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

Aug 8, 2016 – 04:21 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 5L5L |
| Title | : | Plexin A4 full extracellular region, domains 1 to 8 modeled, data to 8 angstrom, spacegroup P2(1) |
| Authors | : | Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y. |
| Deposited on | : | 2016-05-28 |
| Resolution | : | 8.00 Å(reported) |

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

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

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

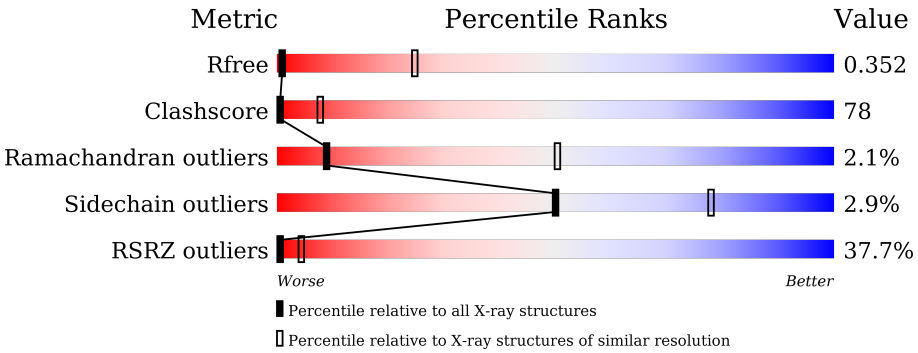
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20027939 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20027939 |

# 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 8.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1015 (11.50-3.66) |
| Clashscore | 102246 | 1064 (11.50-3.70) |
| Ramachandran outliers | 100387 | 1036 (11.50-3.66) |
| Sidechain outliers | 100360 | 1006 (11.50-3.66) |
| RSRZ outliers | 91569 | 1014 (11.50-3.66) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 | 1207 | 33% 27% 52% · 17% |
| 1 | B | 1207 | 27% 25% 47% · 24% |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15030 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 Plexin-A4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1000 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7841 | 4938 | 1356 | 1482 | 65 | | | |
| 1 | B | 915 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7189 | 4533 | 1239 | 1357 | 60 | | | |

There are 26 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 33 | GLU | - | expression tag | UNP Q80UG2 |
| A | 34 | THR | - | expression tag | UNP Q80UG2 |
| A | 35 | GLY | - | expression tag | UNP Q80UG2 |
| A | 1230 | GLY | - | expression tag | UNP Q80UG2 |
| A | 1231 | ARG | - | expression tag | UNP Q80UG2 |
| A | 1232 | THR | - | expression tag | UNP Q80UG2 |
| A | 1233 | LYS | - | expression tag | UNP Q80UG2 |
| A | 1234 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1235 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1236 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1237 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1238 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1239 | HIS | - | expression tag | UNP Q80UG2 |
| B | 33 | GLU | - | expression tag | UNP Q80UG2 |
| B | 34 | THR | - | expression tag | UNP Q80UG2 |
| B | 35 | GLY | - | expression tag | UNP Q80UG2 |
| B | 1230 | GLY | - | expression tag | UNP Q80UG2 |
| B | 1231 | ARG | - | expression tag | UNP Q80UG2 |
| B | 1232 | THR | - | expression tag | UNP Q80UG2 |
| B | 1233 | LYS | - | expression tag | UNP Q80UG2 |
| B | 1234 | HIS | - | expression tag | UNP Q80UG2 |
| B | 1235 | HIS | - | expression tag | UNP Q80UG2 |
| B | 1236 | HIS | - | expression tag | UNP Q80UG2 |
| B | 1237 | HIS | - | expression tag | UNP Q80UG2 |
| B | 1238 | HIS | - | expression tag | UNP Q80UG2 |

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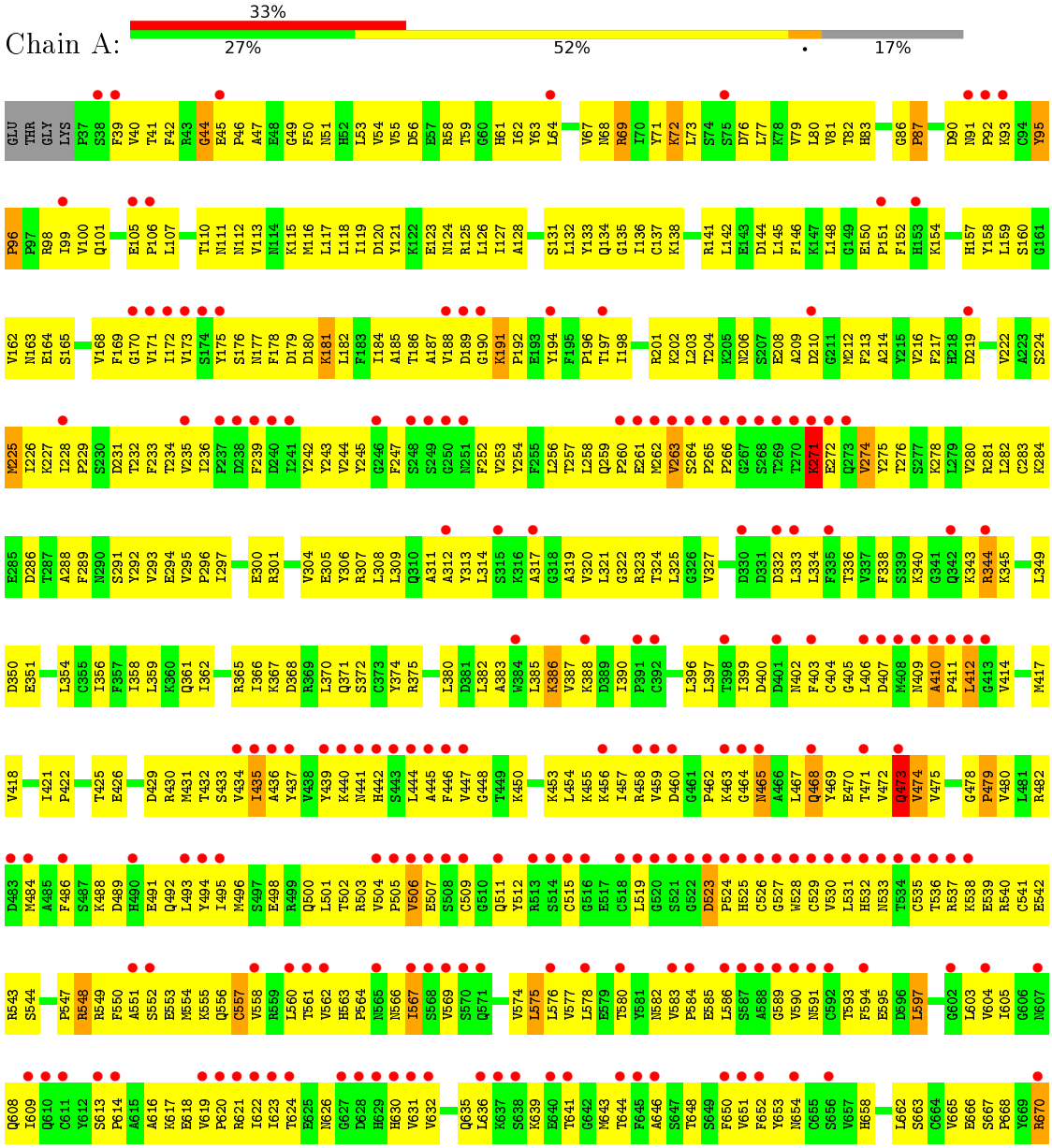
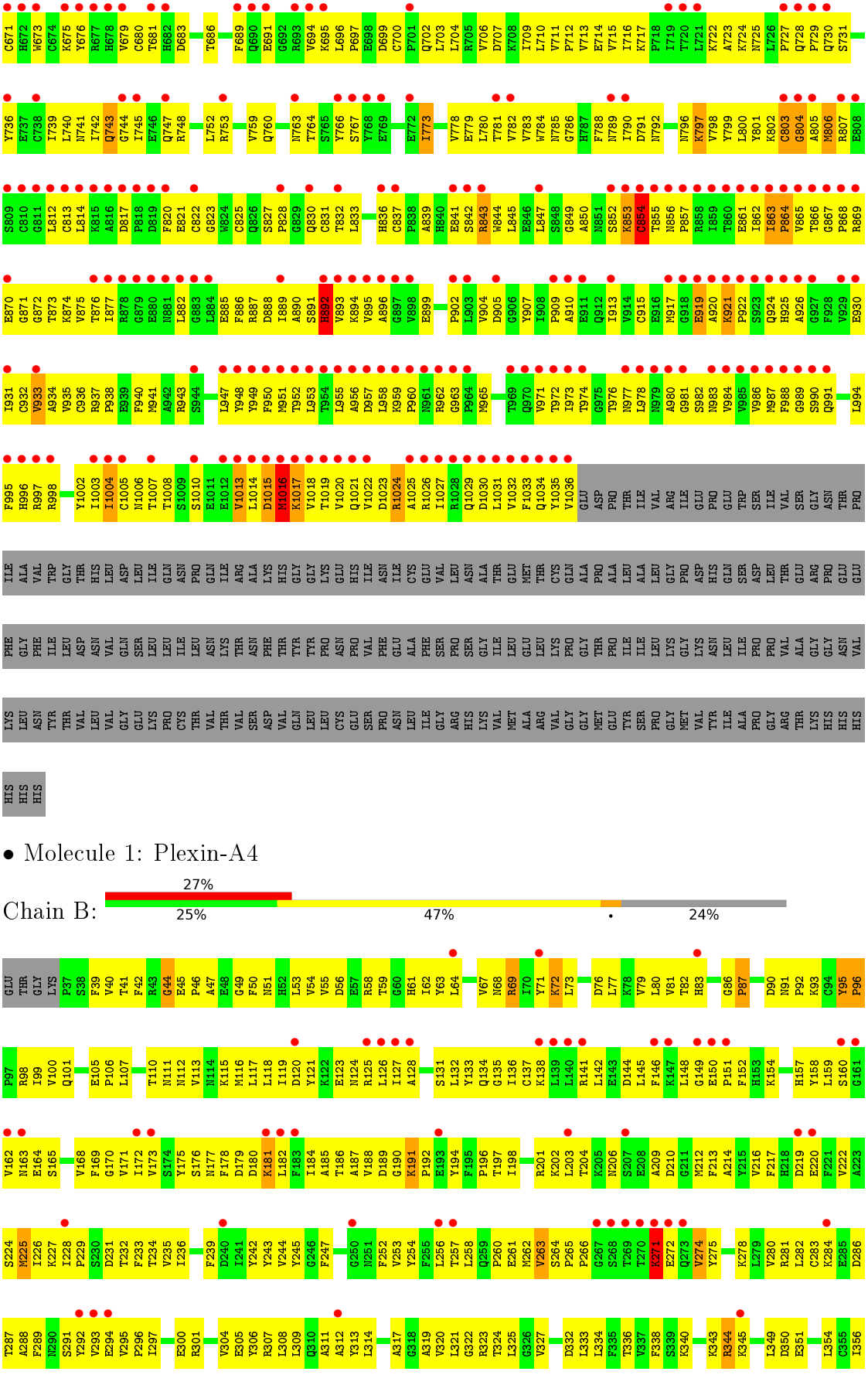
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 1239 | HIS | - | expression tag | UNP Q80UG2 |

# 3 Residue-property plots (i)

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

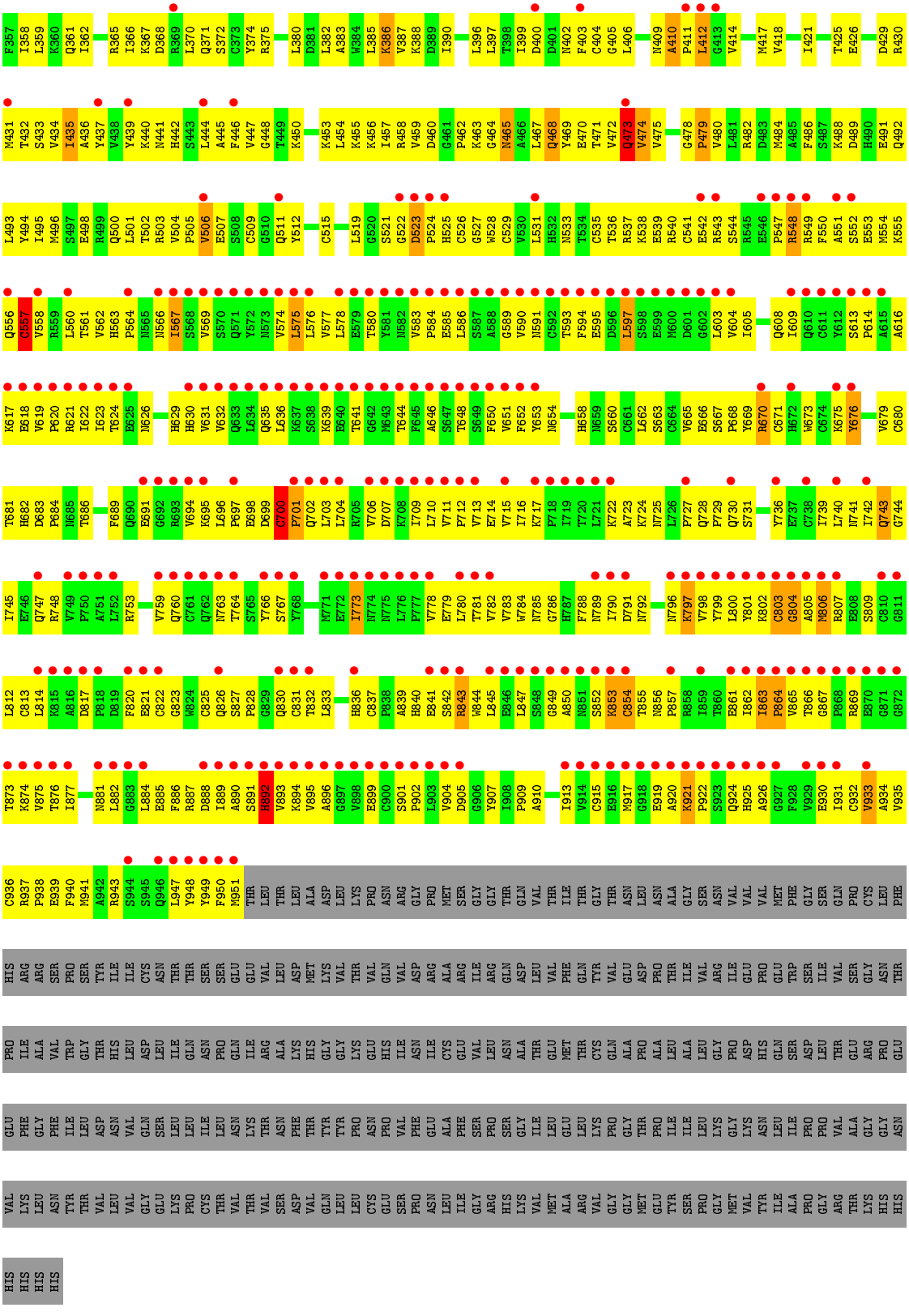
- Molecule 1: Plexin-A4





• Molecule 1: Plexin-A4

Chain B:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 142.18Å 241.00Å 144.07Å<br>90.00° 99.83° 90.00° | Depositor |
| Resolution (Å) | 47.74 – 8.00<br>47.74 – 8.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.1 (47.74-8.00)<br>99.5 (47.74-8.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.16 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.18 (at 8.32Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1309) | Depositor |
| R, $R_{free}$ | 0.349 , 0.349<br>0.344 , 0.352 | Depositor<br>DCC |
| $R_{free}$ test set | 488 reflections (4.86%) | DCC |
| Wilson B-factor (Å$^2$) | 450.9 | Xtriage |
| Anisotropy | 0.543 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.40 , 548.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.43$, $< L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | 0.043 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.70 | EDS |
| Total number of atoms | 15030 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 264.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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

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 | 1.01 | 5/8007 (0.1%) | 1.36 | 27/10846 (0.2%) |
| 1 | B | 1.00 | 5/7344 (0.1%) | 1.32 | 24/9943 (0.2%) |
| All | All | 1.01 | 10/15351 (0.1%) | 1.34 | 51/20789 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 3 |
| 1 | B | 0 | 4 |
| All | All | 0 | 7 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 506 | VAL | C-N | 23.13 | 1.87 | 1.34 |
| 1 | B | 506 | VAL | C-N | 21.10 | 1.82 | 1.34 |
| 1 | A | 557 | CYS | C-N | -20.82 | 0.86 | 1.34 |
| 1 | B | 557 | CYS | C-N | -17.13 | 0.94 | 1.34 |
| 1 | A | 700 | CYS | C-N | -15.63 | 1.04 | 1.34 |
| 1 | B | 700 | CYS | C-N | 15.54 | 1.63 | 1.34 |
| 1 | B | 49 | GLY | CA-C | 6.43 | 1.62 | 1.51 |
| 1 | A | 49 | GLY | CA-C | 6.42 | 1.62 | 1.51 |
| 1 | A | 49 | GLY | C-N | 5.06 | 1.45 | 1.34 |
| 1 | B | 49 | GLY | C-N | 5.05 | 1.45 | 1.34 |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 747 | GLN | CG-CD-OE1 | -38.83 | 43.94 | 121.60 |
| 1 | A | 747 | GLN | CG-CD-OE1 | -38.81 | 43.98 | 121.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 653 | TYR | O-C-N | -33.42 | 69.23 | 122.70 |
| 1 | B | 557 | CYS | O-C-N | -31.89 | 71.68 | 122.70 |
| 1 | A | 653 | TYR | CA-C-N | 23.37 | 168.61 | 117.20 |
| 1 | A | 854 | CYS | O-C-N | -23.21 | 85.56 | 122.70 |
| 1 | A | 557 | CYS | O-C-N | 18.53 | 152.35 | 122.70 |
| 1 | B | 557 | CYS | CA-C-N | 17.95 | 156.70 | 117.20 |
| 1 | B | 700 | CYS | C-N-CD | -17.94 | 81.14 | 120.60 |
| 1 | A | 557 | CYS | CA-C-N | -17.52 | 78.65 | 117.20 |
| 1 | B | 506 | VAL | O-C-N | 17.20 | 150.23 | 122.70 |
| 1 | A | 854 | CYS | C-N-CA | 16.73 | 163.51 | 121.70 |
| 1 | A | 653 | TYR | C-N-CA | 16.67 | 163.37 | 121.70 |
| 1 | B | 506 | VAL | CA-C-N | -16.51 | 80.87 | 117.20 |
| 1 | B | 506 | VAL | C-N-CA | -14.85 | 84.57 | 121.70 |
| 1 | A | 506 | VAL | O-C-N | -14.82 | 98.98 | 122.70 |
| 1 | A | 854 | CYS | CA-C-N | 13.98 | 147.96 | 117.20 |
| 1 | A | 557 | CYS | C-N-CA | -13.97 | 86.77 | 121.70 |
| 1 | B | 557 | CYS | C-N-CA | 11.36 | 150.09 | 121.70 |
| 1 | B | 747 | GLN | CG-CD-NE2 | -9.58 | 93.70 | 116.70 |
| 1 | A | 747 | GLN | CG-CD-NE2 | -9.56 | 93.76 | 116.70 |
| 1 | A | 700 | CYS | O-C-N | -8.60 | 104.76 | 121.10 |
| 1 | A | 479 | PRO | N-CA-C | 8.18 | 133.37 | 112.10 |
| 1 | B | 479 | PRO | N-CA-C | 8.16 | 133.31 | 112.10 |
| 1 | A | 843 | ARG | C-N-CA | 7.76 | 141.10 | 121.70 |
| 1 | B | 843 | ARG | C-N-CA | 7.75 | 141.07 | 121.70 |
| 1 | A | 747 | GLN | OE1-CD-NE2 | 6.89 | 137.74 | 121.90 |
| 1 | A | 478 | GLY | CA-C-O | -6.87 | 108.23 | 120.60 |
| 1 | B | 478 | GLY | CA-C-O | -6.85 | 108.27 | 120.60 |
| 1 | B | 747 | GLN | OE1-CD-NE2 | 6.84 | 137.63 | 121.90 |
| 1 | B | 473 | GLN | C-N-CA | -6.70 | 104.95 | 121.70 |
| 1 | A | 473 | GLN | C-N-CA | -6.69 | 104.97 | 121.70 |
| 1 | B | 892 | HIS | CA-CB-CG | 6.59 | 124.81 | 113.60 |
| 1 | A | 892 | HIS | CA-CB-CG | 6.57 | 124.77 | 113.60 |
| 1 | B | 700 | CYS | CA-C-N | -6.33 | 99.38 | 117.10 |
| 1 | A | 225 | MET | CG-SD-CE | -5.72 | 91.05 | 100.20 |
| 1 | B | 225 | MET | CG-SD-CE | -5.71 | 91.06 | 100.20 |
| 1 | A | 409 | ASN | C-N-CA | 5.67 | 135.87 | 121.70 |
| 1 | B | 409 | ASN | C-N-CA | 5.66 | 135.85 | 121.70 |
| 1 | A | 49 | GLY | C-N-CA | 5.62 | 135.74 | 121.70 |
| 1 | B | 49 | GLY | C-N-CA | 5.57 | 135.63 | 121.70 |
| 1 | B | 700 | CYS | O-C-N | -5.55 | 110.55 | 121.10 |
| 1 | A | 700 | CYS | CA-C-N | 5.48 | 132.43 | 117.10 |
| 1 | B | 274 | VAL | CG1-CB-CG2 | 5.47 | 119.65 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 274 | VAL | CG1-CB-CG2 | 5.45 | 119.61 | 110.90 |
| 1 | B | 919 | GLU | C-N-CA | 5.27 | 134.88 | 121.70 |
| 1 | A | 919 | GLU | C-N-CA | 5.24 | 134.81 | 121.70 |
| 1 | B | 676 | TYR | CA-CB-CG | -5.12 | 103.67 | 113.40 |
| 1 | A | 676 | TYR | CA-CB-CG | -5.11 | 103.70 | 113.40 |
| 1 | A | 803 | CYS | C-N-CA | 5.09 | 132.98 | 122.30 |
| 1 | B | 803 | CYS | C-N-CA | 5.08 | 132.96 | 122.30 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 854 | CYS | Mainchain |
| 1 | A | 863 | ILE | Peptide |
| 1 | A | 95 | TYR | Peptide |
| 1 | B | 557 | CYS | Mainchain |
| 1 | B | 700 | CYS | Mainchain |
| 1 | B | 863 | ILE | Peptide |
| 1 | B | 95 | TYR | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 7841 | 0 | 7710 | 1244 | 29 |
| 1 | B | 7189 | 0 | 7050 | 1075 | 59 |
| All | All | 15030 | 0 | 14760 | 2319 | 61 |

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 78.

All (2319) 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:868:PRO:HD2 | 1:A:981:GLY:CA | 1.32 | 1.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:868:PRO:CD | 1:A:981:GLY:CA | 1.87 | 1.50 |
| 1:A:873:THR:CA | 1:A:982:SER:HB2 | 1.46 | 1.43 |
| 1:A:873:THR:HA | 1:A:982:SER:CB | 1.48 | 1.40 |
| 1:B:506:VAL:HG22 | 1:B:525:HIS:NE2 | 1.33 | 1.38 |
| 1:B:629:HIS:CE1 | 1:B:669:TYR:OH | 1.76 | 1.37 |
| 1:B:629:HIS:ND1 | 1:B:669:TYR:OH | 1.56 | 1.34 |
| 1:A:870:GLU:CD | 1:A:1025:ALA:HB2 | 1.46 | 1.33 |
| 1:A:868:PRO:HD3 | 1:A:981:GLY:N | 1.06 | 1.33 |
| 1:B:506:VAL:N | 1:B:507:GLU:N | 1.77 | 1.29 |
| 1:B:506:VAL:C | 1:B:507:GLU:N | 1.82 | 1.28 |
| 1:A:868:PRO:CD | 1:A:981:GLY:N | 1.88 | 1.27 |
| 1:A:506:VAL:C | 1:A:507:GLU:N | 1.87 | 1.26 |
| 1:B:700:CYS:O | 1:B:725:ASN:HB2 | 1.38 | 1.23 |
| 1:A:870:GLU:HB3 | 1:A:1024:ARG:CG | 1.70 | 1.22 |
| 1:B:809:SER:CB | 1:B:881:ASN:OD1 | 1.89 | 1.19 |
| 1:B:809:SER:HB2 | 1:B:881:ASN:CG | 1.62 | 1.18 |
| 1:A:569:VAL:CG2 | 1:A:654:ASN:HB2 | 1.71 | 1.18 |
| 1:A:867:GLY:HA2 | 1:A:981:GLY:N | 1.59 | 1.17 |
| 1:A:359:LEU:HD12 | 1:A:362:ILE:HD11 | 1.24 | 1.17 |
| 1:B:118:LEU:HD12 | 1:B:172:ILE:HD12 | 1.17 | 1.17 |
| 1:B:456:LYS:HD2 | 1:B:523:ASP:OD2 | 1.44 | 1.17 |
| 1:A:868:PRO:HD3 | 1:A:980:ALA:C | 1.63 | 1.17 |
| 1:B:676:TYR:CE1 | 1:B:730:GLN:HG2 | 1.80 | 1.15 |
| 1:B:295:VAL:HG12 | 1:B:414:VAL:HG11 | 1.27 | 1.14 |
| 1:B:802:LYS:C | 1:B:803:CYS:N | 2.01 | 1.14 |
| 1:A:453:LYS:HG2 | 1:A:472:VAL:HG22 | 1.25 | 1.14 |
| 1:B:359:LEU:HD12 | 1:B:362:ILE:HD11 | 1.24 | 1.14 |
| 1:B:506:VAL:CG2 | 1:B:525:HIS:NE2 | 2.11 | 1.14 |
| 1:A:324:THR:HB | 1:A:462:PRO:HB3 | 1.27 | 1.13 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:HB3 | 1.31 | 1.12 |
| 1:A:118:LEU:HD12 | 1:A:172:ILE:HD12 | 1.17 | 1.12 |
| 1:A:435:ILE:HG22 | 1:A:446:PHE:HB2 | 1.22 | 1.12 |
| 1:A:295:VAL:HG12 | 1:A:414:VAL:HG11 | 1.27 | 1.12 |
| 1:B:453:LYS:HG2 | 1:B:472:VAL:HG22 | 1.25 | 1.12 |
| 1:B:809:SER:HB2 | 1:B:881:ASN:OD1 | 0.95 | 1.11 |
| 1:B:435:ILE:HG22 | 1:B:446:PHE:HB2 | 1.22 | 1.11 |
| 1:A:533:ASN:ND2 | 1:A:644:THR:O | 1.83 | 1.11 |
| 1:A:595:GLU:HB2 | 1:A:597:LEU:HD23 | 1.32 | 1.11 |
| 1:B:676:TYR:CD1 | 1:B:730:GLN:CG | 2.33 | 1.11 |
| 1:B:469:TYR:HB2 | 1:B:523:ASP:OD1 | 1.50 | 1.10 |
| 1:B:595:GLU:HB2 | 1:B:597:LEU:HD23 | 1.32 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:806:MET:H | 1:A:806:MET:HE3 | 1.14 | 1.10 |
| 1:B:324:THR:HB | 1:B:462:PRO:HB3 | 1.27 | 1.09 |
| 1:B:806:MET:HE3 | 1:B:806:MET:H | 1.14 | 1.09 |
| 1:A:868:PRO:CD | 1:A:981:GLY:HA3 | 1.61 | 1.09 |
| 1:A:871:GLY:O | 1:A:1023:ASP:CB | 2.00 | 1.09 |
| 1:B:444:LEU:HD23 | 1:B:524:PRO:CG | 1.83 | 1.08 |
| 1:A:1017:LYS:HE2 | 1:A:1017:LYS:H | 1.18 | 1.08 |
| 1:B:676:TYR:CE1 | 1:B:730:GLN:CG | 2.37 | 1.08 |
| 1:A:868:PRO:HD2 | 1:A:981:GLY:HA2 | 1.17 | 1.08 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:HG23 | 1.33 | 1.08 |
| 1:B:468:GLN:HG3 | 1:B:523:ASP:HA | 1.16 | 1.07 |
| 1:B:469:TYR:CB | 1:B:523:ASP:OD1 | 2.02 | 1.07 |
| 1:B:506:VAL:C | 1:B:507:GLU:CA | 2.21 | 1.07 |
| 1:A:870:GLU:CB | 1:A:1024:ARG:HG2 | 1.84 | 1.07 |
| 1:B:474:VAL:HG12 | 1:B:475:VAL:HG23 | 1.33 | 1.07 |
| 1:A:549:ARG:HD3 | 1:A:584:PRO:CB | 1.84 | 1.06 |
| 1:A:440:LYS:HB2 | 1:A:538:LYS:NZ | 1.68 | 1.06 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:NZ | 2.23 | 1.05 |
| 1:B:506:VAL:CA | 1:B:507:GLU:N | 2.17 | 1.05 |
| 1:B:676:TYR:CD1 | 1:B:730:GLN:HG3 | 1.91 | 1.05 |
| 1:A:569:VAL:HG21 | 1:A:654:ASN:HB2 | 1.32 | 1.04 |
| 1:B:506:VAL:HG22 | 1:B:525:HIS:CE1 | 1.92 | 1.04 |
| 1:B:444:LEU:HD23 | 1:B:524:PRO:HG3 | 1.37 | 1.03 |
| 1:B:494:TYR:HB3 | 1:B:501:LEU:HD21 | 1.40 | 1.03 |
| 1:B:301:ARG:HD2 | 1:B:425:THR:HG21 | 1.37 | 1.03 |
| 1:B:620:PRO:HA | 1:B:623:ILE:HG13 | 1.41 | 1.03 |
| 1:A:46:PRO:HG2 | 1:A:69:ARG:HG3 | 1.41 | 1.02 |
| 1:A:301:ARG:HD2 | 1:A:425:THR:HG21 | 1.37 | 1.02 |
| 1:A:560:LEU:HD23 | 1:A:648:THR:HG23 | 1.37 | 1.02 |
| 1:A:440:LYS:HD2 | 1:A:538:LYS:HD3 | 1.37 | 1.02 |
| 1:A:871:GLY:O | 1:A:1023:ASP:CG | 1.98 | 1.01 |
| 1:A:620:PRO:HA | 1:A:623:ILE:HG13 | 1.41 | 1.01 |
| 1:A:867:GLY:CA | 1:A:981:GLY:H | 1.72 | 1.01 |
| 1:A:494:TYR:HB3 | 1:A:501:LEU:HD21 | 1.40 | 1.01 |
| 1:B:676:TYR:CD1 | 1:B:730:GLN:HG2 | 1.94 | 1.00 |
| 1:B:560:LEU:HD23 | 1:B:648:THR:HG23 | 1.37 | 1.00 |
| 1:B:46:PRO:HG2 | 1:B:69:ARG:HG3 | 1.41 | 1.00 |
| 1:A:873:THR:OG1 | 1:A:981:GLY:HA2 | 1.60 | 0.99 |
| 1:B:117:LEU:HD11 | 1:B:126:LEU:HD21 | 1.45 | 0.99 |
| 1:A:117:LEU:HD11 | 1:A:126:LEU:HD21 | 1.45 | 0.99 |
| 1:A:870:GLU:CB | 1:A:1024:ARG:CG | 2.40 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:623:ILE:HA | 1:B:626:ASN:HD21 | 1.28 | 0.99 |
| 1:A:868:PRO:HD3 | 1:A:981:GLY:CA | 1.73 | 0.99 |
| 1:A:870:GLU:HB3 | 1:A:1024:ARG:HG2 | 1.01 | 0.99 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:CB | 1.92 | 0.98 |
| 1:B:548:ARG:HG3 | 1:B:583:VAL:C | 1.84 | 0.98 |
| 1:B:444:LEU:HD12 | 1:B:446:PHE:CE1 | 1.98 | 0.98 |
| 1:B:862:ILE:HG22 | 1:B:877:ILE:HA | 1.46 | 0.98 |
| 1:A:870:GLU:CD | 1:A:1025:ALA:CB | 2.33 | 0.97 |
| 1:A:444:LEU:HD12 | 1:A:446:PHE:CE1 | 1.98 | 0.97 |
| 1:A:870:GLU:OE1 | 1:A:1025:ALA:HB2 | 1.62 | 0.97 |
| 1:A:563:HIS:HB3 | 1:A:564:PRO:HD3 | 1.44 | 0.97 |
| 1:B:563:HIS:HB3 | 1:B:564:PRO:HD3 | 1.44 | 0.97 |
| 1:A:623:ILE:HA | 1:A:626:ASN:HD21 | 1.28 | 0.96 |
| 1:A:862:ILE:HG22 | 1:A:877:ILE:HA | 1.46 | 0.96 |
| 1:B:662:LEU:HD23 | 1:B:791:ASP:OD2 | 1.65 | 0.96 |
| 1:B:566:ASN:HA | 1:B:651:VAL:HG23 | 1.49 | 0.95 |
| 1:B:458:ARG:HD2 | 1:B:524:PRO:HB3 | 1.45 | 0.95 |
| 1:B:629:HIS:CG | 1:B:669:TYR:OH | 2.15 | 0.95 |
| 1:A:566:ASN:HA | 1:A:651:VAL:HG23 | 1.49 | 0.95 |
| 1:B:506:VAL:C | 1:B:507:GLU:HA | 1.84 | 0.95 |
| 1:A:440:LYS:HB2 | 1:A:538:LYS:HZ2 | 1.27 | 0.94 |
| 1:B:505:PRO:C | 1:B:507:GLU:N | 2.19 | 0.94 |
| 1:A:42:PHE:HE1 | 1:A:79:VAL:HG22 | 1.31 | 0.94 |
| 1:A:870:GLU:OE2 | 1:A:1025:ALA:HB2 | 1.65 | 0.94 |
| 1:A:868:PRO:HD2 | 1:A:981:GLY:HA3 | 1.16 | 0.94 |
| 1:A:994:LEU:HD11 | 1:A:1006:ASN:HD22 | 1.31 | 0.94 |
| 1:A:72:LYS:HE3 | 1:A:80:LEU:HD13 | 1.49 | 0.94 |
| 1:A:871:GLY:O | 1:A:1023:ASP:HB3 | 1.68 | 0.93 |
| 1:B:62:ILE:CG1 | 1:B:73:LEU:HB2 | 1.98 | 0.93 |
| 1:B:42:PHE:HE1 | 1:B:79:VAL:HG22 | 1.31 | 0.93 |
| 1:A:297:ILE:HG22 | 1:A:418:VAL:CG1 | 1.97 | 0.93 |
| 1:A:870:GLU:CG | 1:A:1024:ARG:HG3 | 1.97 | 0.93 |
| 1:B:456:LYS:CD | 1:B:523:ASP:OD2 | 2.15 | 0.93 |
| 1:B:297:ILE:HG22 | 1:B:418:VAL:HG12 | 1.49 | 0.93 |
| 1:B:804:GLY:HA2 | 1:B:806:MET:SD | 2.09 | 0.93 |
| 1:A:62:ILE:CG1 | 1:A:73:LEU:HB2 | 1.98 | 0.93 |
| 1:A:440:LYS:HD2 | 1:A:538:LYS:CD | 1.98 | 0.93 |
| 1:A:804:GLY:HA2 | 1:A:806:MET:SD | 2.09 | 0.93 |
| 1:B:297:ILE:HG22 | 1:B:418:VAL:CG1 | 1.97 | 0.93 |
| 1:B:865:VAL:HG13 | 1:B:866:THR:HG23 | 1.50 | 0.93 |
| 1:A:297:ILE:HG22 | 1:A:418:VAL:HG12 | 1.49 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:863:ILE:HG22 | 1:B:876:THR:HB | 1.48 | 0.92 |
| 1:A:863:ILE:HG22 | 1:A:876:THR:HB | 1.48 | 0.92 |
| 1:A:39:PHE:CE2 | 1:A:473:GLN:HG3 | 2.05 | 0.92 |
| 1:B:72:LYS:HE3 | 1:B:80:LEU:HD13 | 1.49 | 0.92 |
| 1:B:271:LYS:HG3 | 1:B:272:GLU:H | 1.34 | 0.92 |
| 1:A:435:ILE:HD13 | 1:A:436:ALA:H | 1.34 | 0.92 |
| 1:B:527:GLY:HA3 | 1:B:550:PHE:CZ | 2.04 | 0.92 |
| 1:A:239:PHE:HA | 1:A:260:PRO:HG2 | 1.51 | 0.92 |
| 1:A:865:VAL:HG13 | 1:A:866:THR:HG23 | 1.50 | 0.92 |
| 1:B:39:PHE:CE2 | 1:B:473:GLN:HG3 | 2.05 | 0.92 |
| 1:A:933:VAL:HG23 | 1:A:934:ALA:H | 1.35 | 0.91 |
| 1:B:239:PHE:HA | 1:B:260:PRO:HG2 | 1.51 | 0.91 |
| 1:A:870:GLU:HG2 | 1:A:1024:ARG:C | 1.91 | 0.91 |
| 1:B:806:MET:SD | 1:B:807:ARG:HG3 | 2.11 | 0.91 |
| 1:B:435:ILE:HD13 | 1:B:436:ALA:H | 1.34 | 0.91 |
| 1:A:806:MET:SD | 1:A:807:ARG:HG3 | 2.11 | 0.91 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:CZ | 2.05 | 0.90 |
| 1:A:447:VAL:HG22 | 1:A:455:LYS:HB2 | 1.53 | 0.90 |
| 1:A:549:ARG:HD3 | 1:A:584:PRO:HB2 | 1.53 | 0.90 |
| 1:B:933:VAL:HG23 | 1:B:934:ALA:H | 1.36 | 0.90 |
| 1:A:271:LYS:HG3 | 1:A:272:GLU:H | 1.34 | 0.90 |
| 1:A:359:LEU:CD1 | 1:A:362:ILE:HD11 | 2.02 | 0.89 |
| 1:A:447:VAL:CG2 | 1:A:455:LYS:HB2 | 2.03 | 0.89 |
| 1:A:972:THR:HG23 | 1:A:1002:TYR:CE1 | 2.07 | 0.89 |
| 1:A:873:THR:C | 1:A:982:SER:HB2 | 1.91 | 0.89 |
| 1:B:653:TYR:HE2 | 1:B:682:HIS:ND1 | 1.69 | 0.89 |
| 1:A:453:LYS:CG | 1:A:472:VAL:HG22 | 2.03 | 0.88 |
| 1:B:447:VAL:CG2 | 1:B:455:LYS:HB2 | 2.03 | 0.88 |
| 1:B:453:LYS:CG | 1:B:472:VAL:HG22 | 2.03 | 0.88 |
| 1:B:95:TYR:CD2 | 1:B:96:PRO:HD3 | 2.08 | 0.88 |
| 1:B:447:VAL:HG22 | 1:B:455:LYS:HB2 | 1.53 | 0.88 |
| 1:B:802:LYS:O | 1:B:803:CYS:N | 2.06 | 0.88 |
| 1:B:181:LYS:CD | 1:B:202:LYS:HA | 2.04 | 0.88 |
| 1:A:870:GLU:OE2 | 1:A:1025:ALA:CB | 2.22 | 0.88 |
| 1:B:359:LEU:CD1 | 1:B:362:ILE:HD11 | 2.02 | 0.88 |
| 1:A:863:ILE:HG23 | 1:A:864:PRO:HD2 | 1.55 | 0.88 |
| 1:B:892:HIS:HB2 | 1:B:932:CYS:O | 1.74 | 0.88 |
| 1:A:446:PHE:HD2 | 1:A:454:LEU:HD21 | 1.38 | 0.87 |
| 1:B:847:LEU:HG | 1:B:850:ALA:H | 1.39 | 0.87 |
| 1:B:486:PHE:CD1 | 1:B:493:LEU:HD13 | 2.09 | 0.87 |
| 1:A:532:HIS:HA | 1:A:641:THR:OG1 | 1.73 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:892:HIS:HB2 | 1:A:932:CYS:O | 1.73 | 0.87 |
| 1:A:95:TYR:CD2 | 1:A:96:PRO:HD3 | 2.08 | 0.87 |
| 1:A:867:GLY:HA2 | 1:A:981:GLY:H | 0.77 | 0.87 |
| 1:A:486:PHE:CD1 | 1:A:493:LEU:HD13 | 2.09 | 0.87 |
| 1:B:468:GLN:HG3 | 1:B:523:ASP:CA | 2.03 | 0.87 |
| 1:B:863:ILE:HG23 | 1:B:864:PRO:HD2 | 1.56 | 0.86 |
| 1:B:110:THR:CG2 | 1:B:132:LEU:HD21 | 2.05 | 0.86 |
| 1:B:439:TYR:CE2 | 1:B:538:LYS:NZ | 2.42 | 0.86 |
| 1:A:39:PHE:CE1 | 1:A:505:PRO:HD2 | 2.10 | 0.86 |
| 1:A:959:LYS:HB2 | 1:A:972:THR:HB | 1.57 | 0.86 |
| 1:A:110:THR:CG2 | 1:A:132:LEU:HD21 | 2.05 | 0.86 |
| 1:A:181:LYS:CD | 1:A:202:LYS:HA | 2.04 | 0.86 |
| 1:A:833:LEU:HB2 | 1:A:836:HIS:HD2 | 1.39 | 0.86 |
| 1:B:446:PHE:HD2 | 1:B:454:LEU:HD21 | 1.38 | 0.86 |
| 1:B:603:LEU:HD23 | 1:B:604:VAL:N | 1.90 | 0.86 |
| 1:B:699:ASP:HA | 1:B:725:ASN:OD1 | 1.74 | 0.86 |
| 1:A:370:LEU:CD1 | 1:A:399:ILE:HD12 | 2.06 | 0.86 |
| 1:B:256:LEU:HB3 | 1:B:309:LEU:HD22 | 1.56 | 0.86 |
| 1:B:435:ILE:CG2 | 1:B:446:PHE:HB2 | 2.06 | 0.86 |
| 1:B:833:LEU:HB2 | 1:B:836:HIS:HD2 | 1.39 | 0.86 |
| 1:B:295:VAL:HA | 1:B:414:VAL:CG2 | 2.05 | 0.86 |
| 1:A:118:LEU:HD13 | 1:A:119:ILE:N | 1.91 | 0.86 |
| 1:A:295:VAL:HA | 1:A:414:VAL:CG2 | 2.05 | 0.86 |
| 1:B:100:VAL:HG12 | 1:B:101:GLN:HG3 | 1.58 | 0.86 |
| 1:B:473:GLN:CG | 1:B:504:VAL:HG22 | 2.06 | 0.86 |
| 1:B:700:CYS:HB3 | 1:B:701:PRO:CD | 1.92 | 0.86 |
| 1:B:847:LEU:HD12 | 1:B:852:SER:HB3 | 1.58 | 0.86 |
| 1:A:603:LEU:HD23 | 1:A:604:VAL:N | 1.90 | 0.85 |
| 1:B:370:LEU:CD1 | 1:B:399:ILE:HD12 | 2.05 | 0.85 |
| 1:B:531:LEU:O | 1:B:641:THR:OG1 | 1.94 | 0.85 |
| 1:B:847:LEU:HD11 | 1:B:850:ALA:HA | 1.58 | 0.85 |
| 1:A:100:VAL:HG12 | 1:A:101:GLN:HG3 | 1.58 | 0.85 |
| 1:B:676:TYR:HE1 | 1:B:730:GLN:HG2 | 1.41 | 0.85 |
| 1:B:133:TYR:CG | 1:B:136:ILE:HG12 | 2.12 | 0.85 |
| 1:A:882:LEU:HB2 | 1:A:910:ALA:HA | 1.58 | 0.85 |
| 1:A:847:LEU:HD12 | 1:A:852:SER:HB3 | 1.58 | 0.85 |
| 1:A:133:TYR:CG | 1:A:136:ILE:HG12 | 2.12 | 0.85 |
| 1:A:706:VAL:HG22 | 1:A:707:ASP:H | 1.42 | 0.85 |
| 1:A:473:GLN:CG | 1:A:504:VAL:HG22 | 2.06 | 0.85 |
| 1:A:42:PHE:CZ | 1:A:45:GLU:HB2 | 2.12 | 0.84 |
| 1:A:847:LEU:HG | 1:A:850:ALA:H | 1.39 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:118:LEU:HD13 | 1:B:119:ILE:N | 1.91 | 0.84 |
| 1:B:39:PHE:CE1 | 1:B:505:PRO:HD2 | 2.11 | 0.84 |
| 1:A:256:LEU:HB3 | 1:A:309:LEU:HD22 | 1.56 | 0.84 |
| 1:B:548:ARG:HG3 | 1:B:583:VAL:O | 1.77 | 0.84 |
| 1:A:989:GLY:HA2 | 1:A:1017:LYS:HE3 | 1.57 | 0.84 |
| 1:B:42:PHE:CZ | 1:B:45:GLU:HB2 | 2.12 | 0.84 |
| 1:B:356:ILE:CG2 | 1:B:421:ILE:HB | 2.07 | 0.84 |
| 1:B:295:VAL:CG1 | 1:B:414:VAL:HG11 | 2.07 | 0.84 |
| 1:B:50:PHE:HB2 | 1:B:498:GLU:O | 1.78 | 0.84 |
| 1:B:40:VAL:CG1 | 1:B:503:ARG:HB3 | 2.08 | 0.84 |
| 1:B:653:TYR:C | 1:B:654:ASN:N | 2.31 | 0.83 |
| 1:A:40:VAL:CG1 | 1:A:503:ARG:HB3 | 2.08 | 0.83 |
| 1:B:295:VAL:HA | 1:B:414:VAL:HG22 | 1.60 | 0.83 |
| 1:A:229:PRO:O | 1:A:232:THR:HG22 | 1.79 | 0.83 |
| 1:A:356:ILE:CG2 | 1:A:421:ILE:HB | 2.07 | 0.83 |
| 1:A:971:VAL:HG22 | 1:A:1005:CYS:O | 1.78 | 0.83 |
| 1:A:336:THR:O | 1:A:354:LEU:HD12 | 1.78 | 0.83 |
| 1:A:863:ILE:CG2 | 1:A:876:THR:HB | 2.07 | 0.83 |
| 1:B:706:VAL:HG22 | 1:B:707:ASP:H | 1.42 | 0.83 |
| 1:A:118:LEU:HD12 | 1:A:172:ILE:CD1 | 2.05 | 0.83 |
| 1:B:830:GLN:HG2 | 1:B:831:CYS:H | 1.43 | 0.83 |
| 1:B:474:VAL:HG22 | 1:B:495:ILE:HG21 | 1.61 | 0.83 |
| 1:B:118:LEU:HD12 | 1:B:172:ILE:CD1 | 2.05 | 0.83 |
| 1:B:336:THR:O | 1:B:354:LEU:HD12 | 1.78 | 0.83 |
| 1:B:358:ILE:HG23 | 1:B:361:GLN:H | 1.44 | 0.83 |
| 1:A:996:HIS:HB3 | 1:A:1004:ILE:HG23 | 1.59 | 0.83 |
| 1:A:397:LEU:HD23 | 1:A:399:ILE:HD13 | 1.61 | 0.83 |
| 1:A:42:PHE:CE1 | 1:A:79:VAL:HG22 | 2.14 | 0.83 |
| 1:A:847:LEU:HD11 | 1:A:850:ALA:HA | 1.58 | 0.83 |
| 1:B:229:PRO:O | 1:B:232:THR:HG22 | 1.79 | 0.83 |
| 1:A:295:VAL:CG1 | 1:A:414:VAL:HG11 | 2.07 | 0.83 |
| 1:B:133:TYR:CB | 1:B:136:ILE:HG12 | 2.09 | 0.83 |
| 1:A:474:VAL:HG22 | 1:A:495:ILE:HG21 | 1.61 | 0.82 |
| 1:A:440:LYS:CD | 1:A:538:LYS:HD3 | 2.08 | 0.82 |
| 1:B:397:LEU:HD23 | 1:B:399:ILE:HD13 | 1.61 | 0.82 |
| 1:B:53:LEU:HD23 | 1:B:54:VAL:N | 1.94 | 0.82 |
| 1:A:358:ILE:HG23 | 1:A:361:GLN:H | 1.44 | 0.82 |
| 1:A:951:MET:C | 1:A:952:THR:N | 2.32 | 0.82 |
| 1:B:295:VAL:HG12 | 1:B:414:VAL:CG1 | 2.09 | 0.82 |
| 1:A:435:ILE:CG2 | 1:A:446:PHE:HB2 | 2.06 | 0.82 |
| 1:A:548:ARG:HG3 | 1:A:583:VAL:O | 1.79 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:785:ASN:HB3 | 1:B:788:PHE:CD2 | 2.14 | 0.82 |
| 1:B:863:ILE:CG2 | 1:B:876:THR:HB | 2.07 | 0.82 |
| 1:A:987:MET:HB2 | 1:A:1019:THR:CG2 | 2.09 | 0.82 |
| 1:A:44:GLY:HA2 | 1:A:50:PHE:CE2 | 2.15 | 0.82 |
| 1:A:53:LEU:HD23 | 1:A:54:VAL:N | 1.94 | 0.82 |
| 1:A:44:GLY:HA2 | 1:A:50:PHE:HE2 | 1.44 | 0.82 |
| 1:B:44:GLY:HA2 | 1:B:50:PHE:CE2 | 2.15 | 0.82 |
| 1:A:133:TYR:CB | 1:A:136:ILE:HG12 | 2.09 | 0.82 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:CD2 | 2.14 | 0.82 |
| 1:A:295:VAL:HA | 1:A:414:VAL:HG22 | 1.60 | 0.82 |
| 1:A:50:PHE:HB2 | 1:A:498:GLU:O | 1.78 | 0.82 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:CE | 2.63 | 0.82 |
| 1:A:991:GLN:CG | 1:A:1008:THR:HG21 | 2.10 | 0.82 |
| 1:B:185:ALA:HB1 | 1:B:243:TYR:CE1 | 2.15 | 0.82 |
| 1:A:397:LEU:HD23 | 1:A:399:ILE:CD1 | 2.10 | 0.81 |
| 1:B:882:LEU:HB2 | 1:B:910:ALA:HA | 1.58 | 0.81 |
| 1:A:225:MET:HE1 | 1:A:227:LYS:HG3 | 1.63 | 0.81 |
| 1:A:994:LEU:HD11 | 1:A:1006:ASN:HB2 | 1.63 | 0.81 |
| 1:B:356:ILE:HG22 | 1:B:421:ILE:HB | 1.61 | 0.81 |
| 1:B:62:ILE:HG13 | 1:B:73:LEU:HB2 | 1.62 | 0.81 |
| 1:A:889:ILE:HG23 | 1:A:892:HIS:CE1 | 2.16 | 0.81 |
| 1:B:154:LYS:HD3 | 1:B:210:ASP:OD1 | 1.81 | 0.81 |
| 1:B:397:LEU:HD23 | 1:B:399:ILE:CD1 | 2.11 | 0.81 |
| 1:B:863:ILE:HG13 | 1:B:864:PRO:HD3 | 1.62 | 0.81 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:CG | 2.10 | 0.81 |
| 1:B:42:PHE:CE1 | 1:B:79:VAL:HG22 | 2.14 | 0.81 |
| 1:A:440:LYS:CB | 1:A:538:LYS:NZ | 2.44 | 0.81 |
| 1:A:154:LYS:HD3 | 1:A:210:ASP:OD1 | 1.81 | 0.80 |
| 1:B:154:LYS:HB2 | 1:B:157:HIS:CD2 | 2.16 | 0.80 |
| 1:B:324:THR:HB | 1:B:462:PRO:CB | 2.10 | 0.80 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CE1 | 2.15 | 0.80 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:N | 1.96 | 0.80 |
| 1:B:486:PHE:CE1 | 1:B:493:LEU:HD13 | 2.16 | 0.80 |
| 1:B:889:ILE:HG23 | 1:B:892:HIS:CE1 | 2.16 | 0.80 |
| 1:A:830:GLN:HG2 | 1:A:831:CYS:H | 1.43 | 0.80 |
| 1:A:356:ILE:HG22 | 1:A:421:ILE:HB | 1.61 | 0.80 |
| 1:A:486:PHE:CE1 | 1:A:493:LEU:HD13 | 2.16 | 0.80 |
| 1:B:444:LEU:HD13 | 1:B:445:ALA:N | 1.97 | 0.80 |
| 1:B:623:ILE:HD12 | 1:B:624:THR:N | 1.96 | 0.80 |
| 1:A:620:PRO:HA | 1:A:623:ILE:CG1 | 2.12 | 0.80 |
| 1:B:314:LEU:HD11 | 1:B:332:ASP:HB3 | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:192:PRO:HB3 | 1:B:233:PHE:CE1 | 2.17 | 0.80 |
| 1:B:653:TYR:HE2 | 1:B:682:HIS:HD1 | 1.27 | 0.80 |
| 1:A:994:LEU:CD1 | 1:A:1006:ASN:HB2 | 2.12 | 0.79 |
| 1:B:620:PRO:HA | 1:B:623:ILE:CG1 | 2.12 | 0.79 |
| 1:A:192:PRO:HB3 | 1:A:233:PHE:CE1 | 2.17 | 0.79 |
| 1:B:239:PHE:CE1 | 1:B:260:PRO:HD2 | 2.17 | 0.79 |
| 1:B:317:ALA:HB1 | 1:B:321:LEU:HB3 | 1.64 | 0.79 |
| 1:B:380:LEU:HD12 | 1:B:386:LYS:HE3 | 1.64 | 0.79 |
| 1:A:321:LEU:HD12 | 1:A:462:PRO:HG2 | 1.64 | 0.79 |
| 1:A:591:ASN:OD1 | 1:A:639:LYS:HE2 | 1.83 | 0.79 |
| 1:A:926:ALA:HB1 | 1:A:947:LEU:HD12 | 1.63 | 0.79 |
| 1:B:699:ASP:CA | 1:B:725:ASN:OD1 | 2.29 | 0.79 |
| 1:A:154:LYS:HB2 | 1:A:157:HIS:CD2 | 2.16 | 0.79 |
| 1:A:370:LEU:HD12 | 1:A:399:ILE:HD12 | 1.64 | 0.79 |
| 1:A:951:MET:HG2 | 1:A:977:ASN:CG | 2.03 | 0.79 |
| 1:B:370:LEU:HD12 | 1:B:399:ILE:HD12 | 1.63 | 0.79 |
| 1:A:244:VAL:HG13 | 1:A:482:ARG:NH1 | 1.98 | 0.79 |
| 1:A:239:PHE:CE1 | 1:A:260:PRO:HD2 | 2.17 | 0.79 |
| 1:B:244:VAL:HG13 | 1:B:482:ARG:NH1 | 1.98 | 0.79 |
| 1:A:324:THR:HB | 1:A:462:PRO:CB | 2.10 | 0.79 |
| 1:A:444:LEU:HD13 | 1:A:445:ALA:N | 1.97 | 0.79 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:HD3 | 1.62 | 0.79 |
| 1:B:591:ASN:OD1 | 1:B:639:LYS:HE2 | 1.83 | 0.79 |
| 1:A:62:ILE:HG13 | 1:A:73:LEU:HB2 | 1.62 | 0.79 |
| 1:B:319:ALA:H | 1:B:441:ASN:HD22 | 1.31 | 0.79 |
| 1:B:44:GLY:HA2 | 1:B:50:PHE:HE2 | 1.44 | 0.79 |
| 1:B:926:ALA:HB1 | 1:B:947:LEU:HD12 | 1.63 | 0.79 |
| 1:A:715:VAL:HG21 | 1:A:717:LYS:HD2 | 1.65 | 0.78 |
| 1:B:453:LYS:HE3 | 1:B:472:VAL:CG2 | 2.13 | 0.78 |
| 1:B:715:VAL:HG21 | 1:B:717:LYS:HD2 | 1.65 | 0.78 |
| 1:A:319:ALA:H | 1:A:441:ASN:HD22 | 1.31 | 0.78 |
| 1:A:440:LYS:CB | 1:A:538:LYS:HZ3 | 1.96 | 0.78 |
| 1:A:231:ASP:O | 1:A:234:THR:HG22 | 1.84 | 0.78 |
| 1:A:295:VAL:HG12 | 1:A:414:VAL:CG1 | 2.09 | 0.78 |
| 1:A:847:LEU:CG | 1:A:850:ALA:HA | 2.13 | 0.78 |
| 1:B:320:VAL:HG21 | 1:B:442:HIS:CD2 | 2.19 | 0.78 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:CG2 | 2.13 | 0.78 |
| 1:A:320:VAL:HG21 | 1:A:442:HIS:CD2 | 2.19 | 0.78 |
| 1:A:742:ILE:HB | 1:A:745:ILE:O | 1.84 | 0.78 |
| 1:A:873:THR:HA | 1:A:982:SER:HB2 | 0.82 | 0.78 |
| 1:B:469:TYR:HB3 | 1:B:523:ASP:OD1 | 1.81 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:742:ILE:HB | 1:B:745:ILE:O | 1.84 | 0.78 |
| 1:A:380:LEU:HD12 | 1:A:386:LYS:HE3 | 1.64 | 0.78 |
| 1:A:868:PRO:CG | 1:A:981:GLY:HA3 | 2.12 | 0.78 |
| 1:B:56:ASP:OD2 | 1:B:142:LEU:HD11 | 1.83 | 0.78 |
| 1:B:321:LEU:HD12 | 1:B:462:PRO:HG2 | 1.64 | 0.78 |
| 1:A:181:LYS:NZ | 1:A:216:VAL:HG23 | 1.98 | 0.78 |
| 1:A:327:VAL:HG12 | 1:A:358:ILE:HD11 | 1.66 | 0.78 |
| 1:A:972:THR:HA | 1:A:1002:TYR:HE1 | 1.47 | 0.78 |
| 1:B:439:TYR:OH | 1:B:538:LYS:HE3 | 1.83 | 0.78 |
| 1:A:439:TYR:CZ | 1:A:538:LYS:CE | 2.67 | 0.78 |
| 1:A:870:GLU:HG2 | 1:A:1025:ALA:N | 1.98 | 0.78 |
| 1:A:51:ASN:HD21 | 1:A:67:VAL:HG23 | 1.49 | 0.78 |
| 1:A:994:LEU:O | 1:A:994:LEU:HD12 | 1.84 | 0.78 |
| 1:B:847:LEU:CG | 1:B:850:ALA:HA | 2.13 | 0.78 |
| 1:A:314:LEU:HD11 | 1:A:332:ASP:HB3 | 1.64 | 0.77 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:O | 1.84 | 0.77 |
| 1:A:284:LYS:HD3 | 1:A:284:LYS:O | 1.84 | 0.77 |
| 1:B:168:VAL:HG23 | 1:B:185:ALA:O | 1.84 | 0.77 |
| 1:B:51:ASN:HD21 | 1:B:67:VAL:HG23 | 1.50 | 0.77 |
| 1:A:1014:LEU:H | 1:A:1014:LEU:HD22 | 1.48 | 0.77 |
| 1:A:1016:MET:HG2 | 1:A:1035:TYR:CE2 | 2.19 | 0.77 |
| 1:A:327:VAL:CG1 | 1:A:358:ILE:HD11 | 2.14 | 0.77 |
| 1:B:327:VAL:CG1 | 1:B:358:ILE:HD11 | 2.14 | 0.77 |
| 1:A:56:ASP:OD2 | 1:A:142:LEU:HD11 | 1.83 | 0.77 |
| 1:B:710:LEU:O | 1:B:710:LEU:HD12 | 1.84 | 0.77 |
| 1:B:595:GLU:CB | 1:B:597:LEU:HD23 | 2.14 | 0.77 |
| 1:B:231:ASP:O | 1:B:234:THR:HG22 | 1.84 | 0.77 |
| 1:B:327:VAL:HG12 | 1:B:358:ILE:HD11 | 1.65 | 0.77 |
| 1:B:567:ILE:HD13 | 1:B:567:ILE:H | 1.50 | 0.77 |
| 1:A:168:VAL:HG23 | 1:A:185:ALA:O | 1.84 | 0.77 |
| 1:B:662:LEU:HD11 | 1:B:702:GLN:NE2 | 1.99 | 0.77 |
| 1:A:317:ALA:HB1 | 1:A:321:LEU:HB3 | 1.64 | 0.77 |
| 1:A:547:PRO:O | 1:A:548:ARG:HG2 | 1.84 | 0.77 |
| 1:A:870:GLU:HG3 | 1:A:1024:ARG:HG3 | 1.64 | 0.77 |
| 1:B:181:LYS:NZ | 1:B:216:VAL:HG23 | 1.98 | 0.77 |
| 1:B:204:THR:HG21 | 1:B:209:ALA:HB3 | 1.66 | 0.77 |
| 1:B:359:LEU:HD12 | 1:B:362:ILE:CD1 | 2.10 | 0.77 |
| 1:A:1021:GLN:HG2 | 1:A:1026:ARG:HG3 | 1.67 | 0.77 |
| 1:B:403:PHE:CE1 | 1:B:406:LEU:HD23 | 2.20 | 0.77 |
| 1:A:549:ARG:HD3 | 1:A:584:PRO:HB3 | 1.66 | 0.76 |
| 1:A:567:ILE:H | 1:A:567:ILE:HD13 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:284:LYS:O | 1:B:284:LYS:HD3 | 1.84 | 0.76 |
| 1:A:120:ASP:OD2 | 1:A:123:GLU:HG3 | 1.86 | 0.76 |
| 1:A:403:PHE:CE1 | 1:A:406:LEU:HD23 | 2.20 | 0.76 |
| 1:A:439:TYR:OH | 1:A:538:LYS:HE3 | 1.84 | 0.76 |
| 1:A:460:ASP:HB3 | 1:A:464:GLY:N | 2.00 | 0.76 |
| 1:B:780:LEU:O | 1:B:780:LEU:HD12 | 1.86 | 0.76 |
| 1:B:847:LEU:CD1 | 1:B:850:ALA:HA | 2.16 | 0.76 |
| 1:A:873:THR:HA | 1:A:982:SER:CA | 2.15 | 0.76 |
| 1:B:172:ILE:HG12 | 1:B:182:LEU:HD13 | 1.68 | 0.76 |
| 1:B:616:ALA:O | 1:B:620:PRO:HD2 | 1.85 | 0.76 |
| 1:A:359:LEU:HD12 | 1:A:362:ILE:CD1 | 2.09 | 0.76 |
| 1:A:616:ALA:O | 1:A:620:PRO:HD2 | 1.85 | 0.76 |
| 1:A:780:LEU:HD12 | 1:A:780:LEU:O | 1.86 | 0.76 |
| 1:B:120:ASP:OD2 | 1:B:123:GLU:HG3 | 1.86 | 0.76 |
| 1:B:460:ASP:HB3 | 1:B:464:GLY:N | 2.00 | 0.76 |
| 1:B:64:LEU:HD12 | 1:B:496:MET:CE | 2.16 | 0.76 |
| 1:A:873:THR:OG1 | 1:A:981:GLY:CA | 2.34 | 0.76 |
| 1:A:1010:SER:HB2 | 1:A:1035:TYR:CE2 | 2.20 | 0.75 |
| 1:A:256:LEU:CB | 1:A:309:LEU:HD22 | 2.16 | 0.75 |
| 1:A:42:PHE:HZ | 1:A:45:GLU:HB2 | 1.50 | 0.75 |
| 1:A:869:ARG:O | 1:A:920:ALA:HB3 | 1.86 | 0.75 |
| 1:A:172:ILE:HG12 | 1:A:182:LEU:HD13 | 1.68 | 0.75 |
| 1:A:458:ARG:CD | 1:A:524:PRO:HB3 | 2.12 | 0.75 |
| 1:A:868:PRO:HG2 | 1:A:1022:VAL:HG22 | 1.65 | 0.75 |
| 1:A:919:GLU:HB3 | 1:A:1024:ARG:HH11 | 1.51 | 0.75 |
| 1:B:278:LYS:HE3 | 1:B:296:PRO:HG3 | 1.67 | 0.75 |
| 1:B:547:PRO:O | 1:B:548:ARG:HG2 | 1.84 | 0.75 |
| 1:B:806:MET:HE3 | 1:B:806:MET:N | 1.99 | 0.75 |
| 1:B:847:LEU:HD12 | 1:B:852:SER:CB | 2.16 | 0.75 |
| 1:A:874:LYS:N | 1:A:982:SER:HB2 | 2.02 | 0.75 |
| 1:B:506:VAL:HG22 | 1:B:525:HIS:CD2 | 2.21 | 0.75 |
| 1:B:785:ASN:HB3 | 1:B:788:PHE:HD2 | 1.48 | 0.75 |
| 1:B:873:THR:HB | 1:B:917:MET:CE | 2.17 | 0.75 |
| 1:A:204:THR:HG21 | 1:A:209:ALA:HB3 | 1.66 | 0.75 |
| 1:A:847:LEU:CD1 | 1:A:850:ALA:HA | 2.16 | 0.75 |
| 1:A:278:LYS:HE3 | 1:A:296:PRO:HG3 | 1.67 | 0.75 |
| 1:A:473:GLN:CB | 1:A:504:VAL:HG22 | 2.17 | 0.75 |
| 1:B:323:ARG:HG3 | 1:B:324:THR:N | 2.02 | 0.75 |
| 1:B:473:GLN:CB | 1:B:504:VAL:HG22 | 2.17 | 0.75 |
| 1:B:784:TRP:HD1 | 1:B:790:ILE:HD11 | 1.51 | 0.75 |
| 1:B:806:MET:H | 1:B:806:MET:CE | 1.97 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:446:PHE:HB3 | 1:B:454:LEU:HD11 | 1.69 | 0.75 |
| 1:B:448:GLY:HA3 | 1:B:480:VAL:HG21 | 1.68 | 0.75 |
| 1:A:188:VAL:HG22 | 1:A:191:LYS:H | 1.52 | 0.75 |
| 1:A:278:LYS:HG2 | 1:A:296:PRO:HA | 1.69 | 0.75 |
| 1:A:64:LEU:HD12 | 1:A:496:MET:CE | 2.16 | 0.75 |
| 1:A:739:ILE:CD1 | 1:A:748:ARG:HG2 | 2.17 | 0.75 |
| 1:A:847:LEU:HD12 | 1:A:852:SER:CB | 2.16 | 0.75 |
| 1:B:699:ASP:C | 1:B:725:ASN:OD1 | 2.26 | 0.75 |
| 1:B:700:CYS:CB | 1:B:701:PRO:CD | 2.50 | 0.75 |
| 1:A:323:ARG:HG3 | 1:A:324:THR:N | 2.02 | 0.74 |
| 1:A:623:ILE:HA | 1:A:626:ASN:ND2 | 2.01 | 0.74 |
| 1:A:683:ASP:O | 1:A:686:THR:HG22 | 1.87 | 0.74 |
| 1:A:873:THR:HB | 1:A:917:MET:CE | 2.17 | 0.74 |
| 1:B:196:PRO:HB3 | 1:B:225:MET:HE1 | 1.68 | 0.74 |
| 1:A:321:LEU:CD1 | 1:A:462:PRO:HG2 | 2.17 | 0.74 |
| 1:B:202:LYS:HD3 | 1:B:214:ALA:HB3 | 1.69 | 0.74 |
| 1:B:256:LEU:CB | 1:B:309:LEU:HD22 | 2.16 | 0.74 |
| 1:B:321:LEU:CD1 | 1:B:462:PRO:HG2 | 2.17 | 0.74 |
| 1:B:42:PHE:HZ | 1:B:45:GLU:HB2 | 1.50 | 0.74 |
| 1:B:869:ARG:O | 1:B:920:ALA:HB3 | 1.86 | 0.74 |
| 1:A:99:ILE:HD11 | 1:A:152:PHE:HB2 | 1.69 | 0.74 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:HD2 | 1.48 | 0.74 |
| 1:A:151:PRO:HB2 | 1:A:157:HIS:ND1 | 2.02 | 0.74 |
| 1:B:623:ILE:HA | 1:B:626:ASN:ND2 | 2.01 | 0.74 |
| 1:A:868:PRO:HG2 | 1:A:1022:VAL:CG2 | 2.17 | 0.74 |
| 1:A:448:GLY:HA3 | 1:A:480:VAL:HG21 | 1.68 | 0.74 |
| 1:B:151:PRO:HB2 | 1:B:157:HIS:ND1 | 2.03 | 0.74 |
| 1:B:188:VAL:HG22 | 1:B:191:LYS:H | 1.52 | 0.74 |
| 1:A:1010:SER:HB2 | 1:A:1035:TYR:CZ | 2.23 | 0.74 |
| 1:B:814:LEU:HB3 | 1:B:847:LEU:HB2 | 1.70 | 0.74 |
| 1:A:567:ILE:HD12 | 1:A:650:PHE:CZ | 2.22 | 0.74 |
| 1:B:185:ALA:HB1 | 1:B:243:TYR:CZ | 2.23 | 0.74 |
| 1:B:548:ARG:CG | 1:B:584:PRO:HA | 2.16 | 0.74 |
| 1:A:324:THR:HG21 | 1:A:462:PRO:HA | 1.70 | 0.73 |
| 1:B:278:LYS:HG2 | 1:B:296:PRO:HA | 1.68 | 0.73 |
| 1:B:739:ILE:CD1 | 1:B:748:ARG:HG2 | 2.17 | 0.73 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CZ | 2.23 | 0.73 |
| 1:A:569:VAL:CB | 1:A:654:ASN:HB2 | 2.17 | 0.73 |
| 1:B:548:ARG:HG3 | 1:B:584:PRO:N | 2.03 | 0.73 |
| 1:B:562:VAL:HG22 | 1:B:578:LEU:CD2 | 2.18 | 0.73 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:CD2 | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:814:LEU:HB3 | 1:A:847:LEU:HB2 | 1.70 | 0.73 |
| 1:B:324:THR:HG21 | 1:B:462:PRO:HA | 1.70 | 0.73 |
| 1:A:435:ILE:HD13 | 1:A:436:ALA:N | 2.03 | 0.73 |
| 1:A:446:PHE:HB3 | 1:A:454:LEU:HD11 | 1.69 | 0.73 |
| 1:A:704:LEU:HD11 | 1:A:724:LYS:HE3 | 1.69 | 0.73 |
| 1:B:439:TYR:OH | 1:B:538:LYS:CE | 2.37 | 0.73 |
| 1:A:154:LYS:H | 1:A:157:HIS:HD2 | 1.36 | 0.73 |
| 1:A:958:LEU:HD22 | 1:A:960:PRO:O | 1.87 | 0.73 |
| 1:B:683:ASP:O | 1:B:686:THR:HG22 | 1.88 | 0.73 |
| 1:A:225:MET:CE | 1:A:227:LYS:HG3 | 2.19 | 0.73 |
| 1:B:468:GLN:CG | 1:B:523:ASP:HA | 2.08 | 0.73 |
| 1:B:225:MET:CE | 1:B:227:LYS:HG3 | 2.19 | 0.73 |
| 1:A:446:PHE:CD2 | 1:A:454:LEU:HD21 | 2.24 | 0.73 |
| 1:B:225:MET:HE1 | 1:B:227:LYS:HG3 | 1.70 | 0.73 |
| 1:B:435:ILE:HD13 | 1:B:436:ALA:N | 2.03 | 0.73 |
| 1:B:46:PRO:HG2 | 1:B:69:ARG:CG | 2.17 | 0.73 |
| 1:A:548:ARG:O | 1:A:584:PRO:HD3 | 1.88 | 0.73 |
| 1:B:39:PHE:CD2 | 1:B:473:GLN:HG3 | 2.23 | 0.73 |
| 1:B:567:ILE:HD12 | 1:B:650:PHE:CZ | 2.22 | 0.73 |
| 1:B:704:LEU:HD11 | 1:B:724:LYS:HE3 | 1.69 | 0.73 |
| 1:A:670:ARG:HA | 1:A:670:ARG:HE | 1.54 | 0.72 |
| 1:A:46:PRO:HG2 | 1:A:69:ARG:CG | 2.17 | 0.72 |
| 1:B:184:ILE:O | 1:B:184:ILE:HD12 | 1.89 | 0.72 |
| 1:A:1030:ASP:O | 1:A:1032:VAL:HG23 | 1.89 | 0.72 |
| 1:A:181:LYS:HZ3 | 1:A:216:VAL:HG23 | 1.54 | 0.72 |
| 1:A:184:ILE:HD12 | 1:A:184:ILE:O | 1.89 | 0.72 |
| 1:A:73:LEU:HD22 | 1:A:79:VAL:HA | 1.72 | 0.72 |
| 1:A:784:TRP:HD1 | 1:A:790:ILE:HD11 | 1.51 | 0.72 |
| 1:B:99:ILE:HD11 | 1:B:152:PHE:HB2 | 1.69 | 0.72 |
| 1:B:670:ARG:HA | 1:B:670:ARG:HE | 1.55 | 0.72 |
| 1:A:822:CYS:HA | 1:A:833:LEU:HD23 | 1.70 | 0.72 |
| 1:A:994:LEU:HD11 | 1:A:1006:ASN:ND2 | 2.05 | 0.72 |
| 1:B:181:LYS:HD2 | 1:B:202:LYS:HA | 1.71 | 0.72 |
| 1:B:822:CYS:HA | 1:B:833:LEU:HD23 | 1.70 | 0.72 |
| 1:A:558:VAL:HG11 | 1:A:646:ALA:HB2 | 1.71 | 0.72 |
| 1:B:261:GLU:HA | 1:B:264:SER:O | 1.89 | 0.72 |
| 1:A:202:LYS:HD3 | 1:A:214:ALA:HB3 | 1.69 | 0.72 |
| 1:B:115:LYS:HB3 | 1:B:168:VAL:HG11 | 1.71 | 0.72 |
| 1:A:39:PHE:CD2 | 1:A:473:GLN:HG3 | 2.23 | 0.72 |
| 1:A:619:VAL:HB | 1:A:620:PRO:HD3 | 1.72 | 0.72 |
| 1:A:832:THR:CG2 | 1:A:836:HIS:HB2 | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:458:ARG:HG3 | 1:B:468:GLN:OE1 | 1.90 | 0.72 |
| 1:B:704:LEU:HB2 | 1:B:722:LYS:HG3 | 1.72 | 0.72 |
| 1:A:261:GLU:HA | 1:A:264:SER:O | 1.89 | 0.71 |
| 1:A:595:GLU:CB | 1:A:597:LEU:HD23 | 2.14 | 0.71 |
| 1:A:937:ARG:CG | 1:A:938:PRO:HD2 | 2.20 | 0.71 |
| 1:B:93:LYS:HD2 | 1:B:105:GLU:OE1 | 1.90 | 0.71 |
| 1:B:446:PHE:HZ | 1:B:506:VAL:HG23 | 1.55 | 0.71 |
| 1:B:595:GLU:HG2 | 1:B:632:VAL:HG13 | 1.72 | 0.71 |
| 1:A:519:LEU:HD12 | 1:A:552:SER:O | 1.90 | 0.71 |
| 1:A:806:MET:H | 1:A:806:MET:CE | 1.97 | 0.71 |
| 1:B:380:LEU:HB2 | 1:B:386:LYS:CE | 2.20 | 0.71 |
| 1:B:471:THR:HG23 | 1:B:473:GLN:HE22 | 1.55 | 0.71 |
| 1:A:1017:LYS:H | 1:A:1017:LYS:CE | 2.01 | 0.71 |
| 1:A:321:LEU:HG | 1:A:325:LEU:CD1 | 2.20 | 0.71 |
| 1:B:832:THR:CG2 | 1:B:836:HIS:HB2 | 2.20 | 0.71 |
| 1:A:595:GLU:HG2 | 1:A:632:VAL:HG13 | 1.72 | 0.71 |
| 1:A:847:LEU:CD1 | 1:A:852:SER:HB3 | 2.20 | 0.71 |
| 1:B:937:ARG:CG | 1:B:938:PRO:HD2 | 2.20 | 0.71 |
| 1:A:370:LEU:HD21 | 1:A:374:TYR:HE1 | 1.55 | 0.71 |
| 1:A:989:GLY:HA2 | 1:A:1017:LYS:CE | 2.20 | 0.71 |
| 1:B:563:HIS:HB2 | 1:B:577:VAL:CG1 | 2.21 | 0.71 |
| 1:B:619:VAL:HB | 1:B:620:PRO:HD3 | 1.72 | 0.71 |
| 1:B:847:LEU:CD1 | 1:B:852:SER:HB3 | 2.20 | 0.71 |
| 1:A:321:LEU:HG | 1:A:325:LEU:HD11 | 1.71 | 0.71 |
| 1:B:188:VAL:HG13 | 1:B:190:GLY:H | 1.56 | 0.71 |
| 1:B:321:LEU:HG | 1:B:325:LEU:CD1 | 2.20 | 0.71 |
| 1:A:1016:MET:O | 1:A:1032:VAL:HG13 | 1.91 | 0.71 |
| 1:A:304:VAL:HG11 | 1:A:351:GLU:OE2 | 1.91 | 0.71 |
| 1:A:40:VAL:HG12 | 1:A:503:ARG:HB3 | 1.73 | 0.71 |
| 1:B:450:LYS:HA | 1:B:479:PRO:HB3 | 1.73 | 0.71 |
| 1:A:1004:ILE:HD13 | 1:A:1005:CYS:N | 2.06 | 0.71 |
| 1:A:380:LEU:HB2 | 1:A:386:LYS:CE | 2.20 | 0.71 |
| 1:A:474:VAL:HG21 | 1:A:495:ILE:HD13 | 1.72 | 0.71 |
| 1:A:515:CYS:O | 1:A:519:LEU:HD23 | 1.91 | 0.71 |
| 1:A:704:LEU:HB2 | 1:A:722:LYS:HG3 | 1.71 | 0.71 |
| 1:A:806:MET:HE3 | 1:A:806:MET:N | 1.99 | 0.71 |
| 1:B:474:VAL:HG21 | 1:B:495:ILE:HD13 | 1.72 | 0.71 |
| 1:B:575:LEU:HD22 | 1:B:575:LEU:H | 1.56 | 0.71 |
| 1:A:962:ARG:HB3 | 1:A:1034:GLN:HG3 | 1.73 | 0.70 |
| 1:B:154:LYS:H | 1:B:157:HIS:HD2 | 1.36 | 0.70 |
| 1:B:72:LYS:HE3 | 1:B:80:LEU:CD1 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:458:ARG:HG3 | 1:A:468:GLN:OE1 | 1.90 | 0.70 |
| 1:B:321:LEU:HG | 1:B:325:LEU:HD11 | 1.71 | 0.70 |
| 1:A:115:LYS:HB3 | 1:A:168:VAL:HG11 | 1.71 | 0.70 |
| 1:A:480:VAL:HB | 1:A:484:MET:CE | 2.21 | 0.70 |
| 1:A:446:PHE:HZ | 1:A:506:VAL:HG23 | 1.55 | 0.70 |
| 1:A:507:GLU:HG3 | 1:A:537:ARG:HG3 | 1.74 | 0.70 |
| 1:A:556:GLN:O | 1:A:582:ASN:HB3 | 1.91 | 0.70 |
| 1:B:281:ARG:HB3 | 1:B:293:VAL:CG1 | 2.22 | 0.70 |
| 1:B:304:VAL:HG11 | 1:B:351:GLU:OE2 | 1.91 | 0.70 |
| 1:A:281:ARG:HB3 | 1:A:293:VAL:CG1 | 2.22 | 0.70 |
| 1:A:563:HIS:HB2 | 1:A:577:VAL:CG1 | 2.21 | 0.70 |
| 1:B:519:LEU:HD12 | 1:B:552:SER:O | 1.90 | 0.70 |
| 1:A:471:THR:HG23 | 1:A:473:GLN:HE22 | 1.55 | 0.70 |
| 1:B:370:LEU:HD21 | 1:B:374:TYR:HE1 | 1.55 | 0.70 |
| 1:A:63:TYR:C | 1:A:64:LEU:HD22 | 2.12 | 0.70 |
| 1:A:39:PHE:HE1 | 1:A:505:PRO:HD2 | 1.56 | 0.70 |
| 1:A:93:LYS:HD2 | 1:A:105:GLU:OE1 | 1.91 | 0.70 |
| 1:A:1016:MET:HE3 | 1:A:1017:LYS:C | 2.12 | 0.70 |
| 1:A:181:LYS:HD2 | 1:A:202:LYS:HA | 1.71 | 0.70 |
| 1:B:847:LEU:HD21 | 1:B:850:ALA:HA | 1.73 | 0.70 |
| 1:A:42:PHE:HE1 | 1:A:79:VAL:CG2 | 2.05 | 0.70 |
| 1:B:216:VAL:HG12 | 1:B:224:SER:OG | 1.92 | 0.70 |
| 1:B:480:VAL:HB | 1:B:484:MET:CE | 2.21 | 0.70 |
| 1:A:873:THR:HG23 | 1:A:981:GLY:C | 2.11 | 0.70 |
| 1:B:551:ALA:HA | 1:B:556:GLN:OE1 | 1.92 | 0.70 |
| 1:A:367:LYS:HE2 | 1:A:399:ILE:O | 1.91 | 0.69 |
| 1:A:474:VAL:CG1 | 1:A:475:VAL:HG23 | 2.18 | 0.69 |
| 1:A:450:LYS:HA | 1:A:479:PRO:HB3 | 1.73 | 0.69 |
| 1:A:551:ALA:HA | 1:A:556:GLN:OE1 | 1.92 | 0.69 |
| 1:B:558:VAL:HG11 | 1:B:646:ALA:HB2 | 1.71 | 0.69 |
| 1:B:73:LEU:HD22 | 1:B:79:VAL:HA | 1.72 | 0.69 |
| 1:A:739:ILE:HB | 1:A:781:THR:CG2 | 2.22 | 0.69 |
| 1:A:72:LYS:HE3 | 1:A:80:LEU:CD1 | 2.22 | 0.69 |
| 1:B:110:THR:HG22 | 1:B:132:LEU:HD21 | 1.73 | 0.69 |
| 1:B:63:TYR:C | 1:B:64:LEU:HD22 | 2.12 | 0.69 |
| 1:B:367:LYS:HE2 | 1:B:399:ILE:O | 1.91 | 0.69 |
| 1:B:515:CYS:O | 1:B:519:LEU:HD23 | 1.91 | 0.69 |
| 1:A:847:LEU:HD21 | 1:A:850:ALA:HA | 1.73 | 0.69 |
| 1:B:40:VAL:HG12 | 1:B:503:ARG:HB3 | 1.73 | 0.69 |
| 1:A:1016:MET:HG2 | 1:A:1035:TYR:HE2 | 1.57 | 0.69 |
| 1:A:216:VAL:HG12 | 1:A:224:SER:OG | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:380:LEU:HB2 | 1:A:386:LYS:HE3 | 1.74 | 0.69 |
| 1:A:439:TYR:CZ | 1:A:538:LYS:HE3 | 2.28 | 0.69 |
| 1:A:560:LEU:CD2 | 1:A:648:THR:HG23 | 2.19 | 0.69 |
| 1:A:188:VAL:HG13 | 1:A:190:GLY:H | 1.56 | 0.69 |
| 1:A:435:ILE:HD12 | 1:A:486:PHE:CD1 | 2.27 | 0.69 |
| 1:A:473:GLN:OE1 | 1:A:504:VAL:HG13 | 1.93 | 0.69 |
| 1:A:802:LYS:C | 1:A:803:CYS:N | 2.46 | 0.69 |
| 1:A:873:THR:HG23 | 1:A:982:SER:N | 2.07 | 0.69 |
| 1:B:473:GLN:OE1 | 1:B:504:VAL:HG13 | 1.93 | 0.69 |
| 1:A:595:GLU:CG | 1:A:632:VAL:HG13 | 2.22 | 0.69 |
| 1:A:959:LYS:CB | 1:A:972:THR:HB | 2.21 | 0.69 |
| 1:A:988:PHE:HB3 | 1:A:1016:MET:SD | 2.33 | 0.69 |
| 1:B:453:LYS:HE3 | 1:B:472:VAL:HG21 | 1.73 | 0.69 |
| 1:A:958:LEU:HD23 | 1:A:959:LYS:N | 2.08 | 0.69 |
| 1:B:380:LEU:HB2 | 1:B:386:LYS:HE3 | 1.74 | 0.69 |
| 1:A:133:TYR:HB2 | 1:A:136:ILE:HG12 | 1.75 | 0.69 |
| 1:A:133:TYR:CD2 | 1:A:136:ILE:HG12 | 2.28 | 0.69 |
| 1:B:133:TYR:CD2 | 1:B:136:ILE:HG12 | 2.28 | 0.69 |
| 1:A:196:PRO:HB3 | 1:A:225:MET:HE1 | 1.73 | 0.68 |
| 1:B:446:PHE:CD2 | 1:B:454:LEU:HD21 | 2.24 | 0.68 |
| 1:B:507:GLU:HG3 | 1:B:537:ARG:HG3 | 1.74 | 0.68 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:HG21 | 1.73 | 0.68 |
| 1:B:46:PRO:HG3 | 1:B:69:ARG:HD2 | 1.75 | 0.68 |
| 1:A:972:THR:HG23 | 1:A:1002:TYR:CD1 | 2.28 | 0.68 |
| 1:B:739:ILE:HB | 1:B:781:THR:CG2 | 2.23 | 0.68 |
| 1:B:412:LEU:H | 1:B:412:LEU:HD13 | 1.59 | 0.68 |
| 1:A:773:ILE:HD13 | 1:A:773:ILE:H | 1.59 | 0.68 |
| 1:B:474:VAL:CG1 | 1:B:475:VAL:HG23 | 2.18 | 0.68 |
| 1:B:773:ILE:HD13 | 1:B:773:ILE:H | 1.59 | 0.68 |
| 1:A:110:THR:HG22 | 1:A:132:LEU:HD21 | 1.74 | 0.68 |
| 1:A:323:ARG:HG3 | 1:A:324:THR:H | 1.58 | 0.68 |
| 1:A:689:PHE:CD1 | 1:A:691:GLU:HG2 | 2.28 | 0.68 |
| 1:A:703:LEU:HD13 | 1:A:723:ALA:HB2 | 1.76 | 0.68 |
| 1:B:435:ILE:HD12 | 1:B:486:PHE:CD1 | 2.27 | 0.68 |
| 1:A:594:PHE:O | 1:A:595:GLU:HG2 | 1.94 | 0.68 |
| 1:A:867:GLY:HA3 | 1:A:948:TYR:OH | 1.94 | 0.68 |
| 1:B:190:GLY:HA2 | 1:B:233:PHE:CE2 | 2.29 | 0.68 |
| 1:B:548:ARG:NE | 1:B:583:VAL:O | 2.26 | 0.68 |
| 1:B:595:GLU:CG | 1:B:632:VAL:HG13 | 2.22 | 0.68 |
| 1:A:53:LEU:HB2 | 1:A:496:MET:HE1 | 1.76 | 0.68 |
| 1:B:594:PHE:O | 1:B:595:GLU:HG2 | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:700:CYS:O | 1:B:725:ASN:CB | 2.30 | 0.68 |
| 1:A:190:GLY:HA2 | 1:A:233:PHE:CE2 | 2.29 | 0.68 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:NE | 2.09 | 0.68 |
| 1:A:555:LYS:HG3 | 1:A:556:GLN:N | 2.09 | 0.68 |
| 1:A:830:GLN:HG2 | 1:A:831:CYS:N | 2.09 | 0.68 |
| 1:B:689:PHE:CD1 | 1:B:691:GLU:HG2 | 2.28 | 0.68 |
| 1:B:830:GLN:HG2 | 1:B:831:CYS:N | 2.09 | 0.68 |
| 1:B:98:ARG:HE | 1:B:107:LEU:CD1 | 2.07 | 0.68 |
| 1:A:575:LEU:HD22 | 1:A:575:LEU:H | 1.56 | 0.68 |
| 1:A:73:LEU:CD2 | 1:A:79:VAL:HA | 2.23 | 0.68 |
| 1:B:323:ARG:HG3 | 1:B:324:THR:H | 1.58 | 0.68 |
| 1:B:62:ILE:O | 1:B:62:ILE:HG13 | 1.94 | 0.68 |
| 1:B:62:ILE:HD11 | 1:B:73:LEU:HD12 | 1.76 | 0.68 |
| 1:A:867:GLY:C | 1:A:980:ALA:HB1 | 2.14 | 0.67 |
| 1:A:962:ARG:HB3 | 1:A:1034:GLN:CG | 2.23 | 0.67 |
| 1:B:548:ARG:HG3 | 1:B:584:PRO:CA | 2.25 | 0.67 |
| 1:A:1013:VAL:HG22 | 1:A:1014:LEU:H | 1.60 | 0.67 |
| 1:A:532:HIS:O | 1:A:641:THR:HG21 | 1.94 | 0.67 |
| 1:B:42:PHE:HE1 | 1:B:79:VAL:CG2 | 2.05 | 0.67 |
| 1:B:560:LEU:CD2 | 1:B:648:THR:HG23 | 2.19 | 0.67 |
| 1:B:863:ILE:HG23 | 1:B:864:PRO:CD | 2.23 | 0.67 |
| 1:A:46:PRO:HG3 | 1:A:69:ARG:HD2 | 1.75 | 0.67 |
| 1:B:460:ASP:HB3 | 1:B:463:LYS:HB3 | 1.77 | 0.67 |
| 1:B:867:GLY:HA3 | 1:B:948:TYR:OH | 1.94 | 0.67 |
| 1:A:98:ARG:HE | 1:A:107:LEU:HD11 | 1.60 | 0.67 |
| 1:A:531:LEU:HG | 1:A:584:PRO:HG2 | 1.77 | 0.67 |
| 1:A:951:MET:HG3 | 1:A:952:THR:N | 2.09 | 0.67 |
| 1:B:98:ARG:HE | 1:B:107:LEU:HD11 | 1.60 | 0.67 |
| 1:A:137:CYS:HB2 | 1:A:213:PHE:CZ | 2.30 | 0.67 |
| 1:A:321:LEU:O | 1:A:325:LEU:HG | 1.95 | 0.67 |
| 1:A:460:ASP:HB3 | 1:A:463:LYS:HB3 | 1.77 | 0.67 |
| 1:B:555:LYS:HG3 | 1:B:556:GLN:N | 2.09 | 0.67 |
| 1:A:994:LEU:CD1 | 1:A:1006:ASN:HD22 | 2.07 | 0.67 |
| 1:A:863:ILE:HG23 | 1:A:864:PRO:CD | 2.23 | 0.67 |
| 1:B:321:LEU:O | 1:B:325:LEU:HG | 1.95 | 0.67 |
| 1:B:595:GLU:HG2 | 1:B:632:VAL:CG1 | 2.25 | 0.67 |
| 1:B:62:ILE:HD12 | 1:B:64:LEU:HD21 | 1.75 | 0.67 |
| 1:B:73:LEU:CD2 | 1:B:79:VAL:HA | 2.24 | 0.67 |
| 1:A:62:ILE:HD11 | 1:A:73:LEU:HD12 | 1.76 | 0.67 |
| 1:B:53:LEU:HB2 | 1:B:496:MET:HE1 | 1.77 | 0.67 |
| 1:A:62:ILE:HD12 | 1:A:64:LEU:HD21 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:325:LEU:CD1 | 1:B:333:LEU:HD11 | 2.25 | 0.66 |
| 1:A:595:GLU:HG2 | 1:A:632:VAL:CG1 | 2.25 | 0.66 |
| 1:A:847:LEU:HG | 1:A:850:ALA:N | 2.10 | 0.66 |
| 1:A:98:ARG:HE | 1:A:107:LEU:CD1 | 2.07 | 0.66 |
| 1:B:703:LEU:HD13 | 1:B:723:ALA:HB2 | 1.76 | 0.66 |
| 1:B:847:LEU:HG | 1:B:850:ALA:N | 2.10 | 0.66 |
| 1:A:532:HIS:HA | 1:A:641:THR:CG2 | 2.25 | 0.66 |
| 1:A:873:THR:HG1 | 1:A:981:GLY:HA2 | 1.61 | 0.66 |
| 1:B:133:TYR:HB2 | 1:B:136:ILE:HG12 | 1.75 | 0.66 |
| 1:B:863:ILE:HG13 | 1:B:864:PRO:CD | 2.25 | 0.66 |
| 1:B:98:ARG:HH21 | 1:B:107:LEU:HD12 | 1.60 | 0.66 |
| 1:B:40:VAL:HG11 | 1:B:503:ARG:NE | 2.09 | 0.66 |
| 1:A:98:ARG:HH21 | 1:A:107:LEU:HD12 | 1.59 | 0.66 |
| 1:A:239:PHE:CD1 | 1:A:260:PRO:HD2 | 2.30 | 0.66 |
| 1:A:566:ASN:HA | 1:A:651:VAL:CG2 | 2.25 | 0.66 |
| 1:A:955:LEU:HG | 1:A:973:ILE:CG2 | 2.24 | 0.66 |
| 1:B:133:TYR:HB2 | 1:B:136:ILE:H | 1.61 | 0.66 |
| 1:A:446:PHE:CZ | 1:A:486:PHE:HZ | 2.13 | 0.66 |
| 1:B:739:ILE:HD12 | 1:B:748:ARG:HG2 | 1.76 | 0.66 |
| 1:B:854:CYS:C | 1:B:855:THR:N | 2.49 | 0.66 |
| 1:B:809:SER:CB | 1:B:881:ASN:CG | 2.47 | 0.66 |
| 1:A:325:LEU:CD1 | 1:A:333:LEU:HD11 | 2.25 | 0.66 |
| 1:A:739:ILE:HD12 | 1:A:748:ARG:HG2 | 1.76 | 0.66 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:CD | 2.25 | 0.66 |
| 1:A:567:ILE:HD13 | 1:A:651:VAL:O | 1.96 | 0.66 |
| 1:B:181:LYS:HD3 | 1:B:202:LYS:HA | 1.78 | 0.66 |
| 1:B:137:CYS:HB2 | 1:B:213:PHE:CZ | 2.30 | 0.66 |
| 1:B:410:ALA:HB1 | 1:B:411:PRO:HD2 | 1.78 | 0.66 |
| 1:B:548:ARG:HG3 | 1:B:584:PRO:HA | 1.78 | 0.66 |
| 1:A:1016:MET:CE | 1:A:1033:PHE:HB3 | 2.25 | 0.66 |
| 1:A:892:HIS:NE2 | 1:A:931:ILE:HB | 2.11 | 0.66 |
| 1:B:110:THR:HB | 1:B:132:LEU:CD2 | 2.26 | 0.66 |
| 1:B:629:HIS:CE1 | 1:B:669:TYR:CZ | 2.69 | 0.66 |
| 1:A:261:GLU:HG2 | 1:A:264:SER:C | 2.17 | 0.65 |
| 1:A:296:PRO:HD2 | 1:A:414:VAL:CG2 | 2.27 | 0.65 |
| 1:B:261:GLU:HG2 | 1:B:264:SER:C | 2.17 | 0.65 |
| 1:A:216:VAL:HG12 | 1:A:224:SER:CB | 2.26 | 0.65 |
| 1:A:412:LEU:HD13 | 1:A:412:LEU:H | 1.59 | 0.65 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:CG2 | 2.21 | 0.65 |
| 1:A:782:VAL:HG23 | 1:A:790:ILE:HB | 1.78 | 0.65 |
| 1:A:870:GLU:CB | 1:A:1024:ARG:HG3 | 2.17 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:797:LYS:HD2 | 1:A:797:LYS:N | 2.11 | 0.65 |
| 1:B:239:PHE:CD1 | 1:B:260:PRO:HD2 | 2.30 | 0.65 |
| 1:B:782:VAL:HG23 | 1:B:790:ILE:HB | 1.78 | 0.65 |
| 1:A:133:TYR:HB2 | 1:A:136:ILE:H | 1.61 | 0.65 |
| 1:A:62:ILE:HG13 | 1:A:62:ILE:O | 1.94 | 0.65 |
| 1:A:432:THR:OG1 | 1:A:480:VAL:HG23 | 1.96 | 0.65 |
| 1:A:473:GLN:HG2 | 1:A:504:VAL:HG22 | 1.79 | 0.65 |
| 1:B:676:TYR:HD1 | 1:B:730:GLN:CG | 2.08 | 0.65 |
| 1:B:847:LEU:CD2 | 1:B:850:ALA:HA | 2.27 | 0.65 |
| 1:A:181:LYS:HD3 | 1:A:202:LYS:HA | 1.78 | 0.65 |
| 1:A:154:LYS:H | 1:A:157:HIS:CD2 | 2.15 | 0.65 |
| 1:B:265:PRO:HD3 | 1:B:274:VAL:CG2 | 2.27 | 0.65 |
| 1:B:446:PHE:CZ | 1:B:486:PHE:HZ | 2.14 | 0.65 |
| 1:B:675:LYS:HE3 | 1:B:694:VAL:HG22 | 1.79 | 0.65 |
| 1:A:110:THR:HB | 1:A:132:LEU:CD2 | 2.26 | 0.65 |
| 1:A:453:LYS:HG2 | 1:A:472:VAL:CG2 | 2.16 | 0.65 |
| 1:A:706:VAL:HG13 | 1:A:707:ASP:O | 1.96 | 0.65 |
| 1:B:216:VAL:HG12 | 1:B:224:SER:CB | 2.26 | 0.65 |
| 1:A:872:GLY:HA3 | 1:A:1023:ASP:OD1 | 1.97 | 0.65 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:C | 2.18 | 0.65 |
| 1:B:653:TYR:OH | 1:B:682:HIS:CE1 | 2.50 | 0.65 |
| 1:B:807:ARG:HD3 | 1:B:812:LEU:C | 2.17 | 0.65 |
| 1:A:368:ASP:O | 1:A:371:GLN:HG2 | 1.97 | 0.64 |
| 1:A:675:LYS:HE3 | 1:A:694:VAL:HG22 | 1.79 | 0.64 |
| 1:B:432:THR:OG1 | 1:B:480:VAL:HG23 | 1.96 | 0.64 |
| 1:A:405:GLY:O | 1:A:406:LEU:HD22 | 1.98 | 0.64 |
| 1:A:410:ALA:HB1 | 1:A:411:PRO:HD2 | 1.78 | 0.64 |
| 1:B:39:PHE:HE1 | 1:B:505:PRO:HD2 | 1.57 | 0.64 |
| 1:B:405:GLY:O | 1:B:406:LEU:HD22 | 1.98 | 0.64 |
| 1:A:105:GLU:HB3 | 1:A:106:PRO:HD2 | 1.80 | 0.64 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:CG2 | 2.27 | 0.64 |
| 1:A:309:LEU:HD11 | 1:A:311:ALA:O | 1.98 | 0.64 |
| 1:A:926:ALA:HB1 | 1:A:947:LEU:CD1 | 2.27 | 0.64 |
| 1:B:186:THR:HG22 | 1:B:187:ALA:N | 2.12 | 0.64 |
| 1:B:320:VAL:O | 1:B:323:ARG:HG2 | 1.98 | 0.64 |
| 1:B:474:VAL:HG12 | 1:B:475:VAL:CG2 | 2.21 | 0.64 |
| 1:B:53:LEU:HB2 | 1:B:496:MET:CE | 2.28 | 0.64 |
| 1:B:567:ILE:HD13 | 1:B:651:VAL:O | 1.96 | 0.64 |
| 1:A:186:THR:HG22 | 1:A:187:ALA:N | 2.12 | 0.64 |
| 1:A:53:LEU:HB2 | 1:A:496:MET:CE | 2.28 | 0.64 |
| 1:A:620:PRO:CA | 1:A:623:ILE:HG13 | 2.23 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:53:LEU:HG | 1:A:64:LEU:CD1 | 2.28 | 0.64 |
| 1:B:797:LYS:N | 1:B:797:LYS:HD2 | 2.11 | 0.64 |
| 1:B:926:ALA:HB1 | 1:B:947:LEU:CD1 | 2.27 | 0.64 |
| 1:A:175:TYR:HD2 | 1:A:179:ASP:HB3 | 1.63 | 0.64 |
| 1:A:460:ASP:CB | 1:A:463:LYS:HB3 | 2.28 | 0.64 |
| 1:B:469:TYR:HB3 | 1:B:523:ASP:CG | 2.18 | 0.64 |
| 1:B:473:GLN:HG2 | 1:B:504:VAL:HG22 | 1.79 | 0.64 |
| 1:B:175:TYR:HD2 | 1:B:179:ASP:HB3 | 1.63 | 0.64 |
| 1:B:296:PRO:HD2 | 1:B:414:VAL:CG2 | 2.27 | 0.64 |
| 1:B:460:ASP:CB | 1:B:463:LYS:HB3 | 2.28 | 0.64 |
| 1:B:505:PRO:CB | 1:B:507:GLU:O | 2.46 | 0.64 |
| 1:A:566:ASN:HB3 | 1:A:651:VAL:HG21 | 1.80 | 0.64 |
| 1:A:847:LEU:CD2 | 1:A:850:ALA:HA | 2.27 | 0.64 |
| 1:B:56:ASP:OD1 | 1:B:119:ILE:HD12 | 1.98 | 0.64 |
| 1:A:741:ASN:O | 1:A:778:VAL:HG13 | 1.98 | 0.64 |
| 1:B:105:GLU:HB3 | 1:B:106:PRO:HD2 | 1.80 | 0.64 |
| 1:B:473:GLN:HB2 | 1:B:504:VAL:HG22 | 1.80 | 0.64 |
| 1:B:566:ASN:HA | 1:B:651:VAL:CG2 | 2.25 | 0.64 |
| 1:A:56:ASP:OD1 | 1:A:119:ILE:HD12 | 1.98 | 0.64 |
| 1:B:154:LYS:H | 1:B:157:HIS:CD2 | 2.15 | 0.64 |
| 1:B:118:LEU:HG | 1:B:172:ILE:HG13 | 1.80 | 0.64 |
| 1:B:309:LEU:HD11 | 1:B:311:ALA:O | 1.98 | 0.64 |
| 1:B:53:LEU:HG | 1:B:64:LEU:CD1 | 2.28 | 0.64 |
| 1:B:706:VAL:HG13 | 1:B:707:ASP:O | 1.96 | 0.64 |
| 1:B:713:VAL:HG12 | 1:B:714:GLU:HG3 | 1.79 | 0.64 |
| 1:B:806:MET:HG2 | 1:B:807:ARG:HG3 | 1.80 | 0.64 |
| 1:A:405:GLY:C | 1:A:406:LEU:HD22 | 2.19 | 0.63 |
| 1:B:185:ALA:HB1 | 1:B:243:TYR:CD1 | 2.33 | 0.63 |
| 1:B:653:TYR:CE2 | 1:B:682:HIS:ND1 | 2.60 | 0.63 |
| 1:B:892:HIS:NE2 | 1:B:931:ILE:HB | 2.11 | 0.63 |
| 1:B:368:ASP:O | 1:B:371:GLN:HG2 | 1.97 | 0.63 |
| 1:B:405:GLY:C | 1:B:406:LEU:HD22 | 2.19 | 0.63 |
| 1:B:446:PHE:CE1 | 1:B:486:PHE:HZ | 2.16 | 0.63 |
| 1:B:480:VAL:HG11 | 1:B:495:ILE:HD11 | 1.81 | 0.63 |
| 1:B:653:TYR:CE2 | 1:B:682:HIS:CE1 | 2.87 | 0.63 |
| 1:B:894:LYS:HD3 | 1:B:899:GLU:HA | 1.81 | 0.63 |
| 1:A:320:VAL:O | 1:A:323:ARG:HG2 | 1.98 | 0.63 |
| 1:B:181:LYS:HE2 | 1:B:202:LYS:HG2 | 1.80 | 0.63 |
| 1:A:1002:TYR:CZ | 1:A:1004:ILE:HB | 2.32 | 0.63 |
| 1:A:118:LEU:HG | 1:A:172:ILE:HG13 | 1.80 | 0.63 |
| 1:A:713:VAL:HG12 | 1:A:714:GLU:HG3 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:978:LEU:O | 1:A:998:ARG:HD2 | 1.98 | 0.63 |
| 1:B:620:PRO:CA | 1:B:623:ILE:HG13 | 2.23 | 0.63 |
| 1:A:806:MET:HG2 | 1:A:807:ARG:HG3 | 1.80 | 0.63 |
| 1:B:386:LYS:HG3 | 1:B:386:LYS:O | 1.99 | 0.63 |
| 1:B:41:THR:HG22 | 1:B:502:THR:HA | 1.81 | 0.63 |
| 1:B:446:PHE:CZ | 1:B:506:VAL:HG23 | 2.33 | 0.63 |
| 1:B:566:ASN:HB3 | 1:B:651:VAL:HG21 | 1.79 | 0.63 |
| 1:A:933:VAL:HG23 | 1:A:934:ALA:N | 2.10 | 0.63 |
| 1:A:1014:LEU:HD22 | 1:A:1014:LEU:N | 2.14 | 0.63 |
| 1:A:295:VAL:HA | 1:A:414:VAL:HG21 | 1.81 | 0.63 |
| 1:A:446:PHE:CE1 | 1:A:486:PHE:HZ | 2.16 | 0.63 |
| 1:A:894:LYS:HD3 | 1:A:899:GLU:HA | 1.80 | 0.63 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:CZ | 2.29 | 0.63 |
| 1:B:448:GLY:CA | 1:B:480:VAL:HG21 | 2.29 | 0.63 |
| 1:B:575:LEU:N | 1:B:575:LEU:HD22 | 2.14 | 0.63 |
| 1:A:1015:ASP:O | 1:A:1016:MET:HB3 | 1.98 | 0.62 |
| 1:A:197:THR:HG21 | 1:A:228:ILE:HD11 | 1.81 | 0.62 |
| 1:B:741:ASN:O | 1:B:778:VAL:HG13 | 1.98 | 0.62 |
| 1:B:949:TYR:HE2 | 1:B:951:MET:CE | 2.12 | 0.62 |
| 1:A:180:ASP:O | 1:A:181:LYS:HG2 | 1.99 | 0.62 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CD1 | 2.33 | 0.62 |
| 1:A:372:SER:O | 1:A:375:ARG:HB2 | 1.99 | 0.62 |
| 1:B:180:ASP:O | 1:B:181:LYS:HG2 | 1.99 | 0.62 |
| 1:B:295:VAL:HA | 1:B:414:VAL:HG21 | 1.81 | 0.62 |
| 1:B:474:VAL:CG2 | 1:B:495:ILE:HD13 | 2.29 | 0.62 |
| 1:A:949:TYR:HE2 | 1:A:951:MET:CE | 2.12 | 0.62 |
| 1:B:458:ARG:HG3 | 1:B:468:GLN:CD | 2.20 | 0.62 |
| 1:A:382:LEU:HD23 | 1:A:385:LEU:HB3 | 1.81 | 0.62 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:CG | 2.29 | 0.62 |
| 1:A:439:TYR:OH | 1:A:538:LYS:CE | 2.47 | 0.62 |
| 1:B:432:THR:HG1 | 1:B:480:VAL:HG23 | 1.65 | 0.62 |
| 1:B:469:TYR:HE2 | 1:B:471:THR:HB | 1.65 | 0.62 |
| 1:A:446:PHE:CZ | 1:A:506:VAL:HG23 | 2.33 | 0.62 |
| 1:A:448:GLY:CA | 1:A:480:VAL:HG21 | 2.28 | 0.62 |
| 1:A:458:ARG:HG3 | 1:A:468:GLN:CD | 2.20 | 0.62 |
| 1:B:320:VAL:HG21 | 1:B:442:HIS:HD2 | 1.64 | 0.62 |
| 1:A:575:LEU:HD22 | 1:A:575:LEU:N | 2.14 | 0.62 |
| 1:B:933:VAL:HG23 | 1:B:934:ALA:N | 2.10 | 0.62 |
| 1:B:296:PRO:HB2 | 1:B:417:MET:SD | 2.39 | 0.62 |
| 1:B:40:VAL:HG11 | 1:B:503:ARG:CZ | 2.29 | 0.62 |
| 1:A:386:LYS:O | 1:A:386:LYS:HG3 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:696:LEU:N | 1:B:696:LEU:HD12 | 2.15 | 0.62 |
| 1:B:806:MET:CG | 1:B:807:ARG:HG3 | 2.30 | 0.62 |
| 1:B:474:VAL:HG22 | 1:B:495:ILE:CG2 | 2.29 | 0.62 |
| 1:B:492:GLN:HG2 | 1:B:503:ARG:CG | 2.29 | 0.62 |
| 1:B:855:THR:HG23 | 1:B:856:ASN:OD1 | 2.00 | 0.62 |
| 1:A:182:LEU:HG | 1:A:184:ILE:HG23 | 1.82 | 0.61 |
| 1:A:473:GLN:HB2 | 1:A:504:VAL:HG22 | 1.80 | 0.61 |
| 1:A:72:LYS:CD | 1:A:80:LEU:HD12 | 2.30 | 0.61 |
| 1:B:382:LEU:HD23 | 1:B:385:LEU:HB3 | 1.81 | 0.61 |
| 1:B:715:VAL:CG2 | 1:B:717:LYS:HD2 | 2.30 | 0.61 |
| 1:A:855:THR:HG23 | 1:A:856:ASN:OD1 | 1.99 | 0.61 |
| 1:B:372:SER:O | 1:B:375:ARG:HB2 | 1.99 | 0.61 |
| 1:A:110:THR:HG22 | 1:A:111:ASN:N | 2.14 | 0.61 |
| 1:B:204:THR:HG22 | 1:B:212:MET:SD | 2.40 | 0.61 |
| 1:A:181:LYS:HE2 | 1:A:202:LYS:HG2 | 1.80 | 0.61 |
| 1:A:296:PRO:HB2 | 1:A:417:MET:SD | 2.39 | 0.61 |
| 1:A:1016:MET:HE2 | 1:A:1033:PHE:HB3 | 1.82 | 0.61 |
| 1:A:41:THR:HG22 | 1:A:502:THR:HA | 1.81 | 0.61 |
| 1:A:873:THR:HG23 | 1:A:982:SER:CA | 2.30 | 0.61 |
| 1:B:110:THR:HG22 | 1:B:111:ASN:N | 2.14 | 0.61 |
| 1:B:706:VAL:HG22 | 1:B:707:ASP:N | 2.12 | 0.61 |
| 1:A:175:TYR:CD2 | 1:A:179:ASP:HB3 | 2.36 | 0.61 |
| 1:A:204:THR:HG22 | 1:A:212:MET:SD | 2.40 | 0.61 |
| 1:A:410:ALA:HB1 | 1:A:411:PRO:CD | 2.30 | 0.61 |
| 1:A:488:LYS:HG3 | 1:A:489:ASP:N | 2.14 | 0.61 |
| 1:A:480:VAL:HG11 | 1:A:495:ILE:HD11 | 1.81 | 0.61 |
| 1:A:474:VAL:CG2 | 1:A:495:ILE:HD13 | 2.29 | 0.61 |
| 1:A:712:PRO:HG3 | 1:A:801:TYR:OH | 2.01 | 0.61 |
| 1:A:806:MET:CG | 1:A:807:ARG:HG3 | 2.30 | 0.61 |
| 1:B:833:LEU:HB2 | 1:B:836:HIS:CD2 | 2.29 | 0.61 |
| 1:A:119:ILE:HD13 | 1:A:121:TYR:CZ | 2.36 | 0.61 |
| 1:A:532:HIS:HA | 1:A:641:THR:HG21 | 1.82 | 0.61 |
| 1:B:410:ALA:HB1 | 1:B:411:PRO:CD | 2.30 | 0.61 |
| 1:B:41:THR:HG22 | 1:B:502:THR:HG23 | 1.83 | 0.61 |
| 1:A:257:THR:C | 1:A:258:LEU:HD12 | 2.21 | 0.61 |
| 1:A:696:LEU:N | 1:A:696:LEU:HD12 | 2.15 | 0.61 |
| 1:B:175:TYR:CD2 | 1:B:179:ASP:HB3 | 2.36 | 0.61 |
| 1:B:181:LYS:HZ3 | 1:B:216:VAL:HG23 | 1.66 | 0.61 |
| 1:B:333:LEU:CD2 | 1:B:358:ILE:HG13 | 2.31 | 0.61 |
| 1:B:46:PRO:HD2 | 1:B:71:TYR:CE1 | 2.35 | 0.61 |
| 1:B:847:LEU:HD11 | 1:B:850:ALA:CA | 2.29 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:474:VAL:HG22 | 1:A:495:ILE:CG2 | 2.29 | 0.60 |
| 1:A:569:VAL:HB | 1:A:654:ASN:HB2 | 1.83 | 0.60 |
| 1:A:665:VAL:HG12 | 1:A:697:PRO:HG3 | 1.83 | 0.60 |
| 1:A:706:VAL:HG22 | 1:A:707:ASP:N | 2.12 | 0.60 |
| 1:B:488:LYS:HG3 | 1:B:489:ASP:N | 2.14 | 0.60 |
| 1:A:870:GLU:CG | 1:A:1025:ALA:N | 2.64 | 0.60 |
| 1:A:313:TYR:CE1 | 1:A:435:ILE:HG12 | 2.37 | 0.60 |
| 1:A:469:TYR:HE2 | 1:A:471:THR:HB | 1.65 | 0.60 |
| 1:B:444:LEU:CD2 | 1:B:524:PRO:HG3 | 2.23 | 0.60 |
| 1:B:548:ARG:HG2 | 1:B:584:PRO:HA | 1.83 | 0.60 |
| 1:B:95:TYR:CG | 1:B:96:PRO:HD3 | 2.36 | 0.60 |
| 1:A:715:VAL:CG2 | 1:A:717:LYS:HD2 | 2.30 | 0.60 |
| 1:B:257:THR:C | 1:B:258:LEU:HD12 | 2.21 | 0.60 |
| 1:B:99:ILE:HG13 | 1:B:100:VAL:N | 2.16 | 0.60 |
| 1:A:314:LEU:HD12 | 1:A:333:LEU:O | 2.01 | 0.60 |
| 1:B:773:ILE:HD13 | 1:B:773:ILE:N | 2.17 | 0.60 |
| 1:A:919:GLU:HB3 | 1:A:1024:ARG:NH1 | 2.16 | 0.60 |
| 1:A:963:GLY:O | 1:A:1036:VAL:HG22 | 2.01 | 0.60 |
| 1:B:313:TYR:CE1 | 1:B:435:ILE:HG12 | 2.37 | 0.60 |
| 1:B:314:LEU:HD12 | 1:B:333:LEU:O | 2.01 | 0.60 |
| 1:B:712:PRO:HG3 | 1:B:801:TYR:OH | 2.01 | 0.60 |
| 1:A:333:LEU:CD2 | 1:A:358:ILE:HG13 | 2.31 | 0.60 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:CE1 | 2.35 | 0.60 |
| 1:A:773:ILE:HD13 | 1:A:773:ILE:N | 2.17 | 0.60 |
| 1:B:46:PRO:HD2 | 1:B:71:TYR:CZ | 2.36 | 0.60 |
| 1:A:320:VAL:HG21 | 1:A:442:HIS:HD2 | 1.64 | 0.60 |
| 1:A:403:PHE:CZ | 1:A:406:LEU:HD23 | 2.37 | 0.60 |
| 1:A:62:ILE:HD13 | 1:A:77:LEU:CD2 | 2.32 | 0.60 |
| 1:A:630:HIS:HD2 | 1:A:632:VAL:CG2 | 2.15 | 0.60 |
| 1:B:181:LYS:HZ2 | 1:B:216:VAL:HG23 | 1.64 | 0.60 |
| 1:B:495:ILE:CG2 | 1:B:502:THR:HB | 2.32 | 0.60 |
| 1:B:182:LEU:HG | 1:B:184:ILE:HG23 | 1.82 | 0.60 |
| 1:B:323:ARG:HH21 | 1:B:463:LYS:HD2 | 1.67 | 0.60 |
| 1:B:119:ILE:HD13 | 1:B:121:TYR:CZ | 2.36 | 0.60 |
| 1:B:171:VAL:O | 1:B:182:LEU:HD12 | 2.02 | 0.60 |
| 1:B:403:PHE:CZ | 1:B:406:LEU:HD23 | 2.37 | 0.60 |
| 1:B:469:TYR:CE2 | 1:B:471:THR:HB | 2.36 | 0.60 |
| 1:B:665:VAL:HG12 | 1:B:697:PRO:HG3 | 1.83 | 0.60 |
| 1:B:662:LEU:HD11 | 1:B:702:GLN:HE22 | 1.65 | 0.60 |
| 1:B:72:LYS:CD | 1:B:80:LEU:HD12 | 2.30 | 0.60 |
| 1:A:1029:GLN:HG2 | 1:A:1030:ASP:H | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:387:VAL:HG13 | 1:B:388:LYS:HG3 | 1.83 | 0.60 |
| 1:A:1002:TYR:CE2 | 1:A:1004:ILE:HB | 2.37 | 0.59 |
| 1:A:991:GLN:HG3 | 1:A:1008:THR:HG21 | 1.84 | 0.59 |
| 1:B:154:LYS:N | 1:B:157:HIS:HD2 | 2.00 | 0.59 |
| 1:A:99:ILE:HG13 | 1:A:100:VAL:N | 2.16 | 0.59 |
| 1:A:387:VAL:HG13 | 1:A:388:LYS:HG3 | 1.83 | 0.59 |
| 1:A:469:TYR:CE2 | 1:A:471:THR:HB | 2.36 | 0.59 |
| 1:A:566:ASN:CA | 1:A:651:VAL:HG23 | 2.28 | 0.59 |
| 1:A:95:TYR:CG | 1:A:96:PRO:HD3 | 2.36 | 0.59 |
| 1:B:243:TYR:CD2 | 1:B:257:THR:HG22 | 2.37 | 0.59 |
| 1:B:873:THR:HB | 1:B:917:MET:HE2 | 1.84 | 0.59 |
| 1:A:271:LYS:HG3 | 1:A:272:GLU:N | 2.13 | 0.59 |
| 1:A:432:THR:HG1 | 1:A:480:VAL:HG23 | 1.65 | 0.59 |
| 1:A:457:ILE:HG12 | 1:A:467:LEU:HD13 | 1.84 | 0.59 |
| 1:A:560:LEU:HD23 | 1:A:648:THR:CG2 | 2.25 | 0.59 |
| 1:A:847:LEU:HD11 | 1:A:850:ALA:CA | 2.29 | 0.59 |
| 1:B:197:THR:HG21 | 1:B:228:ILE:HD11 | 1.82 | 0.59 |
| 1:B:239:PHE:CA | 1:B:260:PRO:HG2 | 2.30 | 0.59 |
| 1:B:387:VAL:HG13 | 1:B:388:LYS:N | 2.18 | 0.59 |
| 1:B:665:VAL:HG11 | 1:B:697:PRO:HD3 | 1.84 | 0.59 |
| 1:A:243:TYR:CD2 | 1:A:257:THR:HG22 | 2.37 | 0.59 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:CZ | 2.37 | 0.59 |
| 1:A:904:VAL:HG13 | 1:A:905:ASP:N | 2.18 | 0.59 |
| 1:A:931:ILE:O | 1:A:931:ILE:HG13 | 2.02 | 0.59 |
| 1:A:987:MET:HB2 | 1:A:1019:THR:HG23 | 1.83 | 0.59 |
| 1:A:40:VAL:HG13 | 1:A:503:ARG:HB3 | 1.85 | 0.59 |
| 1:A:41:THR:HG22 | 1:A:502:THR:HG23 | 1.82 | 0.59 |
| 1:A:62:ILE:HD12 | 1:A:501:LEU:CD1 | 2.33 | 0.59 |
| 1:A:833:LEU:HB2 | 1:A:836:HIS:CD2 | 2.28 | 0.59 |
| 1:A:994:LEU:CG | 1:A:1006:ASN:HB2 | 2.31 | 0.59 |
| 1:B:453:LYS:HG2 | 1:B:472:VAL:CG2 | 2.16 | 0.59 |
| 1:B:548:ARG:CG | 1:B:583:VAL:O | 2.50 | 0.59 |
| 1:B:904:VAL:HG13 | 1:B:905:ASP:N | 2.18 | 0.59 |
| 1:A:196:PRO:HB3 | 1:A:225:MET:CE | 2.33 | 0.59 |
| 1:A:889:ILE:HD12 | 1:A:907:TYR:CZ | 2.38 | 0.59 |
| 1:B:473:GLN:H | 1:B:473:GLN:NE2 | 2.01 | 0.59 |
| 1:B:630:HIS:HD2 | 1:B:632:VAL:CG2 | 2.15 | 0.59 |
| 1:B:931:ILE:HG13 | 1:B:931:ILE:O | 2.02 | 0.59 |
| 1:A:972:THR:HA | 1:A:1002:TYR:CE1 | 2.32 | 0.59 |
| 1:B:62:ILE:HD13 | 1:B:77:LEU:CD2 | 2.32 | 0.59 |
| 1:A:323:ARG:HH21 | 1:A:463:LYS:HD2 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:439:TYR:CZ | 1:A:538:LYS:NZ | 2.70 | 0.59 |
| 1:A:563:HIS:HB3 | 1:A:564:PRO:CD | 2.28 | 0.59 |
| 1:B:349:LEU:HD22 | 1:B:349:LEU:N | 2.18 | 0.59 |
| 1:B:578:LEU:HD13 | 1:B:636:LEU:HD21 | 1.85 | 0.59 |
| 1:A:814:LEU:HD22 | 1:A:847:LEU:N | 2.18 | 0.59 |
| 1:A:959:LYS:CG | 1:A:972:THR:HB | 2.33 | 0.59 |
| 1:B:40:VAL:HG13 | 1:B:503:ARG:HB3 | 1.85 | 0.59 |
| 1:B:937:ARG:HG2 | 1:B:938:PRO:HD2 | 1.85 | 0.59 |
| 1:A:171:VAL:O | 1:A:182:LEU:HD12 | 2.02 | 0.58 |
| 1:A:495:ILE:CG2 | 1:A:502:THR:HB | 2.32 | 0.58 |
| 1:A:530:VAL:HG11 | 1:A:584:PRO:HD2 | 1.84 | 0.58 |
| 1:A:759:VAL:HG12 | 1:A:760:GLN:N | 2.18 | 0.58 |
| 1:A:955:LEU:CD1 | 1:A:973:ILE:HG23 | 2.33 | 0.58 |
| 1:B:457:ILE:HG12 | 1:B:467:LEU:HD13 | 1.84 | 0.58 |
| 1:B:814:LEU:HD22 | 1:B:847:LEU:N | 2.18 | 0.58 |
| 1:A:387:VAL:HG13 | 1:A:388:LYS:N | 2.18 | 0.58 |
| 1:A:62:ILE:HG12 | 1:A:73:LEU:HB2 | 1.84 | 0.58 |
| 1:A:870:GLU:CG | 1:A:1024:ARG:CG | 2.69 | 0.58 |
| 1:B:271:LYS:HG3 | 1:B:272:GLU:N | 2.13 | 0.58 |
| 1:A:349:LEU:N | 1:A:349:LEU:HD22 | 2.18 | 0.58 |
| 1:A:665:VAL:HG11 | 1:A:697:PRO:HD3 | 1.84 | 0.58 |
| 1:B:560:LEU:HD23 | 1:B:648:THR:CG2 | 2.25 | 0.58 |
| 1:A:110:THR:HB | 1:A:132:LEU:HD23 | 1.85 | 0.58 |
| 1:A:506:VAL:HG22 | 1:A:525:HIS:NE2 | 2.18 | 0.58 |
| 1:B:263:VAL:O | 1:B:263:VAL:HG12 | 2.04 | 0.58 |
| 1:B:426:GLU:HA | 1:B:426:GLU:OE1 | 2.04 | 0.58 |
| 1:B:198:ILE:HB | 1:B:226:ILE:CG2 | 2.34 | 0.58 |
| 1:A:350:ASP:HA | 1:A:430:ARG:HB2 | 1.86 | 0.58 |
| 1:A:473:GLN:H | 1:A:473:GLN:NE2 | 2.01 | 0.58 |
| 1:A:949:TYR:CE2 | 1:A:951:MET:HE1 | 2.38 | 0.58 |
| 1:B:188:VAL:HG22 | 1:B:191:LYS:N | 2.18 | 0.58 |
| 1:B:653:TYR:HE2 | 1:B:682:HIS:CE1 | 2.21 | 0.58 |
| 1:B:832:THR:HG23 | 1:B:836:HIS:HB2 | 1.85 | 0.58 |
| 1:B:889:ILE:HD12 | 1:B:907:TYR:CZ | 2.38 | 0.58 |
| 1:A:426:GLU:OE1 | 1:A:426:GLU:HA | 2.04 | 0.58 |
| 1:A:430:ARG:HH21 | 1:A:432:THR:HG22 | 1.68 | 0.58 |
| 1:A:578:LEU:HD13 | 1:A:636:LEU:HD21 | 1.85 | 0.58 |
| 1:A:814:LEU:HD22 | 1:A:847:LEU:H | 1.68 | 0.58 |
| 1:A:873:THR:HA | 1:A:982:SER:N | 2.17 | 0.58 |
| 1:B:110:THR:HB | 1:B:132:LEU:HD23 | 1.85 | 0.58 |
| 1:B:196:PRO:HB3 | 1:B:225:MET:CE | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:51:ASN:HD21 | 1:B:67:VAL:CG2 | 2.15 | 0.58 |
| 1:B:759:VAL:HG12 | 1:B:760:GLN:N | 2.18 | 0.58 |
| 1:A:1021:GLN:CG | 1:A:1026:ARG:HG3 | 2.34 | 0.58 |
| 1:A:456:LYS:O | 1:A:468:GLN:HG2 | 2.04 | 0.58 |
| 1:A:585:GLU:OE1 | 1:A:585:GLU:HA | 2.04 | 0.58 |
| 1:A:873:THR:HG23 | 1:A:982:SER:HA | 1.86 | 0.58 |
| 1:B:254:TYR:CZ | 1:B:281:ARG:HD2 | 2.39 | 0.58 |
| 1:B:430:ARG:HH21 | 1:B:432:THR:HG22 | 1.68 | 0.58 |
| 1:B:62:ILE:HD12 | 1:B:501:LEU:CD1 | 2.33 | 0.58 |
| 1:A:972:THR:CA | 1:A:1002:TYR:HE1 | 2.15 | 0.58 |
| 1:B:456:LYS:O | 1:B:468:GLN:HG2 | 2.04 | 0.58 |
| 1:B:566:ASN:CA | 1:B:651:VAL:HG23 | 2.28 | 0.58 |
| 1:A:254:TYR:CZ | 1:A:281:ARG:HD2 | 2.39 | 0.57 |
| 1:A:703:LEU:HD21 | 1:A:782:VAL:HG21 | 1.86 | 0.57 |
| 1:B:505:PRO:HB2 | 1:B:507:GLU:O | 2.03 | 0.57 |
| 1:A:937:ARG:HG2 | 1:A:938:PRO:HD2 | 1.85 | 0.57 |
| 1:A:994:LEU:HG | 1:A:1006:ASN:HB2 | 1.87 | 0.57 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:HG3 | 1.86 | 0.57 |
| 1:A:1018:VAL:HG13 | 1:A:1018:VAL:O | 2.04 | 0.57 |
| 1:A:892:HIS:CE1 | 1:A:931:ILE:HB | 2.40 | 0.57 |
| 1:A:874:LYS:N | 1:A:982:SER:CB | 2.66 | 0.57 |
| 1:B:350:ASP:HA | 1:B:430:ARG:HB2 | 1.86 | 0.57 |
| 1:A:154:LYS:N | 1:A:157:HIS:HD2 | 2.00 | 0.57 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:HG21 | 1.87 | 0.57 |
| 1:B:370:LEU:HD21 | 1:B:374:TYR:CE1 | 2.39 | 0.57 |
| 1:A:198:ILE:HB | 1:A:226:ILE:CG2 | 2.34 | 0.57 |
| 1:A:262:MET:HG3 | 1:A:262:MET:O | 2.05 | 0.57 |
| 1:A:532:HIS:HA | 1:A:641:THR:CB | 2.35 | 0.57 |
| 1:A:188:VAL:HG22 | 1:A:191:LYS:N | 2.18 | 0.57 |
| 1:A:263:VAL:O | 1:A:263:VAL:HG12 | 2.04 | 0.57 |
| 1:A:324:THR:CG2 | 1:A:462:PRO:HA | 2.34 | 0.57 |
| 1:A:370:LEU:HD21 | 1:A:374:TYR:CE1 | 2.39 | 0.57 |
| 1:A:458:ARG:CG | 1:A:524:PRO:HG3 | 2.34 | 0.57 |
| 1:A:51:ASN:HD21 | 1:A:67:VAL:CG2 | 2.15 | 0.57 |
| 1:A:832:THR:HG23 | 1:A:836:HIS:HB2 | 1.85 | 0.57 |
| 1:B:265:PRO:HD3 | 1:B:274:VAL:HG21 | 1.87 | 0.57 |
| 1:B:42:PHE:CE2 | 1:B:50:PHE:HZ | 2.23 | 0.57 |
| 1:B:433:SER:HB3 | 1:B:484:MET:SD | 2.45 | 0.57 |
| 1:A:239:PHE:CA | 1:A:260:PRO:HG2 | 2.30 | 0.57 |
| 1:A:459:VAL:O | 1:A:459:VAL:HG23 | 2.05 | 0.57 |
| 1:A:45:GLU:HB3 | 1:A:46:PRO:CD | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:434:VAL:HG22 | 1:B:435:ILE:N | 2.20 | 0.57 |
| 1:B:459:VAL:HG23 | 1:B:459:VAL:O | 2.05 | 0.57 |
| 1:A:446:PHE:CE1 | 1:A:486:PHE:CZ | 2.93 | 0.57 |
| 1:B:262:MET:O | 1:B:262:MET:HG3 | 2.05 | 0.57 |
| 1:A:1013:VAL:HG22 | 1:A:1014:LEU:N | 2.19 | 0.56 |
| 1:A:926:ALA:CB | 1:A:947:LEU:HD12 | 2.35 | 0.56 |
| 1:B:665:VAL:CG1 | 1:B:697:PRO:HD3 | 2.35 | 0.56 |
| 1:A:435:ILE:CG2 | 1:A:486:PHE:HE1 | 2.19 | 0.56 |
| 1:A:501:LEU:HD23 | 1:A:502:THR:H | 1.70 | 0.56 |
| 1:A:820:PHE:O | 1:A:821:GLU:HB3 | 2.05 | 0.56 |
| 1:B:444:LEU:HD23 | 1:B:524:PRO:CD | 2.35 | 0.56 |
| 1:A:305:GLU:O | 1:A:340:LYS:HG3 | 2.06 | 0.56 |
| 1:A:434:VAL:HG22 | 1:A:435:ILE:N | 2.20 | 0.56 |
| 1:B:53:LEU:HG | 1:B:64:LEU:HD13 | 1.87 | 0.56 |
| 1:B:882:LEU:N | 1:B:882:LEU:HD12 | 2.21 | 0.56 |
| 1:A:882:LEU:HD12 | 1:A:882:LEU:N | 2.21 | 0.56 |
| 1:B:116:MET:HG3 | 1:B:117:LEU:N | 2.20 | 0.56 |
| 1:B:41:THR:CG2 | 1:B:502:THR:HG23 | 2.36 | 0.56 |
| 1:A:42:PHE:CE2 | 1:A:50:PHE:HZ | 2.23 | 0.56 |
| 1:A:955:LEU:HG | 1:A:973:ILE:HG23 | 1.86 | 0.56 |
| 1:B:305:GLU:O | 1:B:340:LYS:HG3 | 2.06 | 0.56 |
| 1:B:45:GLU:HB3 | 1:B:46:PRO:CD | 2.35 | 0.56 |
| 1:B:785:ASN:HD22 | 1:B:788:PHE:HE2 | 1.54 | 0.56 |
| 1:B:885:GLU:HG3 | 1:B:887:ARG:H | 1.70 | 0.56 |
| 1:A:665:VAL:CG1 | 1:A:697:PRO:HD3 | 2.35 | 0.56 |
| 1:B:585:GLU:OE1 | 1:B:585:GLU:HA | 2.04 | 0.56 |
| 1:B:700:CYS:HB3 | 1:B:701:PRO:HD2 | 1.81 | 0.56 |
| 1:B:710:LEU:HB2 | 1:B:801:TYR:HE1 | 1.70 | 0.56 |
| 1:B:814:LEU:HD22 | 1:B:847:LEU:H | 1.69 | 0.56 |
| 1:A:865:VAL:HG13 | 1:A:866:THR:N | 2.21 | 0.56 |
| 1:B:892:HIS:CE1 | 1:B:931:ILE:HB | 2.40 | 0.56 |
| 1:A:474:VAL:CG2 | 1:A:495:ILE:HG21 | 2.35 | 0.56 |
| 1:A:785:ASN:ND2 | 1:A:788:PHE:HE2 | 2.03 | 0.56 |
| 1:B:324:THR:CG2 | 1:B:462:PRO:HA | 2.34 | 0.56 |
| 1:B:446:PHE:CE1 | 1:B:486:PHE:CZ | 2.93 | 0.56 |
| 1:B:526:CYS:HB3 | 1:B:535:CYS:SG | 2.46 | 0.56 |
| 1:B:804:GLY:HA2 | 1:B:806:MET:CE | 2.36 | 0.56 |
| 1:A:226:ILE:O | 1:A:226:ILE:HG23 | 2.06 | 0.56 |
| 1:A:321:LEU:HD12 | 1:A:462:PRO:CG | 2.34 | 0.56 |
| 1:A:41:THR:CG2 | 1:A:502:THR:HG23 | 2.35 | 0.56 |
| 1:A:549:ARG:HA | 1:A:584:PRO:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:569:VAL:HB | 1:A:654:ASN:CB | 2.36 | 0.56 |
| 1:A:885:GLU:HG3 | 1:A:887:ARG:H | 1.70 | 0.56 |
| 1:B:118:LEU:HB3 | 1:B:127:ILE:CG2 | 2.36 | 0.56 |
| 1:B:435:ILE:CG2 | 1:B:486:PHE:HE1 | 2.19 | 0.56 |
| 1:B:567:ILE:N | 1:B:567:ILE:HD13 | 2.20 | 0.56 |
| 1:B:569:VAL:HG21 | 1:B:654:ASN:HB2 | 1.87 | 0.56 |
| 1:A:983:ASN:O | 1:A:1022:VAL:HG23 | 2.06 | 0.56 |
| 1:A:118:LEU:HB3 | 1:A:127:ILE:CG2 | 2.36 | 0.56 |
| 1:A:42:PHE:HE2 | 1:A:50:PHE:HZ | 1.54 | 0.56 |
| 1:A:526:CYS:HB3 | 1:A:535:CYS:SG | 2.46 | 0.56 |
| 1:A:567:ILE:HD13 | 1:A:567:ILE:N | 2.20 | 0.56 |
| 1:A:447:VAL:HG23 | 1:A:447:VAL:O | 2.06 | 0.56 |
| 1:A:53:LEU:HG | 1:A:64:LEU:HD13 | 1.87 | 0.56 |
| 1:A:46:PRO:CG | 1:A:69:ARG:HD2 | 2.36 | 0.56 |
| 1:B:505:PRO:HB3 | 1:B:507:GLU:O | 2.04 | 0.56 |
| 1:B:785:ASN:ND2 | 1:B:788:PHE:HE2 | 2.03 | 0.56 |
| 1:B:865:VAL:HG13 | 1:B:866:THR:N | 2.21 | 0.56 |
| 1:A:1022:VAL:HG13 | 1:A:1022:VAL:O | 2.06 | 0.55 |
| 1:A:433:SER:HB3 | 1:A:484:MET:SD | 2.45 | 0.55 |
| 1:A:704:LEU:HD11 | 1:A:724:LYS:CE | 2.35 | 0.55 |
| 1:A:710:LEU:HB2 | 1:A:801:TYR:HE1 | 1.70 | 0.55 |
| 1:A:460:ASP:OD2 | 1:A:463:LYS:HB3 | 2.06 | 0.55 |
| 1:A:873:THR:HB | 1:A:917:MET:HE2 | 1.86 | 0.55 |
| 1:A:949:TYR:HE2 | 1:A:951:MET:HE1 | 1.71 | 0.55 |
| 1:B:46:PRO:CG | 1:B:69:ARG:HD2 | 2.36 | 0.55 |
| 1:A:435:ILE:HD12 | 1:A:486:PHE:HD1 | 1.70 | 0.55 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:N | 2.21 | 0.55 |
| 1:A:548:ARG:HG3 | 1:A:583:VAL:C | 2.26 | 0.55 |
| 1:A:619:VAL:CB | 1:A:620:PRO:HD3 | 2.36 | 0.55 |
| 1:A:845:LEU:HD13 | 1:A:845:LEU:C | 2.26 | 0.55 |
| 1:B:412:LEU:N | 1:B:412:LEU:HD13 | 2.21 | 0.55 |
| 1:B:501:LEU:HD23 | 1:B:502:THR:H | 1.70 | 0.55 |
| 1:B:62:ILE:HG12 | 1:B:73:LEU:HB2 | 1.84 | 0.55 |
| 1:B:807:ARG:HD3 | 1:B:812:LEU:O | 2.07 | 0.55 |
| 1:A:382:LEU:HD23 | 1:A:385:LEU:CB | 2.36 | 0.55 |
| 1:B:110:THR:HG22 | 1:B:111:ASN:H | 1.72 | 0.55 |
| 1:B:190:GLY:O | 1:B:192:PRO:HD3 | 2.07 | 0.55 |
| 1:B:359:LEU:HA | 1:B:362:ILE:HG12 | 1.89 | 0.55 |
| 1:B:447:VAL:O | 1:B:447:VAL:HG23 | 2.06 | 0.55 |
| 1:B:474:VAL:CG2 | 1:B:495:ILE:HG21 | 2.34 | 0.55 |
| 1:B:703:LEU:HD21 | 1:B:782:VAL:HG21 | 1.86 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:713:VAL:HG13 | 1:B:766:TYR:O | 2.06 | 0.55 |
| 1:A:448:GLY:HA3 | 1:A:480:VAL:CG2 | 2.37 | 0.55 |
| 1:B:51:ASN:ND2 | 1:B:67:VAL:HG23 | 2.20 | 0.55 |
| 1:B:710:LEU:HB2 | 1:B:801:TYR:CE1 | 2.42 | 0.55 |
| 1:B:820:PHE:O | 1:B:821:GLU:HB3 | 2.06 | 0.55 |
| 1:B:845:LEU:C | 1:B:845:LEU:HD13 | 2.26 | 0.55 |
| 1:B:91:ASN:CG | 1:B:92:PRO:HD2 | 2.27 | 0.55 |
| 1:B:949:TYR:HE2 | 1:B:951:MET:HE2 | 1.71 | 0.55 |
| 1:A:1014:LEU:H | 1:A:1014:LEU:CD2 | 2.17 | 0.55 |
| 1:A:713:VAL:HG13 | 1:A:766:TYR:O | 2.06 | 0.55 |
| 1:A:825:CYS:HB3 | 1:A:828:PRO:HG2 | 1.89 | 0.55 |
| 1:A:861:GLU:HG3 | 1:A:862:ILE:N | 2.21 | 0.55 |
| 1:A:91:ASN:CG | 1:A:92:PRO:HD2 | 2.27 | 0.55 |
| 1:B:280:VAL:HG12 | 1:B:281:ARG:N | 2.22 | 0.55 |
| 1:B:72:LYS:HD2 | 1:B:80:LEU:HB2 | 1.87 | 0.55 |
| 1:A:168:VAL:HG22 | 1:A:169:PHE:N | 2.22 | 0.55 |
| 1:A:190:GLY:O | 1:A:192:PRO:HD3 | 2.07 | 0.55 |
| 1:A:280:VAL:HG12 | 1:A:281:ARG:N | 2.22 | 0.55 |
| 1:A:509:CYS:HB3 | 1:A:535:CYS:SG | 2.47 | 0.55 |
| 1:B:226:ILE:O | 1:B:226:ILE:HG23 | 2.06 | 0.55 |
| 1:B:380:LEU:HB2 | 1:B:386:LYS:HE2 | 1.87 | 0.55 |
| 1:B:42:PHE:HE2 | 1:B:50:PHE:HZ | 1.54 | 0.55 |
| 1:A:116:MET:HG3 | 1:A:117:LEU:N | 2.21 | 0.55 |
| 1:B:242:TYR:CD1 | 1:B:345:LYS:HE2 | 2.41 | 0.55 |
| 1:B:619:VAL:CB | 1:B:620:PRO:HD3 | 2.36 | 0.55 |
| 1:B:937:ARG:HG3 | 1:B:938:PRO:HD2 | 1.89 | 0.55 |
| 1:A:988:PHE:HD2 | 1:A:1016:MET:SD | 2.30 | 0.55 |
| 1:A:242:TYR:CD1 | 1:A:345:LYS:HE2 | 2.41 | 0.55 |
| 1:A:380:LEU:HB2 | 1:A:386:LYS:HE2 | 1.87 | 0.55 |
| 1:B:380:LEU:CD1 | 1:B:386:LYS:HE3 | 2.37 | 0.55 |
| 1:B:501:LEU:HD23 | 1:B:502:THR:N | 2.22 | 0.55 |
| 1:A:239:PHE:HA | 1:A:260:PRO:CG | 2.32 | 0.55 |
| 1:A:370:LEU:HD13 | 1:A:370:LEU:O | 2.07 | 0.55 |
| 1:A:501:LEU:HD23 | 1:A:502:THR:N | 2.22 | 0.55 |
| 1:A:72:LYS:HD2 | 1:A:80:LEU:HB2 | 1.87 | 0.55 |
| 1:A:804:GLY:HA2 | 1:A:806:MET:CE | 2.36 | 0.55 |
| 1:A:1016:MET:HE3 | 1:A:1017:LYS:CA | 2.38 | 0.54 |
| 1:A:597:LEU:HD22 | 1:A:597:LEU:N | 2.21 | 0.54 |
| 1:B:168:VAL:HG22 | 1:B:169:PHE:N | 2.22 | 0.54 |
| 1:B:370:LEU:HD13 | 1:B:370:LEU:O | 2.07 | 0.54 |
| 1:B:597:LEU:N | 1:B:597:LEU:HD22 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:704:LEU:HD11 | 1:B:724:LYS:CE | 2.35 | 0.54 |
| 1:A:785:ASN:HD22 | 1:A:788:PHE:HE2 | 1.54 | 0.54 |
| 1:A:797:LYS:HD2 | 1:A:797:LYS:H | 1.72 | 0.54 |
| 1:B:382:LEU:HD23 | 1:B:385:LEU:CB | 2.37 | 0.54 |
| 1:B:435:ILE:HD12 | 1:B:486:PHE:HD1 | 1.71 | 0.54 |
| 1:B:930:GLU:OE2 | 1:B:941:MET:HG3 | 2.07 | 0.54 |
| 1:A:471:THR:CG2 | 1:A:473:GLN:HE22 | 2.20 | 0.54 |
| 1:A:46:PRO:CG | 1:A:69:ARG:HG3 | 2.27 | 0.54 |
| 1:A:710:LEU:HB2 | 1:A:801:TYR:CE1 | 2.41 | 0.54 |
| 1:A:709:ILE:O | 1:A:799:TYR:HD1 | 1.91 | 0.54 |
| 1:A:72:LYS:HD2 | 1:A:80:LEU:HD12 | 1.90 | 0.54 |
| 1:A:874:LYS:H | 1:A:982:SER:CB | 2.20 | 0.54 |
| 1:B:236:ILE:O | 1:B:236:ILE:HG23 | 2.07 | 0.54 |
| 1:B:370:LEU:C | 1:B:370:LEU:HD13 | 2.27 | 0.54 |
| 1:B:440:LYS:HB2 | 1:B:538:LYS:NZ | 2.22 | 0.54 |
| 1:B:72:LYS:HD2 | 1:B:80:LEU:HD12 | 1.90 | 0.54 |
| 1:A:301:ARG:CD | 1:A:425:THR:HG21 | 2.26 | 0.54 |
| 1:A:556:GLN:O | 1:A:582:ASN:CB | 2.56 | 0.54 |
| 1:A:947:LEU:CD2 | 1:A:947:LEU:H | 2.21 | 0.54 |
| 1:B:460:ASP:OD2 | 1:B:463:LYS:HB3 | 2.06 | 0.54 |
| 1:A:151:PRO:O | 1:A:157:HIS:HB3 | 2.07 | 0.54 |
| 1:A:359:LEU:HA | 1:A:362:ILE:HG12 | 1.89 | 0.54 |
| 1:A:63:TYR:CE2 | 1:A:72:LYS:HG2 | 2.43 | 0.54 |
| 1:B:474:VAL:HG12 | 1:B:475:VAL:N | 2.21 | 0.54 |
| 1:B:509:CYS:HB3 | 1:B:535:CYS:SG | 2.47 | 0.54 |
| 1:A:412:LEU:C | 1:A:412:LEU:HD22 | 2.28 | 0.54 |
| 1:A:994:LEU:HD11 | 1:A:1006:ASN:CB | 2.37 | 0.54 |
| 1:B:412:LEU:HD22 | 1:B:412:LEU:C | 2.28 | 0.54 |
| 1:B:426:GLU:HG2 | 1:B:429:ASP:O | 2.08 | 0.54 |
| 1:A:495:ILE:O | 1:A:495:ILE:HG23 | 2.08 | 0.54 |
| 1:A:699:ASP:HA | 1:A:725:ASN:OD1 | 2.07 | 0.54 |
| 1:A:739:ILE:HB | 1:A:781:THR:HG22 | 1.90 | 0.54 |
| 1:B:154:LYS:HB2 | 1:B:157:HIS:HD2 | 1.70 | 0.54 |
| 1:B:151:PRO:O | 1:B:157:HIS:HB3 | 2.08 | 0.54 |
| 1:B:471:THR:CG2 | 1:B:473:GLN:HE22 | 2.20 | 0.54 |
| 1:A:236:ILE:O | 1:A:236:ILE:HG23 | 2.07 | 0.54 |
| 1:A:370:LEU:HD13 | 1:A:370:LEU:C | 2.27 | 0.54 |
| 1:A:429:ASP:OD1 | 1:A:450:LYS:HB3 | 2.08 | 0.54 |
| 1:A:930:GLU:OE2 | 1:A:941:MET:HG3 | 2.07 | 0.54 |
| 1:B:370:LEU:HD11 | 1:B:399:ILE:HD12 | 1.88 | 0.54 |
| 1:B:797:LYS:HD2 | 1:B:797:LYS:H | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:135:GLY:O | 1:A:159:LEU:HD13 | 2.08 | 0.54 |
| 1:A:175:TYR:HB3 | 1:A:179:ASP:HB3 | 1.89 | 0.54 |
| 1:A:412:LEU:HD13 | 1:A:412:LEU:N | 2.21 | 0.54 |
| 1:A:531:LEU:O | 1:A:641:THR:OG1 | 2.25 | 0.54 |
| 1:A:780:LEU:HD12 | 1:A:780:LEU:C | 2.27 | 0.54 |
| 1:A:662:LEU:HD23 | 1:A:791:ASP:OD2 | 2.08 | 0.54 |
| 1:B:861:GLU:HG3 | 1:B:862:ILE:N | 2.21 | 0.54 |
| 1:A:370:LEU:HD11 | 1:A:399:ILE:HD12 | 1.88 | 0.54 |
| 1:A:51:ASN:ND2 | 1:A:67:VAL:HG23 | 2.20 | 0.54 |
| 1:B:175:TYR:HB3 | 1:B:179:ASP:HB3 | 1.89 | 0.54 |
| 1:B:716:ILE:HG12 | 1:B:763:ASN:HB3 | 1.90 | 0.54 |
| 1:B:780:LEU:C | 1:B:780:LEU:HD12 | 2.27 | 0.54 |
| 1:B:825:CYS:HB3 | 1:B:828:PRO:HG2 | 1.89 | 0.54 |
| 1:B:301:ARG:CD | 1:B:425:THR:HG21 | 2.26 | 0.53 |
| 1:B:921:LYS:N | 1:B:922:PRO:HD2 | 2.23 | 0.53 |
| 1:B:947:LEU:CD2 | 1:B:947:LEU:H | 2.21 | 0.53 |
| 1:A:110:THR:HG22 | 1:A:111:ASN:H | 1.72 | 0.53 |
| 1:A:225:MET:HE1 | 1:A:227:LYS:CG | 2.37 | 0.53 |
| 1:A:955:LEU:CG | 1:A:973:ILE:HG23 | 2.38 | 0.53 |
| 1:A:957:ASP:O | 1:A:974:THR:HG22 | 2.08 | 0.53 |
| 1:B:63:TYR:CE2 | 1:B:72:LYS:HG2 | 2.43 | 0.53 |
| 1:B:926:ALA:CB | 1:B:947:LEU:HD12 | 2.35 | 0.53 |
| 1:B:925:HIS:O | 1:B:950:PHE:HD2 | 1.91 | 0.53 |
| 1:A:739:ILE:HB | 1:A:781:THR:HG23 | 1.90 | 0.53 |
| 1:A:921:LYS:N | 1:A:922:PRO:HD2 | 2.23 | 0.53 |
| 1:A:924:GLN:O | 1:A:925:HIS:HB2 | 2.09 | 0.53 |
| 1:A:426:GLU:HG2 | 1:A:429:ASP:O | 2.08 | 0.53 |
| 1:A:589:GLY:HA3 | 1:A:639:LYS:HG3 | 1.90 | 0.53 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:O | 2.07 | 0.53 |
| 1:A:867:GLY:CA | 1:A:981:GLY:N | 2.49 | 0.53 |
| 1:B:429:ASP:OD1 | 1:B:450:LYS:HB3 | 2.08 | 0.53 |
| 1:B:623:ILE:C | 1:B:623:ILE:HD12 | 2.28 | 0.53 |
| 1:B:924:GLN:O | 1:B:925:HIS:HB2 | 2.09 | 0.53 |
| 1:A:321:LEU:CD2 | 1:A:325:LEU:HD11 | 2.39 | 0.53 |
| 1:A:533:ASN:HD22 | 1:A:643:MET:HB3 | 1.73 | 0.53 |
| 1:A:827:SER:HB2 | 1:A:828:PRO:HD3 | 1.91 | 0.53 |
| 1:B:181:LYS:CE | 1:B:202:LYS:HG2 | 2.39 | 0.53 |
| 1:B:371:GLN:O | 1:B:375:ARG:HG3 | 2.09 | 0.53 |
| 1:B:385:LEU:HD13 | 1:B:385:LEU:C | 2.29 | 0.53 |
| 1:B:578:LEU:HB2 | 1:B:609:ILE:HB | 1.91 | 0.53 |
| 1:B:709:ILE:O | 1:B:799:TYR:HD1 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:185:ALA:HB3 | 1:A:243:TYR:CG | 2.44 | 0.53 |
| 1:A:509:CYS:HB2 | 1:A:536:THR:HA | 1.91 | 0.53 |
| 1:A:623:ILE:HD12 | 1:A:623:ILE:C | 2.29 | 0.53 |
| 1:A:679:VAL:HG12 | 1:A:680:CYS:N | 2.23 | 0.53 |
| 1:A:716:ILE:HG12 | 1:A:763:ASN:HB3 | 1.90 | 0.53 |
| 1:B:278:LYS:HG2 | 1:B:296:PRO:CA | 2.38 | 0.53 |
| 1:B:321:LEU:CD2 | 1:B:325:LEU:HD11 | 2.39 | 0.53 |
| 1:B:563:HIS:HB3 | 1:B:564:PRO:CD | 2.28 | 0.53 |
| 1:A:190:GLY:HA2 | 1:A:233:PHE:HE2 | 1.73 | 0.53 |
| 1:A:549:ARG:CD | 1:A:584:PRO:HB2 | 2.33 | 0.53 |
| 1:A:805:ALA:H | 1:A:806:MET:CE | 2.22 | 0.53 |
| 1:B:39:PHE:CD1 | 1:B:505:PRO:HD2 | 2.44 | 0.53 |
| 1:B:356:ILE:HG22 | 1:B:421:ILE:O | 2.09 | 0.53 |
| 1:B:448:GLY:HA3 | 1:B:480:VAL:CG2 | 2.37 | 0.53 |
| 1:B:739:ILE:HB | 1:B:781:THR:HG22 | 1.90 | 0.53 |
| 1:B:947:LEU:HD23 | 1:B:947:LEU:O | 2.09 | 0.53 |
| 1:A:997:ARG:H | 1:A:1004:ILE:CG2 | 2.22 | 0.53 |
| 1:A:963:GLY:C | 1:A:1036:VAL:HG22 | 2.29 | 0.53 |
| 1:A:119:ILE:O | 1:A:119:ILE:HG23 | 2.09 | 0.53 |
| 1:A:385:LEU:HD13 | 1:A:385:LEU:C | 2.29 | 0.53 |
| 1:A:356:ILE:HG22 | 1:A:421:ILE:O | 2.09 | 0.53 |
| 1:A:925:HIS:O | 1:A:950:PHE:HD2 | 1.91 | 0.53 |
| 1:A:958:LEU:HD23 | 1:A:959:LYS:H | 1.73 | 0.53 |
| 1:B:198:ILE:HB | 1:B:226:ILE:HG22 | 1.91 | 0.53 |
| 1:B:308:LEU:O | 1:B:338:PHE:HA | 2.09 | 0.53 |
| 1:B:716:ILE:HG23 | 1:B:716:ILE:O | 2.09 | 0.53 |
| 1:A:575:LEU:H | 1:A:575:LEU:CD2 | 2.22 | 0.53 |
| 1:A:937:ARG:HG3 | 1:A:938:PRO:HD2 | 1.89 | 0.53 |
| 1:A:1032:VAL:HG12 | 1:A:1033:PHE:N | 2.23 | 0.53 |
| 1:A:308:LEU:O | 1:A:338:PHE:HA | 2.09 | 0.53 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:NH2 | 2.24 | 0.53 |
| 1:A:578:LEU:HB2 | 1:A:609:ILE:HB | 1.91 | 0.53 |
| 1:A:805:ALA:N | 1:A:806:MET:HE3 | 2.24 | 0.53 |
| 1:A:807:ARG:HD2 | 1:A:813:CYS:HA | 1.90 | 0.53 |
| 1:B:882:LEU:HD13 | 1:B:910:ALA:O | 2.09 | 0.53 |
| 1:A:181:LYS:CE | 1:A:202:LYS:HG2 | 2.39 | 0.52 |
| 1:A:580:THR:HG21 | 1:A:583:VAL:HG11 | 1.91 | 0.52 |
| 1:A:806:MET:HG2 | 1:A:807:ARG:CG | 2.39 | 0.52 |
| 1:A:875:VAL:HG22 | 1:A:915:CYS:O | 2.09 | 0.52 |
| 1:A:933:VAL:HG22 | 1:A:940:PHE:HB3 | 1.91 | 0.52 |
| 1:B:40:VAL:HG11 | 1:B:503:ARG:NH2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1019:THR:HG23 | 1:A:1019:THR:O | 2.10 | 0.52 |
| 1:A:716:ILE:HG23 | 1:A:716:ILE:O | 2.09 | 0.52 |
| 1:A:947:LEU:O | 1:A:947:LEU:HD23 | 2.09 | 0.52 |
| 1:A:952:THR:HG23 | 1:A:952:THR:O | 2.08 | 0.52 |
| 1:A:959:LYS:HG2 | 1:A:972:THR:CG2 | 2.39 | 0.52 |
| 1:B:495:ILE:HG23 | 1:B:495:ILE:O | 2.08 | 0.52 |
| 1:B:439:TYR:CZ | 1:B:538:LYS:CE | 2.92 | 0.52 |
| 1:B:64:LEU:N | 1:B:64:LEU:HD22 | 2.24 | 0.52 |
| 1:B:783:VAL:HG12 | 1:B:784:TRP:N | 2.25 | 0.52 |
| 1:B:807:ARG:HD2 | 1:B:813:CYS:HA | 1.90 | 0.52 |
| 1:A:1004:ILE:HG23 | 1:A:1004:ILE:O | 2.08 | 0.52 |
| 1:A:281:ARG:O | 1:A:282:LEU:HD23 | 2.09 | 0.52 |
| 1:A:827:SER:HB2 | 1:A:828:PRO:CD | 2.39 | 0.52 |
| 1:B:135:GLY:O | 1:B:159:LEU:HD13 | 2.08 | 0.52 |
| 1:B:321:LEU:HD12 | 1:B:462:PRO:CG | 2.34 | 0.52 |
| 1:B:679:VAL:HG12 | 1:B:680:CYS:N | 2.23 | 0.52 |
| 1:B:185:ALA:HB3 | 1:B:243:TYR:CG | 2.44 | 0.52 |
| 1:B:589:GLY:HA3 | 1:B:639:LYS:HG3 | 1.90 | 0.52 |
| 1:B:739:ILE:HB | 1:B:781:THR:HG23 | 1.90 | 0.52 |
| 1:B:827:SER:HB2 | 1:B:828:PRO:CD | 2.40 | 0.52 |
| 1:A:42:PHE:HZ | 1:A:45:GLU:CB | 2.22 | 0.52 |
| 1:B:127:ILE:O | 1:B:127:ILE:HG23 | 2.09 | 0.52 |
| 1:B:281:ARG:O | 1:B:282:LEU:HD23 | 2.09 | 0.52 |
| 1:A:868:PRO:CG | 1:A:1022:VAL:HG21 | 2.40 | 0.52 |
| 1:A:296:PRO:HD2 | 1:A:414:VAL:HG22 | 1.92 | 0.52 |
| 1:A:371:GLN:O | 1:A:375:ARG:HG3 | 2.09 | 0.52 |
| 1:A:882:LEU:HD13 | 1:A:910:ALA:O | 2.09 | 0.52 |
| 1:B:630:HIS:HD2 | 1:B:632:VAL:HG23 | 1.73 | 0.52 |
| 1:B:875:VAL:HG22 | 1:B:915:CYS:O | 2.09 | 0.52 |
| 1:A:560:LEU:HG | 1:A:648:THR:HG21 | 1.92 | 0.52 |
| 1:B:396:LEU:C | 1:B:396:LEU:HD13 | 2.30 | 0.52 |
| 1:B:439:TYR:CZ | 1:B:538:LYS:NZ | 2.75 | 0.52 |
| 1:A:566:ASN:HB3 | 1:A:651:VAL:CG2 | 2.40 | 0.52 |
| 1:A:593:THR:HG23 | 1:A:593:THR:O | 2.10 | 0.52 |
| 1:A:64:LEU:N | 1:A:64:LEU:HD22 | 2.24 | 0.52 |
| 1:B:228:ILE:HG22 | 1:B:233:PHE:CE1 | 2.45 | 0.52 |
| 1:B:472:VAL:HG12 | 1:B:472:VAL:O | 2.09 | 0.52 |
| 1:B:575:LEU:CD2 | 1:B:575:LEU:H | 2.22 | 0.52 |
| 1:B:59:THR:HB | 1:B:61:HIS:CE1 | 2.45 | 0.52 |
| 1:A:198:ILE:HB | 1:A:226:ILE:HG22 | 1.91 | 0.52 |
| 1:A:472:VAL:O | 1:A:472:VAL:HG12 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:39:PHE:CD1 | 1:A:505:PRO:HD2 | 2.44 | 0.52 |
| 1:A:553:GLU:HG3 | 1:A:554:MET:N | 2.24 | 0.52 |
| 1:B:322:GLY:CA | 1:B:327:VAL:HG22 | 2.40 | 0.52 |
| 1:B:560:LEU:HG | 1:B:648:THR:HG21 | 1.92 | 0.52 |
| 1:B:806:MET:HG2 | 1:B:807:ARG:CG | 2.39 | 0.52 |
| 1:A:956:ALA:O | 1:A:1031:LEU:HD11 | 2.10 | 0.52 |
| 1:A:322:GLY:CA | 1:A:327:VAL:HG22 | 2.40 | 0.52 |
| 1:A:712:PRO:O | 1:A:715:VAL:HG22 | 2.09 | 0.52 |
| 1:A:873:THR:CG2 | 1:A:981:GLY:C | 2.78 | 0.52 |
| 1:B:171:VAL:HG12 | 1:B:172:ILE:N | 2.25 | 0.52 |
| 1:B:509:CYS:HB2 | 1:B:536:THR:HA | 1.91 | 0.52 |
| 1:B:580:THR:HG21 | 1:B:583:VAL:HG11 | 1.92 | 0.52 |
| 1:B:64:LEU:HD11 | 1:B:501:LEU:HD12 | 1.92 | 0.52 |
| 1:B:827:SER:HB2 | 1:B:828:PRO:HD3 | 1.91 | 0.52 |
| 1:A:171:VAL:HG12 | 1:A:172:ILE:N | 2.26 | 0.51 |
| 1:A:473:GLN:CD | 1:A:504:VAL:HG13 | 2.31 | 0.51 |
| 1:A:54:VAL:HG22 | 1:A:55:VAL:N | 2.25 | 0.51 |
| 1:A:64:LEU:HD11 | 1:A:501:LEU:HD12 | 1.92 | 0.51 |
| 1:A:716:ILE:CG1 | 1:A:763:ASN:HB3 | 2.41 | 0.51 |
| 1:A:870:GLU:CD | 1:A:1025:ALA:CA | 2.78 | 0.51 |
| 1:A:986:VAL:HG12 | 1:A:988:PHE:CE1 | 2.45 | 0.51 |
| 1:B:444:LEU:HD12 | 1:B:446:PHE:CZ | 2.44 | 0.51 |
| 1:A:127:ILE:O | 1:A:127:ILE:HG23 | 2.09 | 0.51 |
| 1:A:154:LYS:HB2 | 1:A:157:HIS:HD2 | 1.71 | 0.51 |
| 1:A:228:ILE:HG22 | 1:A:233:PHE:CE1 | 2.45 | 0.51 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CG | 2.94 | 0.51 |
| 1:B:712:PRO:O | 1:B:715:VAL:HG22 | 2.09 | 0.51 |
| 1:B:805:ALA:H | 1:B:806:MET:CE | 2.22 | 0.51 |
| 1:A:712:PRO:HG3 | 1:A:801:TYR:CZ | 2.45 | 0.51 |
| 1:A:93:LYS:HD3 | 1:A:105:GLU:OE2 | 2.10 | 0.51 |
| 1:B:119:ILE:HG23 | 1:B:119:ILE:O | 2.09 | 0.51 |
| 1:B:553:GLU:HG3 | 1:B:554:MET:N | 2.24 | 0.51 |
| 1:B:567:ILE:CD1 | 1:B:650:PHE:CE2 | 2.94 | 0.51 |
| 1:A:468:GLN:HG3 | 1:A:523:ASP:HA | 1.92 | 0.51 |
| 1:B:418:VAL:O | 1:B:418:VAL:HG13 | 2.11 | 0.51 |
| 1:B:519:LEU:N | 1:B:519:LEU:HD22 | 2.26 | 0.51 |
| 1:B:468:GLN:HB2 | 1:B:522:GLY:C | 2.30 | 0.51 |
| 1:B:695:LYS:CB | 1:B:696:LEU:HD12 | 2.41 | 0.51 |
| 1:B:727:PRO:O | 1:B:729:PRO:HD3 | 2.10 | 0.51 |
| 1:A:216:VAL:HG13 | 1:A:217:PHE:N | 2.26 | 0.51 |
| 1:A:53:LEU:HG | 1:A:64:LEU:HD11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:695:LYS:CB | 1:A:696:LEU:HD12 | 2.41 | 0.51 |
| 1:A:984:VAL:HG11 | 1:A:998:ARG:HD3 | 1.91 | 0.51 |
| 1:B:265:PRO:HD3 | 1:B:274:VAL:HG22 | 1.92 | 0.51 |
| 1:B:541:CYS:SG | 1:B:550:PHE:HD2 | 2.33 | 0.51 |
| 1:B:712:PRO:HG3 | 1:B:801:TYR:CZ | 2.45 | 0.51 |
| 1:B:716:ILE:CG1 | 1:B:763:ASN:HB3 | 2.40 | 0.51 |
| 1:B:933:VAL:HG22 | 1:B:940:PHE:HB3 | 1.91 | 0.51 |
| 1:A:805:ALA:H | 1:A:806:MET:HE3 | 1.75 | 0.51 |
| 1:B:184:ILE:C | 1:B:184:ILE:HD12 | 2.31 | 0.51 |
| 1:B:53:LEU:HD23 | 1:B:53:LEU:C | 2.31 | 0.51 |
| 1:B:54:VAL:HG22 | 1:B:55:VAL:N | 2.25 | 0.51 |
| 1:A:278:LYS:HG2 | 1:A:296:PRO:CA | 2.39 | 0.51 |
| 1:A:370:LEU:HD11 | 1:A:374:TYR:CE1 | 2.46 | 0.51 |
| 1:A:790:ILE:HD12 | 1:A:790:ILE:N | 2.25 | 0.51 |
| 1:A:889:ILE:CD1 | 1:A:907:TYR:CE1 | 2.94 | 0.51 |
| 1:A:997:ARG:H | 1:A:1004:ILE:HG23 | 1.75 | 0.51 |
| 1:B:426:GLU:HG3 | 1:B:429:ASP:H | 1.75 | 0.51 |
| 1:B:548:ARG:O | 1:B:584:PRO:HD3 | 2.11 | 0.51 |
| 1:B:823:GLY:HA3 | 1:B:844:TRP:CZ2 | 2.46 | 0.51 |
| 1:B:930:GLU:HG3 | 1:B:941:MET:SD | 2.51 | 0.51 |
| 1:A:133:TYR:O | 1:A:134:GLN:HB2 | 2.11 | 0.51 |
| 1:A:396:LEU:C | 1:A:396:LEU:HD13 | 2.30 | 0.51 |
| 1:A:473:GLN:HB2 | 1:A:504:VAL:CG2 | 2.40 | 0.51 |
| 1:B:239:PHE:HA | 1:B:260:PRO:CG | 2.33 | 0.51 |
| 1:B:284:LYS:HD3 | 1:B:284:LYS:C | 2.31 | 0.51 |
| 1:B:370:LEU:HD11 | 1:B:374:TYR:CE1 | 2.46 | 0.51 |
| 1:A:418:VAL:O | 1:A:418:VAL:HG13 | 2.10 | 0.51 |
| 1:A:519:LEU:N | 1:A:519:LEU:HD22 | 2.26 | 0.51 |
| 1:A:567:ILE:CD1 | 1:A:650:PHE:CE2 | 2.94 | 0.51 |
| 1:A:59:THR:HB | 1:A:61:HIS:CE1 | 2.45 | 0.51 |
| 1:A:630:HIS:HD2 | 1:A:632:VAL:HG23 | 1.73 | 0.51 |
| 1:A:727:PRO:O | 1:A:729:PRO:HD3 | 2.10 | 0.51 |
| 1:A:76:ASP:O | 1:A:77:LEU:HB2 | 2.11 | 0.51 |
| 1:A:847:LEU:HG | 1:A:850:ALA:HA | 1.91 | 0.51 |
| 1:B:296:PRO:HD2 | 1:B:414:VAL:HG22 | 1.92 | 0.51 |
| 1:B:527:GLY:HA3 | 1:B:550:PHE:CE1 | 2.45 | 0.51 |
| 1:B:53:LEU:HG | 1:B:64:LEU:HD11 | 1.92 | 0.51 |
| 1:B:703:LEU:N | 1:B:703:LEU:HD22 | 2.26 | 0.51 |
| 1:B:847:LEU:HG | 1:B:850:ALA:HA | 1.91 | 0.51 |
| 1:A:507:GLU:HG3 | 1:A:537:ARG:CG | 2.41 | 0.51 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:HB3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:185:ALA:CB | 1:B:243:TYR:CG | 2.94 | 0.51 |
| 1:B:93:LYS:HD3 | 1:B:105:GLU:OE2 | 2.10 | 0.51 |
| 1:A:870:GLU:OE2 | 1:A:1025:ALA:CA | 2.58 | 0.50 |
| 1:A:358:ILE:CG2 | 1:A:361:GLN:HB2 | 2.41 | 0.50 |
| 1:A:541:CYS:SG | 1:A:550:PHE:HD2 | 2.33 | 0.50 |
| 1:A:823:GLY:HA3 | 1:A:844:TRP:CZ2 | 2.46 | 0.50 |
| 1:A:987:MET:HB2 | 1:A:1019:THR:HG22 | 1.91 | 0.50 |
| 1:B:204:THR:HG23 | 1:B:206:ASN:O | 2.11 | 0.50 |
| 1:B:228:ILE:CG2 | 1:B:233:PHE:CE1 | 2.94 | 0.50 |
| 1:B:566:ASN:HB3 | 1:B:651:VAL:CG2 | 2.40 | 0.50 |
| 1:B:689:PHE:CE1 | 1:B:691:GLU:CG | 2.94 | 0.50 |
| 1:B:790:ILE:HD12 | 1:B:790:ILE:N | 2.25 | 0.50 |
| 1:B:807:ARG:HD3 | 1:B:812:LEU:HB3 | 1.93 | 0.50 |
| 1:B:895:VAL:O | 1:B:896:ALA:HB3 | 2.11 | 0.50 |
| 1:A:204:THR:HG23 | 1:A:206:ASN:O | 2.11 | 0.50 |
| 1:A:469:TYR:HB2 | 1:A:523:ASP:OD2 | 2.11 | 0.50 |
| 1:A:783:VAL:HG12 | 1:A:784:TRP:N | 2.25 | 0.50 |
| 1:A:798:VAL:O | 1:A:798:VAL:HG13 | 2.10 | 0.50 |
| 1:A:930:GLU:HG3 | 1:A:941:MET:SD | 2.51 | 0.50 |
| 1:B:119:ILE:CG2 | 1:B:121:TYR:CE1 | 2.95 | 0.50 |
| 1:B:300:GLU:HG2 | 1:B:305:GLU:HA | 1.93 | 0.50 |
| 1:B:400:ASP:HB2 | 1:B:402:ASN:OD1 | 2.11 | 0.50 |
| 1:A:1004:ILE:HD13 | 1:A:1004:ILE:C | 2.32 | 0.50 |
| 1:A:1029:GLN:HG2 | 1:A:1030:ASP:N | 2.26 | 0.50 |
| 1:A:228:ILE:CG2 | 1:A:233:PHE:CE1 | 2.94 | 0.50 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:HG22 | 1.92 | 0.50 |
| 1:A:284:LYS:HD3 | 1:A:284:LYS:C | 2.31 | 0.50 |
| 1:A:703:LEU:HD22 | 1:A:703:LEU:N | 2.26 | 0.50 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:CE2 | 2.46 | 0.50 |
| 1:B:370:LEU:HD13 | 1:B:374:TYR:CD1 | 2.46 | 0.50 |
| 1:B:370:LEU:CD1 | 1:B:374:TYR:CD1 | 2.95 | 0.50 |
| 1:B:473:GLN:HB2 | 1:B:504:VAL:CG2 | 2.40 | 0.50 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CD2 | 2.94 | 0.50 |
| 1:A:261:GLU:HG2 | 1:A:265:PRO:N | 2.25 | 0.50 |
| 1:A:53:LEU:HD23 | 1:A:53:LEU:C | 2.31 | 0.50 |
| 1:A:689:PHE:CE1 | 1:A:691:GLU:CG | 2.94 | 0.50 |
| 1:A:782:VAL:CG2 | 1:A:790:ILE:HB | 2.41 | 0.50 |
| 1:A:894:LYS:CD | 1:A:899:GLU:HA | 2.41 | 0.50 |
| 1:B:295:VAL:O | 1:B:295:VAL:HG23 | 2.12 | 0.50 |
| 1:B:785:ASN:HB3 | 1:B:788:PHE:CE2 | 2.46 | 0.50 |
| 1:B:853:LYS:H | 1:B:853:LYS:HD2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:184:ILE:HD12 | 1:A:184:ILE:C | 2.31 | 0.50 |
| 1:A:370:LEU:CD1 | 1:A:374:TYR:CD1 | 2.95 | 0.50 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:HE2 | 2.43 | 0.50 |
| 1:B:412:LEU:HD22 | 1:B:412:LEU:O | 2.11 | 0.50 |
| 1:B:541:CYS:CB | 1:B:544:SER:HB3 | 2.42 | 0.50 |
| 1:B:76:ASP:O | 1:B:77:LEU:HB2 | 2.11 | 0.50 |
| 1:A:1029:GLN:CG | 1:A:1030:ASP:H | 2.24 | 0.50 |
| 1:A:662:LEU:CD2 | 1:A:791:ASP:OD2 | 2.60 | 0.50 |
| 1:A:895:VAL:O | 1:A:896:ALA:HB3 | 2.11 | 0.50 |
| 1:A:868:PRO:CD | 1:A:980:ALA:C | 2.54 | 0.50 |
| 1:B:133:TYR:O | 1:B:134:GLN:HB2 | 2.11 | 0.50 |
| 1:B:185:ALA:CB | 1:B:243:TYR:CD2 | 2.94 | 0.50 |
| 1:B:261:GLU:HG2 | 1:B:265:PRO:N | 2.25 | 0.50 |
| 1:B:403:PHE:CE1 | 1:B:406:LEU:CD2 | 2.94 | 0.50 |
| 1:B:473:GLN:CD | 1:B:504:VAL:HG13 | 2.31 | 0.50 |
| 1:B:491:GLU:O | 1:B:506:VAL:HG12 | 2.11 | 0.50 |
| 1:B:64:LEU:HB2 | 1:B:71:TYR:HD2 | 1.77 | 0.50 |
| 1:A:110:THR:CB | 1:A:132:LEU:HD21 | 2.42 | 0.50 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CE2 | 2.47 | 0.50 |
| 1:A:39:PHE:CD2 | 1:A:473:GLN:CG | 2.95 | 0.50 |
| 1:A:491:GLU:O | 1:A:506:VAL:HG12 | 2.11 | 0.50 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:CE1 | 2.45 | 0.50 |
| 1:A:673:TRP:HB3 | 1:A:694:VAL:HB | 1.94 | 0.50 |
| 1:A:81:VAL:HG12 | 1:A:82:THR:N | 2.26 | 0.50 |
| 1:B:358:ILE:CG2 | 1:B:361:GLN:HB2 | 2.41 | 0.50 |
| 1:B:457:ILE:HG12 | 1:B:467:LEU:CD1 | 2.42 | 0.50 |
| 1:B:798:VAL:HG13 | 1:B:798:VAL:O | 2.10 | 0.50 |
| 1:A:40:VAL:HG21 | 1:A:76:ASP:O | 2.12 | 0.50 |
| 1:A:320:VAL:HG23 | 1:A:441:ASN:HB3 | 1.94 | 0.50 |
| 1:A:736:TYR:CD2 | 1:A:784:TRP:HB3 | 2.47 | 0.50 |
| 1:B:889:ILE:CD1 | 1:B:907:TYR:CE1 | 2.94 | 0.50 |
| 1:A:119:ILE:CG2 | 1:A:121:TYR:CE1 | 2.95 | 0.50 |
| 1:A:300:GLU:HG2 | 1:A:305:GLU:HA | 1.93 | 0.50 |
| 1:A:370:LEU:HD13 | 1:A:374:TYR:CD1 | 2.46 | 0.50 |
| 1:A:433:SER:HB3 | 1:A:484:MET:HE3 | 1.93 | 0.50 |
| 1:A:892:HIS:HD2 | 1:A:893:VAL:N | 2.10 | 0.50 |
| 1:A:986:VAL:CG1 | 1:A:988:PHE:CE1 | 2.94 | 0.50 |
| 1:B:593:THR:O | 1:B:593:THR:HG23 | 2.10 | 0.50 |
| 1:B:736:TYR:CD2 | 1:B:784:TRP:HB3 | 2.47 | 0.50 |
| 1:B:81:VAL:HG12 | 1:B:82:THR:N | 2.26 | 0.50 |
| 1:B:841:GLU:HG3 | 1:B:842:SER:H | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:380:LEU:CD1 | 1:A:386:LYS:HE3 | 2.37 | 0.49 |
| 1:A:457:ILE:HG12 | 1:A:467:LEU:CD1 | 2.42 | 0.49 |
| 1:A:597:LEU:HD22 | 1:A:597:LEU:H | 1.78 | 0.49 |
| 1:B:278:LYS:CE | 1:B:296:PRO:HG3 | 2.41 | 0.49 |
| 1:B:882:LEU:HD23 | 1:B:913:ILE:HD11 | 1.94 | 0.49 |
| 1:A:265:PRO:CD | 1:A:274:VAL:HG22 | 2.42 | 0.49 |
| 1:A:426:GLU:HG3 | 1:A:429:ASP:H | 1.75 | 0.49 |
| 1:A:444:LEU:HD12 | 1:A:446:PHE:CZ | 2.44 | 0.49 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:CA | 2.42 | 0.49 |
| 1:A:976:THR:HG22 | 1:A:977:ASN:N | 2.27 | 0.49 |
| 1:B:623:ILE:HD12 | 1:B:624:THR:CA | 2.42 | 0.49 |
| 1:B:790:ILE:H | 1:B:790:ILE:HD12 | 1.77 | 0.49 |
| 1:B:856:ASN:N | 1:B:857:PRO:HD3 | 2.27 | 0.49 |
| 1:B:892:HIS:HD2 | 1:B:893:VAL:N | 2.10 | 0.49 |
| 1:A:105:GLU:CB | 1:A:106:PRO:HD2 | 2.42 | 0.49 |
| 1:A:234:THR:HG23 | 1:A:235:VAL:N | 2.26 | 0.49 |
| 1:A:400:ASP:HB2 | 1:A:402:ASN:OD1 | 2.11 | 0.49 |
| 1:B:234:THR:HG23 | 1:B:235:VAL:N | 2.27 | 0.49 |
| 1:B:333:LEU:HD21 | 1:B:358:ILE:HG13 | 1.94 | 0.49 |
| 1:B:597:LEU:H | 1:B:597:LEU:CD2 | 2.26 | 0.49 |
| 1:B:59:THR:HB | 1:B:61:HIS:ND1 | 2.27 | 0.49 |
| 1:B:792:ASN:HD21 | 1:B:796:ASN:N | 2.10 | 0.49 |
| 1:B:894:LYS:CD | 1:B:899:GLU:HA | 2.41 | 0.49 |
| 1:A:333:LEU:HD21 | 1:A:358:ILE:HG13 | 1.94 | 0.49 |
| 1:A:792:ASN:HD21 | 1:A:796:ASN:N | 2.10 | 0.49 |
| 1:B:185:ALA:HB1 | 1:B:243:TYR:CE2 | 2.47 | 0.49 |
| 1:B:265:PRO:HB2 | 1:B:266:PRO:HD2 | 1.94 | 0.49 |
| 1:B:713:VAL:HG13 | 1:B:767:SER:HA | 1.94 | 0.49 |
| 1:A:412:LEU:O | 1:A:412:LEU:HD22 | 2.11 | 0.49 |
| 1:A:790:ILE:H | 1:A:790:ILE:HD12 | 1.77 | 0.49 |
| 1:A:955:LEU:HD11 | 1:A:973:ILE:HG23 | 1.94 | 0.49 |
| 1:B:312:ALA:HB1 | 1:B:334:LEU:HD11 | 1.94 | 0.49 |
| 1:B:475:VAL:HG22 | 1:B:500:GLN:OE1 | 2.13 | 0.49 |
| 1:B:40:VAL:HG21 | 1:B:76:ASP:O | 2.12 | 0.49 |
| 1:A:132:LEU:HD11 | 1:A:163:ASN:HD22 | 1.77 | 0.49 |
| 1:A:185:ALA:HA | 1:A:197:THR:O | 2.13 | 0.49 |
| 1:A:475:VAL:HG22 | 1:A:500:GLN:OE1 | 2.13 | 0.49 |
| 1:A:597:LEU:CD2 | 1:A:597:LEU:H | 2.26 | 0.49 |
| 1:A:532:HIS:CA | 1:A:641:THR:HG21 | 2.43 | 0.49 |
| 1:A:782:VAL:HG23 | 1:A:782:VAL:O | 2.12 | 0.49 |
| 1:B:110:THR:CB | 1:B:132:LEU:HD21 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:133:TYR:HB3 | 1:B:136:ILE:HG23 | 1.94 | 0.49 |
| 1:B:265:PRO:CD | 1:B:274:VAL:HG22 | 2.42 | 0.49 |
| 1:B:374:TYR:CE2 | 1:B:397:LEU:HD22 | 2.48 | 0.49 |
| 1:B:782:VAL:HG23 | 1:B:782:VAL:O | 2.12 | 0.49 |
| 1:A:1002:TYR:OH | 1:A:1004:ILE:HB | 2.12 | 0.49 |
| 1:A:1021:GLN:HG2 | 1:A:1026:ARG:CG | 2.41 | 0.49 |
| 1:A:254:TYR:CE2 | 1:A:281:ARG:HD2 | 2.48 | 0.49 |
| 1:A:295:VAL:O | 1:A:295:VAL:HG23 | 2.12 | 0.49 |
| 1:A:374:TYR:CE2 | 1:A:397:LEU:HD22 | 2.48 | 0.49 |
| 1:A:995:PHE:HZ | 1:A:998:ARG:HB2 | 1.77 | 0.49 |
| 1:B:444:LEU:CD2 | 1:B:524:PRO:CD | 2.91 | 0.49 |
| 1:B:548:ARG:CD | 1:B:583:VAL:O | 2.60 | 0.49 |
| 1:A:541:CYS:CB | 1:A:544:SER:HB3 | 2.42 | 0.49 |
| 1:A:841:GLU:HG3 | 1:A:842:SER:H | 1.78 | 0.49 |
| 1:A:889:ILE:O | 1:A:892:HIS:HB3 | 2.13 | 0.49 |
| 1:B:132:LEU:HD11 | 1:B:163:ASN:HD22 | 1.77 | 0.49 |
| 1:B:190:GLY:C | 1:B:192:PRO:HD3 | 2.33 | 0.49 |
| 1:B:216:VAL:HG13 | 1:B:217:PHE:N | 2.26 | 0.49 |
| 1:B:433:SER:HB3 | 1:B:484:MET:HE3 | 1.95 | 0.49 |
| 1:B:889:ILE:O | 1:B:892:HIS:HB3 | 2.13 | 0.49 |
| 1:A:991:GLN:CB | 1:A:1008:THR:HG21 | 2.42 | 0.49 |
| 1:A:265:PRO:HB2 | 1:A:266:PRO:HD2 | 1.94 | 0.49 |
| 1:B:473:GLN:HB3 | 1:B:502:THR:HG21 | 1.94 | 0.49 |
| 1:B:590:VAL:HG12 | 1:B:591:ASN:N | 2.27 | 0.49 |
| 1:B:847:LEU:HG | 1:B:850:ALA:CA | 2.42 | 0.49 |
| 1:A:133:TYR:HB3 | 1:A:136:ILE:HG23 | 1.94 | 0.49 |
| 1:A:853:LYS:HD2 | 1:A:853:LYS:H | 1.76 | 0.49 |
| 1:A:868:PRO:HG2 | 1:A:981:GLY:HA3 | 1.91 | 0.49 |
| 1:B:182:LEU:HD21 | 1:B:184:ILE:HG21 | 1.94 | 0.49 |
| 1:B:190:GLY:HA2 | 1:B:233:PHE:HE2 | 1.73 | 0.49 |
| 1:B:662:LEU:HD23 | 1:B:791:ASP:CG | 2.32 | 0.49 |
| 1:B:809:SER:CB | 1:B:881:ASN:ND2 | 2.75 | 0.49 |
| 1:A:603:LEU:C | 1:A:603:LEU:HD23 | 2.33 | 0.48 |
| 1:A:856:ASN:N | 1:A:857:PRO:HD3 | 2.27 | 0.48 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:N | 2.28 | 0.48 |
| 1:A:99:ILE:HD11 | 1:A:152:PHE:CB | 2.41 | 0.48 |
| 1:B:39:PHE:CD2 | 1:B:473:GLN:CG | 2.95 | 0.48 |
| 1:B:506:VAL:O | 1:B:525:HIS:CE1 | 2.66 | 0.48 |
| 1:B:541:CYS:SG | 1:B:550:PHE:CD2 | 3.06 | 0.48 |
| 1:B:863:ILE:HG13 | 1:B:864:PRO:N | 2.28 | 0.48 |
| 1:B:907:TYR:CZ | 1:B:909:PRO:HA | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:868:PRO:CG | 1:A:1022:VAL:CG2 | 2.88 | 0.48 |
| 1:A:473:GLN:CD | 1:A:504:VAL:HG22 | 2.33 | 0.48 |
| 1:A:59:THR:HB | 1:A:61:HIS:ND1 | 2.27 | 0.48 |
| 1:A:790:ILE:HG22 | 1:A:791:ASP:N | 2.29 | 0.48 |
| 1:A:847:LEU:HG | 1:A:850:ALA:CA | 2.42 | 0.48 |
| 1:B:160:SER:OG | 1:B:162:VAL:HG23 | 2.13 | 0.48 |
| 1:B:949:TYR:CE2 | 1:B:951:MET:CE | 2.95 | 0.48 |
| 1:A:1020:VAL:HG13 | 1:A:1020:VAL:O | 2.13 | 0.48 |
| 1:A:590:VAL:HG12 | 1:A:591:ASN:N | 2.27 | 0.48 |
| 1:A:713:VAL:HG13 | 1:A:767:SER:HA | 1.94 | 0.48 |
| 1:A:882:LEU:HD23 | 1:A:913:ILE:HD11 | 1.94 | 0.48 |
| 1:B:185:ALA:HA | 1:B:197:THR:O | 2.13 | 0.48 |
| 1:B:435:ILE:HG21 | 1:B:486:PHE:CE1 | 2.48 | 0.48 |
| 1:B:603:LEU:HD23 | 1:B:603:LEU:C | 2.33 | 0.48 |
| 1:B:673:TRP:HB3 | 1:B:694:VAL:HB | 1.94 | 0.48 |
| 1:A:239:PHE:CD1 | 1:A:260:PRO:HG2 | 2.48 | 0.48 |
| 1:A:321:LEU:CG | 1:A:325:LEU:HD11 | 2.40 | 0.48 |
| 1:A:991:GLN:HB3 | 1:A:1008:THR:HG21 | 1.96 | 0.48 |
| 1:B:239:PHE:CD1 | 1:B:260:PRO:HG2 | 2.48 | 0.48 |
| 1:B:254:TYR:CE2 | 1:B:281:ARG:HD2 | 2.48 | 0.48 |
| 1:B:320:VAL:HG23 | 1:B:441:ASN:HB3 | 1.94 | 0.48 |
| 1:B:781:THR:HG23 | 1:B:781:THR:O | 2.12 | 0.48 |
| 1:B:807:ARG:HB3 | 1:B:812:LEU:HB2 | 1.95 | 0.48 |
| 1:A:435:ILE:HG21 | 1:A:486:PHE:CE1 | 2.48 | 0.48 |
| 1:A:473:GLN:HB3 | 1:A:502:THR:HG21 | 1.94 | 0.48 |
| 1:A:681:THR:HG21 | 1:A:686:THR:HG21 | 1.94 | 0.48 |
| 1:A:740:LEU:HD12 | 1:A:740:LEU:N | 2.29 | 0.48 |
| 1:A:716:ILE:HD11 | 1:A:763:ASN:HB3 | 1.95 | 0.48 |
| 1:A:781:THR:O | 1:A:781:THR:HG23 | 2.12 | 0.48 |
| 1:B:258:LEU:HD12 | 1:B:258:LEU:N | 2.29 | 0.48 |
| 1:B:453:LYS:HE3 | 1:B:472:VAL:HG22 | 1.94 | 0.48 |
| 1:B:715:VAL:HG23 | 1:B:715:VAL:O | 2.13 | 0.48 |
| 1:A:182:LEU:HD21 | 1:A:184:ILE:HG21 | 1.94 | 0.48 |
| 1:A:567:ILE:HD12 | 1:A:650:PHE:CE2 | 2.49 | 0.48 |
| 1:B:716:ILE:HD11 | 1:B:763:ASN:HB3 | 1.95 | 0.48 |
| 1:B:935:VAL:HG12 | 1:B:936:CYS:N | 2.28 | 0.48 |
| 1:A:190:GLY:C | 1:A:192:PRO:HD3 | 2.33 | 0.48 |
| 1:A:312:ALA:HB1 | 1:A:334:LEU:HD11 | 1.94 | 0.48 |
| 1:A:144:ASP:O | 1:A:145:LEU:HB2 | 2.13 | 0.48 |
| 1:A:543:ARG:HH11 | 1:A:549:ARG:HH22 | 1.62 | 0.48 |
| 1:A:626:ASN:ND2 | 1:A:630:HIS:HB2 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:64:LEU:HB2 | 1:A:71:TYR:HD2 | 1.77 | 0.48 |
| 1:A:807:ARG:HB3 | 1:A:812:LEU:HB2 | 1.95 | 0.48 |
| 1:A:935:VAL:HG12 | 1:A:936:CYS:N | 2.28 | 0.48 |
| 1:B:144:ASP:O | 1:B:145:LEU:HB2 | 2.13 | 0.48 |
| 1:B:42:PHE:HZ | 1:B:45:GLU:CB | 2.22 | 0.48 |
| 1:B:626:ASN:ND2 | 1:B:630:HIS:HB2 | 2.29 | 0.48 |
| 1:B:783:VAL:HG13 | 1:B:788:PHE:O | 2.13 | 0.48 |
| 1:B:782:VAL:CG2 | 1:B:790:ILE:HB | 2.41 | 0.48 |
| 1:B:471:THR:HG23 | 1:B:473:GLN:NE2 | 2.27 | 0.48 |
| 1:A:710:LEU:HD13 | 1:A:801:TYR:OH | 2.13 | 0.48 |
| 1:A:1010:SER:HB2 | 1:A:1035:TYR:CD2 | 2.49 | 0.47 |
| 1:A:361:GLN:HE21 | 1:A:365:ARG:HH21 | 1.61 | 0.47 |
| 1:A:469:TYR:CB | 1:A:523:ASP:OD2 | 2.62 | 0.47 |
| 1:A:704:LEU:H | 1:A:723:ALA:HA | 1.79 | 0.47 |
| 1:A:987:MET:HE3 | 1:A:990:SER:HA | 1.95 | 0.47 |
| 1:B:440:LYS:O | 1:B:440:LYS:HG2 | 2.14 | 0.47 |
| 1:B:561:THR:HG22 | 1:B:562:VAL:N | 2.29 | 0.47 |
| 1:B:681:THR:HG21 | 1:B:686:THR:HG21 | 1.95 | 0.47 |
| 1:B:710:LEU:HD13 | 1:B:801:TYR:OH | 2.13 | 0.47 |
| 1:A:124:ASN:OD1 | 1:A:142:LEU:HB3 | 2.14 | 0.47 |
| 1:A:258:LEU:HD12 | 1:A:258:LEU:N | 2.28 | 0.47 |
| 1:A:440:LYS:HG2 | 1:A:440:LYS:O | 2.14 | 0.47 |
| 1:A:541:CYS:SG | 1:A:550:PHE:CD2 | 3.07 | 0.47 |
| 1:A:862:ILE:CG2 | 1:A:877:ILE:HG23 | 2.44 | 0.47 |
| 1:A:907:TYR:CZ | 1:A:909:PRO:HA | 2.48 | 0.47 |
| 1:A:991:GLN:HA | 1:A:991:GLN:OE1 | 2.13 | 0.47 |
| 1:B:124:ASN:OD1 | 1:B:142:LEU:HB3 | 2.15 | 0.47 |
| 1:B:430:ARG:HG2 | 1:B:431:MET:O | 2.14 | 0.47 |
| 1:B:814:LEU:HD11 | 1:B:845:LEU:CD1 | 2.44 | 0.47 |
| 1:A:468:GLN:HB3 | 1:A:468:GLN:HE21 | 1.47 | 0.47 |
| 1:A:695:LYS:HB2 | 1:A:696:LEU:HD12 | 1.97 | 0.47 |
| 1:A:728:GLN:HA | 1:A:753:ARG:NH2 | 2.30 | 0.47 |
| 1:A:953:LEU:HB3 | 1:A:977:ASN:O | 2.14 | 0.47 |
| 1:B:113:VAL:HG11 | 1:B:165:SER:HB3 | 1.97 | 0.47 |
| 1:B:361:GLN:HE21 | 1:B:365:ARG:HH21 | 1.61 | 0.47 |
| 1:B:473:GLN:CD | 1:B:504:VAL:HG22 | 2.34 | 0.47 |
| 1:B:507:GLU:HG3 | 1:B:537:ARG:CG | 2.40 | 0.47 |
| 1:B:698:GLU:O | 1:B:725:ASN:OD1 | 2.32 | 0.47 |
| 1:B:728:GLN:HA | 1:B:753:ARG:NH2 | 2.29 | 0.47 |
| 1:A:991:GLN:HG2 | 1:A:1008:THR:HG21 | 1.96 | 0.47 |
| 1:A:783:VAL:HG13 | 1:A:788:PHE:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:984:VAL:HG23 | 1:A:984:VAL:O | 2.14 | 0.47 |
| 1:A:997:ARG:HG2 | 1:A:998:ARG:N | 2.30 | 0.47 |
| 1:B:98:ARG:NH2 | 1:B:107:LEU:HD12 | 2.29 | 0.47 |
| 1:B:175:TYR:CG | 1:B:176:SER:N | 2.82 | 0.47 |
| 1:B:543:ARG:HH11 | 1:B:549:ARG:HH22 | 1.62 | 0.47 |
| 1:A:264:SER:HA | 1:A:265:PRO:HA | 1.53 | 0.47 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:HE | 1.79 | 0.47 |
| 1:A:458:ARG:CD | 1:A:524:PRO:HG3 | 2.44 | 0.47 |
| 1:A:702:GLN:O | 1:A:723:ALA:HB1 | 2.14 | 0.47 |
| 1:A:715:VAL:HG23 | 1:A:715:VAL:O | 2.13 | 0.47 |
| 1:A:863:ILE:CG1 | 1:A:864:PRO:HD3 | 2.39 | 0.47 |
| 1:A:175:TYR:CG | 1:A:176:SER:N | 2.82 | 0.47 |
| 1:A:430:ARG:HG2 | 1:A:431:MET:O | 2.14 | 0.47 |
| 1:A:77:LEU:HD22 | 1:A:501:LEU:HD13 | 1.96 | 0.47 |
| 1:A:68:ASN:ND2 | 1:A:87:PRO:HD3 | 2.29 | 0.47 |
| 1:B:118:LEU:HD13 | 1:B:118:LEU:C | 2.34 | 0.47 |
| 1:B:380:LEU:HD12 | 1:B:390:ILE:CG2 | 2.45 | 0.47 |
| 1:B:480:VAL:HB | 1:B:484:MET:HE1 | 1.94 | 0.47 |
| 1:B:469:TYR:HB3 | 1:B:523:ASP:OD2 | 2.15 | 0.47 |
| 1:B:597:LEU:H | 1:B:597:LEU:HD22 | 1.78 | 0.47 |
| 1:B:699:ASP:O | 1:B:725:ASN:CB | 2.63 | 0.47 |
| 1:B:745:ILE:O | 1:B:745:ILE:HG23 | 2.14 | 0.47 |
| 1:A:333:LEU:CD2 | 1:A:358:ILE:HA | 2.45 | 0.47 |
| 1:A:569:VAL:HG23 | 1:A:654:ASN:HB2 | 1.80 | 0.47 |
| 1:A:72:LYS:O | 1:A:80:LEU:HB2 | 2.15 | 0.47 |
| 1:A:745:ILE:O | 1:A:745:ILE:HG23 | 2.15 | 0.47 |
| 1:A:814:LEU:HD11 | 1:A:845:LEU:CD1 | 2.44 | 0.47 |
| 1:A:987:MET:CE | 1:A:990:SER:HA | 2.45 | 0.47 |
| 1:B:372:SER:HA | 1:B:375:ARG:NE | 2.29 | 0.47 |
| 1:B:702:GLN:O | 1:B:723:ALA:HB1 | 2.14 | 0.47 |
| 1:B:704:LEU:H | 1:B:723:ALA:HA | 1.79 | 0.47 |
| 1:B:884:LEU:HD23 | 1:B:884:LEU:HA | 1.75 | 0.47 |
| 1:B:262:MET:O | 1:B:263:VAL:HB | 2.14 | 0.47 |
| 1:B:569:VAL:CG1 | 1:B:620:PRO:HG3 | 2.45 | 0.47 |
| 1:B:947:LEU:HD23 | 1:B:947:LEU:H | 1.80 | 0.47 |
| 1:A:958:LEU:HD13 | 1:A:1033:PHE:HD1 | 1.79 | 0.47 |
| 1:A:253:VAL:O | 1:A:253:VAL:HG23 | 2.15 | 0.47 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:HG22 | 1.94 | 0.47 |
| 1:A:843:ARG:NH1 | 1:A:843:ARG:HB2 | 2.30 | 0.47 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:CG2 | 2.98 | 0.47 |
| 1:B:253:VAL:O | 1:B:253:VAL:HG23 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:403:PHE:HE1 | 1:B:406:LEU:HD23 | 1.75 | 0.47 |
| 1:B:45:GLU:HB3 | 1:B:46:PRO:HD3 | 1.97 | 0.47 |
| 1:B:740:LEU:HD12 | 1:B:740:LEU:N | 2.29 | 0.47 |
| 1:B:790:ILE:HG22 | 1:B:791:ASP:N | 2.28 | 0.47 |
| 1:A:245:TYR:CE2 | 1:A:247:PHE:HD2 | 2.33 | 0.47 |
| 1:A:569:VAL:CG1 | 1:A:620:PRO:HG3 | 2.45 | 0.47 |
| 1:A:873:THR:CG2 | 1:A:982:SER:N | 2.78 | 0.47 |
| 1:B:68:ASN:ND2 | 1:B:87:PRO:HD3 | 2.30 | 0.47 |
| 1:A:1020:VAL:HG13 | 1:A:1027:ILE:HG12 | 1.96 | 0.47 |
| 1:A:160:SER:OG | 1:A:162:VAL:HG23 | 2.14 | 0.47 |
| 1:A:495:ILE:HG22 | 1:A:502:THR:HB | 1.96 | 0.47 |
| 1:A:561:THR:HG22 | 1:A:562:VAL:N | 2.28 | 0.47 |
| 1:A:947:LEU:N | 1:A:947:LEU:HD23 | 2.30 | 0.47 |
| 1:B:105:GLU:CB | 1:B:106:PRO:HD2 | 2.42 | 0.47 |
| 1:B:333:LEU:CD2 | 1:B:358:ILE:HA | 2.45 | 0.47 |
| 1:B:343:LYS:HG2 | 1:B:344:ARG:HG2 | 1.97 | 0.47 |
| 1:B:82:THR:O | 1:B:82:THR:HG23 | 2.14 | 0.47 |
| 1:A:118:LEU:C | 1:A:118:LEU:HD13 | 2.34 | 0.46 |
| 1:A:372:SER:HA | 1:A:375:ARG:NE | 2.30 | 0.46 |
| 1:B:244:VAL:HB | 1:B:309:LEU:HD23 | 1.97 | 0.46 |
| 1:B:783:VAL:HG11 | 1:B:786:GLY:O | 2.15 | 0.46 |
| 1:B:843:ARG:HB2 | 1:B:843:ARG:NH1 | 2.30 | 0.46 |
| 1:B:862:ILE:CG2 | 1:B:877:ILE:HG23 | 2.44 | 0.46 |
| 1:B:863:ILE:CG1 | 1:B:864:PRO:HD3 | 2.39 | 0.46 |
| 1:A:181:LYS:HZ2 | 1:A:216:VAL:HG23 | 1.77 | 0.46 |
| 1:A:403:PHE:HE1 | 1:A:406:LEU:HD23 | 1.75 | 0.46 |
| 1:A:68:ASN:HB3 | 1:A:86:GLY:HA3 | 1.97 | 0.46 |
| 1:A:949:TYR:CE2 | 1:A:951:MET:CE | 2.95 | 0.46 |
| 1:A:873:THR:HG23 | 1:A:981:GLY:O | 2.14 | 0.46 |
| 1:B:567:ILE:HD12 | 1:B:650:PHE:CE2 | 2.49 | 0.46 |
| 1:B:72:LYS:O | 1:B:80:LEU:HB2 | 2.15 | 0.46 |
| 1:A:244:VAL:HB | 1:A:309:LEU:HD23 | 1.97 | 0.46 |
| 1:B:286:ASP:OD1 | 1:B:288:ALA:HB3 | 2.15 | 0.46 |
| 1:B:380:LEU:CB | 1:B:386:LYS:HE3 | 2.44 | 0.46 |
| 1:B:505:PRO:HB2 | 1:B:507:GLU:C | 2.35 | 0.46 |
| 1:A:1007:THR:HG22 | 1:A:1008:THR:O | 2.15 | 0.46 |
| 1:A:532:HIS:CA | 1:A:641:THR:OG1 | 2.57 | 0.46 |
| 1:A:82:THR:O | 1:A:82:THR:HG23 | 2.14 | 0.46 |
| 1:B:321:LEU:CG | 1:B:325:LEU:HD11 | 2.40 | 0.46 |
| 1:A:252:PHE:CD1 | 1:A:283:CYS:HA | 2.50 | 0.46 |
| 1:A:503:ARG:O | 1:A:505:PRO:HD3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:549:ARG:HA | 1:A:584:PRO:HG3 | 1.97 | 0.46 |
| 1:A:549:ARG:CD | 1:A:584:PRO:CB | 2.76 | 0.46 |
| 1:A:862:ILE:HG22 | 1:A:877:ILE:CA | 2.32 | 0.46 |
| 1:A:873:THR:HG22 | 1:A:874:LYS:N | 2.31 | 0.46 |
| 1:B:159:LEU:HG | 1:B:201:ARG:HH12 | 1.81 | 0.46 |
| 1:B:245:TYR:CD2 | 1:B:312:ALA:HB3 | 2.51 | 0.46 |
| 1:B:296:PRO:CD | 1:B:414:VAL:HG22 | 2.45 | 0.46 |
| 1:B:468:GLN:O | 1:B:521:SER:O | 2.34 | 0.46 |
| 1:B:660:SER:HB2 | 1:B:791:ASP:OD1 | 2.16 | 0.46 |
| 1:B:68:ASN:HB3 | 1:B:86:GLY:HA3 | 1.97 | 0.46 |
| 1:B:892:HIS:CD2 | 1:B:893:VAL:CG2 | 2.98 | 0.46 |
| 1:A:1015:ASP:H | 1:A:1035:TYR:H | 1.63 | 0.46 |
| 1:A:265:PRO:CB | 1:A:266:PRO:HD2 | 2.45 | 0.46 |
| 1:A:296:PRO:CD | 1:A:414:VAL:HG22 | 2.46 | 0.46 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:HG2 | 1.98 | 0.46 |
| 1:B:77:LEU:HD22 | 1:B:501:LEU:HD13 | 1.96 | 0.46 |
| 1:B:46:PRO:CG | 1:B:69:ARG:HG3 | 2.27 | 0.46 |
| 1:B:902:PRO:HA | 1:B:915:CYS:HA | 1.97 | 0.46 |
| 1:B:99:ILE:HD11 | 1:B:152:PHE:CB | 2.41 | 0.46 |
| 1:A:113:VAL:HG11 | 1:A:165:SER:HB3 | 1.96 | 0.46 |
| 1:A:226:ILE:HD11 | 1:A:385:LEU:CD2 | 2.46 | 0.46 |
| 1:A:444:LEU:HD13 | 1:A:445:ALA:H | 1.79 | 0.46 |
| 1:A:62:ILE:CD1 | 1:A:77:LEU:CD2 | 2.94 | 0.46 |
| 1:A:62:ILE:HD11 | 1:A:73:LEU:CD1 | 2.45 | 0.46 |
| 1:A:873:THR:OG1 | 1:A:982:SER:N | 2.48 | 0.46 |
| 1:B:295:VAL:CA | 1:B:414:VAL:HG21 | 2.45 | 0.46 |
| 1:A:262:MET:O | 1:A:263:VAL:HB | 2.14 | 0.46 |
| 1:A:274:VAL:HG23 | 1:A:275:TYR:N | 2.30 | 0.46 |
| 1:A:295:VAL:CA | 1:A:414:VAL:HG21 | 2.45 | 0.46 |
| 1:A:343:LYS:HG2 | 1:A:344:ARG:HG2 | 1.97 | 0.46 |
| 1:A:947:LEU:H | 1:A:947:LEU:HD23 | 1.80 | 0.46 |
| 1:B:495:ILE:HG22 | 1:B:502:THR:HB | 1.96 | 0.46 |
| 1:B:594:PHE:CZ | 1:B:614:PRO:HD3 | 2.51 | 0.46 |
| 1:A:403:PHE:CE1 | 1:A:406:LEU:CD2 | 2.94 | 0.46 |
| 1:A:437:TYR:CE2 | 1:A:439:TYR:HB2 | 2.51 | 0.46 |
| 1:B:245:TYR:CE2 | 1:B:247:PHE:HD2 | 2.34 | 0.46 |
| 1:B:278:LYS:HD3 | 1:B:294:GLU:HG2 | 1.98 | 0.46 |
| 1:B:46:PRO:HD2 | 1:B:71:TYR:OH | 2.16 | 0.46 |
| 1:B:91:ASN:OD1 | 1:B:92:PRO:HD2 | 2.16 | 0.46 |
| 1:A:870:GLU:CA | 1:A:1024:ARG:HG2 | 2.43 | 0.46 |
| 1:A:286:ASP:OD1 | 1:A:288:ALA:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:380:LEU:HD12 | 1:A:390:ILE:CG2 | 2.45 | 0.46 |
| 1:A:902:PRO:HA | 1:A:915:CYS:HA | 1.98 | 0.46 |
| 1:B:118:LEU:CD1 | 1:B:172:ILE:HD12 | 2.12 | 0.46 |
| 1:B:225:MET:HE1 | 1:B:227:LYS:CG | 2.45 | 0.46 |
| 1:B:361:GLN:O | 1:B:365:ARG:HG2 | 2.16 | 0.46 |
| 1:A:327:VAL:HG11 | 1:A:358:ILE:HD11 | 1.97 | 0.45 |
| 1:A:624:THR:O | 1:A:624:THR:HG23 | 2.15 | 0.45 |
| 1:A:828:PRO:HG3 | 1:A:837:CYS:SG | 2.56 | 0.45 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:HG22 | 2.51 | 0.45 |
| 1:B:252:PHE:CD1 | 1:B:283:CYS:HA | 2.50 | 0.45 |
| 1:B:435:ILE:HG23 | 1:B:486:PHE:HE1 | 1.81 | 0.45 |
| 1:B:439:TYR:CE2 | 1:B:538:LYS:CE | 2.99 | 0.45 |
| 1:B:689:PHE:CE1 | 1:B:691:GLU:HG2 | 2.50 | 0.45 |
| 1:B:62:ILE:CD1 | 1:B:73:LEU:HB2 | 2.47 | 0.45 |
| 1:B:743:GLN:HG2 | 1:B:744:GLY:N | 2.31 | 0.45 |
| 1:A:110:THR:CB | 1:A:132:LEU:CD2 | 2.95 | 0.45 |
| 1:A:435:ILE:HG23 | 1:A:486:PHE:HE1 | 1.81 | 0.45 |
| 1:A:480:VAL:HB | 1:A:484:MET:HE1 | 1.97 | 0.45 |
| 1:A:563:HIS:CB | 1:A:577:VAL:HG12 | 2.46 | 0.45 |
| 1:A:532:HIS:C | 1:A:641:THR:HG21 | 2.36 | 0.45 |
| 1:A:870:GLU:OE2 | 1:A:1025:ALA:HA | 2.16 | 0.45 |
| 1:A:890:ALA:O | 1:A:891:SER:HB2 | 2.17 | 0.45 |
| 1:B:265:PRO:CB | 1:B:266:PRO:HD2 | 2.45 | 0.45 |
| 1:A:1020:VAL:CG1 | 1:A:1027:ILE:CG1 | 2.95 | 0.45 |
| 1:A:380:LEU:CB | 1:A:386:LYS:HE3 | 2.43 | 0.45 |
| 1:A:45:GLU:HB3 | 1:A:46:PRO:HD3 | 1.97 | 0.45 |
| 1:B:118:LEU:HB3 | 1:B:127:ILE:HG22 | 1.98 | 0.45 |
| 1:B:663:SER:O | 1:B:667:SER:HB2 | 2.17 | 0.45 |
| 1:B:695:LYS:HB2 | 1:B:696:LEU:HD12 | 1.96 | 0.45 |
| 1:A:361:GLN:O | 1:A:365:ARG:HG2 | 2.16 | 0.45 |
| 1:A:458:ARG:HG3 | 1:A:468:GLN:NE2 | 2.32 | 0.45 |
| 1:A:469:TYR:CG | 1:A:470:GLU:N | 2.84 | 0.45 |
| 1:A:689:PHE:CE1 | 1:A:691:GLU:HG2 | 2.50 | 0.45 |
| 1:A:783:VAL:HG11 | 1:A:786:GLY:O | 2.16 | 0.45 |
| 1:B:256:LEU:HD22 | 1:B:256:LEU:N | 2.31 | 0.45 |
| 1:B:435:ILE:HG21 | 1:B:486:PHE:HE1 | 1.81 | 0.45 |
| 1:B:58:ARG:HG2 | 1:B:58:ARG:NH1 | 2.31 | 0.45 |
| 1:B:62:ILE:HD11 | 1:B:73:LEU:CD1 | 2.45 | 0.45 |
| 1:B:828:PRO:HG3 | 1:B:837:CYS:SG | 2.56 | 0.45 |
| 1:B:892:HIS:CD2 | 1:B:893:VAL:N | 2.85 | 0.45 |
| 1:A:159:LEU:HG | 1:A:201:ARG:HH12 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:256:LEU:HD22 | 1:A:256:LEU:N | 2.31 | 0.45 |
| 1:A:288:ALA:O | 1:A:289:PHE:HB2 | 2.17 | 0.45 |
| 1:A:322:GLY:HA2 | 1:A:327:VAL:HG22 | 1.99 | 0.45 |
| 1:A:511:GLN:HG3 | 1:A:512:TYR:CD2 | 2.51 | 0.45 |
| 1:A:743:GLN:HG2 | 1:A:744:GLY:N | 2.31 | 0.45 |
| 1:B:563:HIS:CB | 1:B:577:VAL:HG12 | 2.46 | 0.45 |
| 1:B:624:THR:O | 1:B:624:THR:HG23 | 2.15 | 0.45 |
| 1:B:62:ILE:CD1 | 1:B:77:LEU:CD2 | 2.94 | 0.45 |
| 1:B:805:ALA:N | 1:B:806:MET:HE3 | 2.31 | 0.45 |
| 1:A:1014:LEU:HD12 | 1:A:1035:TYR:O | 2.16 | 0.45 |
| 1:A:118:LEU:HB3 | 1:A:127:ILE:HG22 | 1.98 | 0.45 |
| 1:A:278:LYS:CE | 1:A:296:PRO:HG3 | 2.41 | 0.45 |
| 1:A:245:TYR:CD2 | 1:A:312:ALA:HB3 | 2.51 | 0.45 |
| 1:A:506:VAL:O | 1:A:507:GLU:N | 2.39 | 0.45 |
| 1:A:695:LYS:C | 1:A:696:LEU:HD12 | 2.37 | 0.45 |
| 1:B:442:HIS:CD2 | 1:B:458:ARG:HH21 | 2.35 | 0.45 |
| 1:B:503:ARG:O | 1:B:505:PRO:HD3 | 2.15 | 0.45 |
| 1:B:671:CYS:HB3 | 1:B:680:CYS:SG | 2.57 | 0.45 |
| 1:B:873:THR:HG22 | 1:B:874:LYS:N | 2.31 | 0.45 |
| 1:B:892:HIS:CD2 | 1:B:893:VAL:HG22 | 2.51 | 0.45 |
| 1:B:947:LEU:HD23 | 1:B:947:LEU:N | 2.30 | 0.45 |
| 1:A:358:ILE:CG2 | 1:A:361:GLN:CB | 2.95 | 0.45 |
| 1:A:539:GLU:HG3 | 1:A:540:ARG:N | 2.31 | 0.45 |
| 1:A:53:LEU:HD12 | 1:A:501:LEU:HG | 1.99 | 0.45 |
| 1:A:594:PHE:CZ | 1:A:614:PRO:HD3 | 2.51 | 0.45 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:OH | 2.16 | 0.45 |
| 1:B:118:LEU:O | 1:B:127:ILE:HG22 | 2.17 | 0.45 |
| 1:B:226:ILE:HD11 | 1:B:385:LEU:CD2 | 2.46 | 0.45 |
| 1:B:40:VAL:HG11 | 1:B:503:ARG:HE | 1.80 | 0.45 |
| 1:B:62:ILE:CD1 | 1:B:501:LEU:CD1 | 2.95 | 0.45 |
| 1:B:635:GLN:HB3 | 1:B:644:THR:HB | 1.99 | 0.45 |
| 1:B:890:ALA:O | 1:B:891:SER:HB2 | 2.17 | 0.45 |
| 1:A:182:LEU:HB2 | 1:A:203:LEU:HD11 | 1.99 | 0.45 |
| 1:A:62:ILE:CD1 | 1:A:501:LEU:CD1 | 2.95 | 0.45 |
| 1:A:663:SER:O | 1:A:667:SER:HB2 | 2.16 | 0.45 |
| 1:A:715:VAL:HG21 | 1:A:717:LYS:CD | 2.44 | 0.45 |
| 1:A:841:GLU:HG3 | 1:A:842:SER:N | 2.32 | 0.45 |
| 1:A:955:LEU:CD1 | 1:A:973:ILE:CG2 | 2.94 | 0.45 |
| 1:B:133:TYR:CG | 1:B:136:ILE:CG1 | 2.94 | 0.45 |
| 1:B:464:GLY:O | 1:B:465:ASN:HB3 | 2.17 | 0.45 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:HD2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:873:THR:CB | 1:A:982:SER:N | 2.80 | 0.45 |
| 1:B:192:PRO:HB3 | 1:B:233:PHE:CZ | 2.51 | 0.45 |
| 1:B:288:ALA:O | 1:B:289:PHE:HB2 | 2.17 | 0.45 |
| 1:B:492:GLN:HG2 | 1:B:503:ARG:HG2 | 1.98 | 0.45 |
| 1:B:511:GLN:HG3 | 1:B:512:TYR:CD2 | 2.51 | 0.45 |
| 1:B:539:GLU:HG3 | 1:B:540:ARG:N | 2.31 | 0.45 |
| 1:B:814:LEU:HB2 | 1:B:884:LEU:HD11 | 1.98 | 0.45 |
| 1:A:118:LEU:CD1 | 1:A:172:ILE:HD12 | 2.12 | 0.45 |
| 1:A:531:LEU:HG | 1:A:584:PRO:CG | 2.46 | 0.45 |
| 1:A:91:ASN:OD1 | 1:A:92:PRO:HD2 | 2.16 | 0.45 |
| 1:B:327:VAL:HG11 | 1:B:358:ILE:HD11 | 1.97 | 0.45 |
| 1:B:468:GLN:HB3 | 1:B:468:GLN:HE21 | 1.47 | 0.45 |
| 1:B:862:ILE:HG22 | 1:B:877:ILE:CA | 2.32 | 0.45 |
| 1:A:464:GLY:O | 1:A:465:ASN:HB3 | 2.17 | 0.44 |
| 1:A:703:LEU:CD2 | 1:A:790:ILE:CG2 | 2.95 | 0.44 |
| 1:A:778:VAL:O | 1:A:797:LYS:HB2 | 2.17 | 0.44 |
| 1:B:295:VAL:CB | 1:B:414:VAL:HG21 | 2.48 | 0.44 |
| 1:B:469:TYR:CG | 1:B:470:GLU:N | 2.84 | 0.44 |
| 1:B:586:LEU:HD13 | 1:B:590:VAL:HG21 | 1.99 | 0.44 |
| 1:B:703:LEU:CD2 | 1:B:790:ILE:CG2 | 2.95 | 0.44 |
| 1:B:832:THR:HG21 | 1:B:836:HIS:CB | 2.48 | 0.44 |
| 1:A:151:PRO:HB2 | 1:A:157:HIS:CE1 | 2.52 | 0.44 |
| 1:A:247:PHE:CD1 | 1:A:314:LEU:HD22 | 2.52 | 0.44 |
| 1:A:252:PHE:HD1 | 1:A:283:CYS:HA | 1.82 | 0.44 |
| 1:A:278:LYS:HD3 | 1:A:294:GLU:HG2 | 1.98 | 0.44 |
| 1:A:471:THR:HG23 | 1:A:473:GLN:NE2 | 2.27 | 0.44 |
| 1:A:564:PRO:HB2 | 1:A:576:LEU:CD2 | 2.48 | 0.44 |
| 1:A:567:ILE:HD11 | 1:A:652:PHE:CD1 | 2.53 | 0.44 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:N | 2.85 | 0.44 |
| 1:B:162:VAL:HG21 | 1:B:187:ALA:HB3 | 1.99 | 0.44 |
| 1:B:252:PHE:HD1 | 1:B:283:CYS:HA | 1.82 | 0.44 |
| 1:B:305:GLU:HG2 | 1:B:307:ARG:HG2 | 1.99 | 0.44 |
| 1:B:291:SER:HB3 | 1:B:404:CYS:O | 2.18 | 0.44 |
| 1:B:458:ARG:HG3 | 1:B:468:GLN:NE2 | 2.32 | 0.44 |
| 1:B:492:GLN:HG2 | 1:B:503:ARG:HD2 | 1.98 | 0.44 |
| 1:B:53:LEU:HD12 | 1:B:501:LEU:HG | 1.99 | 0.44 |
| 1:B:566:ASN:CB | 1:B:651:VAL:CG2 | 2.95 | 0.44 |
| 1:A:189:ASP:HB3 | 1:A:191:LYS:HD3 | 1.99 | 0.44 |
| 1:B:597:LEU:HG | 1:B:622:ILE:HG12 | 1.99 | 0.44 |
| 1:A:291:SER:HB3 | 1:A:404:CYS:O | 2.18 | 0.44 |
| 1:A:566:ASN:CB | 1:A:651:VAL:CG2 | 2.94 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:868:PRO:HG2 | 1:A:1022:VAL:HG21 | 1.94 | 0.44 |
| 1:A:995:PHE:CZ | 1:A:998:ARG:HB2 | 2.52 | 0.44 |
| 1:B:182:LEU:HB2 | 1:B:203:LEU:HD11 | 1.99 | 0.44 |
| 1:B:264:SER:HA | 1:B:265:PRO:HA | 1.53 | 0.44 |
| 1:B:247:PHE:CD1 | 1:B:314:LEU:HD22 | 2.52 | 0.44 |
| 1:B:370:LEU:CD2 | 1:B:374:TYR:HE1 | 2.27 | 0.44 |
| 1:B:437:TYR:CE2 | 1:B:439:TYR:HB2 | 2.51 | 0.44 |
| 1:B:567:ILE:HD11 | 1:B:652:PHE:CD1 | 2.53 | 0.44 |
| 1:B:695:LYS:C | 1:B:696:LEU:HD12 | 2.37 | 0.44 |
| 1:B:805:ALA:H | 1:B:806:MET:HE3 | 1.82 | 0.44 |
| 1:A:116:MET:SD | 1:A:169:PHE:HA | 2.57 | 0.44 |
| 1:A:262:MET:SD | 1:A:383:ALA:HB3 | 2.57 | 0.44 |
| 1:A:541:CYS:HB3 | 1:A:544:SER:HB3 | 1.99 | 0.44 |
| 1:A:58:ARG:HG2 | 1:A:58:ARG:NH1 | 2.31 | 0.44 |
| 1:A:53:LEU:CG | 1:A:64:LEU:CD1 | 2.96 | 0.44 |
| 1:A:889:ILE:CD1 | 1:A:907:TYR:CZ | 3.01 | 0.44 |
| 1:A:958:LEU:HD13 | 1:A:1033:PHE:CD1 | 2.53 | 0.44 |
| 1:B:116:MET:SD | 1:B:169:PHE:HA | 2.57 | 0.44 |
| 1:A:281:ARG:NH1 | 1:A:366:ILE:HG21 | 2.33 | 0.44 |
| 1:A:306:TYR:HE1 | 1:A:351:GLU:HG2 | 1.83 | 0.44 |
| 1:A:635:GLN:HB3 | 1:A:644:THR:HB | 1.99 | 0.44 |
| 1:A:671:CYS:HB3 | 1:A:680:CYS:SG | 2.57 | 0.44 |
| 1:A:951:MET:HG2 | 1:A:977:ASN:OD1 | 2.17 | 0.44 |
| 1:B:179:ASP:O | 1:B:180:ASP:HB3 | 2.17 | 0.44 |
| 1:B:185:ALA:CB | 1:B:243:TYR:CD1 | 3.00 | 0.44 |
| 1:B:262:MET:SD | 1:B:383:ALA:HB3 | 2.58 | 0.44 |
| 1:A:98:ARG:NH2 | 1:A:107:LEU:HD12 | 2.29 | 0.44 |
| 1:A:179:ASP:O | 1:A:180:ASP:HB3 | 2.17 | 0.44 |
| 1:A:40:VAL:HG13 | 1:A:40:VAL:O | 2.17 | 0.44 |
| 1:A:421:ILE:HA | 1:A:422:PRO:HD2 | 1.84 | 0.44 |
| 1:A:586:LEU:HD13 | 1:A:590:VAL:HG21 | 1.99 | 0.44 |
| 1:A:597:LEU:HG | 1:A:622:ILE:HG12 | 1.99 | 0.44 |
| 1:A:72:LYS:CE | 1:A:80:LEU:CD1 | 2.95 | 0.44 |
| 1:B:117:LEU:HD11 | 1:B:126:LEU:CD2 | 2.31 | 0.44 |
| 1:B:119:ILE:HG23 | 1:B:121:TYR:CE1 | 2.53 | 0.44 |
| 1:B:173:VAL:O | 1:B:173:VAL:HG23 | 2.18 | 0.44 |
| 1:B:256:LEU:CB | 1:B:309:LEU:CD2 | 2.94 | 0.44 |
| 1:B:281:ARG:NH1 | 1:B:366:ILE:HG21 | 2.33 | 0.44 |
| 1:B:676:TYR:CE1 | 1:B:730:GLN:CD | 2.90 | 0.44 |
| 1:B:699:ASP:O | 1:B:725:ASN:HB3 | 2.18 | 0.44 |
| 1:B:62:ILE:CD1 | 1:B:73:LEU:HD12 | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:118:LEU:O | 1:A:127:ILE:HG22 | 2.17 | 0.44 |
| 1:A:133:TYR:CG | 1:A:136:ILE:CG1 | 2.94 | 0.44 |
| 1:A:162:VAL:HG21 | 1:A:187:ALA:HB3 | 1.99 | 0.44 |
| 1:A:217:PHE:CE2 | 1:A:219:ASP:HB2 | 2.53 | 0.44 |
| 1:A:889:ILE:HA | 1:A:892:HIS:ND1 | 2.33 | 0.44 |
| 1:B:110:THR:CB | 1:B:132:LEU:CD2 | 2.95 | 0.44 |
| 1:B:274:VAL:HG23 | 1:B:275:TYR:N | 2.30 | 0.44 |
| 1:B:322:GLY:HA2 | 1:B:327:VAL:HG22 | 1.99 | 0.44 |
| 1:B:332:ASP:O | 1:B:333:LEU:HD23 | 2.18 | 0.44 |
| 1:B:42:PHE:CZ | 1:B:45:GLU:CB | 2.95 | 0.44 |
| 1:B:55:VAL:HG22 | 1:B:62:ILE:HG22 | 2.00 | 0.44 |
| 1:B:564:PRO:HB2 | 1:B:576:LEU:CD2 | 2.48 | 0.44 |
| 1:A:442:HIS:CD2 | 1:A:458:ARG:HH21 | 2.35 | 0.44 |
| 1:A:528:TRP:HZ2 | 1:A:533:ASN:OD1 | 2.01 | 0.44 |
| 1:A:569:VAL:CG2 | 1:A:654:ASN:CB | 2.65 | 0.44 |
| 1:A:574:VAL:HG22 | 1:A:613:SER:OG | 2.17 | 0.44 |
| 1:A:713:VAL:O | 1:A:714:GLU:HB2 | 2.18 | 0.44 |
| 1:B:358:ILE:CG2 | 1:B:361:GLN:CB | 2.95 | 0.44 |
| 1:B:743:GLN:H | 1:B:743:GLN:CD | 2.21 | 0.44 |
| 1:B:778:VAL:O | 1:B:797:LYS:HB2 | 2.17 | 0.44 |
| 1:B:863:ILE:HG22 | 1:B:876:THR:CB | 2.35 | 0.44 |
| 1:B:889:ILE:CD1 | 1:B:907:TYR:CZ | 3.01 | 0.44 |
| 1:A:332:ASP:O | 1:A:333:LEU:HD23 | 2.18 | 0.43 |
| 1:A:53:LEU:HD11 | 1:A:501:LEU:HD11 | 2.00 | 0.43 |
| 1:A:567:ILE:HD11 | 1:A:650:PHE:CE2 | 2.53 | 0.43 |
| 1:A:574:VAL:CG2 | 1:A:613:SER:HB3 | 2.48 | 0.43 |
| 1:A:62:ILE:CD1 | 1:A:73:LEU:HD12 | 2.45 | 0.43 |
| 1:A:764:THR:CG2 | 1:A:766:TYR:CZ | 3.01 | 0.43 |
| 1:A:874:LYS:H | 1:A:982:SER:HB2 | 1.80 | 0.43 |
| 1:B:189:ASP:HB3 | 1:B:191:LYS:HD3 | 1.99 | 0.43 |
| 1:B:306:TYR:HE1 | 1:B:351:GLU:HG2 | 1.83 | 0.43 |
| 1:B:53:LEU:HD11 | 1:B:501:LEU:HD11 | 2.00 | 0.43 |
| 1:B:711:VAL:HG21 | 1:B:798:VAL:CG2 | 2.48 | 0.43 |
| 1:B:841:GLU:HG3 | 1:B:842:SER:N | 2.32 | 0.43 |
| 1:A:711:VAL:HG21 | 1:A:798:VAL:CG2 | 2.48 | 0.43 |
| 1:A:832:THR:HG21 | 1:A:836:HIS:CB | 2.48 | 0.43 |
| 1:B:541:CYS:HB3 | 1:B:544:SER:HB3 | 1.99 | 0.43 |
| 1:A:119:ILE:HG23 | 1:A:121:TYR:CE1 | 2.53 | 0.43 |
| 1:A:333:LEU:HD23 | 1:A:358:ILE:HG13 | 2.00 | 0.43 |
| 1:A:589:GLY:C | 1:A:639:LYS:HG2 | 2.39 | 0.43 |
| 1:B:151:PRO:HB2 | 1:B:157:HIS:CE1 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:324:THR:HG22 | 1:B:324:THR:O | 2.18 | 0.43 |
| 1:B:555:LYS:NZ | 1:B:556:GLN:HG2 | 2.33 | 0.43 |
| 1:B:574:VAL:HG22 | 1:B:613:SER:OG | 2.17 | 0.43 |
| 1:B:764:THR:CG2 | 1:B:766:TYR:CZ | 3.01 | 0.43 |
| 1:B:889:ILE:HA | 1:B:892:HIS:ND1 | 2.33 | 0.43 |
| 1:A:1031:LEU:HD22 | 1:A:1031:LEU:N | 2.34 | 0.43 |
| 1:A:1016:MET:HE2 | 1:A:1033:PHE:H | 1.84 | 0.43 |
| 1:A:1014:LEU:HA | 1:A:1035:TYR:HB2 | 2.00 | 0.43 |
| 1:A:435:ILE:CD1 | 1:A:486:PHE:HD1 | 2.31 | 0.43 |
| 1:A:590:VAL:CG1 | 1:A:591:ASN:N | 2.82 | 0.43 |
| 1:A:62:ILE:CD1 | 1:A:501:LEU:HD13 | 2.49 | 0.43 |
| 1:A:531:LEU:C | 1:A:641:THR:HG1 | 2.19 | 0.43 |
| 1:A:743:GLN:CD | 1:A:743:GLN:H | 2.22 | 0.43 |
| 1:A:839:ALA:HB1 | 1:A:841:GLU:O | 2.18 | 0.43 |
| 1:B:296:PRO:HB2 | 1:B:417:MET:CE | 2.48 | 0.43 |
| 1:B:370:LEU:HD12 | 1:B:399:ILE:HG23 | 2.00 | 0.43 |
| 1:B:456:LYS:HD3 | 1:B:523:ASP:OD2 | 2.10 | 0.43 |
| 1:B:527:GLY:HA3 | 1:B:550:PHE:HZ | 1.72 | 0.43 |
| 1:B:528:TRP:HZ2 | 1:B:533:ASN:OD1 | 2.01 | 0.43 |
| 1:B:563:HIS:CB | 1:B:577:VAL:CG1 | 2.95 | 0.43 |
| 1:B:589:GLY:C | 1:B:639:LYS:HG2 | 2.39 | 0.43 |
| 1:A:173:VAL:HG23 | 1:A:173:VAL:O | 2.18 | 0.43 |
| 1:A:224:SER:HA | 1:A:289:PHE:CD1 | 2.54 | 0.43 |
| 1:A:501:LEU:CD2 | 1:A:502:THR:N | 2.81 | 0.43 |
| 1:A:832:THR:CG2 | 1:A:836:HIS:CB | 2.95 | 0.43 |
| 1:B:333:LEU:HD23 | 1:B:358:ILE:HG13 | 2.00 | 0.43 |
| 1:B:458:ARG:HB2 | 1:B:468:GLN:HE22 | 1.83 | 0.43 |
| 1:B:574:VAL:CG2 | 1:B:613:SER:HB3 | 2.48 | 0.43 |
| 1:B:839:ALA:HB1 | 1:B:841:GLU:O | 2.18 | 0.43 |
| 1:A:962:ARG:HD3 | 1:A:1034:GLN:HE21 | 1.83 | 0.43 |
| 1:A:128:ALA:O | 1:A:138:LYS:HG2 | 2.19 | 0.43 |
| 1:A:100:VAL:HG21 | 1:A:158:TYR:OH | 2.19 | 0.43 |
| 1:A:162:VAL:HG12 | 1:A:164:GLU:H | 1.84 | 0.43 |
| 1:A:295:VAL:CB | 1:A:414:VAL:HG21 | 2.48 | 0.43 |
| 1:A:296:PRO:HB2 | 1:A:417:MET:CE | 2.48 | 0.43 |
| 1:A:470:GLU:HG2 | 1:A:471:THR:N | 2.34 | 0.43 |
| 1:A:716:ILE:CD1 | 1:A:763:ASN:HB3 | 2.49 | 0.43 |
| 1:A:978:LEU:HD13 | 1:A:1003:ILE:HG13 | 2.01 | 0.43 |
| 1:B:117:LEU:HG | 1:B:126:LEU:HD11 | 2.01 | 0.43 |
| 1:B:217:PHE:CE2 | 1:B:219:ASP:HB2 | 2.53 | 0.43 |
| 1:B:281:ARG:HB3 | 1:B:293:VAL:HG11 | 1.97 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:40:VAL:O | 1:B:40:VAL:HG13 | 2.17 | 0.43 |
| 1:B:435:ILE:CD1 | 1:B:486:PHE:HD1 | 2.31 | 0.43 |
| 1:B:440:LYS:HB2 | 1:B:538:LYS:HZ2 | 1.84 | 0.43 |
| 1:B:764:THR:HG23 | 1:B:766:TYR:CZ | 2.54 | 0.43 |
| 1:B:95:TYR:HA | 1:B:95:TYR:HD1 | 1.70 | 0.43 |
| 1:A:965:MET:HG3 | 1:A:1010:SER:O | 2.18 | 0.43 |
| 1:A:962:ARG:CB | 1:A:1034:GLN:HG3 | 2.45 | 0.43 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CE2 | 3.02 | 0.43 |
| 1:A:305:GLU:HG2 | 1:A:307:ARG:HG2 | 1.99 | 0.43 |
| 1:A:764:THR:HG23 | 1:A:766:TYR:CZ | 2.54 | 0.43 |
| 1:B:119:ILE:HG21 | 1:B:121:TYR:CE1 | 2.54 | 0.43 |
| 1:B:460:ASP:CG | 1:B:463:LYS:HB3 | 2.39 | 0.43 |
| 1:B:542:GLU:HG2 | 1:B:543:ARG:HG3 | 2.01 | 0.43 |
| 1:B:549:ARG:HD3 | 1:B:584:PRO:CB | 2.48 | 0.43 |
| 1:A:1010:SER:HB2 | 1:A:1035:TYR:CE1 | 2.52 | 0.43 |
| 1:A:1016:MET:CE | 1:A:1033:PHE:CB | 2.94 | 0.43 |
| 1:A:555:LYS:NZ | 1:A:556:GLN:HG2 | 2.33 | 0.43 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:HD22 | 1.98 | 0.43 |
| 1:A:620:PRO:O | 1:A:623:ILE:HG13 | 2.18 | 0.43 |
| 1:A:72:LYS:CD | 1:A:80:LEU:CD1 | 2.97 | 0.43 |
| 1:B:506:VAL:CG2 | 1:B:525:HIS:CE1 | 2.81 | 0.43 |
| 1:A:333:LEU:HD23 | 1:A:358:ILE:HA | 2.01 | 0.43 |
| 1:A:62:ILE:CD1 | 1:A:64:LEU:HD21 | 2.46 | 0.43 |
| 1:A:789:ASN:HD22 | 1:A:790:ILE:N | 2.17 | 0.43 |
| 1:B:100:VAL:HG21 | 1:B:158:TYR:OH | 2.19 | 0.43 |
| 1:B:234:THR:CG2 | 1:B:235:VAL:N | 2.82 | 0.43 |
| 1:B:358:ILE:HG23 | 1:B:358:ILE:O | 2.18 | 0.43 |
| 1:B:506:VAL:HG21 | 1:B:525:HIS:NE2 | 2.22 | 0.43 |
| 1:B:620:PRO:O | 1:B:623:ILE:HG13 | 2.18 | 0.43 |
| 1:B:949:TYR:CE2 | 1:B:951:MET:HE2 | 2.53 | 0.43 |
| 1:A:117:LEU:HG | 1:A:126:LEU:HD11 | 2.01 | 0.43 |
| 1:A:112:ASN:ND2 | 1:A:133:TYR:HE2 | 2.17 | 0.43 |
| 1:A:186:THR:CG2 | 1:A:187:ALA:N | 2.81 | 0.43 |
| 1:A:281:ARG:HB3 | 1:A:293:VAL:HG11 | 1.97 | 0.43 |
| 1:A:617:LYS:HG3 | 1:A:618:GLU:N | 2.34 | 0.43 |
| 1:A:55:VAL:HG22 | 1:A:62:ILE:HG22 | 2.00 | 0.43 |
| 1:A:805:ALA:N | 1:A:806:MET:CE | 2.82 | 0.43 |
| 1:A:885:GLU:HG3 | 1:A:886:PHE:N | 2.34 | 0.43 |
| 1:B:123:GLU:HB2 | 1:B:125:ARG:HG2 | 2.01 | 0.43 |
| 1:B:470:GLU:HG2 | 1:B:471:THR:N | 2.34 | 0.43 |
| 1:B:501:LEU:CD2 | 1:B:502:THR:N | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:617:LYS:HG3 | 1:B:618:GLU:N | 2.34 | 0.43 |
| 1:B:789:ASN:HD22 | 1:B:790:ILE:N | 2.17 | 0.43 |
| 1:A:665:VAL:HG11 | 1:A:697:PRO:CD | 2.48 | 0.42 |
| 1:A:98:ARG:HE | 1:A:107:LEU:HD12 | 1.83 | 0.42 |
| 1:B:90:ASP:C | 1:B:107:LEU:HD22 | 2.39 | 0.42 |
| 1:B:128:ALA:O | 1:B:138:LYS:HG2 | 2.19 | 0.42 |
| 1:B:62:ILE:CD1 | 1:B:501:LEU:HD13 | 2.49 | 0.42 |
| 1:B:713:VAL:O | 1:B:714:GLU:HB2 | 2.18 | 0.42 |
| 1:A:90:ASP:C | 1:A:107:LEU:HD22 | 2.39 | 0.42 |
| 1:A:192:PRO:HB3 | 1:A:233:PHE:CZ | 2.51 | 0.42 |
| 1:A:972:THR:HG23 | 1:A:1002:TYR:HE1 | 1.72 | 0.42 |
| 1:B:133:TYR:CB | 1:B:136:ILE:HG23 | 2.49 | 0.42 |
| 1:B:178:PHE:O | 1:B:178:PHE:HD1 | 2.02 | 0.42 |
| 1:B:543:ARG:HB2 | 1:B:549:ARG:NH1 | 2.34 | 0.42 |
| 1:B:567:ILE:HD11 | 1:B:650:PHE:CE2 | 2.53 | 0.42 |
| 1:B:665:VAL:HG11 | 1:B:697:PRO:CD | 2.48 | 0.42 |
| 1:A:1032:VAL:CG1 | 1:A:1033:PHE:N | 2.82 | 0.42 |
| 1:A:110:THR:HG21 | 1:A:132:LEU:HD21 | 1.97 | 0.42 |
| 1:A:458:ARG:HB2 | 1:A:468:GLN:HE22 | 1.83 | 0.42 |
| 1:A:541:CYS:HB2 | 1:A:544:SER:HB3 | 2.01 | 0.42 |
| 1:A:630:HIS:CD2 | 1:A:632:VAL:CG2 | 3.00 | 0.42 |
| 1:A:889:ILE:HG23 | 1:A:892:HIS:NE2 | 2.33 | 0.42 |
| 1:B:185:ALA:CB | 1:B:243:TYR:CE2 | 3.02 | 0.42 |
| 1:B:358:ILE:HG23 | 1:B:361:GLN:N | 2.24 | 0.42 |
| 1:B:605:ILE:O | 1:B:608:GLN:HG2 | 2.20 | 0.42 |
| 1:B:689:PHE:HD1 | 1:B:691:GLU:HG2 | 1.80 | 0.42 |
| 1:A:1029:GLN:CG | 1:A:1030:ASP:N | 2.83 | 0.42 |
| 1:A:119:ILE:HG21 | 1:A:121:TYR:CE1 | 2.54 | 0.42 |
| 1:A:225:MET:CE | 1:A:227:LYS:CG | 2.94 | 0.42 |
| 1:A:370:LEU:HD12 | 1:A:399:ILE:HG23 | 2.00 | 0.42 |
| 1:A:471:THR:HG21 | 1:A:473:GLN:OE1 | 2.19 | 0.42 |
| 1:A:567:ILE:CD1 | 1:A:567:ILE:N | 2.82 | 0.42 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:C | 2.40 | 0.42 |
| 1:A:865:VAL:CG1 | 1:A:866:THR:N | 2.82 | 0.42 |
| 1:A:953:LEU:HD12 | 1:A:978:LEU:HD23 | 2.01 | 0.42 |
| 1:A:868:PRO:CD | 1:A:981:GLY:HA2 | 1.99 | 0.42 |
| 1:B:224:SER:HA | 1:B:289:PHE:CD1 | 2.54 | 0.42 |
| 1:B:662:LEU:HD23 | 1:B:791:ASP:CB | 2.48 | 0.42 |
| 1:A:962:ARG:HD3 | 1:A:1034:GLN:NE2 | 2.34 | 0.42 |
| 1:A:169:PHE:CD2 | 1:A:170:GLY:N | 2.84 | 0.42 |
| 1:A:178:PHE:O | 1:A:178:PHE:HD1 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:358:ILE:HG23 | 1:A:361:GLN:N | 2.24 | 0.42 |
| 1:A:358:ILE:HG23 | 1:A:358:ILE:O | 2.18 | 0.42 |
| 1:A:955:LEU:CG | 1:A:973:ILE:CG2 | 2.95 | 0.42 |
| 1:B:216:VAL:CG1 | 1:B:217:PHE:N | 2.82 | 0.42 |
| 1:B:333:LEU:HD23 | 1:B:358:ILE:HA | 2.01 | 0.42 |
| 1:B:567:ILE:N | 1:B:567:ILE:CD1 | 2.82 | 0.42 |
| 1:B:590:VAL:CG1 | 1:B:591:ASN:N | 2.82 | 0.42 |
| 1:B:759:VAL:CG1 | 1:B:760:GLN:N | 2.81 | 0.42 |
| 1:B:885:GLU:HG3 | 1:B:886:PHE:N | 2.34 | 0.42 |
| 1:B:889:ILE:HG23 | 1:B:892:HIS:NE2 | 2.33 | 0.42 |
| 1:A:1007:THR:HG22 | 1:A:1008:THR:N | 2.33 | 0.42 |
| 1:A:123:GLU:HB2 | 1:A:125:ARG:HG2 | 2.01 | 0.42 |
| 1:A:460:ASP:CG | 1:A:463:LYS:HB3 | 2.39 | 0.42 |
| 1:A:435:ILE:HG21 | 1:A:486:PHE:HE1 | 1.81 | 0.42 |
| 1:A:543:ARG:HB2 | 1:A:549:ARG:NH1 | 2.34 | 0.42 |
| 1:A:959:LYS:HG2 | 1:A:972:THR:HG21 | 2.01 | 0.42 |
| 1:B:112:ASN:ND2 | 1:B:133:TYR:HE2 | 2.17 | 0.42 |
| 1:B:186:THR:CG2 | 1:B:187:ALA:N | 2.81 | 0.42 |
| 1:B:471:THR:HG21 | 1:B:473:GLN:OE1 | 2.19 | 0.42 |
| 1:B:68:ASN:CB | 1:B:86:GLY:HA3 | 2.50 | 0.42 |
| 1:A:256:LEU:CB | 1:A:309:LEU:CD2 | 2.94 | 0.42 |
| 1:A:549:ARG:CD | 1:A:584:PRO:HB3 | 2.42 | 0.42 |
| 1:A:830:GLN:CG | 1:A:831:CYS:H | 2.24 | 0.42 |
| 1:B:321:LEU:HD23 | 1:B:333:LEU:CD1 | 2.50 | 0.42 |
| 1:A:542:GLU:HG2 | 1:A:543:ARG:HG3 | 2.00 | 0.42 |
| 1:A:845:LEU:HD11 | 1:A:852:SER:OG | 2.20 | 0.42 |
| 1:B:458:ARG:HD2 | 1:B:524:PRO:CB | 2.31 | 0.42 |
| 1:B:437:TYR:HH | 1:B:525:HIS:CD2 | 2.37 | 0.42 |
| 1:B:653:TYR:CZ | 1:B:682:HIS:CE1 | 3.07 | 0.42 |
| 1:B:700:CYS:HA | 1:B:701:PRO:HD3 | 1.45 | 0.42 |
| 1:A:234:THR:CG2 | 1:A:235:VAL:N | 2.82 | 0.42 |
| 1:A:324:THR:HG22 | 1:A:324:THR:O | 2.18 | 0.42 |
| 1:A:370:LEU:CD2 | 1:A:374:TYR:HE1 | 2.28 | 0.42 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:HD23 | 1.99 | 0.42 |
| 1:A:566:ASN:CA | 1:A:651:VAL:CG2 | 2.95 | 0.42 |
| 1:A:783:VAL:CG1 | 1:A:784:TRP:N | 2.83 | 0.42 |
| 1:B:446:PHE:CB | 1:B:454:LEU:HD11 | 2.43 | 0.42 |
| 1:B:562:VAL:HG22 | 1:B:578:LEU:HD23 | 1.99 | 0.42 |
| 1:B:563:HIS:HB2 | 1:B:577:VAL:HG13 | 2.01 | 0.42 |
| 1:A:380:LEU:HD22 | 1:A:412:LEU:HB3 | 2.02 | 0.42 |
| 1:A:662:LEU:O | 1:A:666:GLU:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:62:ILE:CD1 | 1:A:73:LEU:HB2 | 2.47 | 0.42 |
| 1:A:888:ASP:OD1 | 1:A:889:ILE:HG13 | 2.20 | 0.42 |
| 1:A:920:ALA:C | 1:A:922:PRO:HD2 | 2.41 | 0.42 |
| 1:B:39:PHE:CZ | 1:B:473:GLN:HG3 | 2.53 | 0.42 |
| 1:B:528:TRP:CZ2 | 1:B:533:ASN:OD1 | 2.73 | 0.42 |
| 1:B:783:VAL:CG1 | 1:B:784:TRP:N | 2.83 | 0.42 |
| 1:B:926:ALA:HB2 | 1:B:949:TYR:CD1 | 2.55 | 0.42 |
| 1:A:412:LEU:CD1 | 1:A:412:LEU:N | 2.83 | 0.41 |
| 1:A:440:LYS:HD2 | 1:A:538:LYS:HD2 | 1.93 | 0.41 |
| 1:A:605:ILE:O | 1:A:608:GLN:HG2 | 2.19 | 0.41 |
| 1:A:67:VAL:CG1 | 1:A:111:ASN:HB3 | 2.50 | 0.41 |
| 1:B:162:VAL:HG12 | 1:B:164:GLU:H | 1.84 | 0.41 |
| 1:B:177:ASN:O | 1:B:178:PHE:CG | 2.73 | 0.41 |
| 1:B:256:LEU:HD12 | 1:B:297:ILE:HD11 | 2.02 | 0.41 |
| 1:B:575:LEU:N | 1:B:575:LEU:CD2 | 2.83 | 0.41 |
| 1:B:623:ILE:HD12 | 1:B:624:THR:HA | 2.02 | 0.41 |
| 1:B:64:LEU:HD12 | 1:B:496:MET:HE3 | 1.98 | 0.41 |
| 1:B:817:ASP:OD1 | 1:B:820:PHE:CD2 | 2.73 | 0.41 |
| 1:A:216:VAL:CG1 | 1:A:217:PHE:N | 2.82 | 0.41 |
| 1:A:44:GLY:O | 1:A:47:ALA:HA | 2.20 | 0.41 |
| 1:A:440:LYS:HB3 | 1:A:538:LYS:HZ3 | 1.79 | 0.41 |
| 1:A:817:ASP:OD1 | 1:A:820:PHE:CD2 | 2.73 | 0.41 |
| 1:A:68:ASN:CB | 1:A:86:GLY:HA3 | 2.50 | 0.41 |
| 1:A:959:LYS:CG | 1:A:972:THR:CB | 2.97 | 0.41 |
| 1:B:159:LEU:HG | 1:B:201:ARG:NH1 | 2.35 | 0.41 |
| 1:B:403:PHE:CE2 | 1:B:405:GLY:HA2 | 2.55 | 0.41 |
| 1:B:492:GLN:HB3 | 1:B:503:ARG:HG3 | 2.02 | 0.41 |
| 1:B:728:GLN:HG3 | 1:B:753:ARG:NH2 | 2.35 | 0.41 |
| 1:B:716:ILE:CD1 | 1:B:763:ASN:HB3 | 2.49 | 0.41 |
| 1:B:72:LYS:CE | 1:B:80:LEU:CD1 | 2.95 | 0.41 |
| 1:A:1016:MET:HE2 | 1:A:1033:PHE:CB | 2.49 | 0.41 |
| 1:A:177:ASN:O | 1:A:178:PHE:CG | 2.73 | 0.41 |
| 1:A:387:VAL:CG1 | 1:A:388:LYS:N | 2.82 | 0.41 |
| 1:A:446:PHE:CD1 | 1:A:446:PHE:N | 2.88 | 0.41 |
| 1:A:569:VAL:HB | 1:A:654:ASN:CG | 2.41 | 0.41 |
| 1:A:728:GLN:HG3 | 1:A:753:ARG:NH2 | 2.35 | 0.41 |
| 1:B:412:LEU:N | 1:B:412:LEU:CD1 | 2.83 | 0.41 |
| 1:B:444:LEU:HD23 | 1:B:524:PRO:HG2 | 1.91 | 0.41 |
| 1:B:619:VAL:HB | 1:B:620:PRO:CD | 2.47 | 0.41 |
| 1:B:865:VAL:CG1 | 1:B:866:THR:N | 2.82 | 0.41 |
| 1:A:111:ASN:O | 1:A:132:LEU:HD13 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:188:VAL:HG22 | 1:A:188:VAL:O | 2.21 | 0.41 |
| 1:A:307:ARG:HA | 1:A:307:ARG:HD3 | 1.88 | 0.41 |
| 1:A:349:LEU:CD2 | 1:A:349:LEU:N | 2.84 | 0.41 |
| 1:A:403:PHE:CE2 | 1:A:405:GLY:HA2 | 2.55 | 0.41 |
| 1:A:563:HIS:HB2 | 1:A:577:VAL:HG13 | 2.01 | 0.41 |
| 1:A:631:VAL:HG13 | 1:A:631:VAL:O | 2.19 | 0.41 |
| 1:A:711:VAL:HB | 1:A:800:LEU:HD23 | 2.02 | 0.41 |
| 1:A:926:ALA:HB2 | 1:A:949:TYR:CD1 | 2.55 | 0.41 |
| 1:A:978:LEU:HA | 1:A:978:LEU:HD23 | 1.93 | 0.41 |
| 1:B:110:THR:HG21 | 1:B:132:LEU:HD21 | 1.97 | 0.41 |
| 1:B:225:MET:CE | 1:B:227:LYS:CG | 2.94 | 0.41 |
| 1:B:446:PHE:CD1 | 1:B:446:PHE:N | 2.89 | 0.41 |
| 1:B:562:VAL:HG22 | 1:B:578:LEU:HD22 | 1.98 | 0.41 |
| 1:B:679:VAL:CG1 | 1:B:680:CYS:N | 2.82 | 0.41 |
| 1:B:862:ILE:HG21 | 1:B:877:ILE:HG12 | 2.03 | 0.41 |
| 1:B:920:ALA:C | 1:B:922:PRO:HD2 | 2.40 | 0.41 |
| 1:A:988:PHE:CB | 1:A:1016:MET:SD | 3.06 | 0.41 |
| 1:A:1031:LEU:H | 1:A:1031:LEU:HD22 | 1.84 | 0.41 |
| 1:A:133:TYR:CB | 1:A:136:ILE:HG23 | 2.49 | 0.41 |
| 1:A:159:LEU:HG | 1:A:201:ARG:NH1 | 2.36 | 0.41 |
| 1:A:226:ILE:HD11 | 1:A:385:LEU:HD23 | 2.03 | 0.41 |
| 1:A:531:LEU:HA | 1:A:531:LEU:HD23 | 1.91 | 0.41 |
| 1:B:137:CYS:SG | 1:B:159:LEU:CD1 | 3.09 | 0.41 |
| 1:B:280:VAL:CG1 | 1:B:281:ARG:N | 2.83 | 0.41 |
| 1:B:380:LEU:HD22 | 1:B:412:LEU:HB3 | 2.02 | 0.41 |
| 1:B:631:VAL:HG13 | 1:B:631:VAL:O | 2.19 | 0.41 |
| 1:B:803:CYS:SG | 1:B:832:THR:HA | 2.61 | 0.41 |
| 1:B:949:TYR:CE2 | 1:B:951:MET:HE1 | 2.55 | 0.41 |
| 1:A:446:PHE:CB | 1:A:454:LEU:HD11 | 2.43 | 0.41 |
| 1:A:703:LEU:HD13 | 1:A:723:ALA:CB | 2.47 | 0.41 |
| 1:A:862:ILE:HG21 | 1:A:877:ILE:HG12 | 2.03 | 0.41 |
| 1:A:958:LEU:HD22 | 1:A:960:PRO:N | 2.35 | 0.41 |
| 1:A:959:LYS:CG | 1:A:972:THR:HG21 | 2.51 | 0.41 |
| 1:B:185:ALA:HB3 | 1:B:243:TYR:CD2 | 2.56 | 0.41 |
| 1:B:444:LEU:HD12 | 1:B:446:PHE:CD1 | 2.51 | 0.41 |
| 1:B:444:LEU:HD13 | 1:B:445:ALA:H | 1.79 | 0.41 |
| 1:B:453:LYS:CE | 1:B:472:VAL:HG22 | 2.51 | 0.41 |
| 1:B:506:VAL:CG1 | 1:B:507:GLU:N | 2.84 | 0.41 |
| 1:B:541:CYS:HB2 | 1:B:544:SER:HB3 | 2.01 | 0.41 |
| 1:B:551:ALA:HB1 | 1:B:556:GLN:HB2 | 2.03 | 0.41 |
| 1:B:778:VAL:HG12 | 1:B:779:GLU:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:805:ALA:N | 1:B:806:MET:CE | 2.82 | 0.41 |
| 1:B:888:ASP:OD1 | 1:B:889:ILE:HG13 | 2.20 | 0.41 |
| 1:A:380:LEU:CB | 1:A:386:LYS:CE | 2.95 | 0.41 |
| 1:A:492:GLN:HB3 | 1:A:503:ARG:HG3 | 2.02 | 0.41 |
| 1:A:679:VAL:CG1 | 1:A:680:CYS:N | 2.82 | 0.41 |
| 1:A:759:VAL:CG1 | 1:A:760:GLN:N | 2.81 | 0.41 |
| 1:A:95:TYR:CG | 1:A:96:PRO:CD | 3.03 | 0.41 |
| 1:B:67:VAL:CG1 | 1:B:111:ASN:HB3 | 2.50 | 0.41 |
| 1:B:137:CYS:O | 1:B:150:GLU:HG3 | 2.20 | 0.41 |
| 1:B:387:VAL:CG1 | 1:B:388:LYS:N | 2.82 | 0.41 |
| 1:B:44:GLY:O | 1:B:47:ALA:HA | 2.20 | 0.41 |
| 1:B:658:HIS:ND1 | 1:B:663:SER:HB3 | 2.36 | 0.41 |
| 1:A:972:THR:CG2 | 1:A:1002:TYR:CE1 | 2.93 | 0.41 |
| 1:A:137:CYS:O | 1:A:150:GLU:HG3 | 2.20 | 0.41 |
| 1:A:188:VAL:CG2 | 1:A:191:LYS:HB2 | 2.51 | 0.41 |
| 1:A:185:ALA:HB3 | 1:A:243:TYR:CD2 | 2.56 | 0.41 |
| 1:A:280:VAL:CG1 | 1:A:281:ARG:N | 2.83 | 0.41 |
| 1:A:988:PHE:CD2 | 1:A:1016:MET:SD | 3.12 | 0.41 |
| 1:B:492:GLN:CG | 1:B:503:ARG:HD2 | 2.51 | 0.41 |
| 1:B:95:TYR:CG | 1:B:96:PRO:CD | 3.03 | 0.41 |
| 1:A:137:CYS:SG | 1:A:159:LEU:CD1 | 3.09 | 0.41 |
| 1:A:236:ILE:CG2 | 1:A:239:PHE:HB2 | 2.51 | 0.41 |
| 1:A:480:VAL:HB | 1:A:484:MET:HE2 | 2.01 | 0.41 |
| 1:A:492:GLN:CG | 1:A:503:ARG:HD2 | 2.51 | 0.41 |
| 1:A:528:TRP:CZ2 | 1:A:533:ASN:OD1 | 2.73 | 0.41 |
| 1:B:188:VAL:CG2 | 1:B:191:LYS:HB2 | 2.51 | 0.41 |
| 1:B:226:ILE:HD11 | 1:B:385:LEU:HD23 | 2.03 | 0.41 |
| 1:B:239:PHE:CD1 | 1:B:260:PRO:CD | 3.03 | 0.41 |
| 1:B:696:LEU:HA | 1:B:697:PRO:HD3 | 1.87 | 0.41 |
| 1:B:710:LEU:C | 1:B:710:LEU:HD12 | 2.40 | 0.41 |
| 1:B:832:THR:HG21 | 1:B:836:HIS:HB2 | 1.99 | 0.41 |
| 1:B:843:ARG:CZ | 1:B:843:ARG:CB | 2.99 | 0.41 |
| 1:A:117:LEU:HD11 | 1:A:126:LEU:CD2 | 2.31 | 0.41 |
| 1:A:619:VAL:HB | 1:A:620:PRO:CD | 2.47 | 0.41 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:HA | 2.01 | 0.41 |
| 1:A:959:LYS:HG2 | 1:A:972:THR:HB | 2.02 | 0.41 |
| 1:A:953:LEU:HA | 1:A:977:ASN:HB2 | 2.02 | 0.41 |
| 1:B:111:ASN:O | 1:B:132:LEU:HD13 | 2.20 | 0.41 |
| 1:B:236:ILE:CG2 | 1:B:239:PHE:HB2 | 2.51 | 0.41 |
| 1:B:349:LEU:CD2 | 1:B:349:LEU:N | 2.84 | 0.41 |
| 1:B:560:LEU:CG | 1:B:648:THR:CG2 | 2.98 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:683:ASP:HA | 1:B:684:PRO:HD3 | 1.83 | 0.41 |
| 1:B:703:LEU:HD13 | 1:B:723:ALA:CB | 2.47 | 0.41 |
| 1:B:901:SER:HA | 1:B:902:PRO:HD2 | 1.89 | 0.41 |
| 1:A:111:ASN:O | 1:A:132:LEU:HD22 | 2.21 | 0.41 |
| 1:A:95:TYR:CE2 | 1:A:194:TYR:CD1 | 3.09 | 0.41 |
| 1:A:252:PHE:HE1 | 1:A:283:CYS:SG | 2.44 | 0.41 |
| 1:A:256:LEU:HD12 | 1:A:297:ILE:HD11 | 2.01 | 0.41 |
| 1:A:321:LEU:HD23 | 1:A:333:LEU:CD1 | 2.50 | 0.41 |
| 1:A:551:ALA:HB1 | 1:A:556:GLN:HB2 | 2.03 | 0.41 |
| 1:A:560:LEU:CG | 1:A:648:THR:CG2 | 2.98 | 0.41 |
| 1:A:658:HIS:ND1 | 1:A:663:SER:HB3 | 2.36 | 0.41 |
| 1:A:778:VAL:HG12 | 1:A:779:GLU:O | 2.20 | 0.41 |
| 1:A:832:THR:HG21 | 1:A:836:HIS:HB2 | 1.99 | 0.41 |
| 1:B:469:TYR:CZ | 1:B:470:GLU:O | 2.74 | 0.41 |
| 1:B:560:LEU:HB3 | 1:B:648:THR:CG2 | 2.51 | 0.41 |
| 1:B:711:VAL:HB | 1:B:800:LEU:HD23 | 2.02 | 0.41 |
| 1:A:313:TYR:CZ | 1:A:435:ILE:CD1 | 3.05 | 0.40 |
| 1:B:141:ARG:HB3 | 1:B:144:ASP:OD1 | 2.21 | 0.40 |
| 1:B:188:VAL:HG22 | 1:B:188:VAL:O | 2.21 | 0.40 |
| 1:B:667:SER:HB3 | 1:B:668:PRO:CD | 2.51 | 0.40 |
| 1:B:832:THR:CG2 | 1:B:836:HIS:CB | 2.95 | 0.40 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CD1 | 3.00 | 0.40 |
| 1:A:469:TYR:CZ | 1:A:470:GLU:O | 2.74 | 0.40 |
| 1:A:45:GLU:CB | 1:A:46:PRO:CD | 3.00 | 0.40 |
| 1:A:667:SER:HB3 | 1:A:668:PRO:CD | 2.51 | 0.40 |
| 1:A:873:THR:OG1 | 1:A:981:GLY:C | 2.59 | 0.40 |
| 1:A:955:LEU:HD23 | 1:A:957:ASP:N | 2.37 | 0.40 |
| 1:B:169:PHE:CD2 | 1:B:170:GLY:N | 2.84 | 0.40 |
| 1:B:219:ASP:HB3 | 1:B:222:VAL:H | 1.86 | 0.40 |
| 1:B:242:TYR:CE1 | 1:B:345:LYS:HE2 | 2.56 | 0.40 |
| 1:B:44:GLY:CA | 1:B:50:PHE:HE2 | 2.23 | 0.40 |
| 1:A:131:SER:O | 1:A:133:TYR:CD2 | 2.74 | 0.40 |
| 1:A:453:LYS:CE | 1:A:472:VAL:HG22 | 2.51 | 0.40 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:HZ | 1.72 | 0.40 |
| 1:B:172:ILE:CG1 | 1:B:182:LEU:HD13 | 2.46 | 0.40 |
| 1:B:282:LEU:HD23 | 1:B:292:TYR:HA | 2.03 | 0.40 |
| 1:B:450:LYS:CA | 1:B:479:PRO:HB3 | 2.49 | 0.40 |
| 1:B:62:ILE:CD1 | 1:B:64:LEU:HD21 | 2.46 | 0.40 |
| 1:B:662:LEU:O | 1:B:666:GLU:HB3 | 2.20 | 0.40 |
| 1:B:95:TYR:CE2 | 1:B:194:TYR:CD1 | 3.09 | 0.40 |
| 1:A:188:VAL:HG13 | 1:A:189:ASP:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:219:ASP:HB3 | 1:A:222:VAL:H | 1.86 | 0.40 |
| 1:A:259:GLN:HA | 1:A:260:PRO:HD3 | 1.82 | 0.40 |
| 1:A:276:THR:HB | 1:A:278:LYS:HZ2 | 1.86 | 0.40 |
| 1:A:455:LYS:HB3 | 1:A:467:LEU:CD1 | 2.52 | 0.40 |
| 1:A:773:ILE:N | 1:A:773:ILE:CD1 | 2.82 | 0.40 |
| 1:A:803:CYS:SG | 1:A:832:THR:HA | 2.61 | 0.40 |
| 1:A:904:VAL:CG1 | 1:A:905:ASP:N | 2.82 | 0.40 |
| 1:A:896:ALA:HB1 | 1:A:924:GLN:OE1 | 2.22 | 0.40 |
| 1:B:313:TYR:CZ | 1:B:435:ILE:CD1 | 3.04 | 0.40 |
| 1:B:410:ALA:CB | 1:B:411:PRO:CD | 2.98 | 0.40 |
| 1:B:660:SER:HB2 | 1:B:791:ASP:OD2 | 2.22 | 0.40 |
| 1:B:904:VAL:CG1 | 1:B:905:ASP:N | 2.82 | 0.40 |
| 1:A:282:LEU:HD23 | 1:A:292:TYR:HA | 2.03 | 0.40 |
| 1:A:242:TYR:CE1 | 1:A:345:LYS:HE2 | 2.56 | 0.40 |
| 1:A:847:LEU:CD1 | 1:A:850:ALA:CA | 2.94 | 0.40 |
| 1:A:943:ARG:HB2 | 1:A:943:ARG:CZ | 2.51 | 0.40 |
| 1:B:131:SER:O | 1:B:133:TYR:CD2 | 2.74 | 0.40 |
| 1:B:53:LEU:CG | 1:B:64:LEU:CD1 | 2.96 | 0.40 |
| 1:B:681:THR:OG1 | 1:B:686:THR:HG21 | 2.21 | 0.40 |
| 1:B:81:VAL:CG1 | 1:B:82:THR:N | 2.85 | 0.40 |
| 1:B:889:ILE:HD12 | 1:B:907:TYR:CE1 | 2.56 | 0.40 |
| 1:B:943:ARG:CZ | 1:B:943:ARG:HB2 | 2.51 | 0.40 |

All (61) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:146:PHE:CE1 | 1:B:730:GLN:CD[1_655] | 0.64 | 1.56 |
| 1:B:287:THR:OG1 | 1:B:840:HIS:CG[1_655] | 0.67 | 1.53 |
| 1:A:146:PHE:CE1 | 1:B:730:GLN:OE1[1_655] | 0.77 | 1.43 |
| 1:A:146:PHE:CD1 | 1:B:730:GLN:OE1[1_655] | 0.78 | 1.42 |
| 1:B:287:THR:CA | 1:B:840:HIS:NE2[1_655] | 0.79 | 1.41 |
| 1:B:287:THR:CB | 1:B:840:HIS:CG[1_655] | 0.85 | 1.35 |
| 1:B:287:THR:CB | 1:B:840:HIS:CD2[1_655] | 0.93 | 1.27 |
| 1:B:287:THR:CA | 1:B:840:HIS:CD2[1_655] | 1.03 | 1.17 |
| 1:A:146:PHE:CZ | 1:B:730:GLN:NE2[1_655] | 1.20 | 1.00 |
| 1:B:287:THR:OG1 | 1:B:840:HIS:ND1[1_655] | 1.52 | 0.68 |
| 1:A:407:ASP:OD2 | 1:A:926:ALA:O[1_554] | 1.55 | 0.65 |
| 1:B:220:GLU:OE2 | 1:B:939:GLU:OE1[1_655] | 1.56 | 0.64 |
| 1:A:148:LEU:O | 1:B:728:GLN:OE1[1_655] | 1.56 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:287:THR:OG1 | 1:B:840:HIS:CB[1_655] | 1.58 | 0.62 |
| 1:B:287:THR:OG1 | 1:B:840:HIS:CD2[1_655] | 1.61 | 0.59 |
| 1:A:83:HIS:CE1 | 1:B:731:SER:OG[1_655] | 1.62 | 0.58 |
| 1:B:219:ASP:OD1 | 1:B:826:GLN:OE1[1_655] | 1.68 | 0.52 |
| 1:B:288:ALA:CB | 1:B:841:GLU:OE1[1_655] | 1.71 | 0.49 |
| 1:B:287:THR:CA | 1:B:840:HIS:CE1[1_655] | 1.74 | 0.46 |
| 1:A:146:PHE:CE1 | 1:B:730:GLN:CG[1_655] | 1.75 | 0.45 |
| 1:A:146:PHE:CZ | 1:B:730:GLN:OE1[1_655] | 1.75 | 0.45 |
| 1:A:146:PHE:CG | 1:B:730:GLN:OE1[1_655] | 1.75 | 0.45 |
| 1:B:287:THR:CG2 | 1:B:840:HIS:CD2[1_655] | 1.77 | 0.43 |
| 1:B:287:THR:CG2 | 1:B:840:HIS:C[1_655] | 1.78 | 0.42 |
| 1:A:728:GLN:OE1 | 1:B:148:LEU:O[2_646] | 1.83 | 0.37 |
| 1:A:730:GLN:OE1 | 1:B:146:PHE:CE1[2_646] | 1.84 | 0.36 |
| 1:A:731:SER:OG | 1:B:83:HIS:ND1[2_646] | 1.85 | 0.35 |
| 1:B:219:ASP:OD1 | 1:B:826:GLN:CG[1_655] | 1.86 | 0.34 |
| 1:A:146:PHE:CE1 | 1:B:730:GLN:NE2[1_655] | 1.88 | 0.32 |
| 1:A:728:GLN:NE2 | 1:B:148:LEU:O[2_646] | 1.89 | 0.31 |
| 1:B:217:PHE:CD1 | 1:B:827:SER:OG[1_655] | 1.90 | 0.30 |
| 1:A:752:LEU:CD2 | 1:B:152:PHE:CE1[2_646] | 1.91 | 0.29 |
| 1:B:287:THR:CB | 1:B:840:HIS:CB[1_655] | 1.91 | 0.29 |
| 1:B:287:THR:CB | 1:B:840:HIS:ND1[1_655] | 1.92 | 0.28 |
| 1:B:217:PHE:CE1 | 1:B:827:SER:OG[1_655] | 1.93 | 0.27 |
| 1:A:208:GLU:OE2 | 1:B:728:GLN:NE2[1_655] | 1.93 | 0.27 |
| 1:A:146:PHE:CD1 | 1:B:730:GLN:CD[1_655] | 1.94 | 0.26 |
| 1:B:220:GLU:OE2 | 1:B:939:GLU:CD[1_655] | 1.96 | 0.24 |
| 1:B:287:THR:N | 1:B:840:HIS:NE2[1_655] | 1.98 | 0.22 |
| 1:A:148:LEU:O | 1:B:728:GLN:CD[1_655] | 1.99 | 0.21 |
| 1:B:220:GLU:OE1 | 1:B:939:GLU:OE2[1_655] | 2.00 | 0.20 |
| 1:B:287:THR:CA | 1:B:840:HIS:CG[1_655] | 2.01 | 0.19 |
| 1:A:730:GLN:NE2 | 1:B:146:PHE:CZ[2_646] | 2.01 | 0.19 |
| 1:B:219:ASP:OD2 | 1:B:826:GLN:OE1[1_655] | 2.01 | 0.19 |
| 1:B:287:THR:CB | 1:B:840:HIS:NE2[1_655] | 2.01 | 0.19 |
| 1:B:219:ASP:CG | 1:B:826:GLN:OE1[1_655] | 2.03 | 0.17 |
| 1:A:731:SER:OG | 1:B:83:HIS:NE2[2_646] | 2.03 | 0.17 |
| 1:B:219:ASP:CG | 1:B:826:GLN:CD[1_655] | 2.04 | 0.16 |
| 1:B:287:THR:O | 1:B:840:HIS:NE2[1_655] | 2.05 | 0.15 |
| 1:A:141:ARG:NH2 | 1:B:691:GLU:OE2[1_655] | 2.06 | 0.14 |
| 1:A:208:GLU:OE2 | 1:B:728:GLN:CD[1_655] | 2.08 | 0.12 |
| 1:A:728:GLN:CD | 1:B:148:LEU:O[2_646] | 2.09 | 0.11 |
| 1:B:287:THR:CG2 | 1:B:840:HIS:O[1_655] | 2.09 | 0.11 |
| 1:A:407:ASP:OD1 | 1:A:924:GLN:OE1[1_554] | 2.11 | 0.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:730:GLN:CD | 1:B:146:PHE:CD1[2_646] | 2.11 | 0.09 |
| 1:B:287:THR:CG2 | 1:B:840:HIS:CG[1_655] | 2.12 | 0.08 |
| 1:B:287:THR:CG2 | 1:B:841:GLU:N[1_655] | 2.13 | 0.07 |
| 1:A:208:GLU:OE1 | 1:B:753:ARG:NH2[1_655] | 2.15 | 0.05 |
| 1:B:219:ASP:OD2 | 1:B:826:GLN:NE2[1_655] | 2.16 | 0.04 |
| 1:A:728:GLN:OE1 | 1:B:148:LEU:C[2_646] | 2.18 | 0.02 |
| 1:A:728:GLN:OE1 | 1:B:149:GLY:CA[2_646] | 2.19 | 0.01 |

## 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 | 994/1207 (82%) | 923 (93%) | 51 (5%) | 20 (2%) | 9 | 51 |
| 1 | B | 907/1207 (75%) | 845 (93%) | 43 (5%) | 19 (2%) | 9 | 50 |
| All | All | 1901/2414 (79%) | 1768 (93%) | 94 (5%) | 39 (2%) | 9 | 50 |

All (39) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 96 | PRO |
| 1 | A | 181 | LYS |
| 1 | A | 191 | LYS |
| 1 | A | 410 | ALA |
| 1 | A | 465 | ASN |
| 1 | A | 804 | GLY |
| 1 | A | 864 | PRO |
| 1 | B | 96 | PRO |
| 1 | B | 181 | LYS |
| 1 | B | 191 | LYS |
| 1 | B | 410 | ALA |
| 1 | B | 465 | ASN |
| 1 | B | 557 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 700 | CYS |
| 1 | B | 701 | PRO |
| 1 | B | 804 | GLY |
| 1 | B | 864 | PRO |
| 1 | A | 87 | PRO |
| 1 | B | 87 | PRO |
| 1 | A | 271 | LYS |
| 1 | A | 474 | VAL |
| 1 | A | 557 | CYS |
| 1 | A | 849 | GLY |
| 1 | A | 1015 | ASP |
| 1 | A | 1016 | MET |
| 1 | B | 271 | LYS |
| 1 | B | 474 | VAL |
| 1 | B | 849 | GLY |
| 1 | A | 263 | VAL |
| 1 | B | 263 | VAL |
| 1 | A | 344 | ARG |
| 1 | B | 344 | ARG |
| 1 | A | 933 | VAL |
| 1 | A | 1013 | VAL |
| 1 | B | 933 | VAL |
| 1 | A | 44 | GLY |
| 1 | A | 921 | LYS |
| 1 | B | 921 | LYS |
| 1 | B | 44 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 888/1067 (83%) | 861 (97%) | 27 (3%) | 48 77 |
| 1 | B | 812/1067 (76%) | 789 (97%) | 23 (3%) | 51 78 |
| All | All | 1700/2134 (80%) | 1650 (97%) | 50 (3%) | 50 78 |

All (50) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 69 | ARG |
| 1 | A | 72 | LYS |
| 1 | A | 271 | LYS |
| 1 | A | 386 | LYS |
| 1 | A | 412 | LEU |
| 1 | A | 435 | ILE |
| 1 | A | 468 | GLN |
| 1 | A | 473 | GLN |
| 1 | A | 523 | ASP |
| 1 | A | 529 | CYS |
| 1 | A | 548 | ARG |
| 1 | A | 567 | ILE |
| 1 | A | 575 | LEU |
| 1 | A | 597 | LEU |
| 1 | A | 621 | ARG |
| 1 | A | 670 | ARG |
| 1 | A | 743 | GLN |
| 1 | A | 773 | ILE |
| 1 | A | 797 | LYS |
| 1 | A | 806 | MET |
| 1 | A | 853 | LYS |
| 1 | A | 854 | CYS |
| 1 | A | 892 | HIS |
| 1 | A | 1004 | ILE |
| 1 | A | 1016 | MET |
| 1 | A | 1017 | LYS |
| 1 | A | 1024 | ARG |
| 1 | B | 69 | ARG |
| 1 | B | 72 | LYS |
| 1 | B | 271 | LYS |
| 1 | B | 386 | LYS |
| 1 | B | 412 | LEU |
| 1 | B | 435 | ILE |
| 1 | B | 468 | GLN |
| 1 | B | 473 | GLN |
| 1 | B | 523 | ASP |
| 1 | B | 529 | CYS |
| 1 | B | 548 | ARG |
| 1 | B | 567 | ILE |
| 1 | B | 575 | LEU |
| 1 | B | 597 | LEU |
| 1 | B | 621 | ARG |
| 1 | B | 670 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 743 | GLN |
| 1 | B | 773 | ILE |
| 1 | B | 797 | LYS |
| 1 | B | 806 | MET |
| 1 | B | 853 | LYS |
| 1 | B | 854 | CYS |
| 1 | B | 892 | HIS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 51 | ASN |
| 1 | A | 101 | GLN |
| 1 | A | 157 | HIS |
| 1 | A | 163 | ASN |
| 1 | A | 273 | GLN |
| 1 | A | 361 | GLN |
| 1 | A | 441 | ASN |
| 1 | A | 442 | HIS |
| 1 | A | 473 | GLN |
| 1 | A | 500 | GLN |
| 1 | A | 533 | ASN |
| 1 | A | 626 | ASN |
| 1 | A | 630 | HIS |
| 1 | A | 672 | HIS |
| 1 | A | 685 | ASN |
| 1 | A | 690 | GLN |
| 1 | A | 702 | GLN |
| 1 | A | 728 | GLN |
| 1 | A | 747 | GLN |
| 1 | A | 789 | ASN |
| 1 | A | 792 | ASN |
| 1 | A | 826 | GLN |
| 1 | A | 836 | HIS |
| 1 | A | 892 | HIS |
| 1 | A | 970 | GLN |
| 1 | A | 983 | ASN |
| 1 | A | 1006 | ASN |
| 1 | B | 51 | ASN |
| 1 | B | 101 | GLN |
| 1 | B | 157 | HIS |
| 1 | B | 163 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 273 | GLN |
| 1 | B | 361 | GLN |
| 1 | B | 441 | ASN |
| 1 | B | 442 | HIS |
| 1 | B | 473 | GLN |
| 1 | B | 500 | GLN |
| 1 | B | 626 | ASN |
| 1 | B | 629 | HIS |
| 1 | B | 630 | HIS |
| 1 | B | 672 | HIS |
| 1 | B | 682 | HIS |
| 1 | B | 685 | ASN |
| 1 | B | 690 | GLN |
| 1 | B | 702 | GLN |
| 1 | B | 728 | GLN |
| 1 | B | 730 | GLN |
| 1 | B | 747 | GLN |
| 1 | B | 789 | ASN |
| 1 | B | 792 | ASN |
| 1 | B | 826 | GLN |
| 1 | B | 836 | HIS |
| 1 | B | 892 | HIS |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | B | 6 |
| 1 | A | 5 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | B | 854:CYS | C | 855:THR | N | 2.49 |
| 1 | A | 802:LYS | C | 803:CYS | N | 2.46 |
| 1 | A | 951:MET | C | 952:THR | N | 2.32 |
| 1 | B | 653:TYR | C | 654:ASN | N | 2.31 |
| 1 | B | 802:LYS | C | 803:CYS | N | 2.01 |
| 1 | A | 506:VAL | C | 507:GLU | N | 1.87 |
| 1 | B | 506:VAL | C | 507:GLU | N | 1.82 |
| 1 | B | 700:CYS | C | 701:PRO | N | 1.63 |
| 1 | A | 700:CYS | C | 701:PRO | N | 1.04 |
| 1 | B | 557:CYS | C | 558:VAL | N | 0.94 |
| 1 | A | 557:CYS | C | 558:VAL | N | 0.86 |

# 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 | 1000/1207 (82%) | 1.99 | 393 (39%) | 0 | 4 | 195, 258, 410, 410 | 0 |
| 1 | B | 915/1207 (75%) | 1.81 | 328 (35%) | 0 | 4 | 209, 257, 329, 329 | 0 |
| All | All | 1915/2414 (79%) | 1.90 | 721 (37%) | 0 | 4 | 195, 257, 329, 410 | 0 |

All (721) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1029 | GLN | 16.5 |
| 1 | A | 269 | THR | 16.2 |
| 1 | A | 1018 | VAL | 14.5 |
| 1 | A | 270 | THR | 13.8 |
| 1 | A | 271 | LYS | 13.1 |
| 1 | B | 852 | SER | 12.8 |
| 1 | A | 268 | SER | 11.8 |
| 1 | B | 922 | PRO | 11.1 |
| 1 | A | 854 | CYS | 10.8 |
| 1 | A | 1031 | LEU | 10.4 |
| 1 | A | 1019 | THR | 10.3 |
| 1 | A | 1027 | ILE | 10.1 |
| 1 | A | 1020 | VAL | 10.0 |
| 1 | B | 854 | CYS | 9.6 |
| 1 | A | 1028 | ARG | 9.2 |
| 1 | B | 921 | LYS | 9.2 |
| 1 | A | 953 | LEU | 9.0 |
| 1 | B | 583 | VAL | 8.7 |
| 1 | A | 506 | VAL | 8.6 |
| 1 | B | 850 | ALA | 8.6 |
| 1 | B | 645 | PHE | 8.4 |
| 1 | A | 842 | SER | 8.3 |
| 1 | B | 923 | SER | 8.2 |
| 1 | B | 924 | GLN | 8.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 525 | HIS | 8.0 |
| 1 | B | 926 | ALA | 8.0 |
| 1 | B | 919 | GLU | 7.9 |
| 1 | B | 636 | LEU | 7.8 |
| 1 | A | 272 | GLU | 7.8 |
| 1 | B | 584 | PRO | 7.7 |
| 1 | A | 505 | PRO | 7.5 |
| 1 | B | 585 | GLU | 7.4 |
| 1 | B | 920 | ALA | 7.4 |
| 1 | B | 637 | LYS | 7.4 |
| 1 | A | 727 | PRO | 7.4 |
| 1 | B | 592 | CYS | 7.3 |
| 1 | A | 267 | GLY | 7.2 |
| 1 | A | 507 | GLU | 7.2 |
| 1 | B | 586 | LEU | 7.1 |
| 1 | B | 925 | HIS | 7.0 |
| 1 | B | 644 | THR | 7.0 |
| 1 | B | 851 | ASN | 6.9 |
| 1 | A | 952 | THR | 6.8 |
| 1 | B | 849 | GLY | 6.7 |
| 1 | A | 883 | GLY | 6.6 |
| 1 | A | 524 | PRO | 6.6 |
| 1 | A | 250 | GLY | 6.6 |
| 1 | B | 853 | LYS | 6.4 |
| 1 | A | 955 | LEU | 6.4 |
| 1 | B | 720 | THR | 6.4 |
| 1 | B | 638 | SER | 6.4 |
| 1 | A | 273 | GLN | 6.3 |
| 1 | B | 437 | TYR | 6.2 |
| 1 | A | 1017 | LYS | 6.2 |
| 1 | A | 645 | PHE | 6.1 |
| 1 | A | 881 | ASN | 6.1 |
| 1 | B | 604 | VAL | 6.1 |
| 1 | B | 412 | LEU | 6.0 |
| 1 | B | 640 | GLU | 6.0 |
| 1 | B | 622 | ILE | 6.0 |
| 1 | B | 591 | ASN | 6.0 |
| 1 | A | 590 | VAL | 5.9 |
| 1 | B | 589 | GLY | 5.9 |
| 1 | B | 862 | ILE | 5.9 |
| 1 | B | 269 | THR | 5.9 |
| 1 | A | 882 | LEU | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 568 | SER | 5.8 |
| 1 | A | 523 | ASP | 5.8 |
| 1 | A | 988 | PHE | 5.8 |
| 1 | A | 1032 | VAL | 5.8 |
| 1 | B | 918 | GLY | 5.7 |
| 1 | A | 240 | ASP | 5.7 |
| 1 | A | 1030 | ASP | 5.6 |
| 1 | B | 646 | ALA | 5.6 |
| 1 | A | 694 | VAL | 5.6 |
| 1 | A | 811 | GLY | 5.6 |
| 1 | A | 853 | LYS | 5.6 |
| 1 | B | 870 | GLU | 5.6 |
| 1 | B | 650 | PHE | 5.6 |
| 1 | B | 590 | VAL | 5.6 |
| 1 | B | 884 | LEU | 5.6 |
| 1 | B | 548 | ARG | 5.6 |
| 1 | B | 847 | LEU | 5.5 |
| 1 | A | 238 | ASP | 5.5 |
| 1 | A | 986 | VAL | 5.5 |
| 1 | A | 927 | GLY | 5.4 |
| 1 | A | 1021 | GLN | 5.4 |
| 1 | B | 814 | LEU | 5.4 |
| 1 | B | 803 | CYS | 5.4 |
| 1 | A | 961 | ASN | 5.4 |
| 1 | B | 271 | LYS | 5.4 |
| 1 | B | 652 | PHE | 5.4 |
| 1 | B | 947 | LEU | 5.4 |
| 1 | A | 957 | ASP | 5.4 |
| 1 | B | 710 | LEU | 5.4 |
| 1 | B | 721 | LEU | 5.3 |
| 1 | B | 711 | VAL | 5.3 |
| 1 | B | 883 | GLY | 5.3 |
| 1 | B | 587 | SER | 5.3 |
| 1 | B | 871 | GLY | 5.3 |
| 1 | A | 249 | SER | 5.2 |
| 1 | B | 712 | PRO | 5.2 |
| 1 | A | 646 | ALA | 5.2 |
| 1 | B | 872 | GLY | 5.2 |
| 1 | B | 268 | SER | 5.2 |
| 1 | B | 873 | THR | 5.2 |
| 1 | B | 948 | TYR | 5.2 |
| 1 | B | 719 | ILE | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 917 | MET | 5.1 |
| 1 | A | 852 | SER | 5.1 |
| 1 | A | 855 | THR | 5.1 |
| 1 | A | 569 | VAL | 5.1 |
| 1 | A | 1033 | PHE | 5.1 |
| 1 | B | 634 | LEU | 5.0 |
| 1 | B | 709 | ILE | 5.0 |
| 1 | B | 875 | VAL | 5.0 |
| 1 | A | 652 | PHE | 5.0 |
| 1 | B | 594 | PHE | 5.0 |
| 1 | B | 580 | THR | 5.0 |
| 1 | B | 877 | ILE | 5.0 |
| 1 | B | 869 | ARG | 5.0 |
| 1 | B | 272 | GLU | 4.9 |
| 1 | B | 571 | GLN | 4.9 |
| 1 | B | 582 | ASN | 4.9 |
| 1 | B | 767 | SER | 4.9 |
| 1 | B | 801 | TYR | 4.9 |
| 1 | A | 960 | PRO | 4.9 |
| 1 | A | 458 | ARG | 4.9 |
| 1 | A | 922 | PRO | 4.9 |
| 1 | A | 1026 | ARG | 4.9 |
| 1 | B | 613 | SER | 4.9 |
| 1 | B | 868 | PRO | 4.9 |
| 1 | A | 410 | ALA | 4.8 |
| 1 | A | 589 | GLY | 4.8 |
| 1 | A | 747 | GLN | 4.8 |
| 1 | A | 920 | ALA | 4.8 |
| 1 | A | 879 | GLY | 4.8 |
| 1 | B | 898 | VAL | 4.8 |
| 1 | A | 958 | LEU | 4.8 |
| 1 | A | 984 | VAL | 4.8 |
| 1 | B | 270 | THR | 4.8 |
| 1 | A | 956 | ALA | 4.8 |
| 1 | B | 950 | PHE | 4.8 |
| 1 | A | 437 | TYR | 4.8 |
| 1 | A | 678 | HIS | 4.8 |
| 1 | B | 413 | GLY | 4.7 |
| 1 | A | 810 | CYS | 4.7 |
| 1 | A | 951 | MET | 4.7 |
| 1 | A | 963 | GLY | 4.7 |
| 1 | B | 619 | VAL | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 868 | PRO | 4.7 |
| 1 | A | 898 | VAL | 4.7 |
| 1 | A | 508 | SER | 4.7 |
| 1 | A | 1036 | VAL | 4.7 |
| 1 | B | 558 | VAL | 4.7 |
| 1 | A | 962 | ARG | 4.7 |
| 1 | A | 814 | LEU | 4.7 |
| 1 | A | 973 | ILE | 4.7 |
| 1 | B | 766 | TYR | 4.6 |
| 1 | A | 1016 | MET | 4.6 |
| 1 | B | 864 | PRO | 4.6 |
| 1 | A | 989 | GLY | 4.6 |
| 1 | B | 802 | LYS | 4.6 |
| 1 | A | 980 | ALA | 4.6 |
| 1 | A | 977 | ASN | 4.6 |
| 1 | A | 526 | CYS | 4.6 |
| 1 | A | 530 | VAL | 4.6 |
| 1 | B | 774 | ASN | 4.6 |
| 1 | B | 882 | LEU | 4.6 |
| 1 | A | 1022 | VAL | 4.6 |
| 1 | A | 803 | CYS | 4.5 |
| 1 | B | 927 | GLY | 4.5 |
| 1 | B | 614 | PRO | 4.5 |
| 1 | A | 251 | ASN | 4.5 |
| 1 | B | 800 | LEU | 4.5 |
| 1 | A | 897 | GLY | 4.5 |
| 1 | B | 707 | ASP | 4.5 |
| 1 | B | 567 | ILE | 4.5 |
| 1 | B | 161 | GLY | 4.5 |
| 1 | A | 950 | PHE | 4.5 |
| 1 | B | 775 | ASN | 4.5 |
| 1 | B | 752 | LEU | 4.5 |
| 1 | A | 676 | TYR | 4.5 |
| 1 | A | 910 | ALA | 4.5 |
| 1 | A | 836 | HIS | 4.5 |
| 1 | B | 525 | HIS | 4.4 |
| 1 | B | 588 | ALA | 4.4 |
| 1 | B | 899 | GLU | 4.4 |
| 1 | A | 521 | SER | 4.4 |
| 1 | A | 640 | GLU | 4.4 |
| 1 | B | 782 | VAL | 4.4 |
| 1 | B | 897 | GLY | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 524 | PRO | 4.4 |
| 1 | A | 591 | ASN | 4.4 |
| 1 | B | 695 | LYS | 4.3 |
| 1 | A | 619 | VAL | 4.3 |
| 1 | B | 776 | LEU | 4.3 |
| 1 | B | 620 | PRO | 4.3 |
| 1 | A | 592 | CYS | 4.3 |
| 1 | A | 987 | MET | 4.3 |
| 1 | B | 635 | GLN | 4.3 |
| 1 | B | 902 | PRO | 4.3 |
| 1 | A | 880 | GLU | 4.3 |
| 1 | B | 718 | PRO | 4.3 |
| 1 | B | 916 | GLU | 4.3 |
| 1 | A | 862 | ILE | 4.3 |
| 1 | B | 717 | LYS | 4.3 |
| 1 | B | 874 | LYS | 4.3 |
| 1 | B | 892 | HIS | 4.2 |
| 1 | A | 695 | LYS | 4.2 |
| 1 | A | 948 | TYR | 4.2 |
| 1 | A | 239 | PHE | 4.2 |
| 1 | A | 636 | LEU | 4.2 |
| 1 | A | 924 | GLN | 4.2 |
| 1 | B | 798 | VAL | 4.2 |
| 1 | A | 613 | SER | 4.2 |
| 1 | A | 409 | ASN | 4.2 |
| 1 | A | 767 | SER | 4.2 |
| 1 | A | 602 | GLY | 4.2 |
| 1 | A | 261 | GLU | 4.2 |
| 1 | B | 473 | GLN | 4.2 |
| 1 | B | 593 | THR | 4.2 |
| 1 | B | 761 | CYS | 4.2 |
| 1 | A | 442 | HIS | 4.2 |
| 1 | A | 895 | VAL | 4.2 |
| 1 | A | 893 | VAL | 4.2 |
| 1 | A | 815 | LYS | 4.2 |
| 1 | B | 207 | SER | 4.2 |
| 1 | A | 1034 | GLN | 4.1 |
| 1 | B | 599 | GLU | 4.1 |
| 1 | B | 747 | GLN | 4.1 |
| 1 | B | 694 | VAL | 4.1 |
| 1 | A | 263 | VAL | 4.1 |
| 1 | A | 411 | PRO | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 609 | ILE | 4.1 |
| 1 | B | 895 | VAL | 4.1 |
| 1 | A | 877 | ILE | 4.1 |
| 1 | B | 267 | GLY | 4.1 |
| 1 | A | 672 | HIS | 4.1 |
| 1 | A | 808 | GLU | 4.0 |
| 1 | A | 954 | THR | 4.0 |
| 1 | A | 1025 | ALA | 4.0 |
| 1 | A | 971 | VAL | 4.0 |
| 1 | B | 642 | GLY | 4.0 |
| 1 | B | 727 | PRO | 4.0 |
| 1 | B | 760 | GLN | 4.0 |
| 1 | B | 639 | LYS | 4.0 |
| 1 | B | 842 | SER | 4.0 |
| 1 | A | 446 | PHE | 4.0 |
| 1 | B | 621 | ARG | 4.0 |
| 1 | A | 190 | GLY | 4.0 |
| 1 | A | 527 | GLY | 4.0 |
| 1 | B | 708 | LYS | 4.0 |
| 1 | A | 522 | GLY | 4.0 |
| 1 | B | 843 | ARG | 4.0 |
| 1 | A | 923 | SER | 4.0 |
| 1 | B | 846 | GLU | 4.0 |
| 1 | A | 913 | ILE | 4.0 |
| 1 | B | 547 | PRO | 4.0 |
| 1 | B | 713 | VAL | 4.0 |
| 1 | B | 531 | LEU | 4.0 |
| 1 | B | 736 | TYR | 4.0 |
| 1 | B | 762 | GLN | 3.9 |
| 1 | B | 790 | ILE | 3.9 |
| 1 | A | 884 | LEU | 3.9 |
| 1 | B | 546 | GLU | 3.9 |
| 1 | A | 509 | CYS | 3.9 |
| 1 | A | 691 | GLU | 3.9 |
| 1 | A | 456 | LYS | 3.9 |
| 1 | A | 931 | ILE | 3.9 |
| 1 | B | 750 | PRO | 3.9 |
| 1 | A | 266 | PRO | 3.9 |
| 1 | B | 820 | PHE | 3.9 |
| 1 | A | 926 | ALA | 3.9 |
| 1 | A | 919 | GLU | 3.9 |
| 1 | A | 611 | CYS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 578 | LEU | 3.9 |
| 1 | B | 411 | PRO | 3.9 |
| 1 | A | 859 | ILE | 3.9 |
| 1 | A | 892 | HIS | 3.9 |
| 1 | B | 777 | PRO | 3.9 |
| 1 | A | 586 | LEU | 3.9 |
| 1 | A | 675 | LYS | 3.9 |
| 1 | A | 864 | PRO | 3.9 |
| 1 | B | 570 | SER | 3.9 |
| 1 | A | 248 | SER | 3.9 |
| 1 | A | 537 | ARG | 3.8 |
| 1 | B | 618 | GLU | 3.8 |
| 1 | A | 650 | PHE | 3.8 |
| 1 | B | 889 | ILE | 3.8 |
| 1 | A | 412 | LEU | 3.8 |
| 1 | A | 495 | ILE | 3.8 |
| 1 | A | 391 | PRO | 3.8 |
| 1 | A | 728 | GLN | 3.8 |
| 1 | A | 1004 | ILE | 3.8 |
| 1 | B | 549 | ARG | 3.8 |
| 1 | B | 848 | SER | 3.8 |
| 1 | B | 643 | MET | 3.8 |
| 1 | A | 970 | GLN | 3.8 |
| 1 | B | 949 | TYR | 3.8 |
| 1 | A | 929 | VAL | 3.8 |
| 1 | B | 566 | ASN | 3.7 |
| 1 | A | 623 | ILE | 3.7 |
| 1 | B | 796 | ASN | 3.7 |
| 1 | B | 915 | CYS | 3.7 |
| 1 | A | 969 | THR | 3.7 |
| 1 | A | 262 | MET | 3.7 |
| 1 | A | 1003 | ILE | 3.7 |
| 1 | A | 330 | ASP | 3.7 |
| 1 | A | 869 | ARG | 3.7 |
| 1 | A | 911 | GLU | 3.7 |
| 1 | A | 983 | ASN | 3.7 |
| 1 | A | 444 | LEU | 3.7 |
| 1 | A | 622 | ILE | 3.7 |
| 1 | A | 473 | GLN | 3.7 |
| 1 | B | 598 | SER | 3.6 |
| 1 | B | 931 | ILE | 3.6 |
| 1 | A | 562 | VAL | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 407 | ASP | 3.6 |
| 1 | A | 997 | ARG | 3.6 |
| 1 | A | 843 | ARG | 3.6 |
| 1 | B | 799 | TYR | 3.6 |
| 1 | B | 552 | SER | 3.6 |
| 1 | B | 543 | ARG | 3.6 |
| 1 | A | 174 | SER | 3.6 |
| 1 | A | 439 | TYR | 3.6 |
| 1 | A | 536 | THR | 3.6 |
| 1 | A | 654 | ASN | 3.6 |
| 1 | A | 443 | SER | 3.6 |
| 1 | A | 638 | SER | 3.5 |
| 1 | A | 809 | SER | 3.5 |
| 1 | A | 949 | TYR | 3.5 |
| 1 | A | 153 | HIS | 3.5 |
| 1 | A | 628 | ASP | 3.5 |
| 1 | A | 693 | ARG | 3.5 |
| 1 | A | 189 | ASP | 3.5 |
| 1 | B | 738 | CYS | 3.5 |
| 1 | A | 804 | GLY | 3.5 |
| 1 | B | 578 | LEU | 3.5 |
| 1 | B | 900 | CYS | 3.5 |
| 1 | B | 602 | GLY | 3.5 |
| 1 | A | 985 | VAL | 3.4 |
| 1 | A | 730 | GLN | 3.4 |
| 1 | B | 273 | GLN | 3.4 |
| 1 | B | 572 | TYR | 3.4 |
| 1 | A | 558 | VAL | 3.4 |
| 1 | B | 293 | VAL | 3.4 |
| 1 | A | 847 | LEU | 3.4 |
| 1 | A | 1012 | GLU | 3.4 |
| 1 | B | 751 | ALA | 3.4 |
| 1 | A | 766 | TYR | 3.4 |
| 1 | A | 92 | PRO | 3.4 |
| 1 | B | 576 | LEU | 3.4 |
| 1 | A | 587 | SER | 3.4 |
| 1 | B | 865 | VAL | 3.4 |
| 1 | A | 1035 | TYR | 3.4 |
| 1 | B | 859 | ILE | 3.4 |
| 1 | B | 675 | LYS | 3.3 |
| 1 | B | 773 | ILE | 3.3 |
| 1 | A | 1015 | ASP | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 93 | LYS | 3.3 |
| 1 | B | 781 | THR | 3.3 |
| 1 | B | 706 | VAL | 3.3 |
| 1 | A | 964 | PRO | 3.3 |
| 1 | B | 149 | GLY | 3.3 |
| 1 | A | 620 | PRO | 3.3 |
| 1 | B | 890 | ALA | 3.3 |
| 1 | A | 609 | ILE | 3.3 |
| 1 | A | 520 | GLY | 3.3 |
| 1 | A | 1014 | LEU | 3.3 |
| 1 | B | 740 | LEU | 3.3 |
| 1 | B | 768 | TYR | 3.3 |
| 1 | B | 867 | GLY | 3.3 |
| 1 | B | 780 | LEU | 3.3 |
| 1 | A | 972 | THR | 3.3 |
| 1 | A | 830 | GLN | 3.2 |
| 1 | A | 930 | GLU | 3.2 |
| 1 | B | 845 | LEU | 3.2 |
| 1 | A | 677 | ARG | 3.2 |
| 1 | A | 624 | THR | 3.2 |
| 1 | A | 921 | LYS | 3.2 |
| 1 | B | 789 | ASN | 3.2 |
| 1 | B | 676 | TYR | 3.2 |
| 1 | A | 998 | ARG | 3.2 |
| 1 | B | 901 | SER | 3.2 |
| 1 | A | 504 | VAL | 3.2 |
| 1 | A | 896 | ALA | 3.2 |
| 1 | B | 439 | TYR | 3.2 |
| 1 | B | 183 | PHE | 3.2 |
| 1 | B | 632 | VAL | 3.2 |
| 1 | B | 929 | VAL | 3.2 |
| 1 | B | 822 | CYS | 3.2 |
| 1 | A | 816 | ALA | 3.2 |
| 1 | A | 614 | PRO | 3.2 |
| 1 | B | 126 | LEU | 3.1 |
| 1 | B | 601 | ASP | 3.1 |
| 1 | B | 778 | VAL | 3.1 |
| 1 | A | 866 | THR | 3.1 |
| 1 | B | 891 | SER | 3.1 |
| 1 | B | 162 | VAL | 3.1 |
| 1 | B | 836 | HIS | 3.1 |
| 1 | A | 408 | MET | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 630 | HIS | 3.1 |
| 1 | A | 995 | PHE | 3.1 |
| 1 | A | 484 | MET | 3.1 |
| 1 | A | 996 | HIS | 3.1 |
| 1 | A | 535 | CYS | 3.1 |
| 1 | A | 990 | SER | 3.1 |
| 1 | B | 163 | ASN | 3.1 |
| 1 | A | 567 | ILE | 3.1 |
| 1 | B | 140 | LEU | 3.1 |
| 1 | B | 600 | MET | 3.1 |
| 1 | B | 219 | ASP | 3.1 |
| 1 | B | 759 | VAL | 3.1 |
| 1 | A | 576 | LEU | 3.1 |
| 1 | A | 981 | GLY | 3.1 |
| 1 | A | 483 | ASP | 3.1 |
| 1 | A | 188 | VAL | 3.1 |
| 1 | A | 413 | GLY | 3.1 |
| 1 | A | 627 | GLY | 3.1 |
| 1 | A | 631 | VAL | 3.1 |
| 1 | B | 821 | GLU | 3.0 |
| 1 | A | 39 | PHE | 3.0 |
| 1 | A | 568 | SER | 3.0 |
| 1 | B | 569 | VAL | 3.0 |
| 1 | B | 64 | LEU | 3.0 |
| 1 | A | 75 | SER | 3.0 |
| 1 | A | 552 | SER | 3.0 |
| 1 | A | 807 | ARG | 3.0 |
| 1 | A | 459 | VAL | 3.0 |
| 1 | A | 679 | VAL | 3.0 |
| 1 | A | 979 | ASN | 3.0 |
| 1 | A | 494 | TYR | 3.0 |
| 1 | A | 528 | TRP | 3.0 |
| 1 | A | 531 | LEU | 3.0 |
| 1 | A | 637 | LYS | 3.0 |
| 1 | B | 292 | TYR | 3.0 |
| 1 | B | 817 | ASP | 3.0 |
| 1 | A | 594 | PHE | 3.0 |
| 1 | B | 506 | VAL | 3.0 |
| 1 | B | 574 | VAL | 3.0 |
| 1 | A | 584 | PRO | 3.0 |
| 1 | B | 573 | ASN | 3.0 |
| 1 | A | 1007 | THR | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 139 | LEU | 3.0 |
| 1 | A | 45 | GLU | 3.0 |
| 1 | A | 812 | LEU | 3.0 |
| 1 | B | 797 | LYS | 3.0 |
| 1 | A | 822 | CYS | 2.9 |
| 1 | B | 597 | LEU | 2.9 |
| 1 | B | 610 | GLN | 2.9 |
| 1 | A | 463 | LYS | 2.9 |
| 1 | A | 959 | LYS | 2.9 |
| 1 | A | 246 | GLY | 2.9 |
| 1 | A | 867 | GLY | 2.9 |
| 1 | B | 810 | CYS | 2.9 |
| 1 | A | 681 | THR | 2.9 |
| 1 | A | 644 | THR | 2.9 |
| 1 | B | 611 | CYS | 2.9 |
| 1 | B | 815 | LYS | 2.9 |
| 1 | B | 446 | PHE | 2.9 |
| 1 | A | 870 | GLU | 2.9 |
| 1 | A | 978 | LEU | 2.9 |
| 1 | A | 925 | HIS | 2.9 |
| 1 | B | 905 | ASP | 2.9 |
| 1 | A | 782 | VAL | 2.9 |
| 1 | A | 832 | THR | 2.9 |
| 1 | B | 722 | LYS | 2.9 |
| 1 | B | 816 | ALA | 2.9 |
| 1 | B | 866 | THR | 2.9 |
| 1 | A | 671 | CYS | 2.9 |
| 1 | B | 128 | ALA | 2.8 |
| 1 | B | 595 | GLU | 2.8 |
| 1 | A | 210 | ASP | 2.8 |
| 1 | B | 806 | MET | 2.8 |
| 1 | B | 913 | ILE | 2.8 |
| 1 | A | 91 | ASN | 2.8 |
| 1 | B | 763 | ASN | 2.8 |
| 1 | A | 769 | GLU | 2.8 |
| 1 | A | 515 | CYS | 2.8 |
| 1 | A | 909 | PRO | 2.8 |
| 1 | B | 764 | THR | 2.8 |
| 1 | B | 138 | LYS | 2.8 |
| 1 | A | 570 | SER | 2.8 |
| 1 | B | 903 | LEU | 2.8 |
| 1 | B | 125 | ARG | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 860 | THR | 2.8 |
| 1 | A | 260 | PRO | 2.8 |
| 1 | B | 703 | LEU | 2.8 |
| 1 | A | 772 | GLU | 2.8 |
| 1 | A | 656 | SER | 2.8 |
| 1 | A | 917 | MET | 2.8 |
| 1 | A | 465 | ASN | 2.7 |
| 1 | A | 534 | THR | 2.7 |
| 1 | B | 951 | MET | 2.7 |
| 1 | A | 532 | HIS | 2.7 |
| 1 | A | 241 | ILE | 2.7 |
| 1 | B | 181 | LYS | 2.7 |
| 1 | B | 564 | PRO | 2.7 |
| 1 | A | 876 | THR | 2.7 |
| 1 | B | 542 | GLU | 2.7 |
| 1 | A | 105 | GLU | 2.7 |
| 1 | A | 106 | PRO | 2.7 |
| 1 | A | 511 | GLN | 2.7 |
| 1 | B | 807 | ARG | 2.7 |
| 1 | A | 689 | PHE | 2.7 |
| 1 | A | 744 | GLY | 2.7 |
| 1 | A | 789 | ASN | 2.7 |
| 1 | A | 1005 | CYS | 2.7 |
| 1 | A | 721 | LEU | 2.7 |
| 1 | A | 670 | ARG | 2.7 |
| 1 | A | 551 | ALA | 2.7 |
| 1 | B | 888 | ASP | 2.7 |
| 1 | B | 603 | LEU | 2.7 |
| 1 | A | 533 | ASN | 2.6 |
| 1 | B | 826 | GLN | 2.6 |
| 1 | A | 471 | THR | 2.6 |
| 1 | A | 493 | LEU | 2.6 |
| 1 | A | 529 | CYS | 2.6 |
| 1 | B | 715 | VAL | 2.6 |
| 1 | A | 38 | SER | 2.6 |
| 1 | A | 445 | ALA | 2.6 |
| 1 | A | 571 | GLN | 2.6 |
| 1 | A | 745 | ILE | 2.6 |
| 1 | A | 403 | PHE | 2.6 |
| 1 | A | 933 | VAL | 2.6 |
| 1 | A | 865 | VAL | 2.6 |
| 1 | A | 736 | TYR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 763 | ASN | 2.6 |
| 1 | A | 170 | GLY | 2.6 |
| 1 | A | 690 | GLN | 2.6 |
| 1 | B | 523 | ASP | 2.6 |
| 1 | B | 560 | LEU | 2.6 |
| 1 | A | 384 | TRP | 2.6 |
| 1 | B | 896 | ALA | 2.6 |
| 1 | B | 944 | SER | 2.6 |
| 1 | B | 630 | HIS | 2.6 |
| 1 | A | 264 | SER | 2.6 |
| 1 | A | 682 | HIS | 2.6 |
| 1 | B | 805 | ALA | 2.5 |
| 1 | B | 893 | VAL | 2.5 |
| 1 | A | 629 | HIS | 2.5 |
| 1 | B | 551 | ALA | 2.5 |
| 1 | B | 173 | VAL | 2.5 |
| 1 | B | 749 | VAL | 2.5 |
| 1 | B | 625 | GLU | 2.5 |
| 1 | B | 203 | LEU | 2.5 |
| 1 | A | 440 | LYS | 2.5 |
| 1 | A | 538 | LYS | 2.5 |
| 1 | A | 436 | ALA | 2.5 |
| 1 | A | 607 | ASN | 2.5 |
| 1 | A | 863 | ILE | 2.5 |
| 1 | B | 400 | ASP | 2.5 |
| 1 | A | 99 | ILE | 2.5 |
| 1 | B | 863 | ILE | 2.5 |
| 1 | B | 581 | TYR | 2.5 |
| 1 | A | 861 | GLU | 2.5 |
| 1 | B | 701 | PRO | 2.5 |
| 1 | B | 693 | ARG | 2.5 |
| 1 | B | 127 | ILE | 2.5 |
| 1 | A | 813 | CYS | 2.5 |
| 1 | A | 991 | GLN | 2.5 |
| 1 | B | 861 | GLU | 2.5 |
| 1 | B | 71 | TYR | 2.5 |
| 1 | A | 172 | ILE | 2.5 |
| 1 | B | 284 | LYS | 2.5 |
| 1 | B | 946 | GLN | 2.5 |
| 1 | B | 818 | PRO | 2.4 |
| 1 | B | 933 | VAL | 2.4 |
| 1 | B | 641 | THR | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 518 | CYS | 2.4 |
| 1 | A | 781 | THR | 2.4 |
| 1 | B | 704 | LEU | 2.4 |
| 1 | A | 673 | TRP | 2.4 |
| 1 | A | 905 | ASP | 2.4 |
| 1 | A | 1013 | VAL | 2.4 |
| 1 | A | 265 | PRO | 2.4 |
| 1 | A | 312 | ALA | 2.4 |
| 1 | A | 588 | ALA | 2.4 |
| 1 | B | 904 | VAL | 2.4 |
| 1 | A | 820 | PHE | 2.4 |
| 1 | B | 431 | MET | 2.4 |
| 1 | B | 647 | SER | 2.4 |
| 1 | B | 146 | PHE | 2.4 |
| 1 | B | 633 | GLN | 2.4 |
| 1 | A | 621 | ARG | 2.4 |
| 1 | A | 237 | PRO | 2.4 |
| 1 | B | 151 | PRO | 2.4 |
| 1 | A | 819 | ASP | 2.4 |
| 1 | A | 918 | GLY | 2.4 |
| 1 | B | 876 | THR | 2.4 |
| 1 | A | 228 | ILE | 2.4 |
| 1 | A | 486 | PHE | 2.4 |
| 1 | A | 947 | LEU | 2.4 |
| 1 | B | 120 | ASP | 2.4 |
| 1 | A | 889 | ILE | 2.4 |
| 1 | B | 150 | GLU | 2.4 |
| 1 | B | 930 | GLU | 2.4 |
| 1 | A | 332 | ASP | 2.4 |
| 1 | A | 315 | SER | 2.4 |
| 1 | B | 830 | GLN | 2.4 |
| 1 | A | 604 | VAL | 2.3 |
| 1 | B | 612 | TYR | 2.3 |
| 1 | A | 333 | LEU | 2.3 |
| 1 | B | 182 | LEU | 2.3 |
| 1 | B | 345 | LYS | 2.3 |
| 1 | B | 742 | ILE | 2.3 |
| 1 | A | 583 | VAL | 2.3 |
| 1 | A | 902 | PRO | 2.3 |
| 1 | A | 856 | ASN | 2.3 |
| 1 | A | 857 | PRO | 2.3 |
| 1 | A | 610 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 175 | TYR | 2.3 |
| 1 | A | 858 | ARG | 2.3 |
| 1 | A | 894 | LYS | 2.3 |
| 1 | A | 560 | LEU | 2.3 |
| 1 | A | 435 | ILE | 2.3 |
| 1 | B | 579 | GLU | 2.3 |
| 1 | B | 83 | HIS | 2.3 |
| 1 | B | 160 | SER | 2.3 |
| 1 | A | 878 | ARG | 2.3 |
| 1 | A | 171 | VAL | 2.3 |
| 1 | A | 738 | CYS | 2.3 |
| 1 | A | 194 | TYR | 2.3 |
| 1 | B | 556 | GLN | 2.3 |
| 1 | A | 701 | PRO | 2.3 |
| 1 | A | 903 | LEU | 2.3 |
| 1 | A | 235 | VAL | 2.3 |
| 1 | B | 881 | ASN | 2.3 |
| 1 | B | 369 | ARG | 2.3 |
| 1 | A | 317 | ALA | 2.2 |
| 1 | B | 648 | THR | 2.2 |
| 1 | A | 790 | ILE | 2.2 |
| 1 | B | 172 | ILE | 2.2 |
| 1 | A | 460 | ASP | 2.2 |
| 1 | B | 730 | GLN | 2.2 |
| 1 | B | 250 | GLY | 2.2 |
| 1 | B | 522 | GLY | 2.2 |
| 1 | B | 617 | LYS | 2.2 |
| 1 | A | 447 | VAL | 2.2 |
| 1 | B | 193 | GLU | 2.2 |
| 1 | B | 653 | TYR | 2.2 |
| 1 | A | 720 | THR | 2.2 |
| 1 | A | 64 | LEU | 2.2 |
| 1 | A | 768 | TYR | 2.2 |
| 1 | A | 513 | ARG | 2.2 |
| 1 | B | 256 | LEU | 2.2 |
| 1 | A | 490 | HIS | 2.2 |
| 1 | B | 771 | MET | 2.2 |
| 1 | A | 151 | PRO | 2.2 |
| 1 | A | 173 | VAL | 2.2 |
| 1 | B | 141 | ARG | 2.2 |
| 1 | B | 257 | THR | 2.2 |
| 1 | A | 828 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 841 | GLU | 2.2 |
| 1 | B | 312 | ALA | 2.2 |
| 1 | B | 811 | GLY | 2.2 |
| 1 | B | 651 | VAL | 2.2 |
| 1 | A | 514 | SER | 2.2 |
| 1 | B | 444 | LEU | 2.2 |
| 1 | A | 729 | PRO | 2.2 |
| 1 | B | 772 | GLU | 2.2 |
| 1 | B | 914 | VAL | 2.2 |
| 1 | A | 1010 | SER | 2.2 |
| 1 | A | 719 | ILE | 2.2 |
| 1 | B | 511 | GLN | 2.2 |
| 1 | A | 441 | ASN | 2.2 |
| 1 | B | 670 | ARG | 2.1 |
| 1 | B | 832 | THR | 2.1 |
| 1 | A | 519 | LEU | 2.1 |
| 1 | A | 651 | VAL | 2.1 |
| 1 | B | 631 | VAL | 2.1 |
| 1 | B | 240 | ASP | 2.1 |
| 1 | B | 857 | PRO | 2.1 |
| 1 | A | 398 | THR | 2.1 |
| 1 | A | 580 | THR | 2.1 |
| 1 | B | 894 | LYS | 2.1 |
| 1 | B | 697 | PRO | 2.1 |
| 1 | B | 791 | ASP | 2.1 |
| 1 | B | 624 | THR | 2.1 |
| 1 | B | 596 | ASP | 2.1 |
| 1 | A | 335 | PHE | 2.1 |
| 1 | A | 805 | ALA | 2.1 |
| 1 | A | 219 | ASP | 2.1 |
| 1 | A | 817 | ASP | 2.1 |
| 1 | A | 388 | LYS | 2.1 |
| 1 | B | 294 | GLU | 2.1 |
| 1 | A | 344 | ARG | 2.1 |
| 1 | A | 434 | VAL | 2.1 |
| 1 | B | 702 | GLN | 2.1 |
| 1 | B | 147 | LYS | 2.1 |
| 1 | A | 837 | CYS | 2.1 |
| 1 | A | 464 | GLY | 2.1 |
| 1 | B | 403 | PHE | 2.1 |
| 1 | B | 841 | GLU | 2.1 |
| 1 | A | 468 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 974 | THR | 2.1 |
| 1 | B | 831 | CYS | 2.1 |
| 1 | A | 197 | THR | 2.1 |
| 1 | B | 692 | GLY | 2.1 |
| 1 | A | 561 | THR | 2.0 |
| 1 | A | 632 | VAL | 2.0 |
| 1 | A | 753 | ARG | 2.0 |
| 1 | B | 228 | ILE | 2.0 |
| 1 | B | 615 | ALA | 2.0 |
| 1 | B | 649 | SER | 2.0 |
| 1 | B | 804 | GLY | 2.0 |
| 1 | A | 392 | CYS | 2.0 |
| 1 | A | 818 | PRO | 2.0 |
| 1 | B | 220 | GLU | 2.0 |
| 1 | A | 401 | ASP | 2.0 |
| 1 | A | 944 | SER | 2.0 |
| 1 | A | 516 | GLY | 2.0 |
| 1 | A | 641 | THR | 2.0 |
| 1 | B | 575 | LEU | 2.0 |
| 1 | A | 342 | GLN | 2.0 |
| 1 | B | 623 | ILE | 2.0 |
| 1 | B | 691 | GLU | 2.0 |
| 1 | A | 565 | ASN | 2.0 |
| 1 | B | 672 | HIS | 2.0 |
| 1 | A | 406 | LEU | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.