.87 |
| 1:A:524:THR:O | 1:A:528:THR:HG23 | 1.75 | 0.87 |
| 1:C:738:ALA:C | 1:C:739:LEU:HD13 | 1.95 | 0.87 |
| 1:B:166:ILE:HG22 | 1:B:175:VAL:HG21 | 1.57 | 0.86 |
| 1:C:74:ASN:HB3 | 1:C:95:GLU:HB2 | 1.57 | 0.86 |
| 2:D:126:LEU:HA | 2:D:129:VAL:HG21 | 1.56 | 0.86 |
| 1:A:488:LEU:HD12 | 1:A:488:LEU:C | 1.93 | 0.86 |
| 1:B:658:ILE:CD1 | 1:B:658:ILE:N | 2.30 | 0.86 |
| 1:C:144:ASN:ND2 | 1:C:149:MET:HG3 | 1.90 | 0.86 |
| 1:C:960:LEU:C | 1:C:960:LEU:CD1 | 2.43 | 0.86 |
| 1:A:519:MET:SD | 1:A:520:PHE:HA | 2.16 | 0.86 |
| 1:C:325:TYR:N | 1:C:325:TYR:HD1 | 1.73 | 0.86 |
| 1:A:496:MET:O | 1:A:497:LEU:HD23 | 1.73 | 0.86 |
| 1:B:234:ILE:C | 1:B:235:ILE:HD13 | 1.96 | 0.86 |
| 1:B:445:ILE:HG21 | 1:B:940:LYS:HG3 | 1.55 | 0.86 |
| 1:A:780:ARG:O | 1:A:780:ARG:HG3 | 1.74 | 0.86 |
| 1:B:137:LEU:HD22 | 1:B:293:LEU:HD12 | 1.58 | 0.86 |
| 1:C:200:PRO:HG2 | 1:C:749:THR:HG22 | 1.56 | 0.86 |
| 1:C:989:LEU:CD2 | 1:C:1000:GLN:HB3 | 2.06 | 0.86 |
| 1:A:358:PHE:HB2 | 1:A:977:MET:HE1 | 1.58 | 0.86 |
| 1:A:498:LYS:CD | 1:A:498:LYS:N | 2.35 | 0.85 |
| 1:B:563:PHE:CA | 1:B:564:LEU:HD12 | 2.06 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:735:LYS:O | 1:C:739:LEU:HD22 | 1.76 | 0.85 |
| 1:A:75:LEU:CD1 | 1:A:76:MET:N | 2.33 | 0.85 |
| 1:C:15:ILE:O | 1:C:19:ILE:HG12 | 1.76 | 0.85 |
| 2:D:49:THR:O | 2:D:53:LEU:HD21 | 1.77 | 0.85 |
| 2:D:56:TYR:O | 2:D:56:TYR:CD1 | 2.29 | 0.85 |
| 1:A:758:TYR:CD1 | 1:A:758:TYR:O | 2.29 | 0.85 |
| 1:B:348:ILE:HG21 | 1:B:369:THR:HG23 | 1.58 | 0.85 |
| 1:B:762:PHE:HE1 | 1:B:764:ASP:HB2 | 1.40 | 0.85 |
| 1:C:211:ASN:HD22 | 1:C:760:ASN:ND2 | 1.74 | 0.85 |
| 1:B:154:ILE:O | 1:B:158:VAL:HG23 | 1.77 | 0.85 |
| 1:C:671:ILE:O | 1:C:674:LEU:CD2 | 2.25 | 0.85 |
| 1:B:196:PHE:C | 1:B:197:GLN:NE2 | 2.30 | 0.85 |
| 1:C:158:VAL:HA | 1:C:162:MET:HE2 | 1.55 | 0.85 |
| 1:C:4:PHE:O | 1:C:4:PHE:CD2 | 2.30 | 0.85 |
| 1:C:154:ILE:HD11 | 1:C:287:SER:HB3 | 1.56 | 0.85 |
| 1:C:237:GLN:O | 1:C:238:THR:HG23 | 1.77 | 0.85 |
| 1:A:749:THR:HG21 | 1:A:791:VAL:HG11 | 1.57 | 0.84 |
| 1:B:495:THR:HG22 | 1:B:496:MET:N | 1.92 | 0.84 |
| 1:B:948:PHE:HE2 | 1:B:971:ARG:NE | 1.73 | 0.84 |
| 1:C:671:ILE:HD12 | 1:C:674:LEU:HD11 | 1.59 | 0.84 |
| 2:E:73:VAL:HG12 | 2:E:104:ALA:HB2 | 1.58 | 0.84 |
| 1:C:447:MET:CE | 1:C:891:LEU:HD23 | 2.07 | 0.84 |
| 2:E:56:TYR:CD1 | 2:E:56:TYR:O | 2.30 | 0.84 |
| 1:A:790:TYR:HB3 | 1:A:798:MET:HB3 | 1.59 | 0.84 |
| 2:E:144:LYS:O | 2:E:145:PHE:CG | 2.31 | 0.84 |
| 1:A:75:LEU:CD1 | 1:A:76:MET:H | 1.87 | 0.84 |
| 1:B:207:ILE:HG22 | 1:B:760:ASN:HD21 | 1.42 | 0.84 |
| 1:B:561:SER:HB2 | 1:B:923:ASN:HB3 | 1.58 | 0.84 |
| 1:C:327:TYR:O | 1:C:327:TYR:CD2 | 2.30 | 0.84 |
| 1:B:658:ILE:H | 1:B:658:ILE:HD13 | 1.42 | 0.84 |
| 2:E:46:VAL:CG1 | 2:E:47:GLY:H | 1.87 | 0.84 |
| 1:B:713:LEU:CD1 | 1:B:713:LEU:N | 2.41 | 0.84 |
| 1:A:758:TYR:C | 1:A:758:TYR:HD1 | 1.80 | 0.84 |
| 1:B:563:PHE:O | 1:B:564:LEU:HD12 | 1.75 | 0.84 |
| 1:B:197:GLN:CD | 1:B:197:GLN:N | 2.30 | 0.83 |
| 2:E:144:LYS:O | 2:E:145:PHE:CD2 | 2.30 | 0.83 |
| 1:B:281:PHE:HD1 | 1:B:610:PHE:HD1 | 1.26 | 0.83 |
| 2:D:56:TYR:CD1 | 2:D:90:ARG:NE | 2.45 | 0.83 |
| 1:A:367:ILE:HB | 1:A:368:PRO:HD3 | 1.60 | 0.83 |
| 1:A:486:LEU:N | 1:A:486:LEU:CD1 | 2.30 | 0.83 |
| 1:A:190:PRO:HG2 | 1:A:779:TYR:HB3 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:974:PRO:O | 1:A:978:THR:HG23 | 1.77 | 0.83 |
| 1:B:229:GLN:OE1 | 1:B:230:LEU:N | 2.11 | 0.83 |
| 1:B:837:THR:O | 1:B:841:MET:HG3 | 1.78 | 0.83 |
| 1:B:1027:VAL:O | 1:B:1031:ARG:HG2 | 1.78 | 0.83 |
| 1:C:810:GLU:C | 1:C:811:TYR:HD2 | 1.81 | 0.83 |
| 2:D:125:HIS:O | 2:D:129:VAL:HG22 | 1.78 | 0.83 |
| 1:B:53:ASP:O | 1:B:57:VAL:HG23 | 1.78 | 0.83 |
| 1:C:11:PHE:O | 1:C:11:PHE:CD1 | 2.30 | 0.83 |
| 1:A:411:VAL:HG21 | 1:A:971:ARG:NH2 | 1.94 | 0.83 |
| 1:B:102:ILE:HG22 | 1:B:103:ALA:H | 1.44 | 0.83 |
| 1:A:488:LEU:CD1 | 1:A:492:LEU:HD13 | 2.09 | 0.83 |
| 1:B:182:TYR:CG | 1:B:270:LEU:HD11 | 2.13 | 0.82 |
| 1:B:254:ASN:ND2 | 1:B:258:SER:HB3 | 1.93 | 0.82 |
| 1:B:671:ILE:O | 1:B:671:ILE:HG23 | 1.77 | 0.82 |
| 2:D:56:TYR:CD1 | 2:D:90:ARG:HG3 | 2.13 | 0.82 |
| 1:C:758:TYR:CE2 | 1:C:770:LYS:HB3 | 2.14 | 0.82 |
| 1:B:562:SER:O | 1:B:924:ASP:CA | 2.25 | 0.82 |
| 1:A:488:LEU:HD12 | 1:A:492:LEU:HD13 | 1.59 | 0.82 |
| 1:A:498:LYS:HE3 | 1:A:498:LYS:N | 1.94 | 0.82 |
| 1:A:971:ARG:C | 1:A:974:PRO:HD2 | 1.99 | 0.82 |
| 1:B:234:ILE:O | 1:B:235:ILE:HD12 | 1.79 | 0.82 |
| 1:B:853:THR:C | 1:B:857:TYR:N | 2.33 | 0.82 |
| 1:C:200:PRO:HG2 | 1:C:749:THR:CG2 | 2.09 | 0.82 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:CA | 2.28 | 0.82 |
| 1:B:989:LEU:CD2 | 1:B:1000:GLN:HG2 | 2.09 | 0.82 |
| 1:A:558:ARG:O | 1:A:558:ARG:HD2 | 1.79 | 0.82 |
| 1:C:733:GLN:NE2 | 1:C:743:ILE:HG21 | 1.94 | 0.82 |
| 1:A:445:ILE:HG21 | 1:A:940:LYS:HE2 | 1.62 | 0.81 |
| 1:A:519:MET:C | 1:A:519:MET:CE | 2.48 | 0.81 |
| 1:B:563:PHE:CB | 1:B:564:LEU:HD12 | 2.10 | 0.81 |
| 1:C:671:ILE:CD1 | 1:C:674:LEU:CD1 | 2.42 | 0.81 |
| 1:A:680:PHE:CZ | 1:A:829:GLY:HA3 | 2.15 | 0.81 |
| 1:B:605:ASN:O | 1:B:631:LEU:HD22 | 1.79 | 0.81 |
| 1:B:731:ILE:O | 1:B:731:ILE:HG12 | 1.79 | 0.81 |
| 2:D:51:LEU:C | 2:D:51:LEU:CD2 | 2.47 | 0.81 |
| 2:D:56:TYR:CD1 | 2:D:90:ARG:CD | 2.63 | 0.81 |
| 1:B:160:ALA:C | 1:B:161:ASN:HD22 | 1.83 | 0.81 |
| 1:B:354:VAL:HG21 | 1:B:981:ALA:HB2 | 1.63 | 0.81 |
| 1:B:587:THR:HG21 | 1:B:622:GLN:O | 1.81 | 0.81 |
| 1:B:674:LEU:O | 1:B:674:LEU:HD13 | 1.80 | 0.81 |
| 1:C:71:GLY:O | 1:C:72:ILE:HG12 | 1.81 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:733:GLN:OE1 | 1:C:743:ILE:HD13 | 1.81 | 0.81 |
| 1:A:1:FME:N | 1:A:2:PRO:CD | 2.43 | 0.81 |
| 1:B:230:LEU:C | 1:B:230:LEU:CD2 | 2.37 | 0.81 |
| 1:C:980:LEU:N | 1:C:980:LEU:HD22 | 1.95 | 0.81 |
| 1:A:685:ILE:HD13 | 1:A:685:ILE:H | 1.45 | 0.81 |
| 1:C:512:PHE:CD1 | 1:C:512:PHE:O | 2.34 | 0.81 |
| 1:B:527:TYR:HE2 | 1:B:968:VAL:HG13 | 1.45 | 0.81 |
| 1:A:182:TYR:CD2 | 1:A:270:LEU:HD23 | 2.14 | 0.80 |
| 1:A:485:ALA:O | 1:A:490:PRO:CD | 2.29 | 0.80 |
| 1:B:649:MET:HA | 1:B:649:MET:HE2 | 1.62 | 0.80 |
| 1:B:775:SER:OG | 1:B:780:ARG:HG2 | 1.80 | 0.80 |
| 1:B:671:ILE:O | 1:B:672:VAL:CG1 | 2.30 | 0.80 |
| 1:B:362:PHE:O | 1:B:365:THR:CG2 | 2.30 | 0.80 |
| 1:B:561:SER:CB | 1:B:923:ASN:HB3 | 2.10 | 0.80 |
| 1:C:85:THR:OG1 | 1:C:87:THR:HG23 | 1.80 | 0.80 |
| 2:D:73:VAL:CG1 | 2:D:74:ASN:OD1 | 2.28 | 0.80 |
| 1:A:379:THR:O | 1:A:383:LEU:CD2 | 2.30 | 0.80 |
| 1:A:483:LEU:O | 1:A:486:LEU:CD2 | 2.30 | 0.80 |
| 1:A:534:ILE:HA | 1:A:541:TYR:CE1 | 2.16 | 0.80 |
| 1:B:668:LEU:C | 1:B:668:LEU:CD1 | 2.46 | 0.80 |
| 2:D:46:VAL:CG2 | 2:D:46:VAL:O | 2.30 | 0.80 |
| 1:A:188:MET:HG2 | 1:A:774:MET:O | 1.82 | 0.80 |
| 1:C:83:ASP:O | 1:C:84:SER:CB | 2.29 | 0.80 |
| 1:C:570:GLY:O | 1:C:571:VAL:CG1 | 2.30 | 0.80 |
| 1:B:278:ILE:HG12 | 1:B:278:ILE:O | 1.82 | 0.80 |
| 1:C:496:MET:CG | 1:C:496:MET:O | 2.30 | 0.80 |
| 1:C:568:ASP:OD2 | 1:C:644:VAL:HG22 | 1.82 | 0.80 |
| 1:C:672:VAL:CG2 | 1:C:673:GLU:OE1 | 2.30 | 0.80 |
| 1:A:498:LYS:H | 1:A:498:LYS:CE | 1.93 | 0.80 |
| 1:B:848:ALA:O | 1:B:851:LEU:CD1 | 2.29 | 0.80 |
| 1:C:88:VAL:HG23 | 1:C:89:GLN:N | 1.95 | 0.80 |
| 1:C:927:PHE:CE2 | 1:C:931:LEU:HD11 | 2.16 | 0.80 |
| 1:C:976:LEU:O | 1:C:980:LEU:CD2 | 2.30 | 0.80 |
| 1:A:647:ILE:O | 1:A:650:ARG:HG2 | 1.81 | 0.80 |
| 1:B:188:MET:HE2 | 1:B:773:VAL:CG2 | 2.02 | 0.80 |
| 1:B:671:ILE:O | 1:B:671:ILE:CD1 | 2.30 | 0.80 |
| 1:B:848:ALA:HA | 1:B:851:LEU:HD13 | 1.62 | 0.79 |
| 1:A:73:ASP:CB | 1:A:74:ASN:OD1 | 2.30 | 0.79 |
| 1:B:848:ALA:HA | 1:B:851:LEU:HD11 | 1.63 | 0.79 |
| 1:C:71:GLY:O | 1:C:72:ILE:CG1 | 2.30 | 0.79 |
| 2:D:53:LEU:N | 2:D:53:LEU:HD22 | 1.95 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:441:ALA:O | 1:B:445:ILE:HG13 | 1.81 | 0.79 |
| 1:B:501:ALA:O | 1:B:504:ASP:HB3 | 1.82 | 0.79 |
| 1:A:558:ARG:O | 1:A:558:ARG:CD | 2.30 | 0.79 |
| 1:A:558:ARG:CD | 1:A:558:ARG:C | 2.50 | 0.79 |
| 1:B:182:TYR:HB3 | 1:B:270:LEU:CD1 | 2.10 | 0.79 |
| 1:C:11:PHE:HD1 | 1:C:11:PHE:C | 1.85 | 0.79 |
| 1:C:566:ASP:OD2 | 1:C:678:THR:HG21 | 1.82 | 0.79 |
| 2:D:73:VAL:HG12 | 2:D:74:ASN:N | 1.96 | 0.79 |
| 1:C:876:LEU:C | 1:C:876:LEU:CD2 | 2.50 | 0.79 |
| 1:C:923:ASN:OD1 | 1:C:927:PHE:CD2 | 2.35 | 0.79 |
| 1:B:966:ASP:O | 1:B:970:MET:HG3 | 1.80 | 0.79 |
| 1:C:144:ASN:ND2 | 1:C:149:MET:CG | 2.45 | 0.79 |
| 1:C:314:GLU:CA | 1:C:317:PHE:CD1 | 2.65 | 0.79 |
| 2:E:93:LEU:HD21 | 2:E:128:ILE:CG1 | 2.13 | 0.79 |
| 1:A:931:LEU:O | 1:A:935:ILE:CG2 | 2.30 | 0.79 |
| 1:B:991:ILE:O | 1:B:991:ILE:CD1 | 2.30 | 0.79 |
| 1:C:88:VAL:CG2 | 1:C:89:GLN:N | 2.45 | 0.79 |
| 1:A:376:LEU:O | 1:A:380:PHE:HD1 | 1.64 | 0.78 |
| 1:A:519:MET:O | 1:A:519:MET:CE | 2.30 | 0.78 |
| 1:B:218:GLN:HB3 | 1:B:232:ALA:O | 1.82 | 0.78 |
| 1:B:874:PRO:CB | 1:B:877:TYR:CD2 | 2.61 | 0.78 |
| 1:A:935:ILE:O | 1:A:935:ILE:CD1 | 2.30 | 0.78 |
| 1:B:24:GLY:O | 1:B:27:ILE:HG22 | 1.83 | 0.78 |
| 1:A:263:ARG:HG3 | 1:A:264:ASP:OD2 | 1.83 | 0.78 |
| 1:C:149:MET:SD | 1:C:321:LEU:CD1 | 2.72 | 0.78 |
| 1:C:758:TYR:HE2 | 1:C:770:LYS:HB3 | 1.48 | 0.78 |
| 2:D:56:TYR:HE1 | 2:D:90:ARG:NE | 1.72 | 0.78 |
| 1:B:182:TYR:CD1 | 1:B:270:LEU:CD1 | 2.66 | 0.78 |
| 1:A:956:GLU:OE2 | 1:A:956:GLU:CA | 2.30 | 0.78 |
| 1:B:302:THR:O | 1:B:306:ILE:HG22 | 1.83 | 0.78 |
| 1:B:449:LEU:O | 1:B:453:PHE:HD1 | 1.66 | 0.78 |
| 1:B:848:ALA:CA | 1:B:851:LEU:CD1 | 2.60 | 0.78 |
| 1:C:960:LEU:O | 1:C:960:LEU:CD1 | 2.30 | 0.78 |
| 2:E:93:LEU:HD21 | 2:E:128:ILE:HG12 | 1.64 | 0.78 |
| 1:B:196:PHE:C | 1:B:197:GLN:CD | 2.42 | 0.78 |
| 2:D:56:TYR:HD1 | 2:D:90:ARG:HG3 | 1.49 | 0.78 |
| 1:A:10:ILE:O | 1:A:14:VAL:HG23 | 1.83 | 0.78 |
| 1:A:485:ALA:C | 1:A:486:LEU:HD13 | 2.03 | 0.78 |
| 1:B:919:ARG:HB3 | 1:B:919:ARG:HH11 | 0.67 | 0.78 |
| 1:C:156:ASP:OD1 | 1:C:182:TYR:HB2 | 1.84 | 0.78 |
| 1:B:156:ASP:CB | 1:B:182:TYR:HE2 | 1.96 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:68:ASN:ND2 | 1:C:114:ALA:HB2 | 1.98 | 0.78 |
| 1:C:724:THR:CB | 1:C:725:PRO:CD | 2.63 | 0.78 |
| 1:B:575:MET:HG3 | 1:B:576:VAL:N | 1.99 | 0.77 |
| 1:B:534:ILE:HA | 1:B:541:TYR:CZ | 2.19 | 0.77 |
| 1:A:67:GLN:NE2 | 1:C:767:ARG:NH1 | 2.32 | 0.77 |
| 1:C:927:PHE:CE2 | 1:C:931:LEU:CD1 | 2.67 | 0.77 |
| 1:A:181:GLN:HE21 | 1:A:769:LYS:HE3 | 1.49 | 0.77 |
| 1:A:348:ILE:O | 1:A:351:VAL:HG12 | 1.84 | 0.77 |
| 1:A:496:MET:O | 1:A:497:LEU:CD2 | 2.30 | 0.77 |
| 1:C:568:ASP:OD2 | 1:C:644:VAL:CG1 | 2.32 | 0.77 |
| 1:C:1:FME:CN | 1:C:2:PRO:HD2 | 2.15 | 0.77 |
| 1:C:157:TYR:C | 1:C:157:TYR:CD2 | 2.58 | 0.77 |
| 2:E:146:GLY:HA2 | 2:E:147:LYS:CB | 2.15 | 0.77 |
| 1:A:150:THR:O | 1:A:154:ILE:HG13 | 1.85 | 0.77 |
| 1:B:218:GLN:NE2 | 1:B:231:ASN:HD21 | 1.82 | 0.77 |
| 1:B:762:PHE:HD2 | 1:B:771:VAL:HG23 | 1.48 | 0.77 |
| 1:C:185:ARG:HH12 | 1:C:774:MET:HE2 | 1.46 | 0.77 |
| 1:B:103:ALA:O | 1:B:107:VAL:HG23 | 1.84 | 0.77 |
| 1:C:669:PRO:HA | 1:C:678:THR:HG22 | 1.66 | 0.77 |
| 2:D:126:LEU:O | 2:D:129:VAL:HG23 | 1.85 | 0.77 |
| 1:A:498:LYS:O | 1:A:498:LYS:CE | 2.30 | 0.76 |
| 1:B:559:LEU:HD12 | 1:B:560:PRO:HD2 | 1.66 | 0.76 |
| 1:B:713:LEU:HD13 | 1:B:713:LEU:N | 1.99 | 0.76 |
| 1:C:155:SER:HB3 | 1:C:287:SER:HB2 | 1.64 | 0.76 |
| 1:A:75:LEU:HD12 | 1:A:75:LEU:C | 1.86 | 0.76 |
| 1:B:5:PHE:O | 1:B:491:ALA:HB2 | 1.85 | 0.76 |
| 1:C:671:ILE:O | 1:C:674:LEU:HD21 | 1.85 | 0.76 |
| 1:B:204:ILE:HG23 | 1:B:759:VAL:CG1 | 2.16 | 0.76 |
| 1:C:502:LYS:HG2 | 1:C:503:GLY:N | 2.00 | 0.76 |
| 1:B:270:LEU:CD2 | 1:B:271:GLY:N | 2.39 | 0.76 |
| 1:B:974:PRO:O | 1:B:978:THR:HG23 | 1.85 | 0.76 |
| 1:B:674:LEU:O | 1:B:674:LEU:CD1 | 2.34 | 0.76 |
| 1:B:874:PRO:O | 1:B:874:PRO:CG | 2.30 | 0.76 |
| 2:D:126:LEU:HA | 2:D:129:VAL:CG2 | 2.15 | 0.76 |
| 1:B:234:ILE:O | 1:B:235:ILE:HD13 | 1.85 | 0.76 |
| 1:C:570:GLY:C | 1:C:571:VAL:CG1 | 2.53 | 0.76 |
| 1:C:623:ASN:C | 1:C:623:ASN:ND2 | 2.34 | 0.76 |
| 1:B:72:ILE:HG22 | 1:B:73:ASP:N | 2.00 | 0.76 |
| 1:B:102:ILE:HG22 | 1:B:103:ALA:N | 1.97 | 0.76 |
| 1:B:196:PHE:HA | 1:B:197:GLN:NE2 | 2.00 | 0.76 |
| 1:C:607:GLU:OE2 | 1:C:632:LYS:CG | 2.29 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:904:VAL:O | 1:A:904:VAL:CG2 | 2.34 | 0.76 |
| 1:C:196:PHE:C | 1:C:197:GLN:CG | 2.54 | 0.76 |
| 1:C:669:PRO:CA | 1:C:678:THR:HG22 | 2.15 | 0.76 |
| 1:B:501:ALA:HB3 | 1:B:504:ASP:CB | 2.17 | 0.75 |
| 1:B:712:MET:O | 1:B:713:LEU:CD1 | 2.30 | 0.75 |
| 2:D:19:LEU:HD23 | 2:D:50:PRO:HG3 | 1.67 | 0.75 |
| 1:A:235:ILE:O | 1:B:728:LYS:HA | 1.87 | 0.75 |
| 1:C:369:THR:O | 1:C:372:VAL:HG13 | 1.86 | 0.75 |
| 1:B:1:FME:N | 1:B:2:PRO:CD | 2.49 | 0.75 |
| 1:C:144:ASN:HD21 | 1:C:149:MET:HG3 | 1.52 | 0.75 |
| 1:C:34:GLN:HB2 | 1:C:333:VAL:HG13 | 1.67 | 0.75 |
| 1:C:876:LEU:CD2 | 1:C:876:LEU:O | 2.34 | 0.75 |
| 1:B:178:PHE:HB2 | 1:B:287:SER:O | 1.86 | 0.75 |
| 1:C:724:THR:HB | 1:C:725:PRO:CD | 2.16 | 0.75 |
| 1:B:415:ASN:O | 1:B:419:VAL:HG23 | 1.87 | 0.75 |
| 1:B:848:ALA:O | 1:B:851:LEU:HD12 | 1.86 | 0.75 |
| 1:A:101:ASP:O | 1:A:105:VAL:HG23 | 1.87 | 0.75 |
| 1:B:204:ILE:HG23 | 1:B:759:VAL:HG12 | 1.69 | 0.75 |
| 1:B:988:PRO:O | 1:B:991:ILE:CG2 | 2.35 | 0.75 |
| 1:C:160:ALA:C | 1:C:161:ASN:OD1 | 2.25 | 0.75 |
| 1:C:327:TYR:HD1 | 1:C:628:PHE:HB3 | 1.50 | 0.75 |
| 1:C:689:GLY:CA | 1:C:690:LEU:HD23 | 2.17 | 0.75 |
| 1:C:200:PRO:CG | 1:C:749:THR:CG2 | 2.65 | 0.75 |
| 1:C:314:GLU:HA | 1:C:317:PHE:HE1 | 1.01 | 0.75 |
| 1:B:10:ILE:HB | 1:C:893:GLU:OE2 | 1.87 | 0.74 |
| 1:B:224:PRO:HA | 1:C:781:MET:HE1 | 1.70 | 0.74 |
| 1:B:799:VAL:HG13 | 1:B:800:PRO:HD3 | 1.68 | 0.74 |
| 1:B:853:THR:CG2 | 1:B:853:THR:O | 2.34 | 0.74 |
| 1:A:542:LEU:O | 1:A:545:TYR:HB3 | 1.87 | 0.74 |
| 1:B:161:ASN:N | 1:B:161:ASN:ND2 | 2.29 | 0.74 |
| 1:A:62:THR:O | 1:A:66:GLU:HG3 | 1.86 | 0.74 |
| 1:C:4:PHE:CD2 | 1:C:4:PHE:C | 2.51 | 0.74 |
| 2:D:18:LEU:O | 2:D:18:LEU:CD2 | 2.30 | 0.74 |
| 1:C:102:ILE:O | 1:C:106:GLN:HG3 | 1.87 | 0.74 |
| 2:E:152:ILE:HG13 | 2:E:153:SER:H | 1.51 | 0.74 |
| 1:B:188:MET:HE1 | 1:B:773:VAL:CG2 | 2.16 | 0.74 |
| 1:B:668:LEU:O | 1:B:668:LEU:CD1 | 2.30 | 0.74 |
| 1:C:587:THR:HG21 | 1:C:622:GLN:O | 1.87 | 0.74 |
| 1:C:742:SER:HB3 | 1:C:745:ASP:H | 1.53 | 0.74 |
| 1:C:891:LEU:HD12 | 1:C:892:TYR:CD1 | 2.23 | 0.74 |
| 2:E:112:ASN:CA | 2:E:144:LYS:HE2 | 2.17 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:229:GLN:OE1 | 1:B:229:GLN:CA | 2.34 | 0.74 |
| 1:A:32:VAL:HG12 | 1:A:390:ILE:O | 1.86 | 0.74 |
| 1:A:242:SER:HB2 | 1:A:244:GLU:HG2 | 1.70 | 0.74 |
| 1:A:428:LYS:O | 1:A:431:THR:CG2 | 2.30 | 0.74 |
| 1:B:670:ALA:O | 1:B:671:ILE:HG22 | 1.87 | 0.74 |
| 1:C:267:LYS:C | 1:C:268:ILE:HD13 | 2.08 | 0.74 |
| 2:E:93:LEU:HD23 | 2:E:128:ILE:HG12 | 1.68 | 0.74 |
| 1:A:942:ALA:O | 1:A:946:VAL:HG12 | 1.87 | 0.74 |
| 1:B:990:VAL:HG12 | 1:B:991:ILE:N | 2.00 | 0.74 |
| 1:A:721:LEU:HD12 | 1:A:814:PRO:HG2 | 1.67 | 0.74 |
| 1:C:671:ILE:CG1 | 1:C:671:ILE:O | 2.29 | 0.74 |
| 1:C:247:GLY:O | 1:C:263:ARG:CG | 2.36 | 0.74 |
| 1:C:910:ILE:CG2 | 1:C:1013:THR:HG21 | 2.17 | 0.74 |
| 1:A:897:ILE:N | 1:A:898:PRO:CD | 2.51 | 0.73 |
| 1:C:327:TYR:CD1 | 1:C:628:PHE:HB3 | 2.23 | 0.73 |
| 1:C:512:PHE:CD1 | 1:C:512:PHE:C | 2.57 | 0.73 |
| 2:E:100:LEU:HD21 | 2:E:106:VAL:CG1 | 2.17 | 0.73 |
| 1:A:580:ALA:HA | 1:A:623:ASN:ND2 | 2.03 | 0.73 |
| 1:B:705:GLU:HB3 | 1:B:847:LEU:HD22 | 1.70 | 0.73 |
| 1:B:365:THR:HG23 | 1:B:366:LEU:HD23 | 1.70 | 0.73 |
| 1:A:721:LEU:CD1 | 1:A:814:PRO:HG2 | 2.13 | 0.73 |
| 1:B:169:THR:HG22 | 1:B:172:VAL:CG1 | 2.17 | 0.73 |
| 1:C:11:PHE:CD1 | 1:C:11:PHE:C | 2.57 | 0.73 |
| 1:C:203:VAL:O | 1:C:207:ILE:HG13 | 1.88 | 0.73 |
| 1:B:59:ASP:O | 1:B:63:GLN:HB2 | 1.89 | 0.73 |
| 1:B:224:PRO:HA | 1:C:781:MET:CE | 2.18 | 0.73 |
| 1:C:247:GLY:O | 1:C:263:ARG:HG3 | 1.88 | 0.73 |
| 1:A:478:MET:O | 1:A:482:VAL:CG2 | 2.30 | 0.73 |
| 1:A:488:LEU:O | 1:A:488:LEU:CD1 | 2.30 | 0.73 |
| 1:B:254:ASN:HB2 | 1:B:258:SER:O | 1.88 | 0.73 |
| 1:C:876:LEU:O | 1:C:876:LEU:HD23 | 1.88 | 0.73 |
| 1:A:621:GLY:HA3 | 1:A:624:THR:HG22 | 1.71 | 0.73 |
| 1:A:808:ARG:NH1 | 1:A:808:ARG:CB | 2.30 | 0.73 |
| 1:C:671:ILE:CD1 | 1:C:674:LEU:CD2 | 2.67 | 0.73 |
| 1:A:754:TRP:CZ3 | 1:C:219:LEU:HD23 | 2.22 | 0.73 |
| 1:A:956:GLU:OE2 | 1:A:956:GLU:HA | 1.87 | 0.73 |
| 1:C:149:MET:SD | 1:C:321:LEU:HD13 | 2.29 | 0.73 |
| 1:C:156:ASP:CG | 1:C:182:TYR:CD2 | 2.62 | 0.73 |
| 1:C:669:PRO:HD3 | 1:C:676:THR:O | 1.89 | 0.73 |
| 1:C:754:TRP:CZ2 | 1:C:786:ILE:HG12 | 2.24 | 0.72 |
| 1:B:161:ASN:HD22 | 1:B:161:ASN:N | 1.87 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:254:ASN:HD22 | 1:B:258:SER:CB | 1.97 | 0.72 |
| 1:A:376:LEU:O | 1:A:380:PHE:CD1 | 2.42 | 0.72 |
| 1:B:986:VAL:O | 1:B:986:VAL:HG12 | 1.89 | 0.72 |
| 1:B:948:PHE:CE2 | 1:B:971:ARG:NE | 2.53 | 0.72 |
| 1:C:259:ARG:HH12 | 2:E:155:ASP:CG | 1.93 | 0.72 |
| 1:B:183:ALA:N | 1:B:271:GLY:O | 2.22 | 0.72 |
| 1:B:771:VAL:O | 1:B:771:VAL:HG12 | 1.88 | 0.72 |
| 1:A:407:ASP:OD1 | 1:A:978:THR:HG21 | 1.90 | 0.72 |
| 1:A:427:PRO:HD3 | 1:A:499:PRO:HB3 | 1.72 | 0.72 |
| 1:A:463:THR:O | 1:A:467:TYR:HD2 | 1.73 | 0.72 |
| 1:A:535:LEU:HD22 | 1:A:1027:VAL:HG21 | 1.71 | 0.72 |
| 1:B:874:PRO:HB3 | 1:B:877:TYR:HD2 | 1.51 | 0.72 |
| 1:C:534:ILE:HG13 | 1:C:541:TYR:CE2 | 2.25 | 0.72 |
| 1:A:151:GLN:HB3 | 1:A:285:PRO:HB3 | 1.71 | 0.72 |
| 1:C:757:SER:O | 1:C:772:TYR:HD1 | 1.70 | 0.72 |
| 1:C:896:SER:HG | 1:C:897:ILE:CD1 | 2.03 | 0.72 |
| 1:C:926:TYR:HD2 | 1:C:1003:VAL:HG22 | 1.55 | 0.72 |
| 1:A:383:LEU:HD11 | 1:A:473:THR:HG22 | 1.70 | 0.72 |
| 1:A:498:LYS:HE3 | 1:A:498:LYS:C | 2.08 | 0.72 |
| 1:B:36:PRO:HG3 | 1:B:391:ASN:ND2 | 2.05 | 0.72 |
| 1:B:394:THR:HG22 | 1:B:473:THR:OG1 | 1.90 | 0.72 |
| 1:B:69:MET:CE | 1:B:72:ILE:CD1 | 2.67 | 0.72 |
| 1:B:254:ASN:C | 1:B:257:GLY:H | 1.93 | 0.72 |
| 1:B:671:ILE:O | 1:B:672:VAL:HG12 | 1.89 | 0.72 |
| 1:C:314:GLU:O | 1:C:317:PHE:CD1 | 2.35 | 0.72 |
| 1:A:519:MET:CG | 1:A:520:PHE:N | 2.52 | 0.72 |
| 1:B:102:ILE:HG23 | 1:B:103:ALA:N | 2.02 | 0.72 |
| 1:B:254:ASN:HB2 | 1:B:258:SER:N | 2.05 | 0.72 |
| 1:C:457:ALA:HB1 | 1:C:468:ARG:HG2 | 1.72 | 0.72 |
| 1:C:513:PHE:O | 1:C:516:PHE:N | 2.23 | 0.72 |
| 1:C:793:ALA:O | 1:C:794:ALA:C | 2.28 | 0.72 |
| 1:C:810:GLU:C | 1:C:811:TYR:CD2 | 2.63 | 0.72 |
| 1:B:557:VAL:CG2 | 1:B:557:VAL:O | 2.38 | 0.71 |
| 1:B:670:ALA:O | 1:B:671:ILE:CB | 2.33 | 0.71 |
| 1:C:204:ILE:HG23 | 1:C:759:VAL:CG2 | 2.20 | 0.71 |
| 2:E:125:HIS:ND1 | 2:E:128:ILE:HG13 | 2.06 | 0.71 |
| 1:C:582:ALA:HB3 | 1:C:623:ASN:HB2 | 1.72 | 0.71 |
| 1:C:891:LEU:HD12 | 1:C:892:TYR:CE1 | 2.25 | 0.71 |
| 1:A:520:PHE:CD2 | 1:A:520:PHE:C | 2.60 | 0.71 |
| 1:C:230:LEU:O | 1:C:230:LEU:HG | 1.89 | 0.71 |
| 1:A:423:GLU:C | 1:A:502:LYS:HG3 | 2.11 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1016:VAL:HG23 | 1:A:1017:LEU:HD12 | 1.71 | 0.71 |
| 1:B:182:TYR:CD1 | 1:B:270:LEU:HD13 | 2.26 | 0.71 |
| 1:B:229:GLN:CD | 1:B:229:GLN:N | 2.32 | 0.71 |
| 1:B:605:ASN:HD21 | 1:B:642:ASN:HB3 | 1.54 | 0.71 |
| 1:C:405:LEU:HD12 | 1:C:405:LEU:O | 1.91 | 0.71 |
| 1:A:489:THR:CB | 1:A:490:PRO:CD | 2.69 | 0.71 |
| 1:A:527:TYR:CD1 | 1:A:972:LEU:HD23 | 2.25 | 0.71 |
| 1:B:702:LEU:HB2 | 1:B:851:LEU:HD21 | 1.73 | 0.71 |
| 1:A:6:ILE:HD13 | 1:A:431:THR:HG21 | 1.72 | 0.71 |
| 1:B:150:THR:OG1 | 1:B:152:GLU:HB2 | 1.91 | 0.71 |
| 1:C:739:LEU:HD22 | 1:C:739:LEU:H | 1.55 | 0.71 |
| 1:A:829:GLY:C | 1:A:830:GLN:OE1 | 2.29 | 0.71 |
| 1:A:73:ASP:C | 1:A:74:ASN:OD1 | 2.30 | 0.70 |
| 1:A:234:ILE:CA | 1:A:235:ILE:HD13 | 2.18 | 0.70 |
| 1:A:504:ASP:C | 1:A:504:ASP:OD1 | 2.30 | 0.70 |
| 1:A:901:VAL:O | 1:A:901:VAL:CG1 | 2.39 | 0.70 |
| 1:B:513:PHE:C | 1:B:515:TRP:H | 1.94 | 0.70 |
| 1:C:937:LEU:O | 1:C:940:LYS:CG | 2.39 | 0.70 |
| 1:B:512:PHE:O | 1:B:513:PHE:CB | 2.36 | 0.70 |
| 1:C:673:GLU:CD | 1:C:673:GLU:N | 2.38 | 0.70 |
| 1:C:795:ASP:C | 1:C:795:ASP:OD1 | 2.30 | 0.70 |
| 1:A:527:TYR:CD1 | 1:A:972:LEU:CD2 | 2.75 | 0.70 |
| 1:B:229:GLN:OE1 | 1:B:229:GLN:C | 2.30 | 0.70 |
| 1:C:429:GLU:C | 1:C:429:GLU:OE1 | 2.29 | 0.70 |
| 1:C:1032:ARG:O | 1:C:1033:PHE:CB | 2.37 | 0.70 |
| 1:A:317:PHE:HB3 | 1:A:321:LEU:HB3 | 1.71 | 0.70 |
| 1:A:489:THR:HB | 1:A:490:PRO:CD | 2.22 | 0.70 |
| 1:C:910:ILE:HG23 | 1:C:1013:THR:HG21 | 1.74 | 0.70 |
| 2:D:129:VAL:O | 2:D:133:LEU:CD1 | 2.30 | 0.70 |
| 1:A:504:ASP:CG | 1:A:504:ASP:O | 2.30 | 0.70 |
| 2:D:61:GLU:O | 2:D:65:VAL:CG2 | 2.34 | 0.70 |
| 1:A:182:TYR:CD2 | 1:A:270:LEU:CD2 | 2.74 | 0.70 |
| 1:C:435:MET:CE | 1:C:435:MET:CA | 2.55 | 0.70 |
| 1:C:724:THR:HB | 1:C:725:PRO:HD2 | 1.73 | 0.70 |
| 1:A:58:GLN:NE2 | 1:A:818:ARG:HH11 | 1.88 | 0.70 |
| 1:B:213:GLN:C | 1:B:213:GLN:OE1 | 2.30 | 0.70 |
| 1:B:534:ILE:HA | 1:B:541:TYR:OH | 1.90 | 0.70 |
| 1:B:818:ARG:NH1 | 1:B:821:GLY:O | 2.25 | 0.70 |
| 1:B:905:VAL:HB | 1:B:906:PRO:HD3 | 1.74 | 0.70 |
| 1:C:325:TYR:HD1 | 1:C:325:TYR:H | 1.39 | 0.70 |
| 1:C:993:THR:O | 1:C:993:THR:CG2 | 2.35 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:73:VAL:HG13 | 2:D:74:ASN:OD1 | 1.92 | 0.70 |
| 1:A:989:LEU:HD22 | 1:A:1000:GLN:HB3 | 1.72 | 0.70 |
| 1:B:672:VAL:O | 1:B:672:VAL:CG2 | 2.30 | 0.70 |
| 1:C:891:LEU:CD1 | 1:C:892:TYR:CE1 | 2.74 | 0.70 |
| 1:B:62:THR:OG1 | 1:B:88:VAL:HG21 | 1.92 | 0.70 |
| 2:D:152:ILE:O | 2:D:156:ASN:HB2 | 1.91 | 0.70 |
| 1:C:531:VAL:HA | 1:C:534:ILE:HG22 | 1.74 | 0.70 |
| 1:B:758:TYR:HB2 | 1:B:772:TYR:CD1 | 2.26 | 0.69 |
| 1:B:901:VAL:O | 1:B:904:VAL:HG22 | 1.92 | 0.69 |
| 1:C:82:SER:O | 1:C:815:ARG:HA | 1.90 | 0.69 |
| 1:C:504:ASP:OD1 | 1:C:507:GLU:HA | 1.92 | 0.69 |
| 1:B:459:PHE:O | 1:B:464:GLY:HA3 | 1.92 | 0.69 |
| 1:C:1:FME:N | 1:C:2:PRO:HD2 | 2.06 | 0.69 |
| 1:B:1:FME:HE1 | 1:B:487:ILE:CD1 | 2.22 | 0.69 |
| 1:B:712:MET:HE1 | 1:B:839:GLU:OE2 | 1.92 | 0.69 |
| 1:B:713:LEU:HD22 | 1:B:843:LEU:HD23 | 1.73 | 0.69 |
| 1:B:780:ARG:HD2 | 1:B:780:ARG:O | 1.92 | 0.69 |
| 1:C:672:VAL:HG23 | 1:C:673:GLU:OE1 | 1.90 | 0.69 |
| 2:D:13:ASP:C | 2:D:13:ASP:OD1 | 2.30 | 0.69 |
| 2:D:56:TYR:CD1 | 2:D:90:ARG:CG | 2.75 | 0.69 |
| 2:E:145:PHE:O | 2:E:145:PHE:HD1 | 1.74 | 0.69 |
| 1:B:765:ARG:HB3 | 1:B:765:ARG:NH1 | 2.07 | 0.69 |
| 1:C:327:TYR:CD1 | 1:C:628:PHE:HD1 | 2.11 | 0.69 |
| 1:B:5:PHE:CE1 | 1:B:487:ILE:HG12 | 2.27 | 0.69 |
| 1:B:182:TYR:CD1 | 1:B:270:LEU:HD11 | 2.27 | 0.69 |
| 1:B:450:SER:O | 1:B:454:VAL:HG12 | 1.92 | 0.69 |
| 1:C:65:ILE:O | 1:C:69:MET:HG2 | 1.92 | 0.69 |
| 1:C:816:LEU:HD12 | 1:C:816:LEU:N | 2.07 | 0.69 |
| 1:B:183:ALA:HB3 | 1:B:271:GLY:O | 1.92 | 0.69 |
| 1:B:274:ASN:OD1 | 1:B:276:ASP:N | 2.22 | 0.69 |
| 1:C:190:PRO:HG3 | 1:C:789:TRP:CH2 | 2.27 | 0.69 |
| 1:A:360:GLN:CG | 1:A:513:PHE:CZ | 2.69 | 0.69 |
| 1:A:537:SER:OG | 1:A:540:ARG:CB | 2.41 | 0.69 |
| 1:A:580:ALA:HA | 1:A:623:ASN:HD22 | 1.56 | 0.69 |
| 1:A:781:MET:SD | 1:C:220:GLY:HA2 | 2.33 | 0.69 |
| 1:B:184:MET:HB3 | 1:B:771:VAL:HG22 | 1.73 | 0.69 |
| 1:C:412:VAL:O | 1:C:416:VAL:HG23 | 1.92 | 0.69 |
| 1:C:429:GLU:HA | 1:C:432:ARG:HG3 | 1.75 | 0.69 |
| 1:C:732:ASP:C | 1:C:732:ASP:OD1 | 2.30 | 0.69 |
| 1:B:99:ASP:C | 1:B:99:ASP:OD1 | 2.30 | 0.69 |
| 1:A:414:GLU:CD | 1:A:974:PRO:HG3 | 2.14 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:463:THR:CG2 | 1:A:467:TYR:CE2 | 2.76 | 0.69 |
| 1:B:143:ILE:HG22 | 1:B:286:ALA:HB2 | 1.74 | 0.69 |
| 1:C:4:PHE:HD2 | 1:C:4:PHE:C | 1.95 | 0.69 |
| 1:C:940:LYS:HG3 | 1:C:941:ASN:N | 2.08 | 0.69 |
| 1:A:780:ARG:O | 1:A:780:ARG:CG | 2.41 | 0.68 |
| 1:B:671:ILE:C | 1:B:672:VAL:HG12 | 2.13 | 0.68 |
| 1:C:924:ASP:O | 1:C:927:PHE:HB3 | 1.92 | 0.68 |
| 2:D:77:ASP:C | 2:D:77:ASP:OD1 | 2.30 | 0.68 |
| 1:A:483:LEU:O | 1:A:486:LEU:HD23 | 1.93 | 0.68 |
| 1:A:966:ASP:HA | 1:A:969:ARG:HD3 | 1.74 | 0.68 |
| 1:B:274:ASN:OD1 | 1:B:274:ASN:C | 2.30 | 0.68 |
| 1:C:94:PHE:O | 1:C:95:GLU:C | 2.30 | 0.68 |
| 1:C:211:ASN:HD22 | 1:C:760:ASN:HD21 | 1.41 | 0.68 |
| 1:B:764:ASP:OD1 | 1:B:765:ARG:CG | 2.40 | 0.68 |
| 1:A:423:GLU:C | 1:A:502:LYS:HE3 | 2.12 | 0.68 |
| 1:A:544:LEU:O | 1:A:548:ILE:HG13 | 1.93 | 0.68 |
| 1:A:860:THR:O | 1:A:861:GLY:C | 2.29 | 0.68 |
| 1:C:237:GLN:O | 1:C:238:THR:CG2 | 2.41 | 0.68 |
| 1:A:423:GLU:O | 1:A:502:LYS:CE | 2.42 | 0.68 |
| 1:A:491:ALA:O | 1:A:495:THR:CG2 | 2.41 | 0.68 |
| 1:C:689:GLY:O | 1:C:690:LEU:CD2 | 2.37 | 0.68 |
| 1:A:194:ASN:ND2 | 1:A:798:MET:HG3 | 2.08 | 0.68 |
| 1:B:795:ASP:OD2 | 1:B:797:GLN:HB2 | 1.94 | 0.68 |
| 1:B:222:THR:CG2 | 1:C:275:TYR:HB3 | 2.24 | 0.68 |
| 1:B:231:ASN:HD22 | 1:B:232:ALA:N | 1.92 | 0.68 |
| 1:B:670:ALA:O | 1:B:671:ILE:CG2 | 2.42 | 0.68 |
| 2:D:14:LEU:HD12 | 2:D:14:LEU:N | 2.08 | 0.68 |
| 1:B:166:ILE:O | 1:B:172:VAL:HG21 | 1.93 | 0.68 |
| 1:B:169:THR:CG2 | 1:B:172:VAL:CG1 | 2.72 | 0.68 |
| 1:B:871:ASN:CB | 1:B:872:GLN:HG2 | 2.19 | 0.68 |
| 1:C:707:ALA:O | 1:C:710:PRO:HD3 | 1.94 | 0.68 |
| 2:D:76:ASP:O | 2:D:77:ASP:HB3 | 1.94 | 0.68 |
| 1:B:403:GLY:HA3 | 1:B:982:PHE:CE1 | 2.28 | 0.68 |
| 1:C:980:LEU:HD22 | 1:C:980:LEU:H | 1.56 | 0.68 |
| 2:D:92:HIS:O | 2:D:96:VAL:HG23 | 1.93 | 0.68 |
| 1:A:218:GLN:HA | 1:A:234:ILE:HG13 | 1.76 | 0.67 |
| 1:B:140:VAL:O | 1:B:288:GLY:HA2 | 1.94 | 0.67 |
| 1:B:815:ARG:HG2 | 1:B:815:ARG:NH1 | 2.09 | 0.67 |
| 1:B:13:TRP:O | 1:B:17:ILE:HG13 | 1.95 | 0.67 |
| 1:B:764:ASP:OD1 | 1:B:765:ARG:HG3 | 1.93 | 0.67 |
| 1:C:336:SER:O | 1:C:340:VAL:HG23 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:77:ASP:OD1 | 2:D:79:LEU:N | 2.26 | 0.67 |
| 1:A:586:ARG:O | 1:A:590:VAL:HG23 | 1.95 | 0.67 |
| 1:B:670:ALA:O | 1:B:671:ILE:HB | 1.94 | 0.67 |
| 1:B:732:ASP:C | 1:B:732:ASP:OD1 | 2.30 | 0.67 |
| 1:B:800:PRO:HD2 | 1:B:800:PRO:O | 1.94 | 0.67 |
| 1:C:733:GLN:CD | 1:C:743:ILE:HD13 | 2.15 | 0.67 |
| 1:C:760:ASN:O | 1:C:771:VAL:HB | 1.95 | 0.67 |
| 1:C:879:ILE:O | 1:C:879:ILE:CD1 | 2.30 | 0.67 |
| 1:A:945:ILE:HG22 | 1:A:946:VAL:N | 2.10 | 0.67 |
| 1:C:629:VAL:CG2 | 1:C:629:VAL:O | 2.43 | 0.67 |
| 1:C:742:SER:O | 1:C:746:ILE:HD13 | 1.93 | 0.67 |
| 1:A:298:ASN:HD22 | 1:A:301:ASP:CB | 2.07 | 0.67 |
| 1:B:939:ALA:O | 1:B:943:ILE:HG13 | 1.95 | 0.67 |
| 1:C:53:ASP:C | 1:C:53:ASP:OD1 | 2.30 | 0.67 |
| 1:A:39:ALA:HB1 | 1:A:40:PRO:HD2 | 1.76 | 0.67 |
| 1:C:200:PRO:CG | 1:C:749:THR:HG23 | 2.23 | 0.67 |
| 1:C:876:LEU:C | 1:C:876:LEU:HD22 | 2.13 | 0.67 |
| 1:A:137:LEU:HD13 | 1:A:293:LEU:HD12 | 1.77 | 0.67 |
| 1:B:10:ILE:CB | 1:C:893:GLU:OE2 | 2.43 | 0.67 |
| 1:B:281:PHE:HD1 | 1:B:610:PHE:CD1 | 2.11 | 0.67 |
| 1:A:358:PHE:CD1 | 1:A:977:MET:HE3 | 2.29 | 0.67 |
| 1:A:721:LEU:HD13 | 1:A:814:PRO:HG3 | 1.71 | 0.67 |
| 2:E:152:ILE:CD1 | 2:E:153:SER:N | 2.58 | 0.67 |
| 1:A:488:LEU:C | 1:A:488:LEU:CD1 | 2.62 | 0.67 |
| 1:B:61:VAL:O | 1:B:65:ILE:CG1 | 2.42 | 0.67 |
| 1:B:1022:VAL:HA | 1:B:1025:PHE:HD1 | 1.60 | 0.67 |
| 1:A:423:GLU:O | 1:A:502:LYS:CD | 2.43 | 0.66 |
| 1:B:512:PHE:O | 1:B:513:PHE:HB2 | 1.94 | 0.66 |
| 1:B:874:PRO:HB3 | 1:B:877:TYR:CD2 | 2.28 | 0.66 |
| 1:C:896:SER:HG | 1:C:897:ILE:HD13 | 1.60 | 0.66 |
| 2:D:79:LEU:HD22 | 2:D:111:HIS:CE1 | 2.29 | 0.66 |
| 1:B:512:PHE:O | 1:B:513:PHE:C | 2.32 | 0.66 |
| 1:A:445:ILE:HD11 | 1:A:943:ILE:HG21 | 1.77 | 0.66 |
| 1:A:534:ILE:HG13 | 1:A:535:LEU:N | 2.10 | 0.66 |
| 1:C:563:PHE:CE2 | 1:C:564:LEU:HD12 | 2.30 | 0.66 |
| 1:C:689:GLY:N | 1:C:690:LEU:HD23 | 2.09 | 0.66 |
| 1:C:757:SER:O | 1:C:772:TYR:CD1 | 2.47 | 0.66 |
| 1:A:74:ASN:OD1 | 1:A:74:ASN:N | 2.28 | 0.66 |
| 1:A:652:THR:HA | 1:A:655:PHE:HD2 | 1.59 | 0.66 |
| 1:B:10:ILE:HG12 | 1:C:893:GLU:OE2 | 1.94 | 0.66 |
| 1:B:561:SER:HA | 1:B:923:ASN:HB3 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:853:THR:O | 1:B:853:THR:HG22 | 1.95 | 0.66 |
| 1:C:463:THR:HG22 | 1:C:467:TYR:CE1 | 2.30 | 0.66 |
| 1:C:972:LEU:HD13 | 1:C:976:LEU:HD23 | 1.78 | 0.66 |
| 1:A:373:PRO:O | 1:A:377:LEU:HG | 1.95 | 0.66 |
| 1:B:38:ILE:HD11 | 1:B:671:ILE:HD11 | 1.78 | 0.66 |
| 1:C:575:MET:O | 1:C:575:MET:CG | 2.30 | 0.66 |
| 1:A:520:PHE:C | 1:A:520:PHE:HD2 | 1.99 | 0.66 |
| 1:B:361:ASN:N | 1:B:361:ASN:ND2 | 2.32 | 0.66 |
| 1:B:583:THR:O | 1:B:587:THR:HG22 | 1.96 | 0.66 |
| 1:B:762:PHE:CD2 | 1:B:771:VAL:HG23 | 2.31 | 0.66 |
| 1:A:360:GLN:CG | 1:A:513:PHE:HZ | 2.00 | 0.66 |
| 1:B:69:MET:HE1 | 1:B:72:ILE:HD11 | 1.78 | 0.66 |
| 1:B:563:PHE:CB | 1:B:564:LEU:CD1 | 2.73 | 0.66 |
| 2:D:57:PHE:H | 2:D:58:GLY:HA2 | 1.60 | 0.66 |
| 1:B:727:PHE:CE1 | 1:B:783:PRO:HB3 | 2.30 | 0.66 |
| 1:C:559:LEU:HD12 | 1:C:560:PRO:HD2 | 1.77 | 0.66 |
| 1:C:671:ILE:CG1 | 1:C:674:LEU:CD2 | 2.62 | 0.66 |
| 2:D:46:VAL:O | 2:D:46:VAL:HG23 | 1.94 | 0.66 |
| 1:B:1:FME:CE | 1:B:487:ILE:CD1 | 2.73 | 0.66 |
| 1:B:63:GLN:O | 1:B:67:GLN:HG3 | 1.96 | 0.66 |
| 1:B:116:PRO:C | 1:B:117:LEU:CD1 | 2.64 | 0.66 |
| 1:C:345:VAL:O | 1:C:349:ILE:HG13 | 1.95 | 0.66 |
| 1:C:497:LEU:HD22 | 1:C:498:LYS:N | 2.09 | 0.66 |
| 1:A:242:SER:OG | 1:A:245:GLU:HG3 | 1.94 | 0.66 |
| 1:B:196:PHE:CA | 1:B:197:GLN:NE2 | 2.59 | 0.66 |
| 1:C:187:TRP:NE1 | 1:C:269:GLU:OE2 | 2.28 | 0.66 |
| 1:C:429:GLU:OE1 | 1:C:430:ALA:N | 2.29 | 0.66 |
| 1:C:573:MET:HE3 | 1:C:626:ILE:HD11 | 1.77 | 0.66 |
| 1:A:463:THR:HG22 | 1:A:467:TYR:CD2 | 2.30 | 0.65 |
| 1:A:568:ASP:OD2 | 1:A:643:LYS:HG3 | 1.96 | 0.65 |
| 1:B:541:TYR:O | 1:B:544:LEU:HB2 | 1.96 | 0.65 |
| 1:C:919:ARG:NH1 | 1:C:990:VAL:HG12 | 2.03 | 0.65 |
| 1:A:463:THR:HG22 | 1:A:467:TYR:CE2 | 2.31 | 0.65 |
| 1:A:483:LEU:O | 1:A:486:LEU:HD22 | 1.96 | 0.65 |
| 1:A:483:LEU:C | 1:A:486:LEU:CD2 | 2.64 | 0.65 |
| 1:C:546:LEU:O | 1:C:550:VAL:HG23 | 1.95 | 0.65 |
| 1:C:937:LEU:O | 1:C:940:LYS:HG3 | 1.96 | 0.65 |
| 1:A:754:TRP:CD1 | 1:A:754:TRP:N | 2.62 | 0.65 |
| 1:B:254:ASN:O | 1:B:257:GLY:N | 2.30 | 0.65 |
| 1:C:563:PHE:HE2 | 1:C:862:MET:HE1 | 1.61 | 0.65 |
| 1:B:229:GLN:OE1 | 1:B:229:GLN:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:365:THR:O | 1:B:368:PRO:HD2 | 1.96 | 0.65 |
| 1:B:848:ALA:CA | 1:B:851:LEU:HD13 | 2.26 | 0.65 |
| 1:C:332:PHE:CE2 | 1:C:569:GLN:NE2 | 2.64 | 0.65 |
| 1:C:640:GLU:OE1 | 1:C:640:GLU:N | 2.29 | 0.65 |
| 1:B:274:ASN:OD1 | 1:B:275:TYR:N | 2.30 | 0.65 |
| 1:C:1:FME:N | 1:C:2:PRO:HD3 | 2.09 | 0.65 |
| 1:C:361:ASN:OD1 | 1:C:362:PHE:N | 2.30 | 0.65 |
| 1:C:982:PHE:CD2 | 1:C:1011:MET:HG3 | 2.30 | 0.65 |
| 2:E:143:ASP:N | 2:E:146:GLY:O | 2.30 | 0.65 |
| 1:A:726:GLN:CG | 1:A:812:GLY:HA3 | 2.26 | 0.65 |
| 1:B:527:TYR:CE2 | 1:B:968:VAL:HG13 | 2.31 | 0.65 |
| 1:C:145:THR:OG1 | 1:C:146:ASP:N | 2.29 | 0.65 |
| 1:C:724:THR:CB | 1:C:725:PRO:HD2 | 2.26 | 0.65 |
| 1:A:489:THR:CB | 1:A:490:PRO:HD3 | 2.27 | 0.65 |
| 1:B:213:GLN:OE1 | 1:B:214:VAL:N | 2.30 | 0.65 |
| 1:C:616:GLY:O | 1:C:619:GLY:N | 2.30 | 0.65 |
| 1:B:1018:ALA:O | 1:B:1022:VAL:HG22 | 1.96 | 0.65 |
| 1:C:55:LYS:O | 1:C:56:THR:C | 2.32 | 0.65 |
| 1:B:407:ASP:OD2 | 1:B:978:THR:HB | 1.97 | 0.65 |
| 1:B:712:MET:HB3 | 1:B:713:LEU:HD13 | 1.79 | 0.65 |
| 1:C:225:VAL:HG12 | 1:C:226:LYS:O | 1.97 | 0.65 |
| 1:A:55:LYS:NZ | 1:A:59:ASP:OD1 | 2.30 | 0.65 |
| 1:A:489:THR:HB | 1:A:490:PRO:HD3 | 1.78 | 0.65 |
| 1:B:628:PHE:N | 1:B:628:PHE:CD2 | 2.64 | 0.65 |
| 1:C:83:ASP:O | 1:C:84:SER:HB3 | 1.95 | 0.65 |
| 1:C:671:ILE:O | 1:C:674:LEU:HD23 | 1.96 | 0.65 |
| 1:B:99:ASP:OD1 | 1:B:101:ASP:N | 2.29 | 0.64 |
| 1:B:633:ASP:OD1 | 1:B:634:TRP:N | 2.29 | 0.64 |
| 1:C:161:ASN:OD1 | 1:C:161:ASN:N | 2.29 | 0.64 |
| 2:E:95:VAL:O | 2:E:99:LEU:HG | 1.98 | 0.64 |
| 1:A:956:GLU:OE2 | 1:A:956:GLU:N | 2.29 | 0.64 |
| 1:B:174:ASP:OD2 | 1:B:175:VAL:N | 2.30 | 0.64 |
| 1:C:743:ILE:O | 1:C:747:ASN:ND2 | 2.30 | 0.64 |
| 1:A:445:ILE:HD11 | 1:A:943:ILE:CG2 | 2.27 | 0.64 |
| 1:B:715:SER:O | 1:B:717:ARG:NH1 | 2.30 | 0.64 |
| 1:C:893:GLU:O | 1:C:894:SER:HB2 | 1.96 | 0.64 |
| 2:E:156:ASN:HD22 | 2:E:156:ASN:C | 2.01 | 0.64 |
| 1:A:463:THR:CG2 | 1:A:467:TYR:HE2 | 2.10 | 0.64 |
| 1:C:761:ASP:HB3 | 1:C:768:VAL:CG1 | 2.28 | 0.64 |
| 1:A:240:LEU:CD1 | 1:A:240:LEU:H | 2.10 | 0.64 |
| 1:A:370:ILE:O | 1:A:374:VAL:HG23 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:210:GLN:OE1 | 1:B:249:ILE:HG23 | 1.97 | 0.64 |
| 1:B:456:MET:HG2 | 1:B:467:TYR:HB3 | 1.80 | 0.64 |
| 1:B:705:GLU:CG | 1:B:847:LEU:HD21 | 2.18 | 0.64 |
| 1:C:230:LEU:HD23 | 1:C:230:LEU:H | 1.62 | 0.64 |
| 2:D:126:LEU:C | 2:D:129:VAL:HG23 | 2.17 | 0.64 |
| 1:B:234:ILE:C | 1:B:235:ILE:CD1 | 2.62 | 0.64 |
| 1:C:736:ALA:HB1 | 1:C:741:VAL:HG11 | 1.80 | 0.64 |
| 1:A:894:SER:HB2 | 1:A:897:ILE:HD12 | 1.79 | 0.64 |
| 1:B:188:MET:HE1 | 1:B:773:VAL:HG21 | 1.79 | 0.64 |
| 1:B:197:GLN:N | 1:B:197:GLN:OE1 | 2.30 | 0.64 |
| 1:B:435:MET:O | 1:B:437:GLN:N | 2.31 | 0.64 |
| 1:B:988:PRO:O | 1:B:991:ILE:HG23 | 1.98 | 0.64 |
| 2:D:77:ASP:OD1 | 2:D:78:SER:N | 2.30 | 0.64 |
| 1:A:236:ALA:HB2 | 1:B:729:ILE:CG2 | 2.28 | 0.64 |
| 1:A:298:ASN:HD22 | 1:A:301:ASP:H | 1.44 | 0.64 |
| 1:A:379:THR:HG22 | 1:A:383:LEU:HD21 | 1.80 | 0.64 |
| 1:A:488:LEU:HD11 | 1:A:492:LEU:CD1 | 2.28 | 0.64 |
| 1:A:696:THR:O | 1:A:700:ASN:ND2 | 2.31 | 0.64 |
| 1:A:754:TRP:HZ3 | 1:C:219:LEU:CD2 | 2.09 | 0.64 |
| 1:B:717:ARG:CG | 1:B:717:ARG:NH1 | 2.43 | 0.64 |
| 1:B:746:ILE:HD13 | 1:B:804:PHE:CE2 | 2.32 | 0.64 |
| 2:E:61:GLU:O | 2:E:65:VAL:HG23 | 1.98 | 0.64 |
| 1:A:527:TYR:O | 1:A:531:VAL:CG2 | 2.43 | 0.64 |
| 1:B:254:ASN:O | 1:B:257:GLY:HA2 | 1.98 | 0.64 |
| 1:A:463:THR:HG23 | 1:A:467:TYR:HE2 | 1.61 | 0.64 |
| 1:B:54:ALA:HB1 | 1:B:82:SER:O | 1.98 | 0.64 |
| 1:B:144:ASN:OD1 | 1:B:149:MET:HG2 | 1.98 | 0.64 |
| 1:B:225:VAL:O | 1:B:225:VAL:CG2 | 2.46 | 0.64 |
| 1:B:225:VAL:O | 1:B:225:VAL:HG23 | 1.96 | 0.64 |
| 1:B:355:MET:HG2 | 1:B:365:THR:HA | 1.80 | 0.64 |
| 1:B:459:PHE:HB2 | 1:B:464:GLY:CA | 2.26 | 0.64 |
| 1:B:800:PRO:CD | 1:B:800:PRO:O | 2.44 | 0.64 |
| 1:B:848:ALA:O | 1:B:851:LEU:HD13 | 1.97 | 0.64 |
| 1:B:871:ASN:HB3 | 1:B:872:GLN:CG | 2.22 | 0.64 |
| 1:C:583:THR:O | 1:C:587:THR:HG22 | 1.98 | 0.64 |
| 2:E:112:ASN:HA | 2:E:144:LYS:CE | 2.22 | 0.64 |
| 1:A:109:ASN:O | 1:A:112:GLN:HG3 | 1.99 | 0.63 |
| 1:A:181:GLN:HE21 | 1:A:769:LYS:CE | 2.10 | 0.63 |
| 1:A:190:PRO:HG3 | 1:A:789:TRP:CZ2 | 2.33 | 0.63 |
| 1:C:163:LYS:HD2 | 1:C:177:LEU:HB2 | 1.79 | 0.63 |
| 1:C:733:GLN:OE1 | 1:C:743:ILE:CD1 | 2.46 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:93:LEU:HD23 | 2:D:128:ILE:HG12 | 1.80 | 0.63 |
| 1:A:218:GLN:HB2 | 1:A:232:ALA:O | 1.98 | 0.63 |
| 1:B:60:THR:OG1 | 1:B:61:VAL:N | 2.29 | 0.63 |
| 1:B:153:ASP:OD2 | 1:B:153:ASP:N | 2.30 | 0.63 |
| 1:C:568:ASP:OD2 | 1:C:644:VAL:CG2 | 2.46 | 0.63 |
| 1:C:98:THR:CG2 | 1:C:99:ASP:N | 2.61 | 0.63 |
| 1:C:989:LEU:HD22 | 1:C:1000:GLN:CB | 2.23 | 0.63 |
| 1:B:150:THR:OG1 | 1:B:152:GLU:N | 2.30 | 0.63 |
| 1:B:501:ALA:HB3 | 1:B:504:ASP:OD2 | 1.98 | 0.63 |
| 1:B:669:PRO:O | 1:B:669:PRO:HG2 | 1.97 | 0.63 |
| 1:B:919:ARG:NH1 | 1:B:919:ARG:CB | 2.30 | 0.63 |
| 1:C:88:VAL:HG23 | 1:C:89:GLN:H | 1.63 | 0.63 |
| 1:B:871:ASN:OD1 | 1:B:871:ASN:N | 2.30 | 0.63 |
| 1:C:435:MET:O | 1:C:439:GLN:HB2 | 1.98 | 0.63 |
| 1:A:531:VAL:O | 1:A:534:ILE:HG12 | 1.99 | 0.63 |
| 1:B:669:PRO:O | 1:B:669:PRO:CG | 2.45 | 0.63 |
| 1:A:897:ILE:O | 1:A:897:ILE:HG22 | 1.97 | 0.63 |
| 1:C:531:VAL:HA | 1:C:534:ILE:CG2 | 2.29 | 0.63 |
| 1:C:681:ASP:HB3 | 1:C:860:THR:HG23 | 1.81 | 0.63 |
| 1:C:730:ASP:N | 1:C:730:ASP:OD1 | 2.30 | 0.63 |
| 1:C:919:ARG:HH12 | 1:C:990:VAL:CG1 | 2.04 | 0.63 |
| 1:A:527:TYR:CE1 | 1:A:972:LEU:HD21 | 2.31 | 0.63 |
| 1:A:899:PHE:O | 1:A:900:SER:C | 2.36 | 0.63 |
| 1:B:150:THR:CG2 | 1:B:153:ASP:OD2 | 2.46 | 0.63 |
| 1:B:278:ILE:O | 1:B:278:ILE:CG1 | 2.47 | 0.63 |
| 1:B:501:ALA:HB3 | 1:B:504:ASP:HB2 | 1.80 | 0.63 |
| 1:C:629:VAL:O | 1:C:629:VAL:HG23 | 1.96 | 0.63 |
| 1:A:498:LYS:NZ | 1:A:500:ILE:HD11 | 2.14 | 0.63 |
| 1:B:561:SER:CA | 1:B:923:ASN:HB3 | 2.29 | 0.63 |
| 1:C:739:LEU:HB2 | 1:C:741:VAL:HG23 | 1.81 | 0.63 |
| 2:D:76:ASP:O | 2:D:77:ASP:CB | 2.44 | 0.63 |
| 1:A:379:THR:HG22 | 1:A:383:LEU:CD2 | 2.29 | 0.62 |
| 1:A:489:THR:CG2 | 1:A:490:PRO:HD3 | 2.29 | 0.62 |
| 1:A:758:TYR:HE1 | 1:A:760:ASN:O | 1.82 | 0.62 |
| 1:B:851:LEU:HB3 | 1:B:852:PRO:HD2 | 1.79 | 0.62 |
| 1:C:143:ILE:HG22 | 1:C:286:ALA:HB2 | 1.80 | 0.62 |
| 1:C:259:ARG:NH1 | 2:E:155:ASP:OD2 | 2.32 | 0.62 |
| 1:C:721:LEU:N | 1:C:721:LEU:CD2 | 2.52 | 0.62 |
| 1:C:884:VAL:O | 1:C:888:LEU:HG | 1.98 | 0.62 |
| 1:A:163:LYS:HG3 | 1:A:164:ASP:N | 2.14 | 0.62 |
| 1:A:971:ARG:O | 1:A:974:PRO:CD | 2.37 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:83:ASP:HA | 1:B:815:ARG:H | 1.64 | 0.62 |
| 1:C:1030:ARG:O | 1:C:1034:SER:HB2 | 1.99 | 0.62 |
| 1:B:765:ARG:HH11 | 1:B:765:ARG:CB | 2.09 | 0.62 |
| 1:C:36:PRO:HG3 | 1:C:391:ASN:HD21 | 1.64 | 0.62 |
| 1:C:237:GLN:C | 1:C:238:THR:HG23 | 2.19 | 0.62 |
| 1:C:926:TYR:CD2 | 1:C:1003:VAL:HG22 | 2.33 | 0.62 |
| 1:A:455:PRO:HG2 | 1:A:880:SER:OG | 2.00 | 0.62 |
| 1:B:270:LEU:HD23 | 1:B:271:GLY:CA | 2.27 | 0.62 |
| 1:B:678:THR:O | 1:B:678:THR:CG2 | 2.39 | 0.62 |
| 1:C:724:THR:CG2 | 1:C:814:PRO:HG3 | 2.29 | 0.62 |
| 1:C:937:LEU:HD13 | 1:C:1011:MET:HG2 | 1.81 | 0.62 |
| 2:D:14:LEU:H | 2:D:14:LEU:CD1 | 2.09 | 0.62 |
| 1:B:1:FME:H | 1:B:2:PRO:HD3 | 1.64 | 0.62 |
| 1:B:412:VAL:HG13 | 1:B:435:MET:SD | 2.40 | 0.62 |
| 1:B:668:LEU:HB2 | 1:B:669:PRO:HD2 | 1.81 | 0.62 |
| 1:C:925:VAL:O | 1:C:926:TYR:C | 2.35 | 0.62 |
| 1:C:53:ASP:CG | 1:C:56:THR:OG1 | 2.38 | 0.62 |
| 1:C:382:VAL:HG11 | 1:C:476:SER:OG | 2.00 | 0.62 |
| 1:C:638:PRO:O | 1:C:642:ASN:ND2 | 2.30 | 0.62 |
| 1:A:392:THR:O | 1:A:396:PHE:HD1 | 1.82 | 0.62 |
| 1:A:782:LEU:HB2 | 1:A:785:ASP:OD1 | 1.99 | 0.62 |
| 1:B:1:FME:N | 1:B:2:PRO:HD3 | 2.15 | 0.62 |
| 1:B:534:ILE:HA | 1:B:541:TYR:CE1 | 2.35 | 0.62 |
| 1:B:575:MET:HG3 | 1:B:576:VAL:H | 1.65 | 0.62 |
| 1:B:990:VAL:HG22 | 1:B:1005:THR:HG22 | 1.82 | 0.62 |
| 1:C:1008:MET:O | 1:C:1012:VAL:HG23 | 2.00 | 0.62 |
| 2:E:121:ALA:HB1 | 2:E:152:ILE:HG12 | 1.82 | 0.62 |
| 1:A:764:ASP:HB3 | 1:A:769:LYS:HD2 | 1.81 | 0.62 |
| 1:B:732:ASP:OD1 | 1:B:734:GLU:N | 2.33 | 0.62 |
| 1:C:268:ILE:N | 1:C:268:ILE:CD1 | 2.58 | 0.62 |
| 1:C:379:THR:O | 1:C:383:LEU:HB2 | 2.00 | 0.62 |
| 2:E:84:LEU:HD22 | 2:E:116:PRO:HB3 | 1.82 | 0.62 |
| 1:A:394:THR:HG23 | 1:A:473:THR:HG21 | 1.81 | 0.62 |
| 1:B:176:GLN:O | 1:B:289:LEU:HD23 | 1.99 | 0.62 |
| 1:B:903:LEU:O | 1:B:906:PRO:HD2 | 1.99 | 0.62 |
| 1:C:566:ASP:OD2 | 1:C:678:THR:CG2 | 2.48 | 0.62 |
| 1:C:815:ARG:C | 1:C:816:LEU:HD12 | 2.20 | 0.62 |
| 1:B:844:MET:HA | 1:B:844:MET:HE3 | 1.81 | 0.62 |
| 1:C:983:ILE:HG23 | 1:C:1008:MET:HG3 | 1.81 | 0.62 |
| 2:E:67:LEU:CD2 | 2:E:73:VAL:HG22 | 2.30 | 0.62 |
| 1:A:378:GLY:O | 1:A:382:VAL:HG23 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:314:GLU:C | 1:C:317:PHE:HD1 | 2.02 | 0.61 |
| 1:A:115:MET:HB2 | 1:A:116:PRO:HD3 | 1.81 | 0.61 |
| 1:A:410:ILE:HD12 | 1:A:978:THR:HG22 | 1.80 | 0.61 |
| 1:A:1024:VAL:O | 1:A:1028:VAL:HG23 | 1.99 | 0.61 |
| 1:B:61:VAL:CG2 | 1:B:122:VAL:HG21 | 2.29 | 0.61 |
| 1:B:197:GLN:C | 1:B:798:MET:HE2 | 2.16 | 0.61 |
| 1:B:324:VAL:HG22 | 1:B:325:TYR:N | 2.15 | 0.61 |
| 1:C:911:GLY:HA3 | 1:C:1013:THR:OG1 | 1.99 | 0.61 |
| 1:A:498:LYS:HD3 | 1:A:498:LYS:N | 1.98 | 0.61 |
| 1:C:324:VAL:HG22 | 1:C:325:TYR:N | 2.14 | 0.61 |
| 1:C:671:ILE:CD1 | 1:C:674:LEU:CG | 2.74 | 0.61 |
| 1:C:952:LEU:N | 1:C:952:LEU:CD1 | 2.61 | 0.61 |
| 1:A:459:PHE:HB2 | 1:A:464:GLY:HA2 | 1.83 | 0.61 |
| 1:B:333:VAL:O | 1:B:337:ILE:HG13 | 1.99 | 0.61 |
| 1:B:402:ILE:O | 1:B:406:VAL:HG23 | 2.00 | 0.61 |
| 1:B:534:ILE:CG1 | 1:B:541:TYR:CZ | 2.78 | 0.61 |
| 1:C:527:TYR:CZ | 1:C:968:VAL:HG13 | 2.35 | 0.61 |
| 1:C:910:ILE:HG23 | 1:C:911:GLY:N | 2.15 | 0.61 |
| 1:B:461:GLY:HA3 | 1:B:868:LEU:HD22 | 1.82 | 0.61 |
| 1:C:200:PRO:CG | 1:C:749:THR:HG22 | 2.24 | 0.61 |
| 1:C:318:PRO:O | 1:C:319:SER:OG | 2.16 | 0.61 |
| 1:A:187:TRP:HH2 | 1:A:275:TYR:HE1 | 1.49 | 0.61 |
| 1:B:775:SER:HG | 1:B:780:ARG:HG2 | 1.64 | 0.61 |
| 2:E:145:PHE:O | 2:E:145:PHE:CD1 | 2.53 | 0.61 |
| 1:C:44:THR:HB | 1:C:132:SER:HG | 1.60 | 0.61 |
| 1:C:225:VAL:HG12 | 1:C:225:VAL:O | 1.93 | 0.61 |
| 1:C:496:MET:O | 1:C:496:MET:HG2 | 1.99 | 0.61 |
| 1:C:876:LEU:C | 1:C:876:LEU:HD23 | 2.20 | 0.61 |
| 2:D:53:LEU:H | 2:D:53:LEU:HD22 | 1.50 | 0.61 |
| 1:A:955:LYS:C | 1:A:956:GLU:OE2 | 2.38 | 0.61 |
| 1:C:36:PRO:HG3 | 1:C:391:ASN:ND2 | 2.14 | 0.61 |
| 1:C:567:GLU:OE2 | 1:C:998:GLY:N | 2.20 | 0.61 |
| 1:C:682:PHE:HE2 | 1:C:684:LEU:HD23 | 1.65 | 0.61 |
| 1:B:988:PRO:O | 1:B:991:ILE:HG22 | 1.98 | 0.61 |
| 1:C:502:LYS:HG2 | 1:C:503:GLY:H | 1.65 | 0.61 |
| 1:A:236:ALA:CB | 1:B:729:ILE:O | 2.49 | 0.60 |
| 1:B:492:LEU:HB3 | 1:B:496:MET:CE | 2.31 | 0.60 |
| 1:B:495:THR:HG22 | 1:B:496:MET:HG3 | 1.82 | 0.60 |
| 1:B:966:ASP:O | 1:B:970:MET:CG | 2.48 | 0.60 |
| 1:C:723:ASP:OD1 | 1:C:723:ASP:N | 2.31 | 0.60 |
| 1:C:937:LEU:O | 1:C:940:LYS:HG2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:937:LEU:HA | 1:C:940:LYS:HG2 | 1.83 | 0.60 |
| 1:B:553:ALA:O | 1:B:557:VAL:HG12 | 2.02 | 0.60 |
| 1:B:730:ASP:OD2 | 1:B:730:ASP:N | 2.30 | 0.60 |
| 1:C:372:VAL:O | 1:C:376:LEU:HB2 | 2.02 | 0.60 |
| 1:C:689:GLY:N | 1:C:690:LEU:CD2 | 2.64 | 0.60 |
| 1:C:736:ALA:HB1 | 1:C:741:VAL:CG1 | 2.31 | 0.60 |
| 1:A:684:LEU:O | 1:A:824:SER:HA | 2.00 | 0.60 |
| 1:B:632:LYS:O | 1:B:637:ARG:NH2 | 2.33 | 0.60 |
| 1:C:482:VAL:O | 1:C:486:LEU:HD12 | 2.02 | 0.60 |
| 1:A:202:ASP:OD2 | 1:A:792:ARG:NH2 | 2.34 | 0.60 |
| 1:A:997:SER:O | 1:A:999:ALA:N | 2.34 | 0.60 |
| 1:B:160:ALA:C | 1:B:161:ASN:ND2 | 2.52 | 0.60 |
| 1:B:859:TRP:HA | 1:B:859:TRP:CE3 | 2.36 | 0.60 |
| 1:C:960:LEU:CD1 | 1:C:1027:VAL:HG22 | 2.26 | 0.60 |
| 2:E:151:ASP:O | 2:E:154:ILE:HG12 | 2.00 | 0.60 |
| 1:A:527:TYR:HE1 | 1:A:972:LEU:HD23 | 1.62 | 0.60 |
| 1:B:513:PHE:C | 1:B:515:TRP:N | 2.53 | 0.60 |
| 1:B:563:PHE:C | 1:B:564:LEU:CG | 2.68 | 0.60 |
| 1:C:150:THR:OG1 | 1:C:151:GLN:N | 2.30 | 0.60 |
| 1:B:348:ILE:CG2 | 1:B:369:THR:HG23 | 2.30 | 0.60 |
| 2:D:49:THR:HB | 2:D:50:PRO:CD | 2.31 | 0.60 |
| 1:A:489:THR:HG22 | 1:A:490:PRO:HD3 | 1.82 | 0.60 |
| 1:B:72:ILE:CG2 | 1:B:73:ASP:N | 2.65 | 0.60 |
| 1:C:155:SER:HB3 | 1:C:287:SER:CB | 2.32 | 0.60 |
| 1:C:596:HIS:NE2 | 1:C:600:THR:HG21 | 2.17 | 0.60 |
| 1:B:715:SER:HB2 | 1:B:830:GLN:HG2 | 1.83 | 0.60 |
| 1:C:464:GLY:HA2 | 1:C:467:TYR:HD1 | 1.66 | 0.60 |
| 2:D:49:THR:HB | 2:D:50:PRO:HD2 | 1.82 | 0.60 |
| 1:A:70:ASN:C | 1:A:70:ASN:OD1 | 2.40 | 0.60 |
| 1:A:905:VAL:HB | 1:A:906:PRO:HD3 | 1.83 | 0.60 |
| 1:B:347:ALA:O | 1:B:351:VAL:HG23 | 2.00 | 0.60 |
| 1:B:421:ALA:HA | 1:B:500:ILE:HG21 | 1.83 | 0.60 |
| 1:B:534:ILE:HG13 | 1:B:541:TYR:CD2 | 2.33 | 0.60 |
| 1:C:640:GLU:H | 1:C:640:GLU:CD | 2.04 | 0.60 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:N | 2.35 | 0.60 |
| 2:E:84:LEU:O | 2:E:84:LEU:HD23 | 2.01 | 0.60 |
| 1:A:964:THR:O | 1:A:968:VAL:HG23 | 2.02 | 0.60 |
| 1:C:71:GLY:C | 1:C:72:ILE:HG13 | 2.22 | 0.60 |
| 1:C:211:ASN:ND2 | 1:C:760:ASN:ND2 | 2.49 | 0.60 |
| 2:E:92:HIS:O | 2:E:96:VAL:CG2 | 2.41 | 0.60 |
| 1:A:457:ALA:HB2 | 1:A:471:SER:CB | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:685:ILE:HD13 | 1:A:685:ILE:N | 2.16 | 0.59 |
| 1:A:694:LYS:HA | 1:A:697:GLN:OE1 | 2.01 | 0.59 |
| 1:A:777:ALA:O | 1:A:781:MET:HG2 | 2.03 | 0.59 |
| 1:B:254:ASN:CB | 1:B:258:SER:O | 2.49 | 0.59 |
| 1:B:842:GLU:O | 1:B:846:GLN:HG3 | 2.02 | 0.59 |
| 1:C:454:VAL:HB | 1:C:455:PRO:HD3 | 1.83 | 0.59 |
| 1:C:259:ARG:NH2 | 2:E:155:ASP:OD2 | 2.35 | 0.59 |
| 1:A:69:MET:O | 1:C:168:ARG:HD3 | 2.02 | 0.59 |
| 1:B:372:VAL:HB | 1:B:373:PRO:HD3 | 1.85 | 0.59 |
| 1:B:382:VAL:O | 1:B:382:VAL:CG2 | 2.48 | 0.59 |
| 1:B:726:GLN:NE2 | 1:B:812:GLY:CA | 2.63 | 0.59 |
| 1:B:739:LEU:HD13 | 1:B:799:VAL:CG2 | 2.31 | 0.59 |
| 1:C:490:PRO:O | 1:C:493:CYS:HB2 | 2.02 | 0.59 |
| 2:E:93:LEU:HD21 | 2:E:128:ILE:HG13 | 1.83 | 0.59 |
| 2:E:145:PHE:CD1 | 2:E:145:PHE:C | 2.75 | 0.59 |
| 1:A:444:GLY:O | 1:A:448:VAL:HG12 | 2.03 | 0.59 |
| 1:A:899:PHE:C | 1:A:901:VAL:N | 2.52 | 0.59 |
| 1:C:496:MET:O | 1:C:496:MET:HG3 | 2.03 | 0.59 |
| 1:C:541:TYR:HA | 1:C:544:LEU:HD23 | 1.85 | 0.59 |
| 2:D:110:ASP:C | 2:D:112:ASN:N | 2.53 | 0.59 |
| 1:A:308:ALA:O | 1:A:312:LYS:HG3 | 2.02 | 0.59 |
| 1:A:795:ASP:OD1 | 1:A:795:ASP:N | 2.30 | 0.59 |
| 1:B:117:LEU:N | 1:B:117:LEU:HD12 | 2.16 | 0.59 |
| 1:B:685:ILE:HG23 | 1:B:686:ASP:N | 2.16 | 0.59 |
| 1:B:714:THR:CG2 | 1:B:832:ALA:HA | 2.31 | 0.59 |
| 1:B:848:ALA:C | 1:B:851:LEU:CD1 | 2.71 | 0.59 |
| 1:C:204:ILE:HG23 | 1:C:759:VAL:HG22 | 1.83 | 0.59 |
| 1:C:506:GLY:C | 1:C:507:GLU:CG | 2.65 | 0.59 |
| 2:D:133:LEU:HA | 2:D:137:ALA:HB2 | 1.84 | 0.59 |
| 1:A:78:MET:O | 1:A:78:MET:CG | 2.50 | 0.59 |
| 1:A:983:ILE:HG23 | 1:A:1008:MET:HG3 | 1.85 | 0.59 |
| 1:B:241:THR:HA | 1:B:763:ILE:O | 2.03 | 0.59 |
| 1:B:254:ASN:O | 1:B:257:GLY:CA | 2.50 | 0.59 |
| 1:C:651:ALA:O | 1:C:655:PHE:CD2 | 2.56 | 0.59 |
| 1:A:412:VAL:HG11 | 1:A:489:THR:HG21 | 1.85 | 0.59 |
| 1:A:485:ALA:O | 1:A:490:PRO:HD2 | 2.00 | 0.59 |
| 1:B:60:THR:O | 1:B:64:VAL:HG23 | 2.03 | 0.59 |
| 1:B:116:PRO:C | 1:B:117:LEU:HD12 | 2.23 | 0.59 |
| 1:B:202:ASP:OD2 | 1:B:792:ARG:NH2 | 2.35 | 0.59 |
| 1:C:225:VAL:CG1 | 1:C:226:LYS:O | 2.51 | 0.59 |
| 1:C:570:GLY:C | 1:C:571:VAL:HG13 | 2.22 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:667:ASN:OD1 | 1:C:668:LEU:N | 2.30 | 0.59 |
| 1:C:793:ALA:O | 1:C:795:ASP:N | 2.35 | 0.59 |
| 1:A:485:ALA:O | 1:A:490:PRO:CG | 2.51 | 0.59 |
| 1:B:250:LEU:HD23 | 1:B:251:LEU:H | 1.55 | 0.59 |
| 1:B:293:LEU:HD11 | 1:B:299:ALA:HB2 | 1.84 | 0.59 |
| 1:B:352:PHE:HD2 | 1:B:353:LEU:HD12 | 1.68 | 0.59 |
| 1:B:715:SER:O | 1:B:829:GLY:HA2 | 2.03 | 0.59 |
| 1:B:759:VAL:HG23 | 1:B:771:VAL:HG12 | 1.84 | 0.59 |
| 1:B:765:ARG:NH1 | 1:B:765:ARG:CB | 2.65 | 0.59 |
| 1:A:971:ARG:CG | 1:A:971:ARG:NH1 | 2.38 | 0.58 |
| 1:B:83:ASP:OD2 | 1:B:83:ASP:N | 2.34 | 0.58 |
| 1:C:927:PHE:CE2 | 1:C:931:LEU:HD12 | 2.38 | 0.58 |
| 1:B:422:GLU:O | 1:B:423:GLU:HG2 | 2.03 | 0.58 |
| 1:B:712:MET:CE | 1:B:839:GLU:OE2 | 2.51 | 0.58 |
| 1:C:1:FME:CN | 1:C:2:PRO:CD | 2.79 | 0.58 |
| 1:C:259:ARG:NH1 | 2:E:155:ASP:CG | 2.55 | 0.58 |
| 1:C:435:MET:O | 1:C:439:GLN:CB | 2.51 | 0.58 |
| 1:A:14:VAL:HG11 | 1:B:886:LEU:O | 2.03 | 0.58 |
| 1:A:894:SER:CB | 1:A:897:ILE:HD12 | 2.34 | 0.58 |
| 1:B:116:PRO:C | 1:B:117:LEU:HD13 | 2.22 | 0.58 |
| 1:B:420:MET:HE3 | 1:B:425:LEU:O | 2.03 | 0.58 |
| 1:B:435:MET:O | 1:B:438:ILE:N | 2.27 | 0.58 |
| 1:C:154:ILE:O | 1:C:154:ILE:CD1 | 2.31 | 0.58 |
| 1:C:731:ILE:CD1 | 1:C:746:ILE:HG21 | 2.33 | 0.58 |
| 1:C:773:VAL:O | 1:C:773:VAL:HG13 | 2.04 | 0.58 |
| 1:C:876:LEU:O | 1:C:876:LEU:HD22 | 2.02 | 0.58 |
| 1:A:183:ALA:O | 1:A:271:GLY:O | 2.22 | 0.58 |
| 1:A:758:TYR:CE1 | 1:A:760:ASN:O | 2.57 | 0.58 |
| 1:B:452:VAL:CG1 | 1:B:932:LEU:HD22 | 2.33 | 0.58 |
| 1:C:115:MET:N | 1:C:116:PRO:HD2 | 2.18 | 0.58 |
| 1:A:146:ASP:HB3 | 1:A:148:THR:HG23 | 1.85 | 0.58 |
| 1:A:366:LEU:O | 1:A:370:ILE:HG13 | 2.03 | 0.58 |
| 1:A:411:VAL:CG2 | 1:A:971:ARG:NH2 | 2.58 | 0.58 |
| 1:B:685:ILE:CG2 | 1:B:686:ASP:H | 2.16 | 0.58 |
| 1:B:991:ILE:HD12 | 1:B:991:ILE:C | 2.11 | 0.58 |
| 1:C:563:PHE:CE2 | 1:C:862:MET:HE1 | 2.39 | 0.58 |
| 2:D:49:THR:CB | 2:D:50:PRO:CD | 2.82 | 0.58 |
| 1:B:724:THR:HB | 1:B:725:PRO:CD | 2.33 | 0.58 |
| 1:C:1016:VAL:HG23 | 1:C:1017:LEU:HD12 | 1.86 | 0.58 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:CG | 2.56 | 0.58 |
| 2:D:63:VAL:O | 2:D:67:LEU:HG | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:972:LEU:O | 1:A:975:ILE:HG22 | 2.04 | 0.58 |
| 1:B:878:ALA:O | 1:B:882:ILE:HG13 | 2.04 | 0.58 |
| 1:A:997:SER:C | 1:A:999:ALA:N | 2.54 | 0.58 |
| 1:B:414:GLU:OE2 | 1:B:974:PRO:HG3 | 2.04 | 0.58 |
| 1:B:671:ILE:O | 1:B:672:VAL:HG13 | 2.03 | 0.58 |
| 1:C:71:GLY:C | 1:C:72:ILE:CG1 | 2.71 | 0.58 |
| 1:C:72:ILE:CG2 | 1:C:94:PHE:HE2 | 2.16 | 0.58 |
| 1:C:98:THR:HG23 | 1:C:99:ASP:N | 2.19 | 0.58 |
| 1:C:447:MET:SD | 1:C:891:LEU:HD23 | 2.44 | 0.58 |
| 1:C:688:ALA:HB2 | 1:C:854:GLY:CA | 2.33 | 0.58 |
| 1:A:359:LEU:HD11 | 1:A:413:VAL:HG11 | 1.86 | 0.58 |
| 1:B:69:MET:HE1 | 1:B:107:VAL:HG13 | 1.85 | 0.58 |
| 1:B:668:LEU:HD13 | 1:B:669:PRO:HD2 | 1.86 | 0.58 |
| 1:B:713:LEU:CD2 | 1:B:843:LEU:HD23 | 2.33 | 0.58 |
| 1:C:733:GLN:NE2 | 1:C:743:ILE:HD13 | 2.18 | 0.58 |
| 1:C:980:LEU:CD2 | 1:C:980:LEU:H | 2.16 | 0.58 |
| 1:A:704:ALA:O | 1:A:708:LYS:HG3 | 2.03 | 0.58 |
| 1:B:10:ILE:HG23 | 1:C:895:TRP:CZ2 | 2.39 | 0.58 |
| 1:C:735:LYS:O | 1:C:739:LEU:CD2 | 2.49 | 0.58 |
| 1:A:188:MET:HE1 | 1:A:203:VAL:HG11 | 1.84 | 0.57 |
| 1:A:423:GLU:O | 1:A:502:LYS:HD2 | 2.03 | 0.57 |
| 1:B:365:THR:HG23 | 1:B:366:LEU:N | 2.19 | 0.57 |
| 1:B:531:VAL:O | 1:B:534:ILE:HG22 | 2.04 | 0.57 |
| 1:B:848:ALA:C | 1:B:851:LEU:HD12 | 2.24 | 0.57 |
| 1:C:324:VAL:C | 1:C:325:TYR:CD1 | 2.76 | 0.57 |
| 1:C:453:PHE:CE1 | 1:C:474:ILE:HG21 | 2.38 | 0.57 |
| 1:C:527:TYR:CE2 | 1:C:968:VAL:HG13 | 2.38 | 0.57 |
| 1:C:531:VAL:HG21 | 1:C:968:VAL:HG11 | 1.84 | 0.57 |
| 2:D:110:ASP:C | 2:D:112:ASN:H | 2.03 | 0.57 |
| 1:A:230:LEU:HD12 | 1:A:231:ASN:H | 1.69 | 0.57 |
| 1:B:449:LEU:O | 1:B:453:PHE:CD1 | 2.53 | 0.57 |
| 1:C:30:LEU:HD13 | 1:C:390:ILE:HG13 | 1.86 | 0.57 |
| 1:C:837:THR:O | 1:C:841:MET:HG3 | 2.04 | 0.57 |
| 1:A:815:ARG:O | 1:A:815:ARG:HG3 | 2.05 | 0.57 |
| 1:B:534:ILE:HG13 | 1:B:541:TYR:CE1 | 2.36 | 0.57 |
| 1:B:578:LEU:HD12 | 1:B:579:PRO:HD3 | 1.87 | 0.57 |
| 1:B:685:ILE:HG23 | 1:B:686:ASP:H | 1.68 | 0.57 |
| 1:C:879:ILE:HG23 | 1:C:880:SER:H | 1.69 | 0.57 |
| 1:A:774:MET:HG2 | 1:A:775:SER:H | 1.69 | 0.57 |
| 1:C:58:GLN:OE1 | 1:C:818:ARG:HD2 | 2.04 | 0.57 |
| 1:A:14:VAL:O | 1:A:14:VAL:HG12 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:949:ALA:O | 1:A:953:MET:HG2 | 2.04 | 0.57 |
| 1:C:230:LEU:HD23 | 1:C:230:LEU:N | 2.19 | 0.57 |
| 1:B:853:THR:CA | 1:B:857:TYR:N | 2.67 | 0.57 |
| 1:A:223:PRO:HD2 | 1:B:780:ARG:NH2 | 2.19 | 0.57 |
| 1:A:315:PRO:HB2 | 1:A:316:PHE:CE1 | 2.39 | 0.57 |
| 1:A:534:ILE:HG22 | 1:A:541:TYR:CE1 | 2.40 | 0.57 |
| 1:A:728:LYS:NZ | 1:C:236:ALA:O | 2.21 | 0.57 |
| 1:C:841:MET:HE3 | 1:C:859:TRP:CE2 | 2.40 | 0.57 |
| 2:D:46:VAL:O | 2:D:46:VAL:HG22 | 2.03 | 0.57 |
| 1:A:36:PRO:HD3 | 1:A:391:ASN:ND2 | 2.19 | 0.57 |
| 1:A:423:GLU:CA | 1:A:502:LYS:HG3 | 2.35 | 0.57 |
| 1:A:449:LEU:O | 1:A:452:VAL:HG22 | 2.05 | 0.57 |
| 1:A:591:LEU:HD12 | 1:A:613:ASN:ND2 | 2.20 | 0.57 |
| 1:A:878:ALA:O | 1:A:882:ILE:HG12 | 2.04 | 0.57 |
| 1:B:47:ALA:HB2 | 1:B:127:VAL:HG13 | 1.85 | 0.57 |
| 1:B:452:VAL:HG12 | 1:B:932:LEU:HD22 | 1.87 | 0.57 |
| 1:B:501:ALA:CB | 1:B:504:ASP:HB2 | 2.33 | 0.57 |
| 1:C:572:PHE:CZ | 1:C:629:VAL:HG21 | 2.39 | 0.57 |
| 1:C:714:THR:HG22 | 1:C:715:SER:N | 2.19 | 0.57 |
| 1:C:927:PHE:CZ | 1:C:931:LEU:HD11 | 2.40 | 0.57 |
| 1:A:558:ARG:HD2 | 1:A:558:ARG:C | 2.23 | 0.57 |
| 1:B:403:GLY:HA3 | 1:B:982:PHE:HE1 | 1.69 | 0.57 |
| 1:B:420:MET:HE1 | 1:B:499:PRO:HA | 1.87 | 0.57 |
| 1:B:493:CYS:O | 1:B:497:LEU:HB2 | 2.04 | 0.57 |
| 1:B:1022:VAL:HA | 1:B:1025:PHE:CD1 | 2.39 | 0.57 |
| 1:C:332:PHE:CD2 | 1:C:569:GLN:NE2 | 2.73 | 0.57 |
| 1:A:243:THR:OG1 | 1:A:244:GLU:N | 2.38 | 0.57 |
| 1:B:11:PHE:HE1 | 1:B:15:ILE:HD11 | 1.70 | 0.57 |
| 1:B:726:GLN:HE22 | 1:B:812:GLY:CA | 2.11 | 0.57 |
| 1:C:156:ASP:OD1 | 1:C:182:TYR:CB | 2.52 | 0.57 |
| 1:C:190:PRO:HG3 | 1:C:789:TRP:CZ3 | 2.39 | 0.57 |
| 1:C:746:ILE:HG22 | 1:C:747:ASN:N | 2.20 | 0.57 |
| 1:B:686:ASP:HB2 | 1:B:695:LEU:HD12 | 1.87 | 0.56 |
| 1:B:775:SER:OG | 1:B:780:ARG:CG | 2.50 | 0.56 |
| 1:C:153:ASP:OD1 | 1:C:182:TYR:OH | 2.23 | 0.56 |
| 1:C:448:VAL:HG11 | 1:C:939:ALA:HB3 | 1.85 | 0.56 |
| 1:A:194:ASN:HD22 | 1:A:798:MET:HG3 | 1.68 | 0.56 |
| 1:A:621:GLY:HA3 | 1:A:624:THR:CG2 | 2.34 | 0.56 |
| 1:A:668:LEU:HD23 | 1:A:668:LEU:N | 2.18 | 0.56 |
| 1:A:892:TYR:OH | 1:A:946:VAL:HG13 | 2.04 | 0.56 |
| 1:B:56:THR:O | 1:B:60:THR:HG23 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:34:GLN:HG2 | 1:C:35:TYR:CD1 | 2.40 | 0.56 |
| 1:C:482:VAL:HG12 | 1:C:486:LEU:CD1 | 2.35 | 0.56 |
| 2:D:87:ALA:O | 2:D:91:GLY:N | 2.37 | 0.56 |
| 2:E:156:ASN:C | 2:E:156:ASN:ND2 | 2.59 | 0.56 |
| 1:A:686:ASP:HB3 | 1:A:823:PRO:HB2 | 1.87 | 0.56 |
| 1:A:742:SER:OG | 1:A:744:ASN:HB2 | 2.05 | 0.56 |
| 1:A:892:TYR:HE2 | 1:A:947:GLU:HA | 1.70 | 0.56 |
| 1:A:943:ILE:O | 1:A:946:VAL:HG13 | 2.06 | 0.56 |
| 1:B:62:THR:O | 1:B:62:THR:HG22 | 2.05 | 0.56 |
| 1:B:596:HIS:CD2 | 1:B:600:THR:OG1 | 2.57 | 0.56 |
| 1:B:958:LYS:NZ | 1:B:966:ASP:OD2 | 2.38 | 0.56 |
| 1:C:247:GLY:O | 1:C:263:ARG:HG2 | 2.04 | 0.56 |
| 1:C:448:VAL:HG21 | 1:C:943:ILE:HD11 | 1.86 | 0.56 |
| 1:C:671:ILE:HD11 | 1:C:674:LEU:HG | 1.84 | 0.56 |
| 1:C:978:THR:OG1 | 1:C:979:SER:N | 2.39 | 0.56 |
| 2:D:34:MET:HA | 2:D:34:MET:CE | 2.35 | 0.56 |
| 1:B:189:ASN:OD1 | 1:B:189:ASN:N | 2.38 | 0.56 |
| 1:C:164:ASP:OD2 | 1:C:767:ARG:NH2 | 2.31 | 0.56 |
| 2:D:27:ASP:OD2 | 2:D:27:ASP:N | 2.39 | 0.56 |
| 2:E:105:ASP:OD1 | 2:E:106:VAL:N | 2.38 | 0.56 |
| 1:A:236:ALA:HB2 | 1:B:729:ILE:HG23 | 1.87 | 0.56 |
| 1:A:488:LEU:HD11 | 1:A:492:LEU:HD13 | 1.88 | 0.56 |
| 1:B:987:MET:HG2 | 1:B:988:PRO:CD | 2.35 | 0.56 |
| 1:C:240:LEU:HD22 | 1:C:245:GLU:HB3 | 1.87 | 0.56 |
| 1:C:879:ILE:HG23 | 1:C:880:SER:N | 2.20 | 0.56 |
| 1:A:469:GLN:OE1 | 1:A:469:GLN:HA | 2.05 | 0.56 |
| 1:A:897:ILE:N | 1:A:898:PRO:HD2 | 2.21 | 0.56 |
| 1:B:712:MET:CB | 1:B:713:LEU:HD13 | 2.36 | 0.56 |
| 1:B:893:GLU:HG3 | 1:B:893:GLU:O | 2.05 | 0.56 |
| 1:B:987:MET:HG2 | 1:B:988:PRO:N | 2.21 | 0.56 |
| 1:C:672:VAL:HG22 | 1:C:673:GLU:OE1 | 2.04 | 0.56 |
| 1:B:10:ILE:CG1 | 1:C:893:GLU:OE2 | 2.54 | 0.56 |
| 1:B:540:ARG:O | 1:B:544:LEU:HD13 | 2.05 | 0.56 |
| 1:C:567:GLU:CD | 1:C:998:GLY:HA3 | 2.26 | 0.56 |
| 1:A:248:LYS:O | 1:A:261:LEU:CD2 | 2.49 | 0.56 |
| 1:B:987:MET:HG2 | 1:B:988:PRO:HD3 | 1.88 | 0.56 |
| 1:C:34:GLN:NE2 | 1:C:333:VAL:HG22 | 2.20 | 0.56 |
| 1:C:903:LEU:O | 1:C:906:PRO:HD2 | 2.06 | 0.56 |
| 2:E:56:TYR:O | 2:E:56:TYR:CG | 2.58 | 0.56 |
| 1:A:205:THR:HG22 | 1:A:206:ALA:N | 2.19 | 0.56 |
| 1:A:694:LYS:C | 1:A:697:GLN:OE1 | 2.44 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:979:SER:O | 1:B:983:ILE:HG13 | 2.07 | 0.56 |
| 1:C:146:ASP:CB | 1:C:148:THR:HG21 | 2.35 | 0.56 |
| 1:C:324:VAL:CG2 | 1:C:325:TYR:N | 2.69 | 0.56 |
| 1:C:902:MET:HE2 | 1:C:902:MET:HA | 1.88 | 0.56 |
| 1:A:277:ILE:C | 1:A:278:ILE:HG12 | 2.27 | 0.55 |
| 1:B:988:PRO:C | 1:B:991:ILE:HG22 | 2.27 | 0.55 |
| 1:C:572:PHE:CE2 | 1:C:629:VAL:HG21 | 2.40 | 0.55 |
| 2:D:44:ASP:OD1 | 2:D:45:HIS:CD2 | 2.60 | 0.55 |
| 2:D:73:VAL:HG12 | 2:D:74:ASN:H | 1.68 | 0.55 |
| 2:E:100:LEU:O | 2:E:103:GLY:HA2 | 2.06 | 0.55 |
| 1:A:23:GLY:O | 1:A:26:ALA:HB3 | 2.05 | 0.55 |
| 1:A:456:MET:HG3 | 1:A:467:TYR:HB3 | 1.88 | 0.55 |
| 1:B:764:ASP:OD1 | 1:B:765:ARG:HG2 | 2.05 | 0.55 |
| 2:E:57:PHE:H | 2:E:58:GLY:HA2 | 1.70 | 0.55 |
| 1:B:1:FME:HE1 | 1:B:487:ILE:CG1 | 2.36 | 0.55 |
| 1:C:810:GLU:O | 1:C:811:TYR:CD2 | 2.59 | 0.55 |
| 1:A:583:THR:H | 1:A:586:ARG:HG3 | 1.72 | 0.55 |
| 1:A:655:PHE:O | 1:A:658:ILE:HG13 | 2.07 | 0.55 |
| 1:A:949:ALA:O | 1:A:953:MET:CG | 2.54 | 0.55 |
| 1:B:328:ASP:OD1 | 1:B:329:THR:N | 2.40 | 0.55 |
| 1:C:637:ARG:N | 1:C:638:PRO:HD3 | 2.21 | 0.55 |
| 1:A:542:LEU:O | 1:A:545:TYR:CB | 2.55 | 0.55 |
| 1:B:72:ILE:HG22 | 1:B:73:ASP:H | 1.70 | 0.55 |
| 1:B:169:THR:CG2 | 1:B:172:VAL:HG11 | 2.36 | 0.55 |
| 1:C:816:LEU:N | 1:C:816:LEU:CD1 | 2.70 | 0.55 |
| 1:C:933:THR:O | 1:C:937:LEU:HG | 2.07 | 0.55 |
| 1:A:391:ASN:O | 1:A:395:MET:HG2 | 2.07 | 0.55 |
| 1:A:555:LEU:CD1 | 1:A:914:LEU:HD23 | 2.37 | 0.55 |
| 1:A:1026:PHE:CD2 | 1:A:1026:PHE:O | 2.59 | 0.55 |
| 1:B:162:MET:O | 1:B:166:ILE:HG12 | 2.07 | 0.55 |
| 1:B:197:GLN:HA | 1:B:798:MET:HE2 | 1.61 | 0.55 |
| 1:B:336:SER:OG | 1:B:395:MET:CE | 2.55 | 0.55 |
| 1:C:327:TYR:CD1 | 1:C:628:PHE:CD1 | 2.94 | 0.55 |
| 1:C:482:VAL:HG12 | 1:C:486:LEU:HD11 | 1.88 | 0.55 |
| 1:C:894:SER:O | 1:C:898:PRO:CD | 2.54 | 0.55 |
| 1:A:139:VAL:O | 1:A:326:PRO:HD2 | 2.07 | 0.55 |
| 1:A:184:MET:HG2 | 1:A:246:PHE:CE1 | 2.42 | 0.55 |
| 1:C:327:TYR:CD2 | 1:C:327:TYR:C | 2.80 | 0.55 |
| 1:C:367:ILE:HB | 1:C:368:PRO:HD3 | 1.87 | 0.55 |
| 1:C:674:LEU:CD2 | 1:C:674:LEU:N | 2.30 | 0.55 |
| 2:D:132:LEU:O | 2:D:136:GLY:O | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:77:ASP:HB3 | 2:E:81:VAL:H | 1.71 | 0.55 |
| 1:A:16:ALA:HB2 | 1:A:488:LEU:HD23 | 1.89 | 0.55 |
| 1:A:749:THR:HG21 | 1:A:791:VAL:CG1 | 2.33 | 0.55 |
| 1:A:792:ARG:HG3 | 1:A:793:ALA:N | 2.21 | 0.55 |
| 1:B:108:GLN:HG3 | 1:C:112:GLN:HG3 | 1.87 | 0.55 |
| 1:B:184:MET:CE | 1:B:268:ILE:CG2 | 2.85 | 0.55 |
| 1:B:952:LEU:O | 1:B:956:GLU:HB2 | 2.07 | 0.55 |
| 2:D:100:LEU:HD21 | 2:D:106:VAL:HG13 | 1.88 | 0.55 |
| 1:A:471:SER:O | 1:A:475:VAL:HG23 | 2.06 | 0.55 |
| 1:B:668:LEU:HB2 | 1:B:669:PRO:CD | 2.36 | 0.55 |
| 1:C:688:ALA:HB2 | 1:C:854:GLY:HA3 | 1.87 | 0.55 |
| 1:C:876:LEU:O | 1:C:880:SER:HB2 | 2.06 | 0.55 |
| 1:C:940:LYS:HG3 | 1:C:941:ASN:H | 1.72 | 0.55 |
| 2:E:46:VAL:HG22 | 2:E:78:SER:HB3 | 1.89 | 0.55 |
| 1:B:671:ILE:C | 1:B:672:VAL:CG1 | 2.74 | 0.55 |
| 1:B:673:GLU:C | 1:B:675:GLY:N | 2.59 | 0.55 |
| 1:C:184:MET:HB3 | 1:C:771:VAL:HG22 | 1.89 | 0.55 |
| 1:C:948:PHE:HD1 | 1:C:967:ALA:HA | 1.71 | 0.55 |
| 2:E:154:ILE:CG1 | 2:E:155:ASP:N | 2.70 | 0.55 |
| 1:A:219:LEU:CD1 | 1:B:783:PRO:HG3 | 2.37 | 0.54 |
| 1:A:528:THR:OG1 | 1:A:529:ASP:N | 2.39 | 0.54 |
| 1:A:572:PHE:CZ | 1:A:629:VAL:HG11 | 2.43 | 0.54 |
| 1:B:634:TRP:O | 1:B:637:ARG:O | 2.25 | 0.54 |
| 1:B:705:GLU:HB3 | 1:B:847:LEU:CD2 | 2.37 | 0.54 |
| 1:B:987:MET:O | 1:B:991:ILE:HG22 | 2.08 | 0.54 |
| 1:C:480:LEU:O | 1:C:484:VAL:HG23 | 2.06 | 0.54 |
| 2:E:49:THR:O | 2:E:52:HIS:HB2 | 2.08 | 0.54 |
| 1:A:380:PHE:CD1 | 1:A:380:PHE:N | 2.75 | 0.54 |
| 1:A:899:PHE:O | 1:A:902:MET:N | 2.30 | 0.54 |
| 1:B:194:ASN:ND2 | 1:B:790:TYR:CB | 2.70 | 0.54 |
| 1:A:598:TYR:HA | 1:A:602:GLU:CB | 2.37 | 0.54 |
| 1:A:898:PRO:O | 1:A:901:VAL:HB | 2.08 | 0.54 |
| 1:C:158:VAL:HA | 1:C:162:MET:CE | 2.33 | 0.54 |
| 1:C:343:THR:HG21 | 1:C:989:LEU:HD23 | 1.90 | 0.54 |
| 1:C:626:ILE:O | 1:C:626:ILE:CG2 | 2.50 | 0.54 |
| 1:C:789:TRP:O | 1:C:801:PHE:HB2 | 2.06 | 0.54 |
| 2:E:66:LEU:O | 2:E:71:ALA:HB2 | 2.07 | 0.54 |
| 1:A:685:ILE:HG12 | 1:A:687:GLN:HE22 | 1.73 | 0.54 |
| 1:B:435:MET:C | 1:B:437:GLN:N | 2.58 | 0.54 |
| 1:B:557:VAL:O | 1:B:557:VAL:HG23 | 2.06 | 0.54 |
| 1:C:811:TYR:CD2 | 1:C:811:TYR:N | 2.76 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:330:THR:N | 1:B:331:PRO:CD | 2.71 | 0.54 |
| 1:B:352:PHE:CD2 | 1:B:353:LEU:HD12 | 2.43 | 0.54 |
| 1:B:776:GLU:O | 1:B:777:ALA:C | 2.45 | 0.54 |
| 1:B:859:TRP:HA | 1:B:859:TRP:HE3 | 1.69 | 0.54 |
| 1:C:169:THR:HG22 | 1:C:170:SER:N | 2.21 | 0.54 |
| 1:C:429:GLU:OE1 | 1:C:429:GLU:CA | 2.55 | 0.54 |
| 1:A:236:ALA:HB1 | 1:B:729:ILE:O | 2.07 | 0.54 |
| 1:C:72:ILE:HG22 | 1:C:94:PHE:HE2 | 1.73 | 0.54 |
| 1:C:327:TYR:HB2 | 1:C:628:PHE:HB3 | 1.89 | 0.54 |
| 1:C:607:GLU:HG3 | 1:C:607:GLU:O | 2.08 | 0.54 |
| 1:C:793:ALA:N | 1:C:797:GLN:O | 2.41 | 0.54 |
| 2:E:115:THR:OG1 | 2:E:118:HIS:CD2 | 2.60 | 0.54 |
| 1:A:423:GLU:C | 1:A:502:LYS:CG | 2.75 | 0.54 |
| 1:A:489:THR:O | 1:A:493:CYS:N | 2.37 | 0.54 |
| 1:A:527:TYR:CD1 | 1:A:972:LEU:HD21 | 2.42 | 0.54 |
| 1:A:598:TYR:HA | 1:A:602:GLU:HB3 | 1.89 | 0.54 |
| 1:B:367:ILE:N | 1:B:368:PRO:CD | 2.71 | 0.54 |
| 1:C:894:SER:O | 1:C:898:PRO:HG2 | 2.08 | 0.54 |
| 2:D:50:PRO:HA | 2:D:53:LEU:CD2 | 2.37 | 0.54 |
| 2:E:152:ILE:HD12 | 2:E:153:SER:N | 2.17 | 0.54 |
| 1:A:527:TYR:HE1 | 1:A:968:VAL:HG12 | 1.72 | 0.54 |
| 1:B:143:ILE:HG22 | 1:B:286:ALA:CB | 2.37 | 0.54 |
| 1:C:361:ASN:OD1 | 1:C:361:ASN:C | 2.46 | 0.54 |
| 1:C:687:GLN:HA | 1:C:822:LEU:HD23 | 1.89 | 0.54 |
| 1:C:36:PRO:HD2 | 1:C:393:LEU:HD12 | 1.90 | 0.54 |
| 1:C:754:TRP:CZ2 | 1:C:786:ILE:CG1 | 2.91 | 0.54 |
| 1:C:910:ILE:CG2 | 1:C:911:GLY:N | 2.70 | 0.54 |
| 2:D:49:THR:C | 2:D:53:LEU:HD21 | 2.28 | 0.54 |
| 1:A:594:VAL:HG22 | 1:A:655:PHE:CE1 | 2.43 | 0.54 |
| 1:B:668:LEU:CD1 | 1:B:669:PRO:HD2 | 2.38 | 0.54 |
| 1:A:6:ILE:HG23 | 1:A:494:ALA:CB | 2.38 | 0.53 |
| 1:A:24:GLY:O | 1:A:28:LEU:HG | 2.08 | 0.53 |
| 1:B:242:SER:HB3 | 1:B:245:GLU:HG3 | 1.89 | 0.53 |
| 1:B:853:THR:HA | 1:B:857:TYR:N | 2.23 | 0.53 |
| 1:C:261:LEU:HD12 | 1:C:263:ARG:HD2 | 1.89 | 0.53 |
| 1:C:681:ASP:HB3 | 1:C:860:THR:CG2 | 2.38 | 0.53 |
| 1:C:815:ARG:O | 1:C:815:ARG:HG2 | 2.09 | 0.53 |
| 2:D:110:ASP:HB3 | 2:D:112:ASN:H | 1.73 | 0.53 |
| 1:A:1:FME:CN | 1:A:2:PRO:HD2 | 2.38 | 0.53 |
| 1:A:466:ILE:HD13 | 1:A:466:ILE:N | 2.22 | 0.53 |
| 1:B:250:LEU:C | 1:B:250:LEU:HD22 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:302:THR:O | 1:C:306:ILE:HG13 | 2.08 | 0.53 |
| 1:C:375:VAL:HB | 1:C:405:LEU:HD13 | 1.88 | 0.53 |
| 1:C:753:ALA:O | 1:C:775:SER:HB3 | 2.08 | 0.53 |
| 1:C:926:TYR:HD2 | 1:C:1003:VAL:CG2 | 2.20 | 0.53 |
| 1:B:419:VAL:O | 1:B:423:GLU:HG3 | 2.08 | 0.53 |
| 1:B:557:VAL:O | 1:B:557:VAL:HG22 | 2.08 | 0.53 |
| 1:C:71:GLY:O | 1:C:72:ILE:HG13 | 2.07 | 0.53 |
| 1:C:754:TRP:HZ2 | 1:C:786:ILE:HG12 | 1.73 | 0.53 |
| 2:D:13:ASP:OD1 | 2:D:14:LEU:N | 2.42 | 0.53 |
| 2:D:13:ASP:O | 2:D:14:LEU:C | 2.44 | 0.53 |
| 2:D:57:PHE:N | 2:D:58:GLY:HA2 | 2.20 | 0.53 |
| 1:A:445:ILE:CG2 | 1:A:940:LYS:HE2 | 2.35 | 0.53 |
| 1:B:988:PRO:HA | 1:B:991:ILE:CG2 | 2.38 | 0.53 |
| 1:C:1:FME:HB2 | 1:C:2:PRO:HD3 | 1.90 | 0.53 |
| 1:C:712:MET:SD | 1:C:835:LYS:HG3 | 2.49 | 0.53 |
| 1:C:720:GLY:C | 1:C:721:LEU:HD23 | 2.27 | 0.53 |
| 1:A:694:LYS:CA | 1:A:697:GLN:OE1 | 2.56 | 0.53 |
| 1:A:815:ARG:O | 1:A:815:ARG:CG | 2.56 | 0.53 |
| 1:B:69:MET:HE3 | 1:B:72:ILE:CD1 | 2.33 | 0.53 |
| 1:B:781:MET:HA | 1:B:781:MET:HE2 | 1.89 | 0.53 |
| 1:C:361:ASN:O | 1:C:365:THR:HG22 | 2.08 | 0.53 |
| 1:C:750:LEU:O | 1:C:750:LEU:CD2 | 2.30 | 0.53 |
| 1:A:539:GLY:O | 1:A:543:VAL:CG2 | 2.57 | 0.53 |
| 1:B:196:PHE:CA | 1:B:197:GLN:HE22 | 2.13 | 0.53 |
| 1:B:777:ALA:HA | 1:B:780:ARG:NH2 | 2.23 | 0.53 |
| 1:C:741:VAL:CG1 | 1:C:746:ILE:HD13 | 2.36 | 0.53 |
| 1:C:923:ASN:OD1 | 1:C:927:PHE:HD2 | 1.90 | 0.53 |
| 1:A:298:ASN:ND2 | 1:A:301:ASP:N | 2.50 | 0.53 |
| 1:A:314:GLU:N | 1:A:315:PRO:CD | 2.72 | 0.53 |
| 1:A:424:GLY:CA | 1:A:502:LYS:HB2 | 2.39 | 0.53 |
| 1:C:880:SER:O | 1:C:884:VAL:HG23 | 2.07 | 0.53 |
| 1:C:926:TYR:CD2 | 1:C:1003:VAL:CG2 | 2.92 | 0.53 |
| 2:E:133:LEU:HA | 2:E:136:GLY:O | 2.09 | 0.53 |
| 1:C:101:ASP:O | 1:C:105:VAL:HG23 | 2.08 | 0.53 |
| 1:C:204:ILE:HG23 | 1:C:759:VAL:HG21 | 1.88 | 0.53 |
| 1:C:323:ILE:HG22 | 1:C:324:VAL:N | 2.24 | 0.53 |
| 1:C:673:GLU:N | 1:C:673:GLU:OE2 | 2.30 | 0.53 |
| 1:C:901:VAL:HG12 | 1:C:946:VAL:HG21 | 1.91 | 0.53 |
| 1:B:1:FME:CE | 1:B:487:ILE:CG1 | 2.87 | 0.53 |
| 1:B:596:HIS:CD2 | 1:B:600:THR:HG1 | 2.27 | 0.53 |
| 1:C:623:ASN:ND2 | 1:C:623:ASN:O | 2.29 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:687:GLN:HA | 1:C:822:LEU:CD2 | 2.39 | 0.53 |
| 1:C:811:TYR:HD2 | 1:C:811:TYR:N | 2.07 | 0.53 |
| 2:D:126:LEU:CA | 2:D:129:VAL:CG2 | 2.86 | 0.53 |
| 1:A:743:ILE:HD12 | 1:A:743:ILE:N | 2.23 | 0.53 |
| 1:B:217:GLY:O | 1:B:234:ILE:HG13 | 2.09 | 0.53 |
| 1:B:714:THR:HG21 | 1:B:832:ALA:HA | 1.90 | 0.53 |
| 1:B:764:ASP:CG | 1:B:765:ARG:HG3 | 2.30 | 0.53 |
| 1:C:207:ILE:HG22 | 1:C:760:ASN:HD21 | 1.72 | 0.53 |
| 2:D:100:LEU:HD21 | 2:D:106:VAL:CG1 | 2.39 | 0.53 |
| 1:B:207:ILE:CG2 | 1:B:207:ILE:O | 2.50 | 0.52 |
| 1:B:443:VAL:O | 1:B:446:ALA:HB3 | 2.09 | 0.52 |
| 1:B:879:ILE:O | 1:B:883:VAL:HG23 | 2.07 | 0.52 |
| 1:C:74:ASN:OD1 | 1:C:74:ASN:N | 2.41 | 0.52 |
| 1:C:695:LEU:O | 1:C:695:LEU:HD23 | 2.09 | 0.52 |
| 1:C:724:THR:HG21 | 1:C:814:PRO:HG3 | 1.91 | 0.52 |
| 2:E:93:LEU:CD2 | 2:E:128:ILE:CG1 | 2.70 | 0.52 |
| 1:A:189:ASN:HD22 | 1:A:192:GLU:CD | 2.12 | 0.52 |
| 1:B:62:THR:O | 1:B:66:GLU:HG3 | 2.09 | 0.52 |
| 1:B:501:ALA:O | 1:B:504:ASP:CB | 2.56 | 0.52 |
| 1:C:157:TYR:CD2 | 1:C:157:TYR:O | 2.62 | 0.52 |
| 1:C:506:GLY:O | 1:C:507:GLU:CG | 2.58 | 0.52 |
| 1:C:567:GLU:CD | 1:C:998:GLY:H | 2.10 | 0.52 |
| 1:A:1:FME:N | 1:A:2:PRO:HD3 | 2.21 | 0.52 |
| 1:A:207:ILE:HG22 | 1:A:760:ASN:HD22 | 1.75 | 0.52 |
| 1:B:1:FME:HE3 | 1:B:487:ILE:HD11 | 1.88 | 0.52 |
| 1:B:173:GLY:CA | 1:B:294:ALA:HB2 | 2.40 | 0.52 |
| 1:C:724:THR:HB | 1:C:725:PRO:HD3 | 1.91 | 0.52 |
| 1:C:793:ALA:C | 1:C:795:ASP:N | 2.59 | 0.52 |
| 2:D:51:LEU:HD22 | 2:D:83:PRO:CG | 2.39 | 0.52 |
| 2:D:63:VAL:HG12 | 2:D:64:GLU:N | 2.23 | 0.52 |
| 1:A:445:ILE:O | 1:A:449:LEU:HB2 | 2.09 | 0.52 |
| 1:B:166:ILE:O | 1:B:169:THR:HB | 2.09 | 0.52 |
| 1:C:924:ASP:OD2 | 1:C:924:ASP:N | 2.35 | 0.52 |
| 1:A:558:ARG:O | 1:A:558:ARG:HD3 | 2.08 | 0.52 |
| 1:A:935:ILE:O | 1:A:935:ILE:CG1 | 2.56 | 0.52 |
| 1:B:926:TYR:HB3 | 1:B:1003:VAL:HG13 | 1.90 | 0.52 |
| 1:C:347:ALA:O | 1:C:351:VAL:HG23 | 2.09 | 0.52 |
| 1:C:667:ASN:CG | 1:C:668:LEU:H | 2.11 | 0.52 |
| 1:C:736:ALA:O | 1:C:741:VAL:CB | 2.49 | 0.52 |
| 1:B:687:GLN:NE2 | 1:B:859:TRP:HB2 | 2.24 | 0.52 |
| 1:C:512:PHE:O | 1:C:512:PHE:HD1 | 1.88 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:681:ASP:O | 1:C:859:TRP:HE3 | 1.93 | 0.52 |
| 2:E:100:LEU:O | 2:E:103:GLY:N | 2.42 | 0.52 |
| 1:A:481:SER:OG | 1:A:482:VAL:N | 2.39 | 0.52 |
| 1:B:61:VAL:HG13 | 1:B:65:ILE:HD11 | 1.91 | 0.52 |
| 1:B:898:PRO:O | 1:B:902:MET:HE2 | 2.09 | 0.52 |
| 1:C:378:GLY:O | 1:C:382:VAL:HG23 | 2.10 | 0.52 |
| 1:A:531:VAL:HA | 1:A:534:ILE:HG12 | 1.92 | 0.52 |
| 1:B:659:LYS:O | 1:B:660:ASP:HB2 | 2.09 | 0.52 |
| 1:C:631:LEU:HD11 | 1:C:644:VAL:HG12 | 1.91 | 0.52 |
| 1:C:952:LEU:O | 1:C:956:GLU:HB3 | 2.09 | 0.52 |
| 2:D:73:VAL:HG13 | 2:D:74:ASN:N | 2.16 | 0.52 |
| 2:E:117:LEU:HD12 | 2:E:132:LEU:HD12 | 1.92 | 0.52 |
| 1:A:236:ALA:HB2 | 1:B:729:ILE:HG22 | 1.92 | 0.52 |
| 1:A:269:GLU:O | 1:A:270:LEU:C | 2.41 | 0.52 |
| 1:A:519:MET:HG3 | 1:A:520:PHE:N | 2.25 | 0.52 |
| 1:B:126:GLY:HA2 | 1:C:116:PRO:HB3 | 1.91 | 0.52 |
| 1:B:564:LEU:CD1 | 1:B:564:LEU:N | 2.63 | 0.52 |
| 1:B:729:ILE:HG13 | 1:B:806:SER:O | 2.10 | 0.52 |
| 1:C:44:THR:HB | 1:C:132:SER:CB | 2.39 | 0.52 |
| 1:C:278:ILE:HD13 | 1:C:278:ILE:H | 1.75 | 0.52 |
| 1:C:330:THR:N | 1:C:331:PRO:CD | 2.73 | 0.52 |
| 1:C:505:HIS:O | 1:C:505:HIS:ND1 | 2.39 | 0.52 |
| 1:C:669:PRO:O | 1:C:669:PRO:CD | 2.53 | 0.52 |
| 1:A:139:VAL:HG13 | 1:A:178:PHE:HE2 | 1.75 | 0.52 |
| 1:A:288:GLY:O | 1:A:289:LEU:HD23 | 2.10 | 0.52 |
| 1:A:1021:PHE:HB3 | 1:A:1025:PHE:CZ | 2.45 | 0.52 |
| 1:B:108:GLN:HG3 | 1:C:112:GLN:CG | 2.40 | 0.52 |
| 1:B:184:MET:CB | 1:B:771:VAL:HG22 | 2.38 | 0.52 |
| 1:C:156:ASP:OD1 | 1:C:182:TYR:CD2 | 2.62 | 0.52 |
| 1:C:169:THR:CG2 | 1:C:170:SER:N | 2.72 | 0.52 |
| 1:A:92:LEU:N | 1:A:92:LEU:HD12 | 2.25 | 0.51 |
| 1:B:489:THR:N | 1:B:490:PRO:CD | 2.74 | 0.51 |
| 1:A:488:LEU:HD11 | 1:A:492:LEU:HD11 | 1.91 | 0.51 |
| 1:B:447:MET:HA | 1:B:447:MET:CE | 2.40 | 0.51 |
| 1:B:905:VAL:O | 1:B:909:VAL:HG23 | 2.10 | 0.51 |
| 1:C:957:GLY:O | 1:C:958:LYS:HG2 | 2.11 | 0.51 |
| 2:E:57:PHE:HB2 | 2:E:58:GLY:HA2 | 1.92 | 0.51 |
| 1:A:489:THR:HG22 | 1:A:490:PRO:CD | 2.40 | 0.51 |
| 1:A:504:ASP:OD1 | 1:A:506:GLY:N | 2.44 | 0.51 |
| 1:B:846:GLN:O | 1:B:849:SER:OG | 2.23 | 0.51 |
| 1:C:74:ASN:HB3 | 1:C:95:GLU:CB | 2.34 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:785:ASP:O | 1:C:788:ASP:HB2 | 2.09 | 0.51 |
| 1:A:213:GLN:HA | 1:A:237:GLN:O | 2.10 | 0.51 |
| 1:A:609:VAL:HG22 | 1:A:629:VAL:HG22 | 1.92 | 0.51 |
| 1:B:26:ALA:O | 1:B:30:LEU:HD22 | 2.10 | 0.51 |
| 1:C:71:GLY:H | 1:C:110:LYS:NZ | 2.09 | 0.51 |
| 1:C:160:ALA:CB | 1:C:161:ASN:OD1 | 2.59 | 0.51 |
| 2:D:93:LEU:CD2 | 2:D:128:ILE:HG12 | 2.39 | 0.51 |
| 1:A:450:SER:O | 1:A:454:VAL:HG23 | 2.10 | 0.51 |
| 1:A:685:ILE:HG12 | 1:A:687:GLN:NE2 | 2.26 | 0.51 |
| 1:B:482:VAL:HG12 | 1:B:486:LEU:HD13 | 1.91 | 0.51 |
| 1:B:516:PHE:C | 1:B:516:PHE:CD1 | 2.83 | 0.51 |
| 1:B:1007:VAL:O | 1:B:1011:MET:HB2 | 2.11 | 0.51 |
| 1:C:889:ALA:O | 1:C:892:TYR:O | 2.29 | 0.51 |
| 1:B:336:SER:OG | 1:B:395:MET:HE1 | 2.10 | 0.51 |
| 1:C:974:PRO:O | 1:C:978:THR:HG23 | 2.11 | 0.51 |
| 1:A:683:GLU:OE2 | 1:A:860:THR:HG21 | 2.11 | 0.51 |
| 1:A:767:ARG:HG3 | 1:A:768:VAL:N | 2.26 | 0.51 |
| 1:B:762:PHE:CE1 | 1:B:764:ASP:HB2 | 2.32 | 0.51 |
| 1:B:776:GLU:HB3 | 1:B:779:TYR:HD1 | 1.76 | 0.51 |
| 1:C:724:THR:HG23 | 1:C:814:PRO:HG3 | 1.92 | 0.51 |
| 1:A:975:ILE:HD13 | 1:A:1019:ILE:CD1 | 2.41 | 0.51 |
| 1:B:184:MET:HB2 | 1:B:762:PHE:CE2 | 2.46 | 0.51 |
| 1:C:686:ASP:O | 1:C:686:ASP:OD1 | 2.29 | 0.51 |
| 1:C:729:ILE:C | 1:C:730:ASP:OD1 | 2.49 | 0.51 |
| 1:A:180:SER:HB3 | 1:A:274:ASN:ND2 | 2.26 | 0.51 |
| 1:A:588:GLN:O | 1:A:589:LYS:C | 2.49 | 0.51 |
| 1:B:188:MET:C | 1:B:189:ASN:OD1 | 2.49 | 0.51 |
| 1:B:310:LEU:HD13 | 1:B:323:ILE:CD1 | 2.41 | 0.51 |
| 1:B:960:LEU:HD21 | 1:B:1027:VAL:HG22 | 1.92 | 0.51 |
| 1:C:616:GLY:O | 1:C:619:GLY:O | 2.29 | 0.51 |
| 1:C:692:HIS:O | 1:C:696:THR:HG22 | 2.11 | 0.51 |
| 1:A:807:SER:O | 1:A:808:ARG:HG3 | 2.11 | 0.51 |
| 1:A:997:SER:O | 1:A:998:GLY:C | 2.48 | 0.51 |
| 1:B:790:TYR:CD1 | 1:B:800:PRO:HA | 2.46 | 0.51 |
| 1:A:183:ALA:N | 1:A:271:GLY:O | 2.39 | 0.50 |
| 1:B:146:ASP:HB2 | 1:B:320:GLY:HA3 | 1.93 | 0.50 |
| 1:C:53:ASP:OD2 | 1:C:56:THR:OG1 | 2.29 | 0.50 |
| 1:C:69:MET:HE2 | 1:C:92:LEU:HD21 | 1.93 | 0.50 |
| 1:C:94:PHE:C | 1:C:95:GLU:O | 2.44 | 0.50 |
| 1:C:196:PHE:O | 1:C:197:GLN:CG | 2.59 | 0.50 |
| 1:C:278:ILE:HD11 | 1:C:613:ASN:HB3 | 1.91 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:328:ASP:OD1 | 1:C:329:THR:N | 2.43 | 0.50 |
| 1:A:33:ALA:O | 1:A:391:ASN:HA | 2.11 | 0.50 |
| 1:A:70:ASN:OD1 | 1:A:70:ASN:O | 2.29 | 0.50 |
| 1:A:498:LYS:HZ2 | 1:A:500:ILE:HD11 | 1.76 | 0.50 |
| 1:A:830:GLN:OE1 | 1:A:830:GLN:N | 2.44 | 0.50 |
| 1:B:61:VAL:CG1 | 1:B:65:ILE:HD11 | 2.42 | 0.50 |
| 1:C:451:ALA:O | 1:C:455:PRO:HD2 | 2.10 | 0.50 |
| 1:C:504:ASP:OD1 | 1:C:504:ASP:O | 2.29 | 0.50 |
| 1:C:686:ASP:OD1 | 1:C:686:ASP:C | 2.48 | 0.50 |
| 1:C:741:VAL:HG12 | 1:C:746:ILE:CD1 | 2.38 | 0.50 |
| 1:A:84:SER:OG | 1:A:814:PRO:HA | 2.12 | 0.50 |
| 1:A:150:THR:HG23 | 1:A:153:ASP:H | 1.76 | 0.50 |
| 1:A:355:MET:CE | 1:A:368:PRO:HG2 | 2.41 | 0.50 |
| 1:A:972:LEU:C | 1:A:972:LEU:CD1 | 2.80 | 0.50 |
| 1:B:175:VAL:CG1 | 1:B:289:LEU:CD2 | 2.89 | 0.50 |
| 1:B:199:THR:HG21 | 1:B:792:ARG:H | 1.77 | 0.50 |
| 1:B:420:MET:CE | 1:B:499:PRO:HA | 2.42 | 0.50 |
| 1:B:595:THR:HG23 | 1:B:609:VAL:HB | 1.93 | 0.50 |
| 1:A:58:GLN:NE2 | 1:A:818:ARG:NH1 | 2.57 | 0.50 |
| 1:A:248:LYS:C | 1:A:261:LEU:HD23 | 2.31 | 0.50 |
| 1:A:394:THR:HG23 | 1:A:473:THR:CG2 | 2.41 | 0.50 |
| 1:A:448:VAL:HG21 | 1:A:888:LEU:HD21 | 1.94 | 0.50 |
| 1:B:158:VAL:CA | 1:B:162:MET:HG3 | 2.27 | 0.50 |
| 1:B:623:ASN:HD22 | 1:B:623:ASN:C | 2.14 | 0.50 |
| 1:B:778:LYS:HG3 | 1:B:778:LYS:O | 2.12 | 0.50 |
| 1:B:799:VAL:HG12 | 1:B:800:PRO:O | 2.11 | 0.50 |
| 1:B:982:PHE:O | 1:B:986:VAL:HG23 | 2.12 | 0.50 |
| 1:C:23:GLY:O | 1:C:27:ILE:HG13 | 2.11 | 0.50 |
| 1:A:354:VAL:O | 1:A:358:PHE:HD1 | 1.93 | 0.50 |
| 1:B:324:VAL:HG22 | 1:B:325:TYR:H | 1.75 | 0.50 |
| 1:B:414:GLU:HG3 | 1:B:977:MET:HE2 | 1.94 | 0.50 |
| 1:B:605:ASN:ND2 | 1:B:642:ASN:HB3 | 2.23 | 0.50 |
| 1:B:682:PHE:N | 1:B:827:ILE:O | 2.38 | 0.50 |
| 1:B:774:MET:CE | 1:B:780:ARG:NH1 | 2.75 | 0.50 |
| 1:B:925:VAL:O | 1:B:929:VAL:HG23 | 2.12 | 0.50 |
| 1:B:988:PRO:HA | 1:B:991:ILE:HG21 | 1.93 | 0.50 |
| 1:C:801:PHE:O | 1:C:805:SER:OG | 2.30 | 0.50 |
| 2:E:49:THR:HG22 | 2:E:52:HIS:CE1 | 2.47 | 0.50 |
| 1:A:431:THR:HG22 | 1:A:432:ARG:N | 2.23 | 0.50 |
| 1:A:528:THR:OG1 | 1:A:529:ASP:OD2 | 2.30 | 0.50 |
| 1:B:194:ASN:O | 1:B:194:ASN:OD1 | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:592:ASN:O | 1:C:596:HIS:HB2 | 2.11 | 0.50 |
| 1:C:761:ASP:HB3 | 1:C:768:VAL:HG13 | 1.92 | 0.50 |
| 1:A:589:LYS:NZ | 1:A:593:GLU:OE2 | 2.45 | 0.50 |
| 1:A:899:PHE:C | 1:A:902:MET:H | 2.13 | 0.50 |
| 1:B:235:ILE:HD13 | 1:B:235:ILE:N | 2.26 | 0.50 |
| 1:B:397:GLY:O | 1:B:474:ILE:HG12 | 2.12 | 0.50 |
| 1:C:157:TYR:C | 1:C:157:TYR:HD2 | 2.13 | 0.50 |
| 1:C:559:LEU:HD12 | 1:C:560:PRO:CD | 2.41 | 0.50 |
| 1:C:664:PHE:HD1 | 1:C:715:SER:HG | 1.60 | 0.50 |
| 1:C:780:ARG:HH11 | 1:C:780:ARG:HG3 | 1.77 | 0.50 |
| 2:D:44:ASP:CG | 2:D:45:HIS:CA | 2.80 | 0.50 |
| 2:D:143:ASP:HB2 | 2:D:147:LYS:O | 2.10 | 0.50 |
| 1:A:1:FME:CN | 1:A:2:PRO:CD | 2.90 | 0.50 |
| 1:A:13:TRP:O | 1:A:17:ILE:HG12 | 2.12 | 0.50 |
| 1:A:36:PRO:HD3 | 1:A:391:ASN:HD22 | 1.77 | 0.50 |
| 1:A:721:LEU:HD11 | 1:A:814:PRO:CB | 2.42 | 0.50 |
| 1:A:829:GLY:O | 1:A:830:GLN:OE1 | 2.30 | 0.50 |
| 1:B:58:GLN:HA | 1:B:62:THR:HB | 1.94 | 0.50 |
| 1:B:324:VAL:O | 1:B:326:PRO:HD3 | 2.11 | 0.50 |
| 1:C:53:ASP:OD1 | 1:C:56:THR:OG1 | 2.30 | 0.50 |
| 1:C:927:PHE:O | 1:C:930:GLY:N | 2.41 | 0.50 |
| 1:B:53:ASP:OD2 | 1:B:56:THR:OG1 | 2.30 | 0.50 |
| 1:B:218:GLN:HE22 | 1:B:231:ASN:HD21 | 1.58 | 0.50 |
| 1:B:231:ASN:HD22 | 1:B:231:ASN:C | 2.14 | 0.50 |
| 1:B:291:ILE:HD12 | 1:B:306:ILE:HD12 | 1.94 | 0.50 |
| 1:C:497:LEU:O | 1:C:499:PRO:HD3 | 2.12 | 0.50 |
| 1:C:531:VAL:CA | 1:C:534:ILE:HG22 | 2.41 | 0.50 |
| 1:A:146:ASP:CB | 1:A:148:THR:HG23 | 2.41 | 0.49 |
| 1:A:488:LEU:CD1 | 1:A:492:LEU:CD1 | 2.81 | 0.49 |
| 1:A:647:ILE:HA | 1:A:650:ARG:HD2 | 1.93 | 0.49 |
| 1:B:6:ILE:HG12 | 1:B:490:PRO:O | 2.11 | 0.49 |
| 1:B:224:PRO:HA | 1:C:781:MET:HE3 | 1.94 | 0.49 |
| 1:B:414:GLU:CD | 1:B:974:PRO:HG3 | 2.32 | 0.49 |
| 1:B:705:GLU:CB | 1:B:847:LEU:CD2 | 2.78 | 0.49 |
| 1:C:186:ILE:HB | 1:C:773:VAL:HG23 | 1.94 | 0.49 |
| 1:C:719:ASN:OD1 | 1:C:719:ASN:O | 2.29 | 0.49 |
| 1:C:732:ASP:OD1 | 1:C:734:GLU:N | 2.45 | 0.49 |
| 2:D:150:PHE:O | 2:D:154:ILE:HG13 | 2.11 | 0.49 |
| 1:A:187:TRP:HD1 | 1:A:267:LYS:O | 1.94 | 0.49 |
| 1:A:412:VAL:CG1 | 1:A:489:THR:HG21 | 2.42 | 0.49 |
| 1:A:424:GLY:HA3 | 1:A:502:LYS:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:944:LEU:CD1 | 1:A:971:ARG:NH2 | 2.76 | 0.49 |
| 1:B:195:LYS:O | 1:B:197:GLN:OE1 | 2.30 | 0.49 |
| 1:B:211:ASN:OD1 | 1:B:211:ASN:O | 2.29 | 0.49 |
| 1:B:250:LEU:HD23 | 1:B:251:LEU:CA | 2.37 | 0.49 |
| 1:B:729:ILE:C | 1:B:730:ASP:OD2 | 2.50 | 0.49 |
| 1:B:897:ILE:N | 1:B:898:PRO:HD2 | 2.26 | 0.49 |
| 1:C:83:ASP:O | 1:C:84:SER:OG | 2.30 | 0.49 |
| 1:C:137:LEU:HD22 | 1:C:293:LEU:HD13 | 1.92 | 0.49 |
| 1:C:138:MET:HE2 | 1:C:140:VAL:HG23 | 1.93 | 0.49 |
| 2:D:61:GLU:HG2 | 2:D:62:ILE:N | 2.28 | 0.49 |
| 2:E:143:ASP:O | 2:E:146:GLY:O | 2.29 | 0.49 |
| 1:A:498:LYS:HE3 | 1:A:498:LYS:CA | 2.43 | 0.49 |
| 1:B:81:ASN:OD1 | 1:B:81:ASN:O | 2.30 | 0.49 |
| 1:B:606:VAL:HA | 1:B:631:LEU:HD23 | 1.93 | 0.49 |
| 1:B:973:ARG:HB3 | 1:B:974:PRO:HD3 | 1.94 | 0.49 |
| 1:C:373:PRO:O | 1:C:377:LEU:HB2 | 2.12 | 0.49 |
| 1:C:607:GLU:OE2 | 1:C:632:LYS:HE3 | 2.12 | 0.49 |
| 1:B:8:ARG:N | 1:B:9:PRO:HD3 | 2.27 | 0.49 |
| 1:B:182:TYR:HD1 | 1:B:270:LEU:CD1 | 2.24 | 0.49 |
| 1:C:312:LYS:HG2 | 1:C:313:MET:N | 2.28 | 0.49 |
| 2:D:19:LEU:CD2 | 2:D:50:PRO:HG3 | 2.41 | 0.49 |
| 2:D:43:SER:O | 2:D:43:SER:OG | 2.30 | 0.49 |
| 1:A:174:ASP:HB3 | 1:A:292:LYS:HB2 | 1.95 | 0.49 |
| 1:B:173:GLY:N | 1:B:294:ALA:HB2 | 2.27 | 0.49 |
| 1:B:340:VAL:HG21 | 1:B:395:MET:HB3 | 1.95 | 0.49 |
| 1:C:92:LEU:N | 1:C:92:LEU:HD12 | 2.26 | 0.49 |
| 1:C:261:LEU:CD1 | 1:C:263:ARG:HD2 | 2.42 | 0.49 |
| 1:C:780:ARG:HG3 | 1:C:780:ARG:O | 2.12 | 0.49 |
| 1:C:782:LEU:O | 1:C:785:ASP:HB2 | 2.12 | 0.49 |
| 1:A:591:LEU:HD12 | 1:A:613:ASN:HD22 | 1.77 | 0.49 |
| 1:B:53:ASP:CG | 1:B:56:THR:OG1 | 2.50 | 0.49 |
| 1:B:504:ASP:C | 1:B:505:HIS:O | 2.41 | 0.49 |
| 1:B:733:GLN:NE2 | 1:B:743:ILE:HD11 | 2.27 | 0.49 |
| 1:C:391:ASN:H | 1:C:394:THR:HG22 | 1.77 | 0.49 |
| 1:C:640:GLU:N | 1:C:640:GLU:CD | 2.66 | 0.49 |
| 1:A:423:GLU:O | 1:A:502:LYS:HE3 | 2.09 | 0.49 |
| 1:B:160:ALA:HB3 | 1:B:161:ASN:ND2 | 2.28 | 0.49 |
| 1:B:281:PHE:CD1 | 1:B:610:PHE:HD1 | 2.17 | 0.49 |
| 1:B:329:THR:O | 1:B:329:THR:OG1 | 2.30 | 0.49 |
| 1:B:808:ARG:HA | 2:D:79:LEU:HD13 | 1.95 | 0.49 |
| 1:C:561:SER:HA | 1:C:923:ASN:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:567:GLU:OE1 | 1:C:998:GLY:CA | 2.47 | 0.49 |
| 1:C:979:SER:O | 1:C:983:ILE:HG13 | 2.12 | 0.49 |
| 2:D:51:LEU:HD22 | 2:D:83:PRO:HG3 | 1.95 | 0.49 |
| 1:B:150:THR:HG1 | 1:B:152:GLU:HB2 | 1.78 | 0.49 |
| 1:B:180:SER:HB2 | 1:B:273:GLU:HG3 | 1.95 | 0.49 |
| 1:C:887:CYS:O | 1:C:891:LEU:HG | 2.13 | 0.49 |
| 1:B:302:THR:O | 1:B:306:ILE:CG2 | 2.58 | 0.49 |
| 1:B:682:PHE:HB3 | 1:B:827:ILE:HB | 1.94 | 0.49 |
| 1:C:1036:LYS:O | 1:C:1037:ASN:C | 2.48 | 0.49 |
| 2:E:146:GLY:CA | 2:E:147:LYS:CB | 2.90 | 0.49 |
| 1:A:539:GLY:HA2 | 1:A:542:LEU:H | 1.78 | 0.49 |
| 1:A:693:GLU:OE1 | 1:A:693:GLU:N | 2.30 | 0.49 |
| 1:A:743:ILE:HD12 | 1:A:743:ILE:H | 1.78 | 0.49 |
| 1:B:53:ASP:OD1 | 1:B:56:THR:OG1 | 2.29 | 0.49 |
| 1:B:382:VAL:O | 1:B:382:VAL:HG23 | 2.13 | 0.49 |
| 1:B:794:ALA:C | 1:B:796:GLY:H | 2.14 | 0.49 |
| 1:C:53:ASP:OD1 | 1:C:56:THR:N | 2.30 | 0.49 |
| 1:C:94:PHE:O | 1:C:95:GLU:O | 2.31 | 0.49 |
| 1:C:431:THR:O | 1:C:435:MET:HG2 | 2.13 | 0.49 |
| 1:C:521:GLU:O | 1:C:525:HIS:HD2 | 1.95 | 0.49 |
| 1:C:616:GLY:N | 1:C:619:GLY:O | 2.37 | 0.49 |
| 1:C:714:THR:CG2 | 1:C:715:SER:N | 2.76 | 0.49 |
| 1:A:223:PRO:HD2 | 1:B:780:ARG:HH22 | 1.78 | 0.48 |
| 1:A:488:LEU:O | 1:A:492:LEU:HD13 | 2.13 | 0.48 |
| 1:B:388:PHE:CE2 | 1:B:472:ILE:HG21 | 2.48 | 0.48 |
| 1:C:754:TRP:CE3 | 1:C:780:ARG:HB2 | 2.48 | 0.48 |
| 1:A:754:TRP:HE3 | 1:C:218:GLN:O | 1.96 | 0.48 |
| 1:B:60:THR:O | 1:B:61:VAL:C | 2.49 | 0.48 |
| 1:B:218:GLN:CB | 1:B:232:ALA:O | 2.57 | 0.48 |
| 1:B:668:LEU:CB | 1:B:669:PRO:CD | 2.91 | 0.48 |
| 1:C:14:VAL:O | 1:C:14:VAL:HG12 | 2.13 | 0.48 |
| 1:C:240:LEU:HB2 | 1:C:246:PHE:CE1 | 2.48 | 0.48 |
| 1:C:278:ILE:CD1 | 1:C:613:ASN:HB3 | 2.44 | 0.48 |
| 2:D:79:LEU:HD22 | 2:D:111:HIS:NE2 | 2.28 | 0.48 |
| 1:A:382:VAL:HG11 | 1:A:476:SER:HB3 | 1.94 | 0.48 |
| 1:A:504:ASP:OD1 | 1:A:504:ASP:O | 2.30 | 0.48 |
| 1:B:222:THR:HG23 | 1:C:275:TYR:CB | 2.36 | 0.48 |
| 1:C:23:GLY:HA3 | 1:C:377:LEU:O | 2.13 | 0.48 |
| 1:C:314:GLU:N | 1:C:317:PHE:HE1 | 2.11 | 0.48 |
| 1:C:448:VAL:HG11 | 1:C:939:ALA:CB | 2.42 | 0.48 |
| 1:C:616:GLY:HA3 | 1:C:624:THR:HG22 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:987:MET:HB3 | 1:C:988:PRO:HD3 | 1.95 | 0.48 |
| 1:A:240:LEU:H | 1:A:240:LEU:HD13 | 1.78 | 0.48 |
| 1:A:457:ALA:HB2 | 1:A:471:SER:HB3 | 1.95 | 0.48 |
| 1:B:115:MET:N | 1:B:116:PRO:CD | 2.76 | 0.48 |
| 1:B:137:LEU:HD22 | 1:B:293:LEU:CD1 | 2.39 | 0.48 |
| 1:B:534:ILE:HG23 | 1:B:535:LEU:HG | 1.95 | 0.48 |
| 1:B:808:ARG:HA | 2:D:79:LEU:CD1 | 2.44 | 0.48 |
| 1:B:903:LEU:HD13 | 1:B:1025:PHE:CD2 | 2.48 | 0.48 |
| 1:C:313:MET:O | 1:C:317:PHE:CE1 | 2.67 | 0.48 |
| 1:A:139:VAL:CG1 | 1:A:178:PHE:HE2 | 2.26 | 0.48 |
| 1:A:164:ASP:OD2 | 1:A:767:ARG:NH2 | 2.44 | 0.48 |
| 1:A:445:ILE:HA | 1:A:448:VAL:CG1 | 2.43 | 0.48 |
| 1:B:166:ILE:HD13 | 1:B:166:ILE:N | 2.28 | 0.48 |
| 1:B:435:MET:O | 1:B:436:GLY:C | 2.47 | 0.48 |
| 1:B:910:ILE:HG23 | 1:B:1013:THR:HG21 | 1.95 | 0.48 |
| 1:C:259:ARG:CZ | 2:E:155:ASP:OD2 | 2.62 | 0.48 |
| 1:C:406:VAL:O | 1:C:410:ILE:HG13 | 2.14 | 0.48 |
| 1:C:447:MET:SD | 1:C:887:CYS:HB3 | 2.53 | 0.48 |
| 1:C:795:ASP:OD1 | 1:C:795:ASP:O | 2.30 | 0.48 |
| 1:A:1013:THR:O | 1:A:1017:LEU:HB2 | 2.13 | 0.48 |
| 1:B:183:ALA:CB | 1:B:271:GLY:O | 2.60 | 0.48 |
| 1:B:324:VAL:CG2 | 1:B:325:TYR:N | 2.76 | 0.48 |
| 1:B:418:ARG:O | 1:B:422:GLU:HG3 | 2.14 | 0.48 |
| 1:B:727:PHE:HE1 | 1:B:783:PRO:HB3 | 1.76 | 0.48 |
| 1:C:598:TYR:HB3 | 1:C:606:VAL:HG21 | 1.95 | 0.48 |
| 2:D:13:ASP:C | 2:D:15:GLY:N | 2.62 | 0.48 |
| 1:A:236:ALA:HB2 | 1:B:729:ILE:O | 2.13 | 0.48 |
| 1:A:410:ILE:CD1 | 1:A:978:THR:HG22 | 2.44 | 0.48 |
| 1:A:459:PHE:CB | 1:A:464:GLY:HA2 | 2.43 | 0.48 |
| 1:B:184:MET:CE | 1:B:268:ILE:HG22 | 2.43 | 0.48 |
| 1:B:222:THR:HG22 | 1:C:275:TYR:CB | 2.24 | 0.48 |
| 1:C:504:ASP:O | 1:C:504:ASP:CG | 2.52 | 0.48 |
| 2:E:84:LEU:CD2 | 2:E:116:PRO:HB3 | 2.44 | 0.48 |
| 1:A:242:SER:HB2 | 1:A:244:GLU:CG | 2.41 | 0.48 |
| 1:A:380:PHE:HD1 | 1:A:380:PHE:H | 1.61 | 0.48 |
| 1:A:527:TYR:CE1 | 1:A:968:VAL:HG12 | 2.48 | 0.48 |
| 1:A:534:ILE:CA | 1:A:541:TYR:CE1 | 2.94 | 0.48 |
| 1:A:987:MET:N | 1:A:988:PRO:CD | 2.77 | 0.48 |
| 1:B:182:TYR:HB3 | 1:B:270:LEU:CG | 2.44 | 0.48 |
| 1:B:198:LEU:N | 1:B:798:MET:CE | 2.76 | 0.48 |
| 1:C:199:THR:HB | 1:C:200:PRO:HD2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:94:GLU:H | 2:D:94:GLU:CD | 2.18 | 0.48 |
| 1:A:190:PRO:HD2 | 1:A:779:TYR:CG | 2.49 | 0.48 |
| 1:A:497:LEU:HB3 | 1:A:498:LYS:HE2 | 1.95 | 0.48 |
| 1:A:758:TYR:O | 1:A:758:TYR:CG | 2.61 | 0.48 |
| 1:B:351:VAL:O | 1:B:355:MET:HB2 | 2.12 | 0.48 |
| 1:B:660:ASP:OD1 | 2:D:16:LYS:NZ | 2.41 | 0.48 |
| 1:C:166:ILE:O | 1:C:166:ILE:CG2 | 2.56 | 0.48 |
| 1:C:210:GLN:NE2 | 1:C:249:ILE:HG23 | 2.29 | 0.48 |
| 1:C:391:ASN:O | 1:C:395:MET:HG2 | 2.14 | 0.48 |
| 1:C:429:GLU:CA | 1:C:432:ARG:HG3 | 2.43 | 0.48 |
| 2:D:77:ASP:CG | 2:D:78:SER:N | 2.67 | 0.48 |
| 1:A:497:LEU:HD22 | 1:A:497:LEU:HA | 1.58 | 0.48 |
| 1:A:751:GLY:O | 1:A:754:TRP:O | 2.32 | 0.48 |
| 1:B:1:FME:HE2 | 1:B:487:ILE:HG13 | 1.94 | 0.48 |
| 1:B:561:SER:O | 1:B:562:SER:OG | 2.30 | 0.48 |
| 1:B:668:LEU:CB | 1:B:669:PRO:HD2 | 2.44 | 0.48 |
| 1:B:729:ILE:O | 1:B:729:ILE:HG23 | 2.14 | 0.48 |
| 2:D:56:TYR:O | 2:D:56:TYR:CG | 2.66 | 0.48 |
| 2:D:61:GLU:HG2 | 2:D:62:ILE:H | 1.78 | 0.48 |
| 2:D:110:ASP:HB3 | 2:D:112:ASN:HB2 | 1.96 | 0.48 |
| 2:D:130:GLU:HG3 | 2:D:131:VAL:N | 2.29 | 0.48 |
| 1:A:448:VAL:HG21 | 1:A:888:LEU:CD2 | 2.44 | 0.47 |
| 1:A:813:SER:HB2 | 1:A:814:PRO:HD2 | 1.95 | 0.47 |
| 1:A:910:ILE:CG2 | 1:A:911:GLY:N | 2.77 | 0.47 |
| 1:B:197:GLN:C | 1:B:798:MET:HE3 | 2.13 | 0.47 |
| 1:B:324:VAL:CG2 | 1:B:325:TYR:H | 2.27 | 0.47 |
| 1:B:790:TYR:CE1 | 1:B:800:PRO:HB3 | 2.49 | 0.47 |
| 1:C:158:VAL:CG2 | 1:C:162:MET:HE3 | 2.35 | 0.47 |
| 2:E:93:LEU:HD11 | 2:E:127:GLU:CB | 2.44 | 0.47 |
| 2:E:143:ASP:H | 2:E:146:GLY:C | 2.16 | 0.47 |
| 1:A:489:THR:N | 1:A:490:PRO:HD2 | 2.30 | 0.47 |
| 1:A:519:MET:CE | 1:A:519:MET:CA | 2.88 | 0.47 |
| 1:A:972:LEU:O | 1:A:972:LEU:CD1 | 2.62 | 0.47 |
| 1:B:231:ASN:OD1 | 1:C:622:GLN:CG | 2.62 | 0.47 |
| 1:B:328:ASP:OD1 | 1:B:328:ASP:C | 2.51 | 0.47 |
| 1:B:716:VAL:O | 1:B:716:VAL:HG13 | 2.13 | 0.47 |
| 1:B:767:ARG:HH22 | 1:C:67:GLN:HE22 | 1.62 | 0.47 |
| 1:C:278:ILE:HD12 | 1:C:584:GLN:OE1 | 2.14 | 0.47 |
| 1:C:948:PHE:HE1 | 1:C:970:MET:SD | 2.37 | 0.47 |
| 2:D:145:PHE:C | 2:D:147:LYS:H | 2.16 | 0.47 |
| 1:A:74:ASN:HB3 | 1:A:95:GLU:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:196:PHE:O | 1:B:197:GLN:C | 2.47 | 0.47 |
| 1:B:480:LEU:HA | 1:B:483:LEU:HD23 | 1.95 | 0.47 |
| 1:B:674:LEU:O | 1:B:674:LEU:HD12 | 2.12 | 0.47 |
| 2:D:44:ASP:CG | 2:D:45:HIS:HA | 2.33 | 0.47 |
| 2:E:154:ILE:HG13 | 2:E:155:ASP:N | 2.30 | 0.47 |
| 1:A:648:THR:O | 1:A:652:THR:HG22 | 2.14 | 0.47 |
| 1:A:650:ARG:CG | 1:A:651:ALA:N | 2.77 | 0.47 |
| 1:B:686:ASP:HB2 | 1:B:695:LEU:CD1 | 2.44 | 0.47 |
| 1:B:687:GLN:NE2 | 1:B:859:TRP:CB | 2.77 | 0.47 |
| 1:C:842:GLU:O | 1:C:846:GLN:HG3 | 2.14 | 0.47 |
| 1:C:960:LEU:C | 1:C:960:LEU:HD12 | 2.31 | 0.47 |
| 1:C:1037:ASN:OD1 | 1:C:1039:ASP:O | 2.32 | 0.47 |
| 1:A:697:GLN:HA | 1:A:700:ASN:HD22 | 1.80 | 0.47 |
| 1:A:1012:VAL:O | 1:A:1016:VAL:HG22 | 2.14 | 0.47 |
| 1:B:2:PRO:O | 1:B:6:ILE:HG13 | 2.14 | 0.47 |
| 1:B:47:ALA:HB3 | 1:B:88:VAL:CG1 | 2.44 | 0.47 |
| 1:B:263:ARG:O | 1:B:263:ARG:HG2 | 2.14 | 0.47 |
| 1:B:378:GLY:HA3 | 1:B:480:LEU:HD23 | 1.95 | 0.47 |
| 1:B:576:VAL:HG22 | 1:B:663:VAL:HG22 | 1.96 | 0.47 |
| 1:C:733:GLN:NE2 | 1:C:743:ILE:CG2 | 2.72 | 0.47 |
| 1:C:1033:PHE:O | 1:C:1034:SER:OG | 2.30 | 0.47 |
| 1:A:181:GLN:NE2 | 1:A:769:LYS:HE3 | 2.25 | 0.47 |
| 1:A:454:VAL:N | 1:A:455:PRO:CD | 2.77 | 0.47 |
| 1:A:971:ARG:HH11 | 1:A:971:ARG:HG2 | 1.69 | 0.47 |
| 1:B:193:LEU:CD2 | 1:B:265:VAL:HB | 2.44 | 0.47 |
| 1:A:78:MET:O | 1:A:78:MET:HG3 | 2.14 | 0.47 |
| 1:A:306:ILE:H | 1:A:306:ILE:HG12 | 1.34 | 0.47 |
| 1:A:492:LEU:CD1 | 1:A:492:LEU:N | 2.78 | 0.47 |
| 1:A:534:ILE:HG22 | 1:A:541:TYR:CZ | 2.50 | 0.47 |
| 1:A:860:THR:O | 1:A:860:THR:OG1 | 2.30 | 0.47 |
| 1:A:987:MET:HB3 | 1:A:988:PRO:HD3 | 1.97 | 0.47 |
| 1:B:255:GLN:C | 1:B:257:GLY:N | 2.64 | 0.47 |
| 1:B:293:LEU:HD11 | 1:B:299:ALA:CB | 2.45 | 0.47 |
| 1:B:504:ASP:OD1 | 1:B:505:HIS:O | 2.33 | 0.47 |
| 1:B:537:SER:O | 1:B:541:TYR:HD1 | 1.97 | 0.47 |
| 1:C:488:LEU:O | 1:C:492:LEU:HG | 2.15 | 0.47 |
| 1:C:669:PRO:N | 1:C:678:THR:HG22 | 2.29 | 0.47 |
| 1:C:727:PHE:CE1 | 1:C:807:SER:HB3 | 2.50 | 0.47 |
| 1:C:908:GLY:HA3 | 1:C:938:SER:OG | 2.14 | 0.47 |
| 2:D:48:TRP:NE1 | 2:D:77:ASP:OD2 | 2.44 | 0.47 |
| 2:D:94:GLU:O | 2:D:98:VAL:HG23 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:110:ASP:CB | 2:D:112:ASN:HB2 | 2.45 | 0.47 |
| 1:A:182:TYR:HD2 | 1:A:270:LEU:CD2 | 2.26 | 0.47 |
| 1:A:423:GLU:N | 1:A:502:LYS:HG3 | 2.29 | 0.47 |
| 1:B:365:THR:HG23 | 1:B:366:LEU:H | 1.79 | 0.47 |
| 1:C:332:PHE:HA | 1:C:335:ILE:HG22 | 1.96 | 0.47 |
| 1:A:41:PRO:HD2 | 1:A:95:GLU:O | 2.15 | 0.47 |
| 1:B:72:ILE:CG2 | 1:B:73:ASP:H | 2.25 | 0.47 |
| 1:B:182:TYR:HD1 | 1:B:270:LEU:CD2 | 2.27 | 0.47 |
| 1:B:243:THR:HG23 | 1:B:244:GLU:N | 2.30 | 0.47 |
| 1:C:631:LEU:HD12 | 1:C:637:ARG:CZ | 2.45 | 0.47 |
| 1:C:885:PHE:HE1 | 1:C:898:PRO:HB2 | 1.80 | 0.47 |
| 2:D:49:THR:O | 2:D:52:HIS:HB2 | 2.15 | 0.47 |
| 2:D:49:THR:O | 2:D:53:LEU:HD23 | 2.10 | 0.47 |
| 2:D:125:HIS:O | 2:D:129:VAL:CG2 | 2.57 | 0.47 |
| 1:A:211:ASN:HA | 1:A:240:LEU:HD13 | 1.97 | 0.47 |
| 1:A:241:THR:HG23 | 1:A:763:ILE:O | 2.15 | 0.47 |
| 1:A:314:GLU:N | 1:A:315:PRO:HD2 | 2.30 | 0.47 |
| 1:A:343:THR:HA | 1:A:346:GLU:HB2 | 1.96 | 0.47 |
| 1:A:423:GLU:C | 1:A:502:LYS:CE | 2.81 | 0.47 |
| 1:A:539:GLY:O | 1:A:543:VAL:HG22 | 2.15 | 0.47 |
| 1:A:570:GLY:N | 1:A:634:TRP:HH2 | 2.13 | 0.47 |
| 1:A:621:GLY:CA | 1:A:624:THR:HG22 | 2.44 | 0.47 |
| 1:C:598:TYR:HB3 | 1:C:606:VAL:HG11 | 1.97 | 0.47 |
| 2:E:57:PHE:N | 2:E:58:GLY:HA2 | 2.30 | 0.47 |
| 1:A:692:HIS:O | 1:A:696:THR:OG1 | 2.33 | 0.46 |
| 1:B:370:ILE:HG21 | 1:B:492:LEU:HD11 | 1.97 | 0.46 |
| 1:B:456:MET:HG2 | 1:B:456:MET:O | 2.14 | 0.46 |
| 1:C:247:GLY:C | 1:C:263:ARG:HG2 | 2.36 | 0.46 |
| 1:C:958:LYS:HD3 | 1:C:962:GLU:CD | 2.36 | 0.46 |
| 2:D:89:ASP:C | 2:D:91:GLY:N | 2.65 | 0.46 |
| 1:A:431:THR:O | 1:A:432:ARG:C | 2.53 | 0.46 |
| 1:A:782:LEU:HB2 | 1:A:785:ASP:CG | 2.35 | 0.46 |
| 1:A:815:ARG:HE | 1:A:815:ARG:HB2 | 1.22 | 0.46 |
| 1:A:944:LEU:HD12 | 1:A:971:ARG:NH2 | 2.29 | 0.46 |
| 1:A:1026:PHE:O | 1:A:1026:PHE:CG | 2.68 | 0.46 |
| 1:B:605:ASN:HD22 | 1:B:647:ILE:HD11 | 1.80 | 0.46 |
| 1:B:733:GLN:HE22 | 1:B:743:ILE:HD11 | 1.80 | 0.46 |
| 1:C:76:MET:HG2 | 1:C:95:GLU:OE2 | 2.15 | 0.46 |
| 1:C:87:THR:C | 1:C:88:VAL:HG12 | 2.35 | 0.46 |
| 1:C:412:VAL:HG23 | 1:C:442:LEU:HD21 | 1.96 | 0.46 |
| 1:C:885:PHE:CE1 | 1:C:898:PRO:HB2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:987:MET:O | 1:C:990:VAL:N | 2.45 | 0.46 |
| 2:D:65:VAL:O | 2:D:69:ASN:ND2 | 2.40 | 0.46 |
| 1:A:212:ALA:O | 1:A:237:GLN:HG2 | 2.15 | 0.46 |
| 1:B:222:THR:HG23 | 1:C:275:TYR:HB3 | 1.95 | 0.46 |
| 1:B:393:LEU:HD12 | 1:B:469:GLN:HG3 | 1.97 | 0.46 |
| 1:B:669:PRO:O | 1:B:669:PRO:CD | 2.63 | 0.46 |
| 1:B:671:ILE:HG23 | 1:B:673:GLU:N | 2.30 | 0.46 |
| 1:C:719:ASN:HB2 | 1:C:828:LEU:CD1 | 2.46 | 0.46 |
| 1:C:722:GLU:HG3 | 1:C:723:ASP:H | 1.81 | 0.46 |
| 1:C:952:LEU:N | 1:C:952:LEU:HD13 | 2.30 | 0.46 |
| 1:A:219:LEU:HD13 | 1:B:783:PRO:HD3 | 1.96 | 0.46 |
| 1:A:427:PRO:HD3 | 1:A:499:PRO:CB | 2.44 | 0.46 |
| 1:A:435:MET:O | 1:A:439:GLN:HB2 | 2.14 | 0.46 |
| 1:A:584:GLN:N | 1:A:622:GLN:OE1 | 2.49 | 0.46 |
| 1:A:754:TRP:N | 1:A:754:TRP:HD1 | 2.12 | 0.46 |
| 1:C:63:GLN:O | 1:C:67:GLN:HG2 | 2.15 | 0.46 |
| 1:C:436:GLY:O | 1:C:439:GLN:HB3 | 2.15 | 0.46 |
| 2:E:67:LEU:HD22 | 2:E:73:VAL:HG22 | 1.97 | 0.46 |
| 1:A:248:LYS:HA | 1:A:261:LEU:HD23 | 1.98 | 0.46 |
| 1:B:341:VAL:O | 1:B:345:VAL:HG23 | 2.15 | 0.46 |
| 1:B:733:GLN:O | 1:B:736:ALA:HB3 | 2.15 | 0.46 |
| 1:A:685:ILE:HA | 1:A:823:PRO:O | 2.16 | 0.46 |
| 1:B:605:ASN:HD21 | 1:B:642:ASN:CB | 2.26 | 0.46 |
| 1:B:774:MET:CE | 1:B:780:ARG:HH11 | 2.28 | 0.46 |
| 1:B:881:LEU:O | 1:B:881:LEU:HD22 | 2.16 | 0.46 |
| 2:D:43:SER:HA | 2:D:49:THR:HA | 1.97 | 0.46 |
| 1:A:229:GLN:OE1 | 1:B:586:ARG:HD2 | 2.15 | 0.46 |
| 1:B:291:ILE:CD1 | 1:B:306:ILE:HD12 | 2.46 | 0.46 |
| 1:B:758:TYR:HB2 | 1:B:772:TYR:HE1 | 1.70 | 0.46 |
| 1:C:466:ILE:H | 1:C:466:ILE:HG12 | 1.40 | 0.46 |
| 1:C:713:LEU:HD21 | 1:C:843:LEU:HD23 | 1.96 | 0.46 |
| 1:C:925:VAL:C | 1:C:927:PHE:N | 2.65 | 0.46 |
| 1:A:449:LEU:HD23 | 1:A:478:MET:SD | 2.56 | 0.46 |
| 1:A:480:LEU:HA | 1:A:480:LEU:HD23 | 1.69 | 0.46 |
| 1:B:88:VAL:HG22 | 1:B:89:GLN:N | 2.30 | 0.46 |
| 1:B:102:ILE:O | 1:B:103:ALA:C | 2.54 | 0.46 |
| 1:B:183:ALA:CA | 1:B:271:GLY:O | 2.64 | 0.46 |
| 1:C:907:LEU:O | 1:C:910:ILE:HG22 | 2.14 | 0.46 |
| 2:D:76:ASP:HB3 | 2:D:80:GLY:HA2 | 1.97 | 0.46 |
| 1:A:17:ILE:O | 1:A:21:LEU:HB2 | 2.16 | 0.46 |
| 1:A:159:ALA:HB1 | 1:A:181:GLN:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:445:ILE:HD13 | 1:B:940:LYS:HG3 | 1.98 | 0.46 |
| 1:B:717:ARG:HG3 | 1:B:828:LEU:HD12 | 1.98 | 0.46 |
| 1:C:925:VAL:O | 1:C:928:GLN:N | 2.49 | 0.46 |
| 1:A:182:TYR:CD2 | 1:A:270:LEU:HD21 | 2.51 | 0.46 |
| 1:A:525:HIS:O | 1:A:528:THR:OG1 | 2.30 | 0.46 |
| 1:A:693:GLU:H | 1:A:693:GLU:CD | 2.16 | 0.46 |
| 1:B:235:ILE:HD12 | 1:B:235:ILE:HA | 1.60 | 0.46 |
| 1:B:350:LEU:O | 1:B:354:VAL:HG13 | 2.16 | 0.46 |
| 1:C:465:ALA:O | 1:C:469:GLN:HG2 | 2.15 | 0.46 |
| 1:C:1015:THR:O | 1:C:1019:ILE:HB | 2.15 | 0.46 |
| 2:E:143:ASP:O | 2:E:146:GLY:N | 2.39 | 0.46 |
| 1:A:1:FME:N | 1:A:2:PRO:HD2 | 2.30 | 0.45 |
| 1:A:182:TYR:HD2 | 1:A:270:LEU:HD21 | 1.81 | 0.45 |
| 1:A:519:MET:SD | 1:A:519:MET:O | 2.67 | 0.45 |
| 1:A:813:SER:CB | 1:A:814:PRO:HD2 | 2.45 | 0.45 |
| 1:B:733:GLN:HE22 | 1:B:743:ILE:CD1 | 2.28 | 0.45 |
| 1:B:746:ILE:C | 1:B:748:THR:H | 2.20 | 0.45 |
| 1:C:672:VAL:HG23 | 1:C:673:GLU:N | 2.30 | 0.45 |
| 2:D:13:ASP:O | 2:D:16:LYS:N | 2.50 | 0.45 |
| 1:A:470:PHE:O | 1:A:474:ILE:HG13 | 2.16 | 0.45 |
| 1:A:781:MET:HE1 | 1:C:228:GLN:CB | 2.46 | 0.45 |
| 1:B:903:LEU:HD13 | 1:B:1025:PHE:HD2 | 1.81 | 0.45 |
| 1:C:62:THR:O | 1:C:66:GLU:HB2 | 2.15 | 0.45 |
| 2:D:80:GLY:O | 2:D:82:THR:HG23 | 2.15 | 0.45 |
| 2:E:97:GLU:OE1 | 2:E:97:GLU:CA | 2.46 | 0.45 |
| 1:A:351:VAL:HG23 | 1:A:981:ALA:HB1 | 1.98 | 0.45 |
| 1:A:908:GLY:HA2 | 1:A:1014:ALA:HB2 | 1.98 | 0.45 |
| 1:B:44:THR:HG21 | 1:B:89:GLN:NE2 | 2.31 | 0.45 |
| 1:B:733:GLN:H | 1:B:733:GLN:HG2 | 1.53 | 0.45 |
| 1:B:815:ARG:NH1 | 1:B:815:ARG:CG | 2.73 | 0.45 |
| 1:B:908:GLY:HA2 | 1:B:1014:ALA:HB2 | 1.99 | 0.45 |
| 1:C:446:ALA:CB | 1:C:482:VAL:HG22 | 2.46 | 0.45 |
| 1:C:801:PHE:O | 1:C:801:PHE:CD1 | 2.70 | 0.45 |
| 1:C:876:LEU:HD11 | 1:C:932:LEU:HD11 | 1.98 | 0.45 |
| 1:C:879:ILE:HD12 | 1:C:883:VAL:HG23 | 1.91 | 0.45 |
| 2:D:56:TYR:HD1 | 2:D:90:ARG:CG | 2.19 | 0.45 |
| 2:E:106:VAL:HG21 | 2:E:136:GLY:HA3 | 1.98 | 0.45 |
| 1:A:55:LYS:O | 1:A:56:THR:C | 2.50 | 0.45 |
| 1:A:650:ARG:HG2 | 1:A:651:ALA:N | 2.32 | 0.45 |
| 1:B:214:VAL:CG1 | 1:B:215:ALA:N | 2.79 | 0.45 |
| 1:C:269:GLU:O | 1:C:269:GLU:HG3 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:514:GLY:O | 1:C:518:ARG:HG3 | 2.17 | 0.45 |
| 1:C:555:LEU:HD23 | 1:C:555:LEU:HA | 1.84 | 0.45 |
| 1:C:616:GLY:HA3 | 1:C:624:THR:CG2 | 2.47 | 0.45 |
| 1:C:894:SER:O | 1:C:898:PRO:CG | 2.64 | 0.45 |
| 1:C:986:VAL:O | 1:C:986:VAL:HG13 | 2.16 | 0.45 |
| 2:D:57:PHE:N | 2:D:58:GLY:CA | 2.79 | 0.45 |
| 2:E:82:THR:O | 2:E:85:HIS:HB2 | 2.16 | 0.45 |
| 1:A:219:LEU:HD11 | 1:B:783:PRO:HG3 | 1.98 | 0.45 |
| 1:A:943:ILE:O | 1:A:946:VAL:CG1 | 2.64 | 0.45 |
| 1:B:76:MET:HG2 | 1:B:95:GLU:OE2 | 2.17 | 0.45 |
| 1:B:178:PHE:HE2 | 1:B:290:GLY:N | 2.15 | 0.45 |
| 1:B:197:GLN:C | 1:B:798:MET:HE1 | 2.31 | 0.45 |
| 1:C:154:ILE:HG13 | 1:C:155:SER:N | 2.30 | 0.45 |
| 1:C:506:GLY:O | 1:C:507:GLU:HG2 | 2.13 | 0.45 |
| 1:A:58:GLN:HE21 | 1:A:818:ARG:HH11 | 1.60 | 0.45 |
| 1:A:189:ASN:HD22 | 1:A:192:GLU:CG | 2.29 | 0.45 |
| 1:A:199:THR:O | 1:A:199:THR:HG23 | 2.17 | 0.45 |
| 1:A:244:GLU:HG2 | 1:A:244:GLU:H | 1.36 | 0.45 |
| 1:A:378:GLY:HA3 | 1:A:480:LEU:CD1 | 2.47 | 0.45 |
| 1:A:578:LEU:HD13 | 1:A:587:THR:HG23 | 1.99 | 0.45 |
| 1:A:888:LEU:HD13 | 1:A:901:VAL:HB | 1.97 | 0.45 |
| 1:B:21:LEU:HD13 | 1:B:21:LEU:HA | 1.81 | 0.45 |
| 1:B:522:LYS:O | 1:B:525:HIS:HB2 | 2.15 | 0.45 |
| 1:B:588:GLN:HB2 | 1:B:613:ASN:HD22 | 1.80 | 0.45 |
| 1:B:713:LEU:HD12 | 1:B:713:LEU:HA | 1.64 | 0.45 |
| 1:C:318:PRO:C | 1:C:319:SER:HG | 2.16 | 0.45 |
| 1:C:444:GLY:O | 1:C:448:VAL:HG23 | 2.16 | 0.45 |
| 1:C:542:LEU:O | 1:C:546:LEU:HD13 | 2.16 | 0.45 |
| 1:C:586:ARG:O | 1:C:590:VAL:HG23 | 2.17 | 0.45 |
| 1:C:695:LEU:C | 1:C:695:LEU:CD2 | 2.85 | 0.45 |
| 1:A:40:PRO:HA | 1:A:41:PRO:HD3 | 1.82 | 0.45 |
| 1:A:264:ASP:OD2 | 1:A:264:ASP:N | 2.48 | 0.45 |
| 1:A:427:PRO:CG | 1:A:497:LEU:O | 2.65 | 0.45 |
| 1:A:972:LEU:O | 1:A:972:LEU:HD13 | 2.16 | 0.45 |
| 1:B:892:TYR:OH | 1:B:943:ILE:HA | 2.17 | 0.45 |
| 1:C:335:ILE:HD12 | 1:C:338:HIS:HB3 | 1.98 | 0.45 |
| 1:C:775:SER:HG | 1:C:789:TRP:HZ2 | 1.64 | 0.45 |
| 1:C:937:LEU:CA | 1:C:940:LYS:HG2 | 2.47 | 0.45 |
| 2:E:100:LEU:O | 2:E:103:GLY:CA | 2.65 | 0.45 |
| 2:E:112:ASN:HB2 | 2:E:114:PHE:HD2 | 1.82 | 0.45 |
| 1:A:144:ASN:OD1 | 1:A:149:MET:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:753:ALA:HB3 | 1:A:754:TRP:HD1 | 1.82 | 0.45 |
| 1:A:913:LEU:HD23 | 1:A:927:PHE:HZ | 1.82 | 0.45 |
| 1:A:1008:MET:O | 1:A:1012:VAL:HG23 | 2.17 | 0.45 |
| 1:B:169:THR:CG2 | 1:B:172:VAL:HG13 | 2.34 | 0.45 |
| 1:B:456:MET:O | 1:B:467:TYR:HB3 | 2.17 | 0.45 |
| 1:B:1013:THR:CG2 | 1:B:1017:LEU:HD12 | 2.47 | 0.45 |
| 1:C:98:THR:HG23 | 1:C:99:ASP:H | 1.80 | 0.45 |
| 1:C:447:MET:HE3 | 1:C:891:LEU:CD2 | 2.40 | 0.45 |
| 1:C:472:ILE:HG23 | 1:C:473:THR:N | 2.31 | 0.45 |
| 1:C:567:GLU:OE2 | 1:C:997:SER:N | 2.50 | 0.45 |
| 1:C:725:PRO:CD | 1:C:725:PRO:O | 2.64 | 0.45 |
| 1:C:750:LEU:CD2 | 1:C:751:GLY:N | 2.77 | 0.45 |
| 1:A:230:LEU:HD23 | 1:B:782:LEU:HD22 | 1.99 | 0.45 |
| 1:A:910:ILE:HG23 | 1:A:911:GLY:N | 2.32 | 0.45 |
| 1:B:118:LEU:O | 1:B:123:GLN:OE1 | 2.33 | 0.45 |
| 1:B:435:MET:C | 1:B:437:GLN:H | 2.18 | 0.45 |
| 1:B:575:MET:O | 1:B:576:VAL:HG23 | 2.16 | 0.45 |
| 2:D:14:LEU:O | 2:D:15:GLY:C | 2.52 | 0.45 |
| 2:D:50:PRO:HA | 2:D:53:LEU:HD23 | 1.98 | 0.45 |
| 1:A:316:PHE:CD2 | 1:B:687:GLN:HB3 | 2.52 | 0.45 |
| 1:A:694:LYS:O | 1:A:697:GLN:HB2 | 2.17 | 0.45 |
| 1:A:908:GLY:CA | 1:A:1014:ALA:HB2 | 2.47 | 0.45 |
| 1:B:62:THR:O | 1:B:62:THR:CG2 | 2.63 | 0.45 |
| 1:B:98:THR:HG22 | 1:B:99:ASP:N | 2.32 | 0.45 |
| 1:B:293:LEU:CD1 | 1:B:299:ALA:HB2 | 2.46 | 0.45 |
| 1:B:488:LEU:O | 1:B:492:LEU:HG | 2.17 | 0.45 |
| 1:B:501:ALA:HB3 | 1:B:504:ASP:CG | 2.38 | 0.45 |
| 1:B:698:ALA:O | 1:B:851:LEU:HD23 | 2.16 | 0.45 |
| 1:C:719:ASN:HD22 | 1:C:828:LEU:HD11 | 1.82 | 0.45 |
| 1:B:10:ILE:HD12 | 1:C:895:TRP:NE1 | 2.32 | 0.44 |
| 1:B:813:SER:HB3 | 1:B:816:LEU:CD2 | 2.48 | 0.44 |
| 1:C:5:PHE:CE2 | 1:C:487:ILE:HG23 | 2.53 | 0.44 |
| 1:C:5:PHE:CE2 | 1:C:487:ILE:HG12 | 2.51 | 0.44 |
| 1:C:53:ASP:OD1 | 1:C:53:ASP:O | 2.35 | 0.44 |
| 2:D:73:VAL:HG11 | 2:D:103:GLY:O | 2.17 | 0.44 |
| 2:E:77:ASP:HB2 | 2:E:81:VAL:O | 2.17 | 0.44 |
| 1:A:427:PRO:HG2 | 1:A:497:LEU:O | 2.17 | 0.44 |
| 1:A:483:LEU:HA | 1:A:486:LEU:HD23 | 1.99 | 0.44 |
| 1:B:340:VAL:O | 1:B:344:LEU:HG | 2.17 | 0.44 |
| 1:B:416:VAL:HG22 | 1:B:434:SER:CB | 2.47 | 0.44 |
| 1:C:9:PRO:HD2 | 1:C:10:ILE:H | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:559:LEU:HA | 1:C:560:PRO:HD3 | 1.87 | 0.44 |
| 1:A:899:PHE:O | 1:A:903:LEU:HD12 | 2.17 | 0.44 |
| 1:A:997:SER:C | 1:A:999:ALA:H | 2.20 | 0.44 |
| 1:B:406:VAL:C | 1:B:408:ASP:H | 2.19 | 0.44 |
| 1:C:45:ILE:HD11 | 1:C:107:VAL:CG1 | 2.47 | 0.44 |
| 1:C:367:ILE:CB | 1:C:368:PRO:HD3 | 2.47 | 0.44 |
| 1:C:568:ASP:HA | 1:C:644:VAL:CG2 | 2.47 | 0.44 |
| 2:D:164:ILE:H | 2:D:164:ILE:HG13 | 1.57 | 0.44 |
| 1:A:725:PRO:HA | 1:A:810:GLU:O | 2.17 | 0.44 |
| 1:A:726:GLN:HB3 | 1:C:235:ILE:HG12 | 1.99 | 0.44 |
| 1:B:416:VAL:HG22 | 1:B:434:SER:HB3 | 1.99 | 0.44 |
| 1:B:673:GLU:C | 1:B:675:GLY:H | 2.18 | 0.44 |
| 1:B:911:GLY:C | 1:B:1010:GLY:HA2 | 2.37 | 0.44 |
| 1:B:1020:PHE:O | 1:B:1023:PRO:HD2 | 2.18 | 0.44 |
| 1:C:733:GLN:O | 1:C:734:GLU:C | 2.55 | 0.44 |
| 1:C:886:LEU:O | 1:C:887:CYS:C | 2.55 | 0.44 |
| 1:C:952:LEU:HA | 1:C:952:LEU:HD12 | 1.40 | 0.44 |
| 1:A:987:MET:C | 1:A:989:LEU:H | 2.20 | 0.44 |
| 1:B:33:ALA:O | 1:B:391:ASN:HA | 2.18 | 0.44 |
| 1:B:62:THR:OG1 | 1:B:88:VAL:CG2 | 2.65 | 0.44 |
| 1:B:365:THR:C | 1:B:368:PRO:HD2 | 2.37 | 0.44 |
| 1:B:508:GLY:C | 1:B:510:LYS:N | 2.63 | 0.44 |
| 1:B:754:TRP:CE3 | 1:B:780:ARG:HB2 | 2.52 | 0.44 |
| 1:B:853:THR:O | 1:B:853:THR:HG23 | 2.14 | 0.44 |
| 1:C:342:LYS:O | 1:C:343:THR:C | 2.53 | 0.44 |
| 1:C:390:ILE:O | 1:C:390:ILE:HG22 | 2.17 | 0.44 |
| 1:C:999:ALA:O | 1:C:1000:GLN:C | 2.55 | 0.44 |
| 2:E:44:ASP:HA | 2:E:45:HIS:HA | 1.50 | 0.44 |
| 2:E:57:PHE:H | 2:E:58:GLY:CA | 2.31 | 0.44 |
| 2:E:126:LEU:HA | 2:E:129:VAL:HG22 | 2.00 | 0.44 |
| 1:A:239:ARG:C | 1:A:240:LEU:HD12 | 2.31 | 0.44 |
| 1:A:388:PHE:CE1 | 1:A:469:GLN:OE1 | 2.71 | 0.44 |
| 1:A:401:ALA:O | 1:A:405:LEU:HD13 | 2.18 | 0.44 |
| 1:A:519:MET:HE2 | 1:A:519:MET:HB2 | 1.34 | 0.44 |
| 1:C:48:SER:HB3 | 1:C:125:GLN:HG2 | 1.99 | 0.44 |
| 1:C:367:ILE:HG23 | 1:C:492:LEU:HD12 | 1.99 | 0.44 |
| 1:A:190:PRO:HG3 | 1:A:789:TRP:CE2 | 2.52 | 0.44 |
| 1:A:263:ARG:HG3 | 1:A:264:ASP:N | 2.32 | 0.44 |
| 1:A:753:ALA:HB3 | 1:A:754:TRP:CD1 | 2.52 | 0.44 |
| 1:B:702:LEU:HD11 | 1:B:844:MET:CE | 2.48 | 0.44 |
| 1:B:724:THR:HB | 1:B:725:PRO:HD2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:69:MET:HA | 1:C:69:MET:HE3 | 2.00 | 0.44 |
| 1:C:172:VAL:HG13 | 1:C:291:ILE:HG23 | 2.00 | 0.44 |
| 1:C:527:TYR:CZ | 1:C:1019:ILE:HG13 | 2.53 | 0.44 |
| 1:C:952:LEU:N | 1:C:952:LEU:HD12 | 2.27 | 0.44 |
| 2:D:18:LEU:C | 2:D:18:LEU:HD22 | 2.36 | 0.44 |
| 1:A:462:SER:OG | 1:A:463:THR:N | 2.49 | 0.44 |
| 1:A:531:VAL:O | 1:A:534:ILE:CG1 | 2.66 | 0.44 |
| 1:A:721:LEU:HD11 | 1:A:814:PRO:HG2 | 1.85 | 0.44 |
| 1:B:166:ILE:CG2 | 1:B:175:VAL:HG21 | 2.38 | 0.44 |
| 1:B:534:ILE:HG23 | 1:B:535:LEU:N | 2.32 | 0.44 |
| 1:B:578:LEU:CD1 | 1:B:579:PRO:HD3 | 2.48 | 0.44 |
| 1:C:448:VAL:HG12 | 1:C:936:GLY:HA2 | 2.00 | 0.44 |
| 2:E:101:LYS:O | 2:E:102:ASN:C | 2.50 | 0.44 |
| 1:A:72:ILE:HD13 | 1:A:107:VAL:HG22 | 1.99 | 0.44 |
| 1:A:159:ALA:O | 1:A:163:LYS:HE2 | 2.18 | 0.44 |
| 1:A:492:LEU:N | 1:A:492:LEU:HD12 | 2.32 | 0.44 |
| 1:A:645:GLU:O | 1:A:649:MET:HG3 | 2.18 | 0.44 |
| 1:B:960:LEU:HD22 | 1:B:961:ILE:HD13 | 1.99 | 0.44 |
| 1:C:163:LYS:O | 1:C:164:ASP:C | 2.56 | 0.44 |
| 1:C:281:PHE:O | 1:C:282:ASN:HB2 | 2.18 | 0.44 |
| 1:C:431:THR:HG22 | 1:C:435:MET:HG3 | 1.98 | 0.44 |
| 1:C:471:SER:O | 1:C:475:VAL:HG23 | 2.17 | 0.44 |
| 1:A:1013:THR:C | 1:A:1015:THR:H | 2.21 | 0.43 |
| 1:C:144:ASN:ND2 | 1:C:149:MET:N | 2.66 | 0.43 |
| 1:C:151:GLN:HA | 1:C:154:ILE:HG23 | 2.00 | 0.43 |
| 1:C:672:VAL:HG23 | 1:C:673:GLU:CD | 2.37 | 0.43 |
| 1:C:737:GLN:O | 1:C:738:ALA:C | 2.53 | 0.43 |
| 1:A:98:THR:CG2 | 1:A:103:ALA:HB2 | 2.47 | 0.43 |
| 1:A:190:PRO:HD2 | 1:A:779:TYR:CD2 | 2.53 | 0.43 |
| 1:A:897:ILE:O | 1:A:897:ILE:CG2 | 2.64 | 0.43 |
| 1:B:139:VAL:HG22 | 1:B:327:TYR:HB3 | 1.99 | 0.43 |
| 1:B:187:TRP:HD1 | 1:B:267:LYS:O | 2.00 | 0.43 |
| 1:B:561:SER:HA | 1:B:923:ASN:CB | 2.48 | 0.43 |
| 1:C:358:PHE:CG | 1:C:977:MET:HG2 | 2.54 | 0.43 |
| 1:C:404:LEU:HD22 | 1:C:404:LEU:N | 2.33 | 0.43 |
| 1:C:594:VAL:CG1 | 1:C:598:TYR:HE2 | 2.31 | 0.43 |
| 1:C:648:THR:HA | 1:C:651:ALA:HB3 | 2.00 | 0.43 |
| 1:C:724:THR:HG23 | 1:C:814:PRO:CG | 2.48 | 0.43 |
| 1:C:741:VAL:HG11 | 1:C:746:ILE:HD11 | 1.84 | 0.43 |
| 2:D:126:LEU:C | 2:D:129:VAL:CG2 | 2.86 | 0.43 |
| 2:D:148:THR:H | 2:D:151:ASP:HB2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:25:GLY:CA | 2:E:59:HIS:CE1 | 3.01 | 0.43 |
| 1:A:184:MET:HG2 | 1:A:246:PHE:CD1 | 2.53 | 0.43 |
| 1:A:189:ASN:ND2 | 1:A:192:GLU:HG3 | 2.34 | 0.43 |
| 1:A:534:ILE:HD12 | 1:A:1024:VAL:CG2 | 2.48 | 0.43 |
| 1:B:157:TYR:C | 1:B:157:TYR:CD2 | 2.91 | 0.43 |
| 1:B:531:VAL:HA | 1:B:534:ILE:HG22 | 2.00 | 0.43 |
| 1:B:531:VAL:C | 1:B:534:ILE:HG22 | 2.38 | 0.43 |
| 1:B:699:ARG:HD3 | 1:B:825:MET:HG2 | 2.00 | 0.43 |
| 1:B:733:GLN:HA | 1:B:736:ALA:HB3 | 2.00 | 0.43 |
| 1:C:226:LYS:HD3 | 1:C:226:LYS:HA | 1.83 | 0.43 |
| 1:C:372:VAL:H | 1:C:373:PRO:HD2 | 1.83 | 0.43 |
| 1:C:415:ASN:HD22 | 1:C:434:SER:HB3 | 1.84 | 0.43 |
| 1:C:521:GLU:O | 1:C:525:HIS:CD2 | 2.71 | 0.43 |
| 1:C:563:PHE:CE2 | 1:C:862:MET:CE | 3.01 | 0.43 |
| 1:C:993:THR:HA | 1:C:997:SER:CB | 2.49 | 0.43 |
| 1:A:485:ALA:HB3 | 1:A:486:LEU:CD1 | 2.49 | 0.43 |
| 1:A:739:LEU:HD13 | 1:A:799:VAL:HG11 | 2.00 | 0.43 |
| 1:B:310:LEU:HD13 | 1:B:323:ILE:HD12 | 2.00 | 0.43 |
| 1:C:194:ASN:O | 1:C:194:ASN:ND2 | 2.52 | 0.43 |
| 1:C:391:ASN:H | 1:C:394:THR:CG2 | 2.31 | 0.43 |
| 1:C:780:ARG:O | 1:C:780:ARG:CG | 2.66 | 0.43 |
| 2:D:50:PRO:C | 2:D:53:LEU:HD23 | 2.39 | 0.43 |
| 1:A:185:ARG:HA | 1:A:185:ARG:HD2 | 1.86 | 0.43 |
| 1:A:587:THR:HB | 1:A:613:ASN:HD21 | 1.82 | 0.43 |
| 1:B:11:PHE:CD1 | 1:B:11:PHE:O | 2.72 | 0.43 |
| 1:B:223:PRO:HA | 1:B:224:PRO:HD3 | 1.78 | 0.43 |
| 1:B:746:ILE:HG23 | 1:B:801:PHE:CE1 | 2.53 | 0.43 |
| 1:B:869:SER:C | 1:B:871:ASN:N | 2.66 | 0.43 |
| 1:C:177:LEU:HD13 | 1:C:179:GLY:N | 2.34 | 0.43 |
| 1:C:207:ILE:HG22 | 1:C:760:ASN:ND2 | 2.33 | 0.43 |
| 1:A:140:VAL:HG22 | 1:A:140:VAL:O | 2.17 | 0.43 |
| 1:A:379:THR:CG2 | 1:A:383:LEU:HD21 | 2.47 | 0.43 |
| 1:A:696:THR:O | 1:A:699:ARG:HB3 | 2.18 | 0.43 |
| 1:B:83:ASP:HA | 1:B:815:ARG:N | 2.30 | 0.43 |
| 1:B:353:LEU:C | 1:B:355:MET:H | 2.20 | 0.43 |
| 1:B:495:THR:HG22 | 1:B:496:MET:CG | 2.48 | 0.43 |
| 1:B:497:LEU:HD12 | 1:B:497:LEU:HA | 1.73 | 0.43 |
| 1:B:754:TRP:CH2 | 1:B:780:ARG:HA | 2.54 | 0.43 |
| 1:B:997:SER:O | 1:B:1000:GLN:N | 2.52 | 0.43 |
| 1:C:263:ARG:HG3 | 1:C:263:ARG:H | 1.57 | 0.43 |
| 1:C:577:GLN:HE22 | 1:C:623:ASN:HD21 | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:614:GLY:HA2 | 1:C:621:GLY:O | 2.19 | 0.43 |
| 1:C:741:VAL:HG12 | 1:C:746:ILE:HD13 | 1.97 | 0.43 |
| 2:D:50:PRO:CA | 2:D:53:LEU:HD23 | 2.49 | 0.43 |
| 2:E:28:ASP:O | 2:E:32:ILE:HG13 | 2.19 | 0.43 |
| 2:E:143:ASP:O | 2:E:144:LYS:C | 2.55 | 0.43 |
| 1:A:52:ALA:C | 1:A:53:ASP:O | 2.54 | 0.43 |
| 1:A:431:THR:HG22 | 1:A:432:ARG:H | 1.82 | 0.43 |
| 1:A:538:THR:C | 1:A:540:ARG:N | 2.69 | 0.43 |
| 1:B:351:VAL:O | 1:B:355:MET:CB | 2.66 | 0.43 |
| 1:B:391:ASN:O | 1:B:395:MET:HG3 | 2.19 | 0.43 |
| 1:B:448:VAL:O | 1:B:452:VAL:HG23 | 2.19 | 0.43 |
| 1:B:774:MET:SD | 1:B:780:ARG:NH1 | 2.91 | 0.43 |
| 1:C:5:PHE:C | 1:C:7:ASP:N | 2.69 | 0.43 |
| 1:C:522:LYS:HG2 | 1:C:526:HIS:HE1 | 1.83 | 0.43 |
| 1:C:1019:ILE:HD12 | 1:C:1019:ILE:HA | 1.84 | 0.43 |
| 2:E:100:LEU:HA | 2:E:100:LEU:HD23 | 1.64 | 0.43 |
| 1:A:187:TRP:O | 1:A:266:ALA:HA | 2.18 | 0.43 |
| 1:A:961:ILE:O | 1:A:961:ILE:HD13 | 2.19 | 0.43 |
| 1:B:351:VAL:HG13 | 1:B:410:ILE:HD11 | 2.00 | 0.43 |
| 1:B:566:ASP:OD1 | 1:B:566:ASP:N | 2.52 | 0.43 |
| 1:C:822:LEU:N | 1:C:822:LEU:HD12 | 2.33 | 0.43 |
| 1:C:925:VAL:O | 1:C:927:PHE:N | 2.51 | 0.43 |
| 1:A:14:VAL:HG13 | 1:B:886:LEU:HD12 | 2.01 | 0.43 |
| 1:A:314:GLU:C | 1:A:316:PHE:H | 2.22 | 0.43 |
| 1:A:497:LEU:CA | 1:A:498:LYS:HE2 | 2.49 | 0.43 |
| 1:A:973:ARG:O | 1:A:977:MET:CG | 2.53 | 0.43 |
| 1:B:753:ALA:HB1 | 1:B:789:TRP:CZ2 | 2.54 | 0.43 |
| 1:C:213:GLN:HG2 | 1:C:239:ARG:HD3 | 2.00 | 0.43 |
| 1:C:318:PRO:C | 1:C:319:SER:OG | 2.55 | 0.43 |
| 1:C:578:LEU:N | 1:C:578:LEU:HD12 | 2.33 | 0.43 |
| 1:C:604:ASN:HD22 | 1:C:604:ASN:HA | 1.60 | 0.43 |
| 1:C:669:PRO:HG3 | 1:C:675:GLY:O | 2.19 | 0.43 |
| 1:C:945:ILE:HD11 | 1:C:1019:ILE:HD12 | 2.00 | 0.43 |
| 2:D:56:TYR:HD1 | 2:D:90:ARG:HE | 1.61 | 0.43 |
| 1:A:886:LEU:HB3 | 1:C:14:VAL:HG13 | 2.00 | 0.43 |
| 1:A:996:GLY:O | 1:A:999:ALA:HB3 | 2.19 | 0.43 |
| 1:B:102:ILE:O | 1:B:105:VAL:HG12 | 2.18 | 0.43 |
| 1:B:909:VAL:O | 1:B:912:ALA:HB3 | 2.18 | 0.43 |
| 1:C:185:ARG:HG3 | 1:C:271:GLY:HA3 | 2.00 | 0.43 |
| 1:C:911:GLY:CA | 1:C:1013:THR:OG1 | 2.64 | 0.43 |
| 1:A:45:ILE:HG12 | 1:A:111:LEU:HD12 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:158:VAL:CG1 | 1:A:289:LEU:HD21 | 2.49 | 0.42 |
| 1:A:360:GLN:CD | 1:A:513:PHE:CE1 | 2.93 | 0.42 |
| 1:B:353:LEU:HD12 | 1:B:353:LEU:N | 2.34 | 0.42 |
| 1:B:674:LEU:CD1 | 1:B:674:LEU:C | 2.85 | 0.42 |
| 1:B:702:LEU:HD11 | 1:B:844:MET:HE1 | 2.00 | 0.42 |
| 1:A:275:TYR:CD1 | 1:C:223:PRO:HD3 | 2.55 | 0.42 |
| 1:A:570:GLY:N | 1:A:634:TRP:CH2 | 2.87 | 0.42 |
| 1:B:107:VAL:HG23 | 1:B:107:VAL:H | 1.44 | 0.42 |
| 1:B:687:GLN:HE22 | 1:B:859:TRP:CB | 2.32 | 0.42 |
| 1:B:814:PRO:O | 1:B:815:ARG:C | 2.57 | 0.42 |
| 1:B:871:ASN:HA | 1:B:872:GLN:HA | 1.35 | 0.42 |
| 1:B:1022:VAL:N | 1:B:1023:PRO:CD | 2.82 | 0.42 |
| 1:C:372:VAL:N | 1:C:373:PRO:HD2 | 2.34 | 0.42 |
| 1:C:719:ASN:HB2 | 1:C:828:LEU:HD11 | 2.00 | 0.42 |
| 2:D:44:ASP:CG | 2:D:45:HIS:HB3 | 2.37 | 0.42 |
| 1:A:489:THR:CG2 | 1:A:490:PRO:CD | 2.95 | 0.42 |
| 1:A:814:PRO:HG2 | 1:A:815:ARG:H | 1.85 | 0.42 |
| 1:B:5:PHE:CD1 | 1:B:487:ILE:HG12 | 2.55 | 0.42 |
| 1:B:11:PHE:CE2 | 1:C:890:ALA:HB1 | 2.54 | 0.42 |
| 1:B:160:ALA:HB3 | 1:B:161:ASN:HD21 | 1.85 | 0.42 |
| 1:B:371:ALA:HB2 | 1:B:489:THR:CG2 | 2.48 | 0.42 |
| 1:B:915:ALA:HB2 | 1:B:1009:GLY:HA3 | 2.00 | 0.42 |
| 1:C:231:ASN:O | 1:C:231:ASN:CG | 2.56 | 0.42 |
| 1:C:742:SER:HB3 | 1:C:745:ASP:HB2 | 2.00 | 0.42 |
| 1:C:793:ALA:HB3 | 1:C:797:GLN:H | 1.84 | 0.42 |
| 1:A:60:THR:HG22 | 1:A:61:VAL:HG23 | 2.01 | 0.42 |
| 1:A:912:ALA:O | 1:A:927:PHE:CE2 | 2.73 | 0.42 |
| 1:B:199:THR:CG2 | 1:B:792:ARG:H | 2.33 | 0.42 |
| 1:B:799:VAL:HG12 | 1:B:800:PRO:HD2 | 1.84 | 0.42 |
| 1:B:991:ILE:HG23 | 1:B:992:SER:N | 2.33 | 0.42 |
| 1:C:597:TYR:CD2 | 1:C:597:TYR:C | 2.93 | 0.42 |
| 2:D:27:ASP:HB3 | 2:D:62:ILE:CG1 | 2.49 | 0.42 |
| 1:A:302:THR:O | 1:A:306:ILE:HG12 | 2.20 | 0.42 |
| 1:A:355:MET:HE2 | 1:A:368:PRO:HG2 | 2.01 | 0.42 |
| 1:A:539:GLY:O | 1:A:540:ARG:C | 2.58 | 0.42 |
| 1:A:912:ALA:O | 1:A:927:PHE:HE2 | 2.03 | 0.42 |
| 1:A:975:ILE:O | 1:A:979:SER:HB2 | 2.18 | 0.42 |
| 1:A:990:VAL:HG11 | 1:A:1008:MET:HE2 | 2.02 | 0.42 |
| 1:B:212:ALA:O | 1:B:237:GLN:HG3 | 2.20 | 0.42 |
| 1:B:931:LEU:O | 1:B:935:ILE:HG13 | 2.19 | 0.42 |
| 1:C:412:VAL:HA | 1:C:438:ILE:CD1 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:431:THR:O | 1:C:435:MET:CG | 2.67 | 0.42 |
| 1:C:943:ILE:O | 1:C:947:GLU:HB3 | 2.19 | 0.42 |
| 2:E:25:GLY:HA3 | 2:E:59:HIS:CE1 | 2.55 | 0.42 |
| 1:A:66:GLU:O | 1:C:168:ARG:NH1 | 2.53 | 0.42 |
| 1:A:537:SER:HB3 | 1:A:541:TYR:CD1 | 2.55 | 0.42 |
| 1:B:377:LEU:HD12 | 1:B:377:LEU:HA | 1.63 | 0.42 |
| 1:B:690:LEU:HD11 | 1:B:857:TYR:CB | 2.50 | 0.42 |
| 1:B:961:ILE:HG22 | 1:B:965:LEU:HD13 | 2.02 | 0.42 |
| 1:C:65:ILE:O | 1:C:69:MET:CG | 2.65 | 0.42 |
| 1:C:162:MET:O | 1:C:163:LYS:C | 2.55 | 0.42 |
| 1:C:453:PHE:O | 1:C:456:MET:HG2 | 2.20 | 0.42 |
| 1:C:632:LYS:O | 1:C:633:ASP:C | 2.58 | 0.42 |
| 1:A:74:ASN:O | 1:A:95:GLU:HG2 | 2.20 | 0.42 |
| 1:A:570:GLY:HA3 | 1:A:634:TRP:CH2 | 2.54 | 0.42 |
| 1:B:182:TYR:HB3 | 1:B:270:LEU:HD21 | 2.02 | 0.42 |
| 1:B:184:MET:HE3 | 1:B:268:ILE:HG22 | 2.02 | 0.42 |
| 1:B:764:ASP:HB3 | 1:B:769:LYS:HD2 | 2.02 | 0.42 |
| 1:B:828:LEU:HD12 | 1:B:828:LEU:O | 2.20 | 0.42 |
| 1:C:254:ASN:C | 1:C:256:ASP:H | 2.23 | 0.42 |
| 1:C:980:LEU:HA | 1:C:980:LEU:HD13 | 1.73 | 0.42 |
| 2:D:53:LEU:HD23 | 2:D:53:LEU:N | 2.03 | 0.42 |
| 1:A:600:THR:O | 1:A:603:LYS:HG2 | 2.20 | 0.42 |
| 1:A:841:MET:O | 1:A:844:MET:HB2 | 2.20 | 0.42 |
| 1:B:156:ASP:CB | 1:B:182:TYR:CD2 | 2.98 | 0.42 |
| 1:B:519:MET:CG | 1:B:520:PHE:N | 2.78 | 0.42 |
| 1:B:671:ILE:CG2 | 1:B:673:GLU:N | 2.82 | 0.42 |
| 1:B:777:ALA:HA | 1:B:780:ARG:HH21 | 1.85 | 0.42 |
| 1:C:142:VAL:HG13 | 1:C:322:LYS:O | 2.20 | 0.42 |
| 1:C:277:ILE:N | 1:C:277:ILE:HD12 | 2.34 | 0.42 |
| 1:C:507:GLU:HB2 | 1:C:508:GLY:H | 1.58 | 0.42 |
| 1:C:571:VAL:HB | 1:C:629:VAL:O | 2.19 | 0.42 |
| 1:B:511:GLY:HA2 | 1:B:512:PHE:C | 2.40 | 0.42 |
| 1:C:222:THR:HA | 1:C:224:PRO:HD3 | 2.02 | 0.42 |
| 1:C:567:GLU:OE2 | 1:C:996:GLY:CA | 2.68 | 0.42 |
| 1:C:898:PRO:O | 1:C:902:MET:HB2 | 2.20 | 0.42 |
| 1:A:470:PHE:CD1 | 1:A:929:VAL:HG11 | 2.55 | 0.42 |
| 1:A:580:ALA:CA | 1:A:623:ASN:ND2 | 2.81 | 0.42 |
| 1:A:973:ARG:HB3 | 1:A:974:PRO:HD3 | 2.01 | 0.42 |
| 1:B:575:MET:CG | 1:B:576:VAL:N | 2.76 | 0.42 |
| 1:B:623:ASN:O | 1:B:623:ASN:ND2 | 2.50 | 0.42 |
| 1:B:864:TYR:O | 1:B:865:GLN:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:342:LYS:O | 1:C:344:LEU:N | 2.53 | 0.42 |
| 1:C:454:VAL:HB | 1:C:455:PRO:CD | 2.48 | 0.42 |
| 1:C:528:THR:HG22 | 1:C:529:ASP:N | 2.34 | 0.42 |
| 1:C:761:ASP:HB3 | 1:C:768:VAL:HG12 | 1.99 | 0.42 |
| 1:C:988:PRO:O | 1:C:992:SER:HB3 | 2.20 | 0.42 |
| 1:A:310:LEU:HD12 | 1:A:313:MET:HE3 | 2.01 | 0.41 |
| 1:A:376:LEU:O | 1:A:379:THR:HB | 2.20 | 0.41 |
| 1:B:672:VAL:O | 1:B:672:VAL:HG13 | 2.19 | 0.41 |
| 1:B:715:SER:CB | 1:B:830:GLN:HE21 | 2.33 | 0.41 |
| 1:C:54:ALA:N | 1:C:84:SER:HA | 2.35 | 0.41 |
| 1:C:153:ASP:OD1 | 1:C:153:ASP:N | 2.52 | 0.41 |
| 1:C:154:ILE:HD12 | 1:C:155:SER:N | 2.24 | 0.41 |
| 1:C:185:ARG:HH22 | 1:C:774:MET:HE1 | 1.86 | 0.41 |
| 1:C:896:SER:OG | 1:C:897:ILE:HD13 | 2.04 | 0.41 |
| 1:C:934:THR:HA | 1:C:937:LEU:HD12 | 2.02 | 0.41 |
| 1:A:111:LEU:HD23 | 1:A:111:LEU:O | 2.20 | 0.41 |
| 1:A:900:SER:HA | 1:A:1025:PHE:HB3 | 2.02 | 0.41 |
| 1:A:971:ARG:HA | 1:A:971:ARG:HD2 | 1.49 | 0.41 |
| 1:A:975:ILE:O | 1:A:979:SER:CB | 2.68 | 0.41 |
| 1:A:1016:VAL:HG23 | 1:A:1017:LEU:CD1 | 2.45 | 0.41 |
| 1:B:74:ASN:OD1 | 1:B:74:ASN:N | 2.52 | 0.41 |
| 1:B:631:LEU:HD23 | 1:B:631:LEU:HA | 1.77 | 0.41 |
| 1:B:813:SER:HA | 1:B:814:PRO:HD2 | 1.90 | 0.41 |
| 1:C:555:LEU:HD11 | 1:C:914:LEU:CD2 | 2.49 | 0.41 |
| 1:C:795:ASP:OD1 | 1:C:797:GLN:HG2 | 2.20 | 0.41 |
| 1:C:987:MET:O | 1:C:989:LEU:N | 2.53 | 0.41 |
| 1:A:405:LEU:HD11 | 1:A:477:ALA:HB1 | 2.02 | 0.41 |
| 1:A:774:MET:CG | 1:A:775:SER:H | 2.33 | 0.41 |
| 1:B:25:LEU:HD12 | 1:B:25:LEU:O | 2.19 | 0.41 |
| 1:B:254:ASN:ND2 | 1:B:258:SER:CB | 2.69 | 0.41 |
| 1:B:938:SER:HB3 | 1:B:1014:ALA:HB1 | 2.02 | 0.41 |
| 1:C:177:LEU:HD23 | 1:C:289:LEU:CD1 | 2.51 | 0.41 |
| 1:C:199:THR:HB | 1:C:200:PRO:CD | 2.50 | 0.41 |
| 2:D:106:VAL:O | 2:D:116:PRO:HD2 | 2.20 | 0.41 |
| 1:A:189:ASN:OD1 | 1:A:779:TYR:CZ | 2.73 | 0.41 |
| 1:B:352:PHE:HD2 | 1:B:353:LEU:CD1 | 2.31 | 0.41 |
| 1:B:456:MET:CG | 1:B:467:TYR:HB3 | 2.49 | 0.41 |
| 1:C:72:ILE:HG21 | 1:C:94:PHE:HE2 | 1.85 | 0.41 |
| 1:C:564:LEU:HA | 1:C:565:PRO:HD3 | 1.86 | 0.41 |
| 1:C:569:GLN:C | 1:C:634:TRP:HZ2 | 2.24 | 0.41 |
| 1:A:198:LEU:HD23 | 1:A:198:LEU:HA | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:487:ILE:HG22 | 1:A:488:LEU:N | 2.36 | 0.41 |
| 1:A:535:LEU:HD23 | 1:A:535:LEU:HA | 1.80 | 0.41 |
| 1:A:789:TRP:C | 1:A:790:TYR:HD2 | 2.23 | 0.41 |
| 1:C:682:PHE:CE2 | 1:C:684:LEU:HD23 | 2.51 | 0.41 |
| 1:A:67:GLN:NE2 | 1:C:767:ARG:HH11 | 2.15 | 0.41 |
| 1:B:10:ILE:HD12 | 1:C:895:TRP:HE1 | 1.86 | 0.41 |
| 1:B:138:MET:HE3 | 1:B:325:TYR:CD2 | 2.56 | 0.41 |
| 1:B:184:MET:HE3 | 1:B:268:ILE:CG2 | 2.51 | 0.41 |
| 1:B:876:LEU:H | 1:B:876:LEU:HG | 1.30 | 0.41 |
| 1:C:454:VAL:O | 1:C:455:PRO:C | 2.58 | 0.41 |
| 1:C:572:PHE:CE2 | 1:C:631:LEU:HD21 | 2.56 | 0.41 |
| 1:A:331:PRO:O | 1:A:335:ILE:HG13 | 2.20 | 0.41 |
| 1:A:393:LEU:HD13 | 1:A:466:ILE:HG23 | 2.03 | 0.41 |
| 1:A:492:LEU:O | 1:A:493:CYS:C | 2.57 | 0.41 |
| 1:A:731:ILE:H | 1:A:731:ILE:HG12 | 1.67 | 0.41 |
| 1:A:949:ALA:O | 1:A:953:MET:HG3 | 2.20 | 0.41 |
| 1:B:540:ARG:O | 1:B:544:LEU:CD1 | 2.69 | 0.41 |
| 1:B:971:ARG:O | 1:B:975:ILE:HG13 | 2.21 | 0.41 |
| 1:B:1013:THR:C | 1:B:1015:THR:H | 2.24 | 0.41 |
| 1:C:582:ALA:HB3 | 1:C:623:ASN:CB | 2.48 | 0.41 |
| 1:C:588:GLN:NE2 | 1:C:613:ASN:HD22 | 2.17 | 0.41 |
| 1:C:873:ALA:N | 1:C:874:PRO:CD | 2.83 | 0.41 |
| 1:A:131:LYS:O | 1:A:295:THR:OG1 | 2.36 | 0.41 |
| 1:A:330:THR:N | 1:A:331:PRO:CD | 2.84 | 0.41 |
| 1:A:505:HIS:CE1 | 1:A:973:ARG:HH12 | 2.39 | 0.41 |
| 1:A:569:GLN:O | 1:A:571:VAL:HG23 | 2.21 | 0.41 |
| 1:A:591:LEU:CD1 | 1:A:613:ASN:HD22 | 2.33 | 0.41 |
| 1:A:652:THR:HA | 1:A:655:PHE:CD2 | 2.48 | 0.41 |
| 1:B:303:ALA:O | 1:B:307:ARG:HB2 | 2.21 | 0.41 |
| 1:B:498:LYS:HA | 1:B:499:PRO:HD3 | 1.85 | 0.41 |
| 1:B:870:GLY:C | 1:B:871:ASN:OD1 | 2.59 | 0.41 |
| 1:B:937:LEU:O | 1:B:937:LEU:HD23 | 2.21 | 0.41 |
| 1:C:36:PRO:CD | 1:C:393:LEU:HD12 | 2.51 | 0.41 |
| 1:C:156:ASP:OD1 | 1:C:182:TYR:CG | 2.74 | 0.41 |
| 2:D:27:ASP:OD1 | 2:D:61:GLU:HG3 | 2.21 | 0.41 |
| 1:A:108:GLN:HE22 | 1:B:113:LEU:HG | 1.85 | 0.41 |
| 1:A:219:LEU:HD13 | 1:B:783:PRO:HG3 | 2.02 | 0.41 |
| 1:A:913:LEU:HD23 | 1:A:913:LEU:HA | 1.78 | 0.41 |
| 1:A:946:VAL:HG23 | 1:A:1026:PHE:CD1 | 2.56 | 0.41 |
| 1:B:246:PHE:O | 1:B:249:ILE:HG13 | 2.21 | 0.41 |
| 1:B:408:ASP:O | 1:B:412:VAL:HG23 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:420:MET:O | 1:B:423:GLU:O | 2.38 | 0.41 |
| 1:B:578:LEU:HD13 | 1:B:578:LEU:HA | 1.96 | 0.41 |
| 1:B:681:ASP:HB3 | 1:B:863:SER:O | 2.20 | 0.41 |
| 1:B:693:GLU:HA | 1:B:696:THR:HG22 | 2.03 | 0.41 |
| 1:B:846:GLN:O | 1:B:847:LEU:C | 2.58 | 0.41 |
| 1:B:851:LEU:HD12 | 1:B:851:LEU:H | 1.85 | 0.41 |
| 1:C:9:PRO:CD | 1:C:10:ILE:H | 2.34 | 0.41 |
| 1:C:158:VAL:HG12 | 1:C:159:ALA:N | 2.27 | 0.41 |
| 1:C:180:SER:CB | 1:C:274:ASN:H | 2.33 | 0.41 |
| 1:C:513:PHE:O | 1:C:514:GLY:C | 2.58 | 0.41 |
| 1:C:569:GLN:HE21 | 1:C:569:GLN:HB3 | 1.47 | 0.41 |
| 2:D:123:ILE:O | 2:D:123:ILE:HG12 | 2.21 | 0.41 |
| 2:E:46:VAL:CG1 | 2:E:47:GLY:N | 2.56 | 0.41 |
| 2:E:133:LEU:HD23 | 2:E:137:ALA:HA | 2.02 | 0.41 |
| 1:A:416:VAL:HG12 | 1:A:420:MET:HE2 | 2.03 | 0.41 |
| 1:A:454:VAL:N | 1:A:455:PRO:HD2 | 2.35 | 0.41 |
| 1:A:519:MET:HG3 | 1:A:520:PHE:H | 1.84 | 0.41 |
| 1:A:910:ILE:HD12 | 1:A:910:ILE:HA | 1.88 | 0.41 |
| 1:A:991:ILE:HD12 | 1:A:991:ILE:HA | 1.81 | 0.41 |
| 1:B:58:GLN:CG | 1:B:59:ASP:N | 2.82 | 0.41 |
| 1:B:187:TRP:O | 1:B:266:ALA:HA | 2.21 | 0.41 |
| 1:B:193:LEU:H | 1:B:193:LEU:CD2 | 2.06 | 0.41 |
| 1:B:249:ILE:O | 1:B:262:LEU:N | 2.48 | 0.41 |
| 1:C:115:MET:N | 1:C:116:PRO:CD | 2.84 | 0.41 |
| 1:C:351:VAL:O | 1:C:352:PHE:C | 2.57 | 0.41 |
| 2:E:121:ALA:CB | 2:E:152:ILE:HG12 | 2.50 | 0.41 |
| 1:A:293:LEU:HD11 | 1:A:299:ALA:HA | 2.03 | 0.40 |
| 1:B:537:SER:O | 1:B:541:TYR:CD1 | 2.73 | 0.40 |
| 1:B:582:ALA:HB3 | 1:B:623:ASN:HB3 | 2.02 | 0.40 |
| 1:B:919:ARG:HD3 | 1:B:1005:THR:HG21 | 2.03 | 0.40 |
| 1:B:987:MET:N | 1:B:988:PRO:CD | 2.83 | 0.40 |
| 1:B:1021:PHE:O | 1:B:1024:VAL:HB | 2.20 | 0.40 |
| 1:C:80:SER:HB3 | 1:C:90:ILE:HG23 | 2.02 | 0.40 |
| 1:C:154:ILE:CG1 | 1:C:155:SER:N | 2.81 | 0.40 |
| 1:C:632:LYS:O | 1:C:633:ASP:O | 2.38 | 0.40 |
| 2:D:112:ASN:HB3 | 2:D:114:PHE:CD2 | 2.56 | 0.40 |
| 1:A:542:LEU:O | 1:A:545:TYR:N | 2.48 | 0.40 |
| 1:A:637:ARG:N | 1:A:638:PRO:HD3 | 2.36 | 0.40 |
| 1:B:414:GLU:HG3 | 1:B:977:MET:CE | 2.51 | 0.40 |
| 1:B:543:VAL:O | 1:B:547:ILE:HG13 | 2.21 | 0.40 |
| 1:B:781:MET:HA | 1:B:781:MET:CE | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:869:SER:OG | 1:B:870:GLY:N | 2.54 | 0.40 |
| 1:C:314:GLU:C | 1:C:317:PHE:CD1 | 2.85 | 0.40 |
| 1:C:571:VAL:HG23 | 1:C:572:PHE:N | 2.37 | 0.40 |
| 1:A:150:THR:OG1 | 1:A:151:GLN:N | 2.55 | 0.40 |
| 1:A:158:VAL:HG12 | 1:A:289:LEU:HD21 | 2.03 | 0.40 |
| 1:A:306:ILE:HD13 | 1:A:306:ILE:HG23 | 1.71 | 0.40 |
| 1:A:489:THR:HB | 1:A:490:PRO:HD2 | 1.99 | 0.40 |
| 1:C:213:GLN:HE22 | 1:C:238:THR:HG22 | 1.86 | 0.40 |
| 1:C:483:LEU:O | 1:C:487:ILE:HB | 2.21 | 0.40 |
| 1:C:502:LYS:CG | 1:C:503:GLY:N | 2.77 | 0.40 |
| 1:C:568:ASP:HA | 1:C:644:VAL:HG22 | 2.02 | 0.40 |
| 2:D:44:ASP:HA | 2:D:45:HIS:HA | 1.53 | 0.40 |
| 2:E:79:LEU:HD22 | 2:E:111:HIS:NE2 | 2.36 | 0.40 |
| 1:A:109:ASN:O | 1:A:113:LEU:HD12 | 2.21 | 0.40 |
| 1:A:228:GLN:C | 1:B:583:THR:HG21 | 2.41 | 0.40 |
| 1:A:306:ILE:O | 1:A:307:ARG:C | 2.60 | 0.40 |
| 1:B:104:GLN:NE2 | 1:B:129:VAL:O | 2.54 | 0.40 |
| 1:B:142:VAL:HG13 | 1:B:321:LEU:HD11 | 2.03 | 0.40 |
| 1:B:734:GLU:O | 1:B:735:LYS:C | 2.58 | 0.40 |
| 1:B:790:TYR:CD1 | 1:B:800:PRO:CA | 3.04 | 0.40 |
| 1:C:457:ALA:CB | 1:C:468:ARG:HG2 | 2.49 | 0.40 |
| 1:C:733:GLN:HE22 | 1:C:743:ILE:HD13 | 1.85 | 0.40 |
| 2:D:52:HIS:NE2 | 2:D:83:PRO:HD3 | 2.37 | 0.40 |
| 1:A:309:GLU:O | 1:A:309:GLU:HG3 | 2.22 | 0.40 |
| 1:A:314:GLU:HA | 1:A:317:PHE:CE2 | 2.56 | 0.40 |
| 1:A:390:ILE:H | 1:A:390:ILE:HG12 | 1.73 | 0.40 |
| 1:A:531:VAL:O | 1:A:532:GLY:C | 2.59 | 0.40 |
| 1:A:699:ARG:O | 1:A:702:LEU:HB3 | 2.22 | 0.40 |
| 1:B:379:THR:O | 1:B:383:LEU:HG | 2.21 | 0.40 |
| 1:B:799:VAL:CG1 | 1:B:804:PHE:HE1 | 2.35 | 0.40 |
| 1:B:851:LEU:HD12 | 1:B:851:LEU:N | 2.36 | 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 | A | 1004/1049 (96%) | 919 (92%) | 78 (8%) | 7 (1%) | 22 | 57 |
| 1 | B | 1022/1049 (97%) | 941 (92%) | 73 (7%) | 8 (1%) | 19 | 53 |
| 1 | C | 1038/1049 (99%) | 954 (92%) | 80 (8%) | 4 (0%) | 34 | 68 |
| 2 | D | 152/169 (90%) | 141 (93%) | 10 (7%) | 1 (1%) | 22 | 57 |
| 2 | E | 147/169 (87%) | 136 (92%) | 10 (7%) | 1 (1%) | 22 | 57 |
| All | All | 3363/3485 (96%) | 3091 (92%) | 251 (8%) | 21 (1%) | 25 | 60 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 638 | PRO |
| 1 | B | 671 | ILE |
| 1 | C | 224 | PRO |
| 1 | B | 1014 | ALA |
| 1 | A | 315 | PRO |
| 1 | C | 633 | ASP |
| 2 | D | 70 | GLY |
| 1 | A | 184 | MET |
| 1 | B | 200 | PRO |
| 1 | B | 747 | ASN |
| 1 | B | 864 | TYR |
| 1 | C | 36 | PRO |
| 1 | B | 448 | VAL |
| 2 | E | 50 | PRO |
| 1 | A | 746 | ILE |
| 1 | A | 852 | PRO |
| 1 | A | 998 | GLY |
| 1 | A | 560 | PRO |
| 1 | B | 436 | GLY |
| 1 | A | 988 | PRO |
| 1 | C | 771 | VAL |

### 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 | A | 770/854 (90%) | 685 (89%) | 85 (11%) | 6 25 |
| 1 | B | 772/854 (90%) | 656 (85%) | 116 (15%) | 3 13 |
| 1 | C | 802/854 (94%) | 695 (87%) | 107 (13%) | 4 17 |
| 2 | D | 103/133 (77%) | 90 (87%) | 13 (13%) | 4 19 |
| 2 | E | 88/133 (66%) | 81 (92%) | 7 (8%) | 12 40 |
| All | All | 2535/2828 (90%) | 2207 (87%) | 328 (13%) | 4 18 |

All (328) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 25 | LEU |
| 1 | A | 30 | LEU |
| 1 | A | 32 | VAL |
| 1 | A | 46 | SER |
| 1 | A | 48 | SER |
| 1 | A | 65 | ILE |
| 1 | A | 74 | ASN |
| 1 | A | 75 | LEU |
| 1 | A | 78 | MET |
| 1 | A | 79 | SER |
| 1 | A | 82 | SER |
| 1 | A | 127 | VAL |
| 1 | A | 140 | VAL |
| 1 | A | 144 | ASN |
| 1 | A | 180 | SER |
| 1 | A | 197 | GLN |
| 1 | A | 205 | THR |
| 1 | A | 235 | ILE |
| 1 | A | 237 | GLN |
| 1 | A | 241 | THR |
| 1 | A | 244 | GLU |
| 1 | A | 262 | LEU |
| 1 | A | 264 | ASP |
| 1 | A | 269 | GLU |
| 1 | A | 278 | ILE |
| 1 | A | 295 | THR |
| 1 | A | 306 | ILE |
| 1 | A | 312 | LYS |
| 1 | A | 321 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 390 | ILE |
| 1 | A | 478 | MET |
| 1 | A | 486 | LEU |
| 1 | A | 488 | LEU |
| 1 | A | 489 | THR |
| 1 | A | 495 | THR |
| 1 | A | 497 | LEU |
| 1 | A | 498 | LYS |
| 1 | A | 519 | MET |
| 1 | A | 520 | PHE |
| 1 | A | 543 | VAL |
| 1 | A | 558 | ARG |
| 1 | A | 583 | THR |
| 1 | A | 586 | ARG |
| 1 | A | 587 | THR |
| 1 | A | 601 | LYS |
| 1 | A | 602 | GLU |
| 1 | A | 605 | ASN |
| 1 | A | 612 | VAL |
| 1 | A | 622 | GLN |
| 1 | A | 640 | GLU |
| 1 | A | 650 | ARG |
| 1 | A | 658 | ILE |
| 1 | A | 685 | ILE |
| 1 | A | 687 | GLN |
| 1 | A | 696 | THR |
| 1 | A | 717 | ARG |
| 1 | A | 723 | ASP |
| 1 | A | 754 | TRP |
| 1 | A | 757 | SER |
| 1 | A | 758 | TYR |
| 1 | A | 775 | SER |
| 1 | A | 780 | ARG |
| 1 | A | 795 | ASP |
| 1 | A | 807 | SER |
| 1 | A | 811 | TYR |
| 1 | A | 813 | SER |
| 1 | A | 815 | ARG |
| 1 | A | 822 | LEU |
| 1 | A | 823 | PRO |
| 1 | A | 830 | GLN |
| 1 | A | 847 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 860 | THR |
| 1 | A | 893 | GLU |
| 1 | A | 894 | SER |
| 1 | A | 900 | SER |
| 1 | A | 917 | THR |
| 1 | A | 932 | LEU |
| 1 | A | 935 | ILE |
| 1 | A | 953 | MET |
| 1 | A | 956 | GLU |
| 1 | A | 961 | ILE |
| 1 | A | 971 | ARG |
| 1 | A | 972 | LEU |
| 1 | A | 976 | LEU |
| 1 | A | 978 | THR |
| 1 | B | 21 | LEU |
| 1 | B | 46 | SER |
| 1 | B | 49 | TYR |
| 1 | B | 53 | ASP |
| 1 | B | 58 | GLN |
| 1 | B | 60 | THR |
| 1 | B | 75 | LEU |
| 1 | B | 79 | SER |
| 1 | B | 80 | SER |
| 1 | B | 82 | SER |
| 1 | B | 87 | THR |
| 1 | B | 99 | ASP |
| 1 | B | 108 | GLN |
| 1 | B | 111 | LEU |
| 1 | B | 117 | LEU |
| 1 | B | 128 | SER |
| 1 | B | 143 | ILE |
| 1 | B | 150 | THR |
| 1 | B | 153 | ASP |
| 1 | B | 161 | ASN |
| 1 | B | 162 | MET |
| 1 | B | 163 | LYS |
| 1 | B | 166 | ILE |
| 1 | B | 170 | SER |
| 1 | B | 189 | ASN |
| 1 | B | 193 | LEU |
| 1 | B | 197 | GLN |
| 1 | B | 207 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 218 | GLN |
| 1 | B | 229 | GLN |
| 1 | B | 230 | LEU |
| 1 | B | 231 | ASN |
| 1 | B | 233 | SER |
| 1 | B | 235 | ILE |
| 1 | B | 237 | GLN |
| 1 | B | 250 | LEU |
| 1 | B | 253 | VAL |
| 1 | B | 259 | ARG |
| 1 | B | 274 | ASN |
| 1 | B | 278 | ILE |
| 1 | B | 284 | GLN |
| 1 | B | 289 | LEU |
| 1 | B | 306 | ILE |
| 1 | B | 321 | LEU |
| 1 | B | 329 | THR |
| 1 | B | 361 | ASN |
| 1 | B | 365 | THR |
| 1 | B | 366 | LEU |
| 1 | B | 369 | THR |
| 1 | B | 377 | LEU |
| 1 | B | 382 | VAL |
| 1 | B | 399 | VAL |
| 1 | B | 405 | LEU |
| 1 | B | 408 | ASP |
| 1 | B | 423 | GLU |
| 1 | B | 425 | LEU |
| 1 | B | 462 | SER |
| 1 | B | 493 | CYS |
| 1 | B | 495 | THR |
| 1 | B | 497 | LEU |
| 1 | B | 507 | GLU |
| 1 | B | 513 | PHE |
| 1 | B | 519 | MET |
| 1 | B | 540 | ARG |
| 1 | B | 555 | LEU |
| 1 | B | 557 | VAL |
| 1 | B | 566 | ASP |
| 1 | B | 577 | GLN |
| 1 | B | 587 | THR |
| 1 | B | 623 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 628 | PHE |
| 1 | B | 649 | MET |
| 1 | B | 658 | ILE |
| 1 | B | 669 | PRO |
| 1 | B | 671 | ILE |
| 1 | B | 674 | LEU |
| 1 | B | 687 | GLN |
| 1 | B | 695 | LEU |
| 1 | B | 705 | GLU |
| 1 | B | 712 | MET |
| 1 | B | 713 | LEU |
| 1 | B | 714 | THR |
| 1 | B | 717 | ARG |
| 1 | B | 723 | ASP |
| 1 | B | 731 | ILE |
| 1 | B | 733 | GLN |
| 1 | B | 757 | SER |
| 1 | B | 759 | VAL |
| 1 | B | 763 | ILE |
| 1 | B | 765 | ARG |
| 1 | B | 771 | VAL |
| 1 | B | 780 | ARG |
| 1 | B | 808 | ARG |
| 1 | B | 815 | ARG |
| 1 | B | 822 | LEU |
| 1 | B | 824 | SER |
| 1 | B | 825 | MET |
| 1 | B | 844 | MET |
| 1 | B | 853 | THR |
| 1 | B | 859 | TRP |
| 1 | B | 862 | MET |
| 1 | B | 867 | ARG |
| 1 | B | 871 | ASN |
| 1 | B | 874 | PRO |
| 1 | B | 876 | LEU |
| 1 | B | 888 | LEU |
| 1 | B | 894 | SER |
| 1 | B | 919 | ARG |
| 1 | B | 968 | VAL |
| 1 | B | 971 | ARG |
| 1 | B | 972 | LEU |
| 1 | B | 987 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 989 | LEU |
| 1 | B | 990 | VAL |
| 1 | B | 991 | ILE |
| 1 | B | 1028 | VAL |
| 1 | C | 4 | PHE |
| 1 | C | 11 | PHE |
| 1 | C | 49 | TYR |
| 1 | C | 56 | THR |
| 1 | C | 58 | GLN |
| 1 | C | 81 | ASN |
| 1 | C | 84 | SER |
| 1 | C | 85 | THR |
| 1 | C | 88 | VAL |
| 1 | C | 98 | THR |
| 1 | C | 127 | VAL |
| 1 | C | 133 | SER |
| 1 | C | 143 | ILE |
| 1 | C | 145 | THR |
| 1 | C | 148 | THR |
| 1 | C | 150 | THR |
| 1 | C | 154 | ILE |
| 1 | C | 157 | TYR |
| 1 | C | 161 | ASN |
| 1 | C | 167 | SER |
| 1 | C | 182 | TYR |
| 1 | C | 197 | GLN |
| 1 | C | 218 | GLN |
| 1 | C | 226 | LYS |
| 1 | C | 233 | SER |
| 1 | C | 241 | THR |
| 1 | C | 263 | ARG |
| 1 | C | 268 | ILE |
| 1 | C | 278 | ILE |
| 1 | C | 289 | LEU |
| 1 | C | 298 | ASN |
| 1 | C | 310 | LEU |
| 1 | C | 321 | LEU |
| 1 | C | 325 | TYR |
| 1 | C | 329 | THR |
| 1 | C | 372 | VAL |
| 1 | C | 404 | LEU |
| 1 | C | 429 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 435 | MET |
| 1 | C | 437 | GLN |
| 1 | C | 452 | VAL |
| 1 | C | 466 | ILE |
| 1 | C | 473 | THR |
| 1 | C | 497 | LEU |
| 1 | C | 505 | HIS |
| 1 | C | 507 | GLU |
| 1 | C | 510 | LYS |
| 1 | C | 512 | PHE |
| 1 | C | 528 | THR |
| 1 | C | 542 | LEU |
| 1 | C | 561 | SER |
| 1 | C | 566 | ASP |
| 1 | C | 567 | GLU |
| 1 | C | 569 | GLN |
| 1 | C | 571 | VAL |
| 1 | C | 575 | MET |
| 1 | C | 587 | THR |
| 1 | C | 604 | ASN |
| 1 | C | 623 | ASN |
| 1 | C | 626 | ILE |
| 1 | C | 631 | LEU |
| 1 | C | 640 | GLU |
| 1 | C | 641 | GLU |
| 1 | C | 674 | LEU |
| 1 | C | 684 | LEU |
| 1 | C | 690 | LEU |
| 1 | C | 695 | LEU |
| 1 | C | 712 | MET |
| 1 | C | 715 | SER |
| 1 | C | 717 | ARG |
| 1 | C | 721 | LEU |
| 1 | C | 723 | ASP |
| 1 | C | 730 | ASP |
| 1 | C | 732 | ASP |
| 1 | C | 739 | LEU |
| 1 | C | 742 | SER |
| 1 | C | 743 | ILE |
| 1 | C | 744 | ASN |
| 1 | C | 749 | THR |
| 1 | C | 757 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 774 | MET |
| 1 | C | 782 | LEU |
| 1 | C | 805 | SER |
| 1 | C | 815 | ARG |
| 1 | C | 830 | GLN |
| 1 | C | 862 | MET |
| 1 | C | 869 | SER |
| 1 | C | 875 | SER |
| 1 | C | 876 | LEU |
| 1 | C | 879 | ILE |
| 1 | C | 880 | SER |
| 1 | C | 891 | LEU |
| 1 | C | 910 | ILE |
| 1 | C | 917 | THR |
| 1 | C | 922 | THR |
| 1 | C | 924 | ASP |
| 1 | C | 947 | GLU |
| 1 | C | 951 | ASP |
| 1 | C | 956 | GLU |
| 1 | C | 960 | LEU |
| 1 | C | 976 | LEU |
| 1 | C | 978 | THR |
| 1 | C | 979 | SER |
| 1 | C | 990 | VAL |
| 1 | C | 993 | THR |
| 1 | C | 1011 | MET |
| 1 | C | 1035 | ARG |
| 2 | D | 18 | LEU |
| 2 | D | 27 | ASP |
| 2 | D | 41 | ASN |
| 2 | D | 45 | HIS |
| 2 | D | 46 | VAL |
| 2 | D | 53 | LEU |
| 2 | D | 73 | VAL |
| 2 | D | 77 | ASP |
| 2 | D | 78 | SER |
| 2 | D | 83 | PRO |
| 2 | D | 84 | LEU |
| 2 | D | 111 | HIS |
| 2 | D | 129 | VAL |
| 2 | E | 99 | LEU |
| 2 | E | 102 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 145 | PHE |
| 2 | E | 152 | ILE |
| 2 | E | 154 | ILE |
| 2 | E | 155 | ASP |
| 2 | E | 156 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 58 | GLN |
| 1 | A | 67 | GLN |
| 1 | A | 123 | GLN |
| 1 | A | 176 | GLN |
| 1 | A | 181 | GLN |
| 1 | A | 189 | ASN |
| 1 | A | 191 | ASN |
| 1 | A | 194 | ASN |
| 1 | A | 197 | GLN |
| 1 | A | 231 | ASN |
| 1 | A | 274 | ASN |
| 1 | A | 284 | GLN |
| 1 | A | 298 | ASN |
| 1 | A | 361 | ASN |
| 1 | A | 577 | GLN |
| 1 | A | 613 | ASN |
| 1 | A | 687 | GLN |
| 1 | A | 700 | ASN |
| 1 | A | 737 | GLN |
| 1 | A | 760 | ASN |
| 1 | A | 1000 | GLN |
| 1 | A | 1001 | ASN |
| 1 | B | 81 | ASN |
| 1 | B | 108 | GLN |
| 1 | B | 123 | GLN |
| 1 | B | 124 | GLN |
| 1 | B | 125 | GLN |
| 1 | B | 161 | ASN |
| 1 | B | 176 | GLN |
| 1 | B | 197 | GLN |
| 1 | B | 218 | GLN |
| 1 | B | 254 | ASN |
| 1 | B | 284 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 361 | ASN |
| 1 | B | 569 | GLN |
| 1 | B | 577 | GLN |
| 1 | B | 592 | ASN |
| 1 | B | 596 | HIS |
| 1 | B | 605 | ASN |
| 1 | B | 623 | ASN |
| 1 | B | 687 | GLN |
| 1 | B | 701 | GLN |
| 1 | B | 726 | GLN |
| 1 | B | 733 | GLN |
| 1 | B | 747 | ASN |
| 1 | B | 760 | ASN |
| 1 | B | 830 | GLN |
| 1 | B | 923 | ASN |
| 1 | B | 941 | ASN |
| 1 | C | 34 | GLN |
| 1 | C | 67 | GLN |
| 1 | C | 68 | ASN |
| 1 | C | 104 | GLN |
| 1 | C | 125 | GLN |
| 1 | C | 144 | ASN |
| 1 | C | 181 | GLN |
| 1 | C | 194 | ASN |
| 1 | C | 197 | GLN |
| 1 | C | 213 | GLN |
| 1 | C | 298 | ASN |
| 1 | C | 415 | ASN |
| 1 | C | 525 | HIS |
| 1 | C | 569 | GLN |
| 1 | C | 588 | GLN |
| 1 | C | 604 | ASN |
| 1 | C | 623 | ASN |
| 1 | C | 701 | GLN |
| 1 | C | 719 | ASN |
| 1 | C | 747 | ASN |
| 1 | C | 760 | ASN |
| 1 | C | 830 | GLN |
| 1 | C | 865 | GLN |
| 2 | D | 45 | HIS |
| 2 | D | 52 | HIS |
| 2 | D | 111 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 118 | HIS |
| 2 | E | 69 | ASN |
| 2 | E | 118 | HIS |
| 2 | E | 156 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | FME | B | 1 | 1 | 8,9,10 | 0.53 | 0 | 7,9,11 | 0.95 | 0 |
| 1 | FME | C | 1 | 1 | 8,9,10 | 0.59 | 0 | 7,9,11 | 0.61 | 0 |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.30 | 0 | 7,9,11 | 0.92 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | FME | B | 1 | 1 | - | 4/7/9/11 | - |
| 1 | FME | C | 1 | 1 | - | 3/7/9/11 | - |
| 1 | FME | A | 1 | 1 | - | 2/7/9/11 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | A | 1 | FME | O1-CN-N-CA |
| 1 | B | 1 | FME | O1-CN-N-CA |
| 1 | B | 1 | FME | CB-CA-N-CN |
| 1 | C | 1 | FME | CB-CG-SD-CE |
| 1 | C | 1 | FME | N-CA-CB-CG |
| 1 | A | 1 | FME | CB-CG-SD-CE |
| 1 | C | 1 | FME | C-CA-CB-CG |
| 1 | B | 1 | FME | N-CA-CB-CG |
| 1 | B | 1 | FME | C-CA-CB-CG |

There are no ring outliers.

3 monomers are involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | B | 1 | FME | 11 | 0 |
| 1 | C | 1 | FME | 6 | 0 |
| 1 | A | 1 | FME | 5 | 0 |

## 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

## 6.1 Protein, DNA and RNA chains

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 | A | 1007/1049 (95%) | -0.33 | 6 (0%) 89 90 | 30, 72, 139, 274 | 1 (0%) |
| 1 | B | 1027/1049 (97%) | -0.28 | 17 (1%) 70 69 | 26, 71, 142, 330 | 0 |
| 1 | C | 1037/1049 (98%) | -0.35 | 14 (1%) 75 75 | 26, 63, 126, 198 | 0 |
| 2 | D | 154/169 (91%) | 0.13 | 10 (6%) 18 20 | 30, 85, 134, 207 | 1 (0%) |
| 2 | E | 148/169 (87%) | 1.26 | 39 (26%) 0 0 | 70, 147, 256, 372 | 1 (0%) |
| All | All | 3373/3485 (96%) | -0.23 | 86 (2%) 57 56 | 26, 71, 152, 372 | 3 (0%) |

All (86) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | E | 32 | ILE | 5.3 |
| 2 | E | 36 | ASN | 5.2 |
| 1 | B | 134 | SER | 5.1 |
| 2 | E | 35 | ALA | 5.0 |
| 2 | D | 139 | VAL | 5.0 |
| 1 | B | 675 | GLY | 5.0 |
| 1 | B | 509 | LYS | 4.5 |
| 2 | E | 145 | PHE | 4.4 |
| 2 | E | 144 | LYS | 4.1 |
| 2 | E | 158 | ASN | 4.0 |
| 2 | E | 162 | ALA | 3.9 |
| 2 | D | 150 | PHE | 3.8 |
| 2 | E | 33 | LEU | 3.8 |
| 1 | C | 501 | ALA | 3.8 |
| 2 | E | 124 | GLY | 3.7 |
| 1 | B | 216 | ALA | 3.6 |
| 2 | E | 38 | ALA | 3.5 |
| 2 | E | 34 | MET | 3.5 |
| 2 | E | 82 | THR | 3.5 |
| 1 | A | 833 | PRO | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | D | 158 | ASN | 3.2 |
| 1 | B | 859 | TRP | 3.2 |
| 2 | D | 140 | ASN | 3.2 |
| 2 | E | 111 | HIS | 3.2 |
| 2 | D | 126 | LEU | 3.2 |
| 2 | E | 137 | ALA | 3.2 |
| 2 | E | 31 | ARG | 3.2 |
| 2 | E | 163 | GLU | 3.1 |
| 2 | E | 114 | PHE | 3.1 |
| 1 | B | 407 | ASP | 3.0 |
| 1 | C | 701 | GLN | 3.0 |
| 2 | E | 159 | GLU | 2.9 |
| 2 | D | 141 | ALA | 2.9 |
| 1 | C | 730 | ASP | 2.9 |
| 2 | E | 76 | ASP | 2.8 |
| 1 | A | 254 | ASN | 2.8 |
| 2 | E | 37 | GLY | 2.8 |
| 1 | C | 425 | LEU | 2.7 |
| 2 | E | 117 | LEU | 2.7 |
| 2 | D | 148 | THR | 2.7 |
| 1 | B | 361 | ASN | 2.7 |
| 1 | B | 674 | LEU | 2.7 |
| 2 | E | 166 | GLN | 2.7 |
| 2 | E | 66 | LEU | 2.6 |
| 1 | C | 424 | GLY | 2.6 |
| 1 | B | 628 | PHE | 2.5 |
| 1 | A | 860 | THR | 2.5 |
| 1 | A | 836 | SER | 2.5 |
| 1 | A | 678 | THR | 2.4 |
| 1 | C | 851 | LEU | 2.4 |
| 1 | A | 872 | GLN | 2.4 |
| 2 | E | 143 | ASP | 2.4 |
| 1 | B | 858 | ASP | 2.4 |
| 2 | D | 138 | ASP | 2.3 |
| 1 | B | 326 | PRO | 2.3 |
| 2 | E | 154 | ILE | 2.3 |
| 1 | C | 502 | LYS | 2.3 |
| 1 | C | 804 | PHE | 2.3 |
| 1 | C | 423 | GLU | 2.3 |
| 2 | E | 99 | LEU | 2.2 |
| 1 | B | 996 | GLY | 2.2 |
| 2 | E | 75 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | E | 54 | ALA | 2.2 |
| 2 | E | 69 | ASN | 2.2 |
| 2 | E | 64 | GLU | 2.2 |
| 1 | B | 771 | VAL | 2.2 |
| 2 | D | 137 | ALA | 2.2 |
| 2 | D | 161 | LEU | 2.2 |
| 2 | E | 126 | LEU | 2.1 |
| 2 | E | 141 | ALA | 2.1 |
| 1 | C | 791 | VAL | 2.1 |
| 2 | E | 122 | ASN | 2.1 |
| 1 | B | 617 | PHE | 2.1 |
| 2 | E | 45 | HIS | 2.1 |
| 2 | E | 48 | TRP | 2.1 |
| 1 | B | 599 | LEU | 2.1 |
| 2 | E | 112 | ASN | 2.1 |
| 1 | B | 501 | ALA | 2.1 |
| 2 | E | 87 | ALA | 2.1 |
| 1 | C | 193 | LEU | 2.1 |
| 1 | C | 806 | SER | 2.0 |
| 1 | C | 811 | TYR | 2.0 |
| 1 | B | 848 | ALA | 2.0 |
| 1 | C | 513 | PHE | 2.0 |
| 2 | E | 155 | ASP | 2.0 |
| 2 | E | 30 | VAL | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | FME | B | 1 | 10/11 | 0.85 | 0.24 | 68,71,78,80 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.87 | 0.18 | 87,88,108,109 | 0 |
| 1 | FME | C | 1 | 10/11 | 0.94 | 0.13 | 62,64,181,181 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.