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

Feb 1, 2016 – 05:29 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 2QVW |
| Title | : | Structure of Giardia Dicer refined against twinned data |
| Authors | : | Doudna, J.A.; MacRae, I.J |
| Deposited on | : | 2007-08-09 |
| Resolution | : | 3.00 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

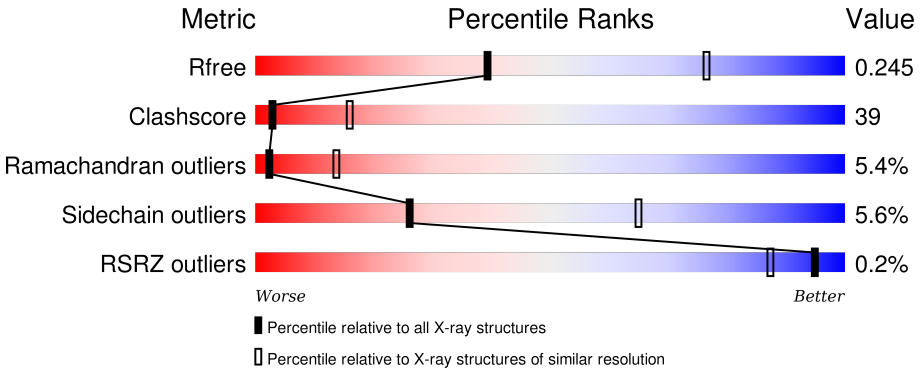
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1578 (3.00-3.00) |
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 | 756 | 41% 49% 7% • |
| 1 | B | 756 | 41% 50% 5% • |
| 1 | C | 756 | 42% 48% 5% 5% |
| 1 | D | 756 | % 40% 47% 7% • 5% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | MN | C | 760 | - | - | - | X |

# 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22372 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 GLP_546_48378_50642.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 732 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5630 | 3614 | 957 | 1029 | 30 | | | |
| 1 | B | 726 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5590 | 3589 | 950 | 1021 | 30 | | | |
| 1 | C | 718 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5539 | 3560 | 941 | 1008 | 30 | | | |
| 1 | D | 720 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5574 | 3586 | 942 | 1016 | 30 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -1 | GLY | - | EXPRESSION TAG | UNP Q7R2M2 |
| A | 0 | ALA | - | EXPRESSION TAG | UNP Q7R2M2 |
| B | -1 | GLY | - | EXPRESSION TAG | UNP Q7R2M2 |
| B | 0 | ALA | - | EXPRESSION TAG | UNP Q7R2M2 |
| C | -1 | GLY | - | EXPRESSION TAG | UNP Q7R2M2 |
| C | 0 | ALA | - | EXPRESSION TAG | UNP Q7R2M2 |
| D | -1 | GLY | - | EXPRESSION TAG | UNP Q7R2M2 |
| D | 0 | ALA | - | EXPRESSION TAG | UNP Q7R2M2 |

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

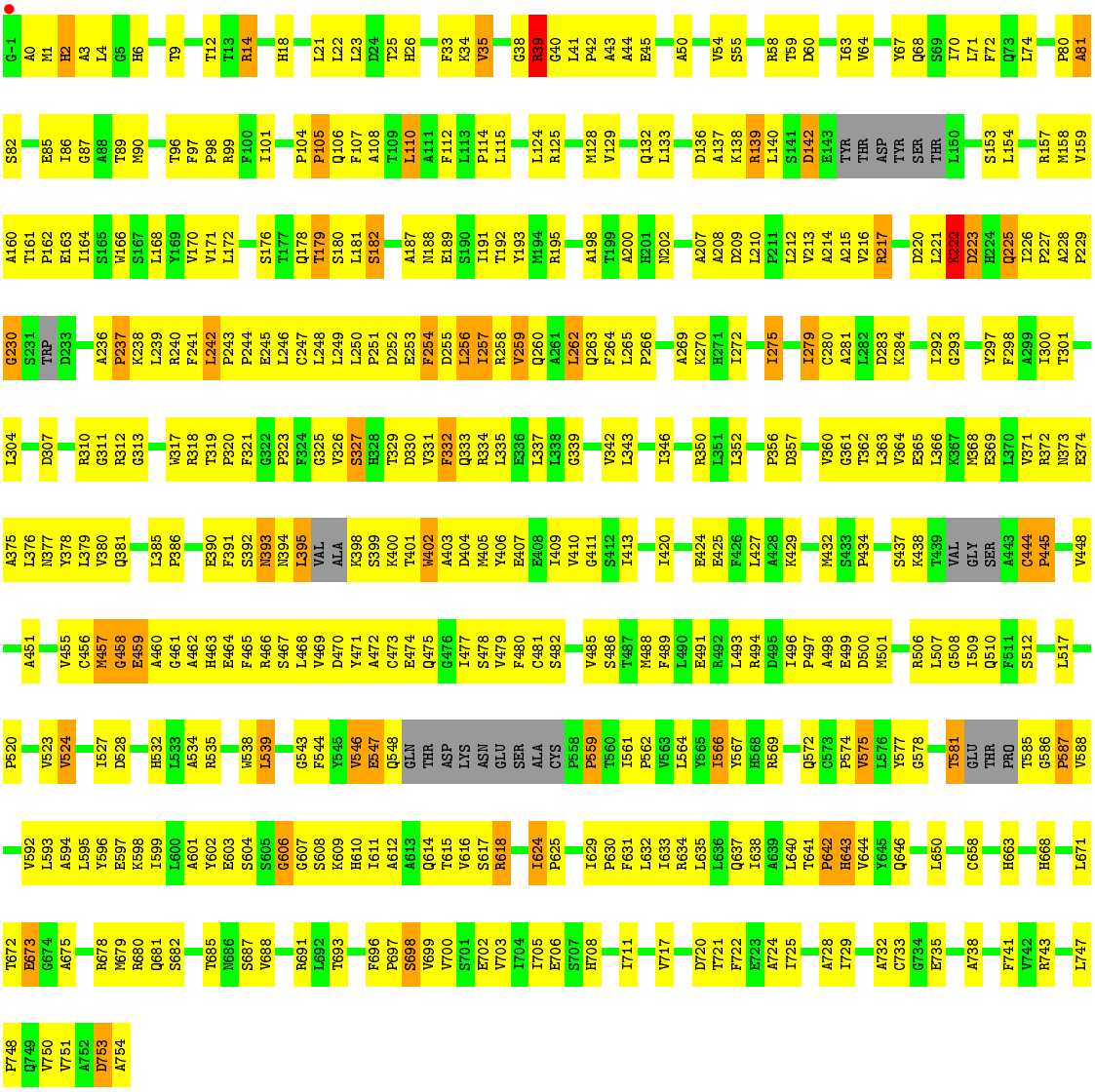
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | B | 9 | Total | Mn | 0 | 0 |
| | | | 9 | 9 | | |
| 2 | A | 12 | Total | Mn | 0 | 0 |
| | | | 12 | 12 | | |
| 2 | D | 9 | Total | Mn | 0 | 0 |
| | | | 9 | 9 | | |
| 2 | C | 9 | Total | Mn | 0 | 0 |
| | | | 9 | 9 | | |

# 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.

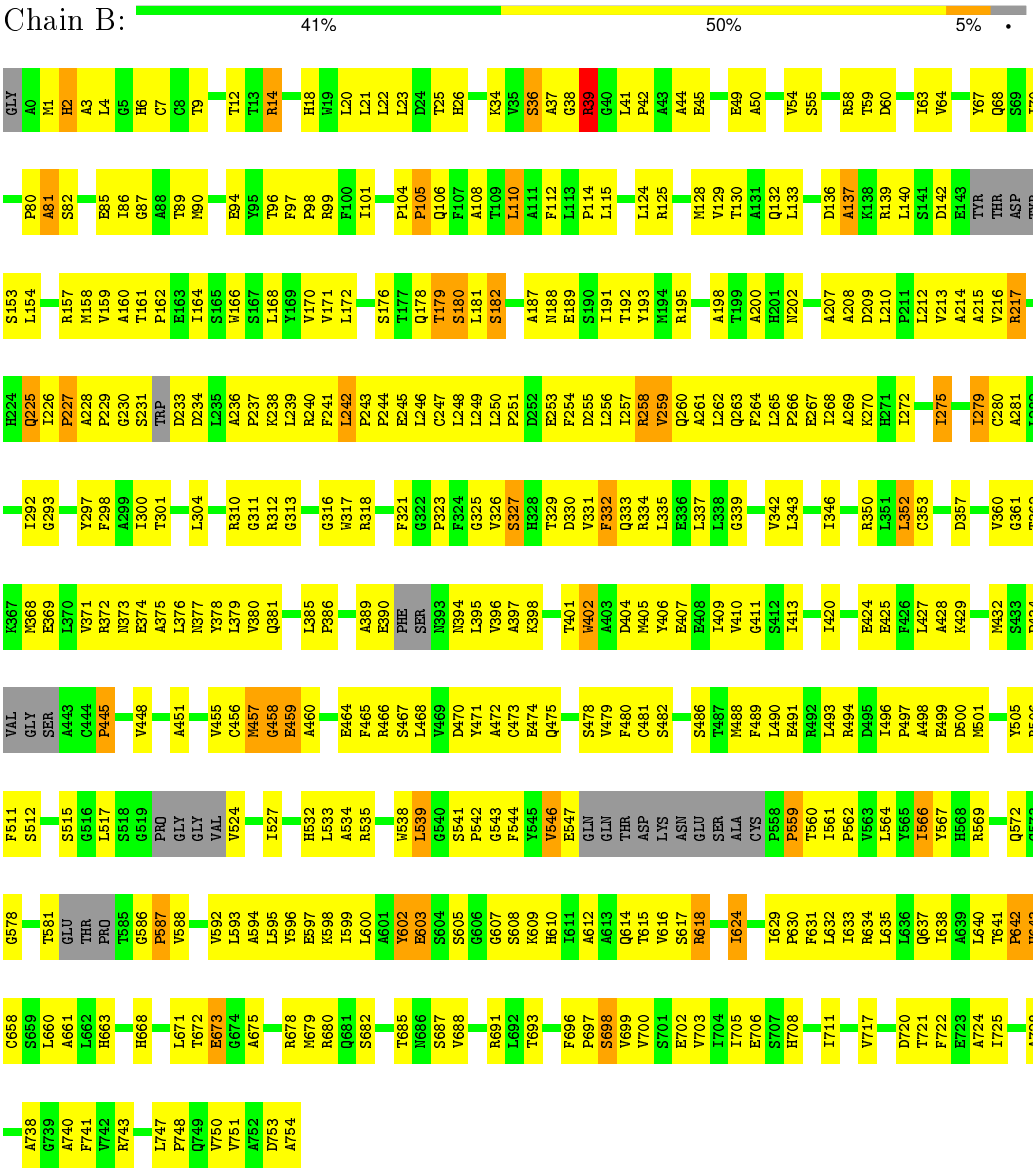
- Molecule 1: GLP_546_48378_50642

Chain A:

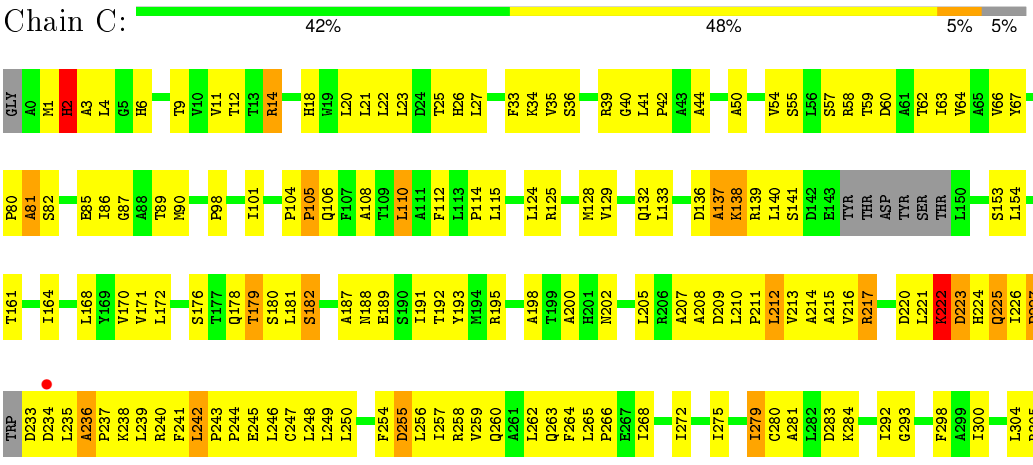
- Molecule 1: GLP_546_48378_50642

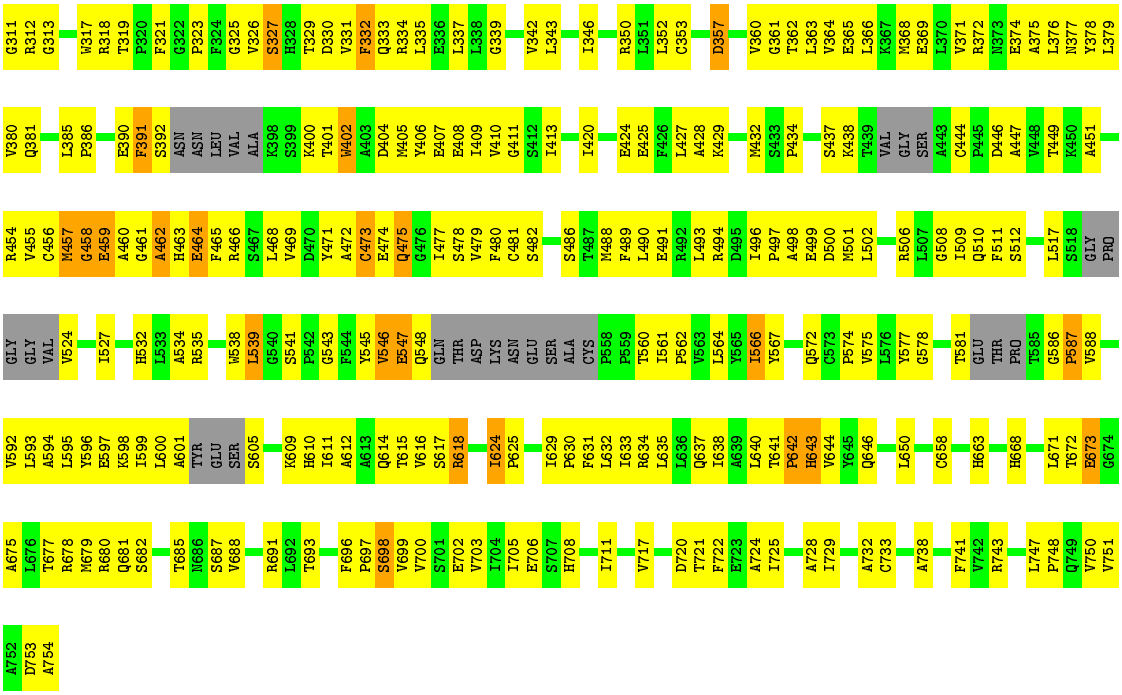
Chain B:




- Molecule 1: GLP_546_48378_50642

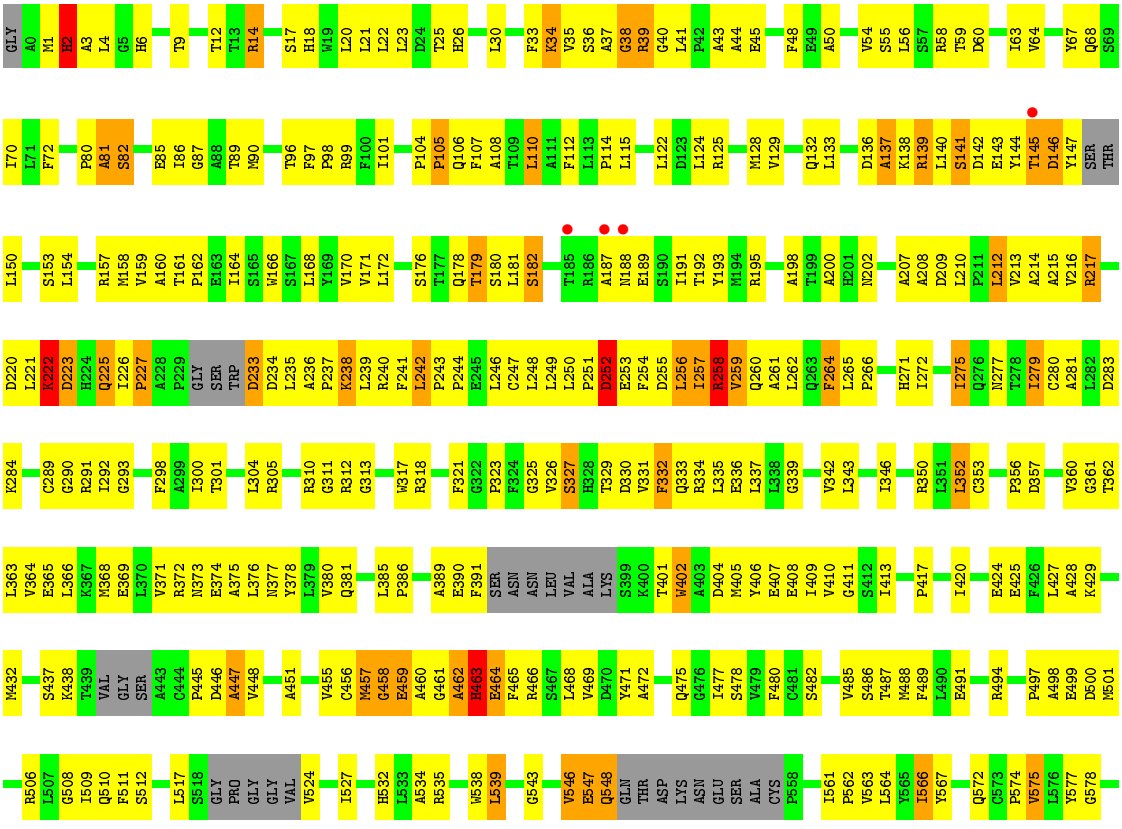
Chain C:

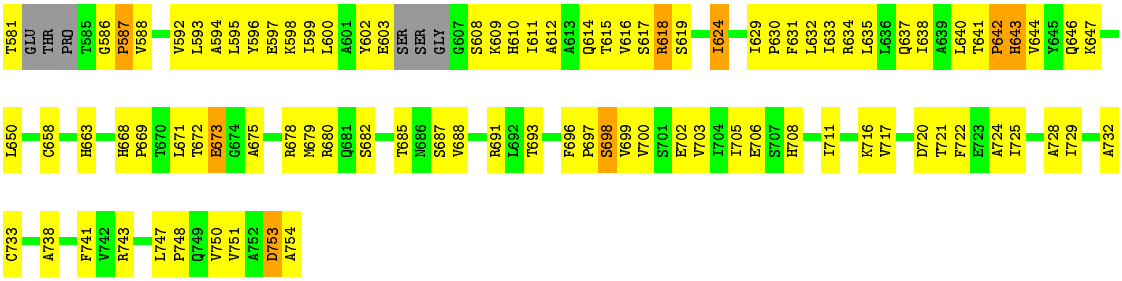




• Molecule 1: GLP_546_48378_50642

Chain D:


T581 GLU THR PRO T585 G586 P587 V588 V592 L593 A594 L595 Y596 E597 K598 I599 L600 A601 Y602 E603 SER SER GLY G607 S608 K609 H610 I611 A612 A613 Q614 T615 V616 S617 R618 S619 I624 I629 P630 F631 L632 I633 R634 L635 L636 Q637 I638 A639 L640 T641 P642 H643 V644 Y645 Q646 K647
L650 C658 H663 H668 P669 T670 L671 T672 E673 G674 A675 R678 M679 R680 Q681 S682 T685 N686 S687 V688 R691 L692 T693 F696 P697 S698 V699 V700 S701 E702 V703 I704 I705 E706 S707 H708 I711 K716 V717 D720 T721 F722 E723 A724 I725 A728 I729 A732
C733 A738 F741 V742 R743 L747 P748 Q749 V750 V751 A752 D753 A754

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 155.41Å 173.49Å 155.45Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.00<br>49.16 – 3.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.9 (50.00-3.00)<br>97.8 (49.16-3.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.08 | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| $< I/\sigma(I) >$ [1] | 4.84 (at 3.01Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.221 , 0.263<br>0.216 , 0.245 | Depositor<br>DCC |
| $R_{free}$ test set | 3938 reflections (5.00%) | DCC |
| Wilson B-factor (Å$^2$) | 53.2 | Xtriage |
| Anisotropy | 0.137 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 8.3 | EDS |
| Estimated twinning fraction | 0.478 for l,-k,h | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.40$, $< L^2 > = 0.22$ | Xtriage |
| Outliers | 0 of 82722 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 22372 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 39.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.37 | 0/5761 | 0.60 | 0/7836 |
| 1 | B | 0.36 | 0/5718 | 0.60 | 0/7777 |
| 1 | C | 0.36 | 0/5666 | 0.60 | 0/7704 |
| 1 | D | 0.36 | 0/5704 | 0.60 | 0/7759 |
| All | All | 0.36 | 0/22849 | 0.60 | 0/31076 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5630 | 0 | 5672 | 434 | 0 |
| 1 | B | 5590 | 0 | 5640 | 438 | 0 |
| 1 | C | 5539 | 0 | 5592 | 460 | 0 |
| 1 | D | 5574 | 0 | 5611 | 449 | 0 |
| 2 | A | 12 | 0 | 0 | 0 | 0 |
| 2 | B | 9 | 0 | 0 | 0 | 0 |
| 2 | C | 9 | 0 | 0 | 0 | 0 |
| 2 | D | 9 | 0 | 0 | 0 | 0 |
| All | All | 22372 | 0 | 22515 | 1769 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1769) 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:B:465:PHE:HE2 | 1:B:533:LEU:HD21 | 1.23 | 1.03 |
| 1:C:597:GLU:HA | 1:C:600:LEU:HD12 | 1.40 | 1.02 |
| 1:C:114:PRO:HA | 1:C:258:ARG:HH12 | 1.21 | 1.01 |
| 1:C:465:PHE:HE1 | 1:C:502:LEU:HB2 | 1.29 | 0.97 |
| 1:B:373:ASN:HD21 | 1:B:401:THR:HG21 | 1.26 | 0.97 |
| 1:D:110:LEU:HD13 | 1:D:272:ILE:HD12 | 1.44 | 0.96 |
| 1:A:373:ASN:HD21 | 1:A:401:THR:HG21 | 1.32 | 0.94 |
| 1:B:99:ARG:HH12 | 1:B:390:GLU:C | 1.70 | 0.94 |
| 1:B:466:ARG:NE | 1:B:498:ALA:HB2 | 1.81 | 0.93 |
| 1:C:115:LEU:H | 1:C:258:ARG:HH22 | 0.94 | 0.93 |
| 1:A:220:ASP:HB3 | 1:A:238:LYS:HD3 | 1.53 | 0.91 |
| 1:A:39:ARG:HD2 | 1:A:317:TRP:CZ2 | 2.06 | 0.91 |
| 1:A:104:PRO:HB3 | 1:A:280:CYS:SG | 2.10 | 0.90 |
| 1:B:466:ARG:HH21 | 1:B:498:ALA:H | 1.18 | 0.89 |
| 1:C:138:LYS:O | 1:C:139:ARG:HD2 | 1.73 | 0.87 |
| 1:D:258:ARG:HH11 | 1:D:258:ARG:HA | 1.40 | 0.87 |
| 1:C:110:LEU:HD13 | 1:C:272:ILE:HD12 | 1.57 | 0.87 |
| 1:C:115:LEU:H | 1:C:258:ARG:NH2 | 1.73 | 0.86 |
| 1:A:743:ARG:HA | 1:A:747:LEU:HB2 | 1.59 | 0.85 |
| 1:C:178:GLN:HE21 | 1:C:212:LEU:HD12 | 1.41 | 0.84 |
| 1:D:178:GLN:HE21 | 1:D:212:LEU:HD12 | 1.42 | 0.84 |
| 1:D:104:PRO:HB3 | 1:D:280:CYS:SG | 2.17 | 0.84 |
| 1:D:279:ILE:O | 1:D:283:ASP:HB2 | 1.77 | 0.84 |
| 1:B:377:ASN:HD21 | 1:B:395:LEU:HD21 | 1.42 | 0.84 |
| 1:C:743:ARG:HA | 1:C:747:LEU:HB2 | 1.57 | 0.84 |
| 1:B:178:GLN:HE21 | 1:B:212:LEU:HD12 | 1.43 | 0.83 |
| 1:C:233:ASP:HB3 | 1:C:236:ALA:HB2 | 1.60 | 0.83 |
| 1:D:743:ARG:HA | 1:D:747:LEU:HB2 | 1.58 | 0.83 |
| 1:B:743:ARG:HA | 1:B:747:LEU:HB2 | 1.61 | 0.83 |
| 1:B:279:ILE:O | 1:B:283:ASP:HB2 | 1.80 | 0.82 |
| 1:C:279:ILE:O | 1:C:283:ASP:HB2 | 1.79 | 0.82 |
| 1:A:279:ILE:O | 1:A:283:ASP:HB2 | 1.78 | 0.82 |
| 1:C:381:GLN:NE2 | 1:C:402:TRP:HD1 | 1.77 | 0.81 |
| 1:C:508:GLY:HA3 | 1:C:532:HIS:O | 1.79 | 0.81 |
| 1:D:1:MET:HG3 | 1:D:55:SER:HB3 | 1.61 | 0.81 |
| 1:C:104:PRO:HB3 | 1:C:280:CYS:SG | 2.21 | 0.81 |
| 1:B:220:ASP:HB3 | 1:B:238:LYS:HD3 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:350:ARG:HD3 | 1:C:538:TRP:O | 1.81 | 0.81 |
| 1:B:36:SER:O | 1:B:38:GLY:N | 2.15 | 0.80 |
| 1:C:543:GLY:HA3 | 1:C:561:ILE:O | 1.82 | 0.80 |
| 1:A:178:GLN:HE21 | 1:A:212:LEU:HD12 | 1.43 | 0.80 |
| 1:C:465:PHE:HA | 1:C:468:LEU:HD12 | 1.64 | 0.79 |
| 1:D:543:GLY:HA3 | 1:D:561:ILE:O | 1.82 | 0.79 |
| 1:A:39:ARG:HD2 | 1:A:317:TRP:CE2 | 2.17 | 0.79 |
| 1:D:508:GLY:HA3 | 1:D:532:HIS:O | 1.82 | 0.79 |
| 1:C:305:ARG:HD2 | 1:C:390:GLU:HB3 | 1.64 | 0.79 |
| 1:D:747:LEU:O | 1:D:750:VAL:HG12 | 1.83 | 0.79 |
| 1:D:333:GLN:NE2 | 1:D:672:THR:HB | 1.98 | 0.79 |
| 1:D:362:THR:O | 1:D:366:LEU:HG | 1.83 | 0.79 |
| 1:B:85:GLU:O | 1:B:89:THR:HG23 | 1.83 | 0.78 |
| 1:A:110:LEU:HD13 | 1:A:272:ILE:HD12 | 1.64 | 0.78 |
| 1:C:85:GLU:O | 1:C:89:THR:HG23 | 1.83 | 0.78 |
| 1:B:362:THR:O | 1:B:366:LEU:HG | 1.83 | 0.78 |
| 1:D:3:ALA:HB3 | 1:D:54:VAL:O | 1.82 | 0.78 |
| 1:A:609:LYS:HD3 | 1:A:641:THR:HG22 | 1.65 | 0.78 |
| 1:C:362:THR:O | 1:C:366:LEU:HG | 1.83 | 0.78 |
| 1:A:432:MET:HE2 | 1:A:534:ALA:HB1 | 1.66 | 0.78 |
| 1:A:85:GLU:O | 1:A:89:THR:HG23 | 1.84 | 0.78 |
| 1:C:747:LEU:O | 1:C:750:VAL:HG12 | 1.85 | 0.77 |
| 1:D:180:SER:HB2 | 1:D:208:ALA:O | 1.84 | 0.77 |
| 1:A:596:TYR:O | 1:A:599:ILE:HG22 | 1.85 | 0.77 |
| 1:B:747:LEU:O | 1:B:750:VAL:HG12 | 1.84 | 0.77 |
| 1:A:362:THR:O | 1:A:366:LEU:HG | 1.84 | 0.77 |
| 1:A:399:SER:HA | 1:B:395:LEU:HD12 | 1.66 | 0.77 |
| 1:D:38:GLY:H | 1:D:41:LEU:HD12 | 1.49 | 0.77 |
| 1:D:172:LEU:HD12 | 1:D:239:LEU:HD13 | 1.67 | 0.77 |
| 1:C:471:TYR:O | 1:C:475:GLN:HB2 | 1.85 | 0.77 |
| 1:B:465:PHE:HA | 1:B:468:LEU:HD12 | 1.66 | 0.76 |
| 1:D:147:TYR:CG | 1:D:150:LEU:HB2 | 2.20 | 0.76 |
| 1:C:205:LEU:HB3 | 1:C:245:GLU:OE2 | 1.86 | 0.76 |
| 1:D:139:ARG:NH1 | 1:D:162:PRO:HG3 | 2.00 | 0.76 |
| 1:D:369:GLU:HG2 | 1:D:485:VAL:HG23 | 1.66 | 0.76 |
| 1:A:508:GLY:HA3 | 1:A:532:HIS:O | 1.85 | 0.76 |
| 1:D:337:LEU:HD22 | 1:D:673:GLU:HA | 1.67 | 0.76 |
| 1:C:21:LEU:HD21 | 1:C:272:ILE:HD11 | 1.66 | 0.76 |
| 1:C:159:VAL:HG23 | 1:C:248:LEU:O | 1.85 | 0.76 |
| 1:B:115:LEU:H | 1:B:258:ARG:HH22 | 1.33 | 0.76 |
| 1:A:3:ALA:HB3 | 1:A:54:VAL:O | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:352:LEU:HD11 | 1:D:650:LEU:HD23 | 1.67 | 0.76 |
| 1:C:596:TYR:O | 1:C:599:ILE:HG22 | 1.85 | 0.76 |
| 1:A:392:SER:O | 1:A:394:ASN:N | 2.17 | 0.76 |
| 1:D:1:MET:HG3 | 1:D:55:SER:CB | 2.15 | 0.76 |
| 1:D:160:ALA:HB2 | 1:D:168:LEU:HD23 | 1.68 | 0.76 |
| 1:A:99:ARG:HH11 | 1:A:390:GLU:CD | 1.89 | 0.76 |
| 1:A:310:ARG:HH22 | 1:A:392:SER:HB3 | 1.49 | 0.76 |
| 1:B:3:ALA:HB3 | 1:B:54:VAL:O | 1.86 | 0.76 |
| 1:B:300:ILE:HG23 | 1:B:304:LEU:HD12 | 1.68 | 0.76 |
| 1:A:747:LEU:O | 1:A:750:VAL:HG12 | 1.85 | 0.75 |
| 1:B:160:ALA:HB2 | 1:B:168:LEU:HD23 | 1.66 | 0.75 |
| 1:C:465:PHE:CE1 | 1:C:502:LEU:HB2 | 2.19 | 0.75 |
| 1:C:158:MET:HE3 | 1:C:256:LEU:HB2 | 1.68 | 0.75 |
| 1:D:300:ILE:HG23 | 1:D:304:LEU:HD12 | 1.69 | 0.75 |
| 1:C:160:ALA:HB2 | 1:C:168:LEU:HD23 | 1.67 | 0.75 |
| 1:A:300:ILE:HG23 | 1:A:304:LEU:HD12 | 1.68 | 0.75 |
| 1:C:705:ILE:HG12 | 1:C:711:ILE:HD11 | 1.69 | 0.75 |
| 1:C:180:SER:HB2 | 1:C:208:ALA:O | 1.87 | 0.75 |
| 1:D:635:LEU:HD12 | 1:D:732:ALA:HB2 | 1.68 | 0.75 |
| 1:A:635:LEU:HD12 | 1:A:732:ALA:HB2 | 1.66 | 0.74 |
| 1:D:596:TYR:O | 1:D:599:ILE:HG22 | 1.87 | 0.74 |
| 1:A:160:ALA:HB2 | 1:A:168:LEU:HD23 | 1.69 | 0.74 |
| 1:C:255:ASP:O | 1:C:259:VAL:HG23 | 1.86 | 0.74 |
| 1:B:508:GLY:HA3 | 1:B:532:HIS:O | 1.87 | 0.74 |
| 1:D:343:LEU:HD13 | 1:D:427:LEU:HD21 | 1.69 | 0.74 |
| 1:C:635:LEU:HD12 | 1:C:732:ALA:HB2 | 1.69 | 0.74 |
| 1:C:115:LEU:N | 1:C:258:ARG:HH22 | 1.78 | 0.74 |
| 1:D:180:SER:HA | 1:D:212:LEU:HD21 | 1.70 | 0.74 |
| 1:B:596:TYR:O | 1:B:599:ILE:HG22 | 1.88 | 0.74 |
| 1:A:180:SER:HA | 1:A:212:LEU:HD21 | 1.70 | 0.74 |
| 1:C:180:SER:HA | 1:C:212:LEU:HD21 | 1.70 | 0.74 |
| 1:A:180:SER:HB2 | 1:A:208:ALA:O | 1.88 | 0.74 |
| 1:B:466:ARG:CZ | 1:B:498:ALA:HB2 | 2.17 | 0.74 |
| 1:B:180:SER:HB2 | 1:B:208:ALA:O | 1.87 | 0.74 |
| 1:A:379:LEU:HD21 | 1:A:481:CYS:HB3 | 1.70 | 0.73 |
| 1:B:465:PHE:CE2 | 1:B:533:LEU:HD21 | 2.15 | 0.73 |
| 1:C:138:LYS:C | 1:C:139:ARG:HD2 | 2.08 | 0.73 |
| 1:B:139:ARG:HG3 | 1:B:247:CYS:O | 1.88 | 0.73 |
| 1:D:259:VAL:O | 1:D:262:LEU:HB3 | 1.89 | 0.73 |
| 1:B:346:ILE:HG21 | 1:B:427:LEU:HD13 | 1.71 | 0.73 |
| 1:B:350:ARG:HD3 | 1:B:538:TRP:O | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:139:ARG:HG2 | 1:B:245:GLU:O | 1.87 | 0.73 |
| 1:A:158:MET:HG3 | 1:A:259:VAL:HG21 | 1.70 | 0.73 |
| 1:B:39:ARG:HG3 | 1:B:317:TRP:CZ2 | 2.24 | 0.73 |
| 1:C:634:ARG:O | 1:C:638:ILE:HG13 | 1.88 | 0.72 |
| 1:B:178:GLN:HB2 | 1:B:182:SER:OG | 1.89 | 0.72 |
| 1:A:432:MET:HA | 1:A:479:VAL:O | 1.90 | 0.72 |
| 1:B:394:ASN:OD1 | 1:B:396:VAL:HG12 | 1.88 | 0.72 |
| 1:B:180:SER:HA | 1:B:212:LEU:HD21 | 1.70 | 0.72 |
| 1:B:561:ILE:HD12 | 1:B:561:ILE:H | 1.54 | 0.72 |
| 1:A:634:ARG:O | 1:A:638:ILE:HG13 | 1.90 | 0.72 |
| 1:A:352:LEU:HD12 | 1:A:363:LEU:HD13 | 1.70 | 0.72 |
| 1:B:264:PHE:O | 1:B:268:ILE:HG13 | 1.90 | 0.72 |
| 1:B:635:LEU:HD12 | 1:B:732:ALA:HB2 | 1.71 | 0.72 |
| 1:D:609:LYS:NZ | 1:D:641:THR:HG21 | 2.05 | 0.72 |
| 1:C:14:ARG:NH2 | 1:C:224:HIS:O | 2.22 | 0.72 |
| 1:A:310:ARG:HB2 | 1:A:310:ARG:NH1 | 2.05 | 0.72 |
| 1:D:342:VAL:HG12 | 1:D:658:CYS:SG | 2.29 | 0.72 |
| 1:C:114:PRO:CA | 1:C:258:ARG:HH12 | 2.01 | 0.72 |
| 1:C:14:ARG:HD2 | 1:C:260:GLN:OE1 | 1.89 | 0.72 |
| 1:A:561:ILE:HD12 | 1:A:561:ILE:H | 1.53 | 0.72 |
| 1:C:133:LEU:O | 1:C:137:ALA:N | 2.23 | 0.71 |
| 1:B:602:TYR:HD2 | 1:B:634:ARG:NH1 | 1.86 | 0.71 |
| 1:D:705:ILE:HG12 | 1:D:711:ILE:HD11 | 1.72 | 0.71 |
| 1:A:705:ILE:HG12 | 1:A:711:ILE:HD11 | 1.72 | 0.71 |
| 1:C:178:GLN:HB2 | 1:C:182:SER:OG | 1.90 | 0.71 |
| 1:A:228:ALA:O | 1:A:230:GLY:N | 2.23 | 0.71 |
| 1:C:310:ARG:HB2 | 1:C:310:ARG:NH1 | 2.05 | 0.71 |
| 1:A:624:ILE:HD13 | 1:A:624:ILE:H | 1.55 | 0.71 |
| 1:D:624:ILE:H | 1:D:624:ILE:HD13 | 1.54 | 0.71 |
| 1:B:705:ILE:HG12 | 1:B:711:ILE:HD11 | 1.73 | 0.71 |
| 1:D:448:VAL:HG13 | 1:D:468:LEU:HD23 | 1.72 | 0.71 |
| 1:A:41:LEU:O | 1:A:41:LEU:HD12 | 1.90 | 0.71 |
| 1:A:98:PRO:HA | 1:A:101:ILE:HD11 | 1.73 | 0.71 |
| 1:D:561:ILE:H | 1:D:561:ILE:HD12 | 1.55 | 0.71 |
| 1:B:437:SER:HB3 | 1:B:478:SER:O | 1.90 | 0.71 |
| 1:C:466:ARG:NH2 | 1:C:498:ALA:H | 1.89 | 0.71 |
| 1:D:236:ALA:N | 1:D:237:PRO:HD2 | 2.06 | 0.71 |
| 1:C:98:PRO:HA | 1:C:101:ILE:HD11 | 1.73 | 0.70 |
| 1:B:634:ARG:O | 1:B:638:ILE:HG13 | 1.90 | 0.70 |
| 1:A:520:PRO:HD2 | 1:D:698:SER:OG | 1.92 | 0.70 |
| 1:B:98:PRO:HA | 1:B:101:ILE:HD11 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:178:GLN:HB2 | 1:D:182:SER:OG | 1.91 | 0.70 |
| 1:D:463:HIS:O | 1:D:466:ARG:HB3 | 1.91 | 0.70 |
| 1:C:596:TYR:O | 1:C:600:LEU:HG | 1.90 | 0.70 |
| 1:C:597:GLU:HA | 1:C:600:LEU:CD1 | 2.19 | 0.70 |
| 1:D:98:PRO:HA | 1:D:101:ILE:HD11 | 1.73 | 0.70 |
| 1:D:37:ALA:HB2 | 1:D:43:ALA:HB2 | 1.72 | 0.70 |
| 1:D:85:GLU:O | 1:D:89:THR:HG23 | 1.91 | 0.70 |
| 1:D:310:ARG:NH1 | 1:D:310:ARG:HB2 | 2.07 | 0.70 |
| 1:B:21:LEU:HD21 | 1:B:272:ILE:HD11 | 1.72 | 0.70 |
| 1:A:67:TYR:OH | 1:A:114:PRO:HG3 | 1.92 | 0.70 |
| 1:B:129:VAL:O | 1:B:133:LEU:HG | 1.90 | 0.70 |
| 1:D:602:TYR:O | 1:D:634:ARG:NH1 | 2.25 | 0.69 |
| 1:C:300:ILE:HG23 | 1:C:304:LEU:HD12 | 1.73 | 0.69 |
| 1:A:337:LEU:HD22 | 1:A:673:GLU:HA | 1.74 | 0.69 |
| 1:A:158:MET:HE1 | 1:A:256:LEU:HD13 | 1.73 | 0.69 |
| 1:A:137:ALA:CB | 1:A:248:LEU:HD21 | 2.22 | 0.69 |
| 1:B:352:LEU:HD12 | 1:B:363:LEU:HD13 | 1.73 | 0.69 |
| 1:B:432:MET:HE2 | 1:B:534:ALA:HB1 | 1.73 | 0.69 |
| 1:C:158:MET:HG3 | 1:C:259:VAL:HG21 | 1.74 | 0.69 |
| 1:B:466:ARG:NH2 | 1:B:498:ALA:H | 1.89 | 0.69 |
| 1:C:343:LEU:HD13 | 1:C:427:LEU:HD21 | 1.75 | 0.69 |
| 1:C:624:ILE:HD13 | 1:C:624:ILE:H | 1.56 | 0.69 |
| 1:D:352:LEU:HD12 | 1:D:363:LEU:HD13 | 1.75 | 0.69 |
| 1:D:172:LEU:HB2 | 1:D:214:ALA:O | 1.92 | 0.69 |
| 1:D:172:LEU:HD12 | 1:D:239:LEU:CD1 | 2.23 | 0.69 |
| 1:C:129:VAL:O | 1:C:133:LEU:HG | 1.93 | 0.69 |
| 1:B:310:ARG:HB2 | 1:B:310:ARG:NH1 | 2.07 | 0.69 |
| 1:C:561:ILE:HD12 | 1:C:561:ILE:H | 1.58 | 0.68 |
| 1:D:634:ARG:O | 1:D:638:ILE:HG13 | 1.93 | 0.68 |
| 1:A:610:HIS:CD2 | 1:A:614:GLN:HE21 | 2.11 | 0.68 |
| 1:B:618:ARG:HH11 | 1:B:618:ARG:HB2 | 1.57 | 0.68 |
| 1:B:624:ILE:H | 1:B:624:ILE:HD13 | 1.57 | 0.68 |
| 1:B:110:LEU:HD13 | 1:B:272:ILE:HD12 | 1.74 | 0.68 |
| 1:D:432:MET:HE2 | 1:D:534:ALA:HB1 | 1.76 | 0.68 |
| 1:C:36:SER:HB3 | 1:C:317:TRP:HB3 | 1.76 | 0.68 |
| 1:A:138:LYS:HD3 | 1:A:142:ASP:HB3 | 1.73 | 0.68 |
| 1:C:180:SER:O | 1:C:193:TYR:HB2 | 1.93 | 0.68 |
| 1:A:369:GLU:HG3 | 1:A:482:SER:OG | 1.93 | 0.68 |
| 1:C:284:LYS:HD2 | 1:C:284:LYS:H | 1.58 | 0.68 |
| 1:C:125:ARG:HG2 | 1:C:125:ARG:HH11 | 1.58 | 0.68 |
| 1:D:609:LYS:HE3 | 1:D:637:GLN:HB3 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:235:LEU:C | 1:C:237:PRO:HD2 | 2.14 | 0.68 |
| 1:A:178:GLN:HB2 | 1:A:182:SER:OG | 1.93 | 0.68 |
| 1:C:198:ALA:O | 1:C:202:ASN:HA | 1.94 | 0.68 |
| 1:B:333:GLN:HE21 | 1:B:673:GLU:HB3 | 1.58 | 0.68 |
| 1:B:139:ARG:HH21 | 1:B:162:PRO:HG3 | 1.58 | 0.68 |
| 1:A:548:GLN:HA | 1:A:548:GLN:HE21 | 1.57 | 0.68 |
| 1:A:307:ASP:HB3 | 1:A:391:PHE:HB2 | 1.75 | 0.68 |
| 1:D:602:TYR:CE1 | 1:D:603:GLU:HG2 | 2.28 | 0.68 |
| 1:C:420:ILE:O | 1:C:424:GLU:HG3 | 1.94 | 0.68 |
| 1:C:67:TYR:OH | 1:C:114:PRO:HG3 | 1.94 | 0.68 |
| 1:A:543:GLY:HA3 | 1:A:561:ILE:O | 1.94 | 0.67 |
| 1:D:615:THR:HA | 1:D:618:ARG:HH12 | 1.59 | 0.67 |
| 1:D:139:ARG:HH12 | 1:D:162:PRO:HG3 | 1.54 | 0.67 |
| 1:A:618:ARG:HH11 | 1:A:618:ARG:HB2 | 1.58 | 0.67 |
| 1:A:129:VAL:O | 1:A:133:LEU:HG | 1.94 | 0.67 |
| 1:C:114:PRO:HA | 1:C:258:ARG:NH1 | 2.02 | 0.67 |
| 1:B:377:ASN:HD21 | 1:B:395:LEU:CD2 | 2.05 | 0.67 |
| 1:C:618:ARG:HB2 | 1:C:618:ARG:HH11 | 1.60 | 0.67 |
| 1:D:437:SER:HB3 | 1:D:478:SER:O | 1.95 | 0.67 |
| 1:B:284:LYS:HD2 | 1:B:284:LYS:H | 1.60 | 0.67 |
| 1:C:193:TYR:CE2 | 1:C:241:PHE:HB2 | 2.30 | 0.67 |
| 1:B:236:ALA:N | 1:B:237:PRO:HD2 | 2.10 | 0.67 |
| 1:A:284:LYS:H | 1:A:284:LYS:HD2 | 1.60 | 0.67 |
| 1:A:339:GLY:HA3 | 1:A:407:GLU:O | 1.95 | 0.67 |
| 1:D:180:SER:O | 1:D:193:TYR:HB2 | 1.95 | 0.67 |
| 1:B:39:ARG:HD2 | 1:B:39:ARG:N | 2.09 | 0.67 |
| 1:C:260:GLN:O | 1:C:263:GLN:HG2 | 1.95 | 0.67 |
| 1:A:523:VAL:HG11 | 1:D:618:ARG:HB2 | 1.77 | 0.67 |
| 1:D:608:SER:HA | 1:D:611:ILE:HG12 | 1.77 | 0.67 |
| 1:B:373:ASN:ND2 | 1:B:401:THR:HG21 | 2.07 | 0.66 |
| 1:C:3:ALA:HB3 | 1:C:54:VAL:O | 1.94 | 0.66 |
| 1:C:381:GLN:NE2 | 1:C:402:TRP:CD1 | 2.61 | 0.66 |
| 1:A:420:ILE:O | 1:A:424:GLU:HG3 | 1.95 | 0.66 |
| 1:C:466:ARG:NH1 | 1:C:501:MET:HE1 | 2.10 | 0.66 |
| 1:B:679:MET:O | 1:B:750:VAL:HG23 | 1.96 | 0.66 |
| 1:C:687:SER:O | 1:C:691:ARG:HG3 | 1.95 | 0.66 |
| 1:C:333:GLN:NE2 | 1:C:672:THR:HB | 2.10 | 0.66 |
| 1:D:527:ILE:HD12 | 1:D:527:ILE:H | 1.59 | 0.66 |
| 1:A:432:MET:HE1 | 1:A:534:ALA:C | 2.15 | 0.66 |
| 1:A:527:ILE:H | 1:A:527:ILE:HD12 | 1.61 | 0.66 |
| 1:B:527:ILE:H | 1:B:527:ILE:HD12 | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:213:VAL:O | 1:D:241:PHE:HA | 1.95 | 0.66 |
| 1:D:432:MET:HE1 | 1:D:534:ALA:C | 2.15 | 0.66 |
| 1:C:337:LEU:HD22 | 1:C:673:GLU:HA | 1.76 | 0.66 |
| 1:C:305:ARG:CD | 1:C:390:GLU:HG2 | 2.25 | 0.66 |
| 1:D:129:VAL:O | 1:D:133:LEU:HG | 1.95 | 0.66 |
| 1:B:180:SER:O | 1:B:193:TYR:HB2 | 1.95 | 0.66 |
| 1:C:615:THR:HA | 1:C:618:ARG:HH12 | 1.59 | 0.66 |
| 1:D:610:HIS:CD2 | 1:D:614:GLN:HE21 | 2.13 | 0.66 |
| 1:D:198:ALA:O | 1:D:202:ASN:HA | 1.95 | 0.66 |
| 1:D:67:TYR:OH | 1:D:114:PRO:HG3 | 1.94 | 0.66 |
| 1:B:172:LEU:HB2 | 1:B:214:ALA:O | 1.96 | 0.66 |
| 1:C:332:PHE:CZ | 1:C:400:LYS:HE2 | 2.31 | 0.66 |
| 1:B:90:MET:CE | 1:B:318:ARG:HH22 | 2.09 | 0.65 |
| 1:B:610:HIS:CD2 | 1:B:614:GLN:HE21 | 2.14 | 0.65 |
| 1:D:409:ILE:O | 1:D:413:ILE:HG12 | 1.97 | 0.65 |
| 1:C:39:ARG:O | 1:C:41:LEU:N | 2.29 | 0.65 |
| 1:B:228:ALA:O | 1:B:230:GLY:N | 2.30 | 0.65 |
| 1:D:138:LYS:HD3 | 1:D:142:ASP:HB3 | 1.77 | 0.65 |
| 1:D:172:LEU:HD11 | 1:D:216:VAL:HG23 | 1.78 | 0.65 |
| 1:D:14:ARG:HD3 | 1:D:257:ILE:HD13 | 1.76 | 0.65 |
| 1:A:717:VAL:O | 1:A:721:THR:HG23 | 1.97 | 0.65 |
| 1:C:610:HIS:CD2 | 1:C:614:GLN:HE21 | 2.13 | 0.65 |
| 1:C:172:LEU:HB2 | 1:C:214:ALA:O | 1.97 | 0.65 |
| 1:B:420:ILE:O | 1:B:424:GLU:HG3 | 1.95 | 0.65 |
| 1:A:180:SER:O | 1:A:193:TYR:HB2 | 1.97 | 0.65 |
| 1:B:1:MET:HG3 | 1:B:55:SER:HB3 | 1.77 | 0.65 |
| 1:C:527:ILE:HD12 | 1:C:527:ILE:H | 1.62 | 0.65 |
| 1:D:251:PRO:HG2 | 1:D:254:PHE:CD1 | 2.31 | 0.65 |
| 1:D:679:MET:O | 1:D:750:VAL:HG23 | 1.97 | 0.65 |
| 1:B:255:ASP:OD1 | 1:B:258:ARG:HB2 | 1.95 | 0.65 |
| 1:B:615:THR:HA | 1:B:618:ARG:HH12 | 1.62 | 0.65 |
| 1:A:629:ILE:O | 1:A:633:ILE:HG12 | 1.96 | 0.65 |
| 1:A:469:VAL:O | 1:A:473:CYS:HB2 | 1.96 | 0.65 |
| 1:D:125:ARG:HH11 | 1:D:125:ARG:HG2 | 1.62 | 0.65 |
| 1:A:642:PRO:O | 1:A:644:VAL:N | 2.30 | 0.65 |
| 1:C:115:LEU:O | 1:C:258:ARG:NH2 | 2.29 | 0.64 |
| 1:C:137:ALA:CB | 1:C:248:LEU:HD21 | 2.26 | 0.64 |
| 1:A:1:MET:HG3 | 1:A:55:SER:HB3 | 1.80 | 0.64 |
| 1:C:44:ALA:HB3 | 1:C:264:PHE:CE2 | 2.31 | 0.64 |
| 1:B:140:LEU:HD21 | 1:B:249:LEU:HB2 | 1.77 | 0.64 |
| 1:B:629:ILE:O | 1:B:633:ILE:HG12 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:226:ILE:N | 1:A:226:ILE:HD12 | 2.12 | 0.64 |
| 1:C:466:ARG:NE | 1:C:498:ALA:HB2 | 2.10 | 0.64 |
| 1:A:4:LEU:HD22 | 1:A:25:THR:O | 1.97 | 0.64 |
| 1:A:60:ASP:O | 1:A:64:VAL:HG23 | 1.97 | 0.64 |
| 1:B:225:GLN:H | 1:B:225:GLN:NE2 | 1.95 | 0.64 |
| 1:A:310:ARG:HB2 | 1:A:310:ARG:HH11 | 1.62 | 0.64 |
| 1:B:157:ARG:HE | 1:B:249:LEU:HD21 | 1.62 | 0.64 |
| 1:A:343:LEU:HD13 | 1:A:427:LEU:HD21 | 1.79 | 0.64 |
| 1:B:198:ALA:O | 1:B:202:ASN:HA | 1.97 | 0.64 |
| 1:D:1:MET:HA | 1:D:56:LEU:H | 1.63 | 0.64 |
| 1:C:172:LEU:HD11 | 1:C:216:VAL:HG23 | 1.78 | 0.64 |
| 1:A:352:LEU:HD11 | 1:A:650:LEU:HD23 | 1.78 | 0.64 |
| 1:A:140:LEU:HB2 | 1:A:244:PRO:O | 1.96 | 0.64 |
| 1:A:198:ALA:O | 1:A:202:ASN:HA | 1.97 | 0.64 |
| 1:C:352:LEU:HD12 | 1:C:363:LEU:HD13 | 1.78 | 0.64 |
| 1:C:381:GLN:HE21 | 1:C:402:TRP:HD1 | 1.43 | 0.64 |
| 1:D:140:LEU:HB3 | 1:D:144:TYR:HE2 | 1.63 | 0.64 |
| 1:A:444:CYS:SG | 1:A:448:VAL:HB | 2.36 | 0.64 |
| 1:C:82:SER:O | 1:C:86:ILE:HG13 | 1.97 | 0.64 |
| 1:B:139:ARG:NH2 | 1:B:162:PRO:HG3 | 2.13 | 0.64 |
| 1:D:284:LYS:HD2 | 1:D:284:LYS:H | 1.62 | 0.64 |
| 1:D:226:ILE:HD12 | 1:D:226:ILE:N | 2.13 | 0.64 |
| 1:B:67:TYR:OH | 1:B:114:PRO:HG3 | 1.97 | 0.64 |
| 1:D:420:ILE:O | 1:D:424:GLU:HG3 | 1.96 | 0.64 |
| 1:D:4:LEU:HD22 | 1:D:25:THR:O | 1.98 | 0.64 |
| 1:D:191:ILE:HG23 | 1:D:195:ARG:HD3 | 1.79 | 0.64 |
| 1:B:373:ASN:HD21 | 1:B:401:THR:CG2 | 2.08 | 0.64 |
| 1:D:637:GLN:O | 1:D:641:THR:HG23 | 1.98 | 0.64 |
| 1:A:561:ILE:HD12 | 1:A:561:ILE:N | 2.13 | 0.64 |
| 1:B:409:ILE:O | 1:B:413:ILE:HG12 | 1.98 | 0.64 |
| 1:A:125:ARG:HG2 | 1:A:125:ARG:HH11 | 1.63 | 0.64 |
| 1:A:402:TRP:CH2 | 1:B:396:VAL:HG23 | 2.34 | 0.63 |
| 1:A:615:THR:HA | 1:A:618:ARG:HH12 | 1.62 | 0.63 |
| 1:D:386:PRO:O | 1:D:389:ALA:HB3 | 1.98 | 0.63 |
| 1:B:4:LEU:HD22 | 1:B:25:THR:O | 1.98 | 0.63 |
| 1:C:4:LEU:HD22 | 1:C:25:THR:O | 1.99 | 0.63 |
| 1:A:494:ARG:NH1 | 1:A:494:ARG:HG2 | 2.13 | 0.63 |
| 1:C:114:PRO:HB3 | 1:C:258:ARG:NH1 | 2.12 | 0.63 |
| 1:C:310:ARG:HB2 | 1:C:310:ARG:HH11 | 1.63 | 0.63 |
| 1:B:125:ARG:HG2 | 1:B:125:ARG:HH11 | 1.62 | 0.63 |
| 1:C:717:VAL:O | 1:C:721:THR:HG23 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:679:MET:O | 1:A:750:VAL:HG23 | 1.98 | 0.63 |
| 1:C:1:MET:HG3 | 1:C:55:SER:HB3 | 1.80 | 0.63 |
| 1:C:191:ILE:HG23 | 1:C:195:ARG:HD3 | 1.79 | 0.63 |
| 1:B:191:ILE:HG23 | 1:B:195:ARG:HD3 | 1.81 | 0.63 |
| 1:D:159:VAL:HG23 | 1:D:248:LEU:C | 2.19 | 0.63 |
| 1:B:561:ILE:N | 1:B:561:ILE:HD12 | 2.13 | 0.63 |
| 1:D:236:ALA:N | 1:D:237:PRO:CD | 2.62 | 0.63 |
| 1:B:310:ARG:HB2 | 1:B:310:ARG:HH11 | 1.64 | 0.63 |
| 1:B:226:ILE:HD12 | 1:B:226:ILE:N | 2.13 | 0.63 |
| 1:C:41:LEU:HD13 | 1:C:264:PHE:CE2 | 2.33 | 0.63 |
| 1:B:687:SER:O | 1:B:691:ARG:HG3 | 1.98 | 0.63 |
| 1:A:307:ASP:OD1 | 1:A:391:PHE:HA | 1.97 | 0.63 |
| 1:C:256:LEU:O | 1:C:259:VAL:N | 2.29 | 0.63 |
| 1:B:265:LEU:N | 1:B:266:PRO:CD | 2.62 | 0.63 |
| 1:A:310:ARG:NH2 | 1:A:392:SER:HB3 | 2.14 | 0.63 |
| 1:A:137:ALA:HB1 | 1:A:248:LEU:HD21 | 1.78 | 0.63 |
| 1:A:243:PRO:HD2 | 1:A:246:LEU:HD12 | 1.81 | 0.63 |
| 1:D:687:SER:O | 1:D:691:ARG:HG3 | 1.98 | 0.63 |
| 1:A:82:SER:O | 1:A:86:ILE:HG13 | 1.99 | 0.62 |
| 1:C:226:ILE:N | 1:C:226:ILE:HD12 | 2.14 | 0.62 |
| 1:D:494:ARG:HG2 | 1:D:494:ARG:HH11 | 1.64 | 0.62 |
| 1:A:472:ALA:HA | 1:A:477:ILE:HD12 | 1.81 | 0.62 |
| 1:C:187:ALA:O | 1:C:188:ASN:HB2 | 1.99 | 0.62 |
| 1:B:94:GLU:HG2 | 1:B:316:GLY:CA | 2.29 | 0.62 |
| 1:B:60:ASP:O | 1:B:64:VAL:HG23 | 1.99 | 0.62 |
| 1:B:90:MET:HE3 | 1:B:318:ARG:HH22 | 1.63 | 0.62 |
| 1:D:251:PRO:HG2 | 1:D:254:PHE:CE1 | 2.35 | 0.62 |
| 1:A:494:ARG:HG2 | 1:A:494:ARG:HH11 | 1.64 | 0.62 |
| 1:B:187:ALA:O | 1:B:188:ASN:HB2 | 2.00 | 0.62 |
| 1:A:678:ARG:NH2 | 1:A:753:ASP:OD1 | 2.33 | 0.62 |
| 1:B:434:PRO:HA | 1:B:527:ILE:CG2 | 2.28 | 0.62 |
| 1:A:395:LEU:N | 1:A:395:LEU:HD23 | 2.15 | 0.62 |
| 1:D:225:GLN:NE2 | 1:D:225:GLN:H | 1.97 | 0.62 |
| 1:D:260:GLN:O | 1:D:264:PHE:HE1 | 1.83 | 0.62 |
| 1:A:705:ILE:HG23 | 1:A:711:ILE:HD11 | 1.82 | 0.62 |
| 1:D:618:ARG:HH11 | 1:D:618:ARG:HB2 | 1.64 | 0.62 |
| 1:D:243:PRO:HD2 | 1:D:246:LEU:HD12 | 1.82 | 0.62 |
| 1:B:717:VAL:O | 1:B:721:THR:HG23 | 1.98 | 0.62 |
| 1:A:38:GLY:HA3 | 1:A:317:TRP:CZ3 | 2.35 | 0.62 |
| 1:C:679:MET:O | 1:C:750:VAL:HG23 | 2.00 | 0.62 |
| 1:C:305:ARG:NE | 1:C:390:GLU:HG2 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:172:LEU:HD11 | 1:A:216:VAL:HG23 | 1.82 | 0.62 |
| 1:B:434:PRO:HA | 1:B:527:ILE:HG22 | 1.81 | 0.62 |
| 1:C:747:LEU:HB3 | 1:C:748:PRO:HD3 | 1.81 | 0.62 |
| 1:A:172:LEU:HB2 | 1:A:214:ALA:O | 2.00 | 0.62 |
| 1:C:60:ASP:O | 1:C:64:VAL:HG23 | 2.00 | 0.62 |
| 1:C:372:ARG:HD2 | 1:C:374:GLU:OE1 | 1.99 | 0.62 |
| 1:B:394:ASN:O | 1:B:395:LEU:HB2 | 1.98 | 0.62 |
| 1:C:346:ILE:HG21 | 1:C:427:LEU:HD13 | 1.80 | 0.62 |
| 1:B:104:PRO:HB3 | 1:B:280:CYS:SG | 2.40 | 0.62 |
| 1:C:629:ILE:O | 1:C:633:ILE:HG12 | 1.99 | 0.62 |
| 1:D:494:ARG:NH1 | 1:D:494:ARG:HG2 | 2.14 | 0.61 |
| 1:A:225:GLN:NE2 | 1:A:225:GLN:H | 1.98 | 0.61 |
| 1:A:405:MET:O | 1:A:409:ILE:HD13 | 1.99 | 0.61 |
| 1:D:642:PRO:O | 1:D:644:VAL:N | 2.33 | 0.61 |
| 1:C:699:VAL:O | 1:C:703:VAL:HG23 | 2.00 | 0.61 |
| 1:C:361:GLY:O | 1:C:365:GLU:HG3 | 2.00 | 0.61 |
| 1:D:147:TYR:HB3 | 1:D:150:LEU:HD22 | 1.82 | 0.61 |
| 1:B:721:THR:O | 1:B:725:ILE:HG12 | 2.01 | 0.61 |
| 1:A:687:SER:O | 1:A:691:ARG:HG3 | 2.01 | 0.61 |
| 1:A:191:ILE:HG23 | 1:A:195:ARG:HD3 | 1.83 | 0.61 |
| 1:C:642:PRO:O | 1:C:644:VAL:N | 2.33 | 0.61 |
| 1:A:71:LEU:HD22 | 1:A:262:LEU:HD13 | 1.81 | 0.61 |
| 1:D:60:ASP:CG | 1:D:124:LEU:HD13 | 2.21 | 0.61 |
| 1:A:747:LEU:HB3 | 1:A:748:PRO:HD3 | 1.81 | 0.61 |
| 1:C:178:GLN:HE21 | 1:C:212:LEU:CD1 | 2.14 | 0.61 |
| 1:C:159:VAL:HG23 | 1:C:248:LEU:C | 2.20 | 0.61 |
| 1:B:139:ARG:HH21 | 1:B:162:PRO:CG | 2.13 | 0.61 |
| 1:D:629:ILE:O | 1:D:633:ILE:HG12 | 2.01 | 0.61 |
| 1:B:243:PRO:HD2 | 1:B:246:LEU:HD12 | 1.82 | 0.61 |
| 1:C:262:LEU:HB3 | 1:C:263:GLN:NE2 | 2.16 | 0.61 |
| 1:B:154:LEU:HA | 1:B:157:ARG:HD3 | 1.83 | 0.61 |
| 1:D:717:VAL:O | 1:D:721:THR:HG23 | 2.00 | 0.61 |
| 1:A:310:ARG:O | 1:A:312:ARG:HG2 | 2.01 | 0.61 |
| 1:B:705:ILE:HG23 | 1:B:711:ILE:HD11 | 1.81 | 0.61 |
| 1:A:217:ARG:HB3 | 1:A:220:ASP:OD2 | 2.01 | 0.61 |
| 1:B:432:MET:HA | 1:B:479:VAL:O | 2.01 | 0.61 |
| 1:D:60:ASP:O | 1:D:64:VAL:HG23 | 2.01 | 0.61 |
| 1:D:310:ARG:HH11 | 1:D:310:ARG:HB2 | 1.64 | 0.60 |
| 1:D:693:THR:OG1 | 1:D:722:PHE:HB2 | 2.01 | 0.60 |
| 1:D:561:ILE:N | 1:D:561:ILE:HD12 | 2.16 | 0.60 |
| 1:D:369:GLU:HG3 | 1:D:482:SER:CB | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:489:PHE:CZ | 1:A:534:ALA:HA | 2.36 | 0.60 |
| 1:D:699:VAL:O | 1:D:703:VAL:HG23 | 2.00 | 0.60 |
| 1:B:172:LEU:HD11 | 1:B:216:VAL:HG23 | 1.81 | 0.60 |
| 1:B:217:ARG:HB3 | 1:B:220:ASP:OD2 | 2.00 | 0.60 |
| 1:A:115:LEU:O | 1:A:258:ARG:NH2 | 2.34 | 0.60 |
| 1:A:535:ARG:O | 1:A:539:LEU:HD12 | 2.01 | 0.60 |
| 1:A:33:PHE:CD2 | 1:A:318:ARG:HB2 | 2.36 | 0.60 |
| 1:B:432:MET:HE1 | 1:B:534:ALA:C | 2.22 | 0.60 |
| 1:B:372:ARG:HD2 | 1:B:374:GLU:OE1 | 2.02 | 0.60 |
| 1:A:346:ILE:HG21 | 1:A:427:LEU:HD13 | 1.81 | 0.60 |
| 1:B:564:LEU:HB3 | 1:B:592:VAL:HG11 | 1.83 | 0.60 |
| 1:C:605:SER:HB3 | 1:C:634:ARG:HH12 | 1.66 | 0.60 |
| 1:D:41:LEU:HD12 | 1:D:41:LEU:O | 2.00 | 0.60 |
| 1:B:437:SER:HB3 | 1:B:478:SER:H | 1.65 | 0.60 |
| 1:D:37:ALA:HB2 | 1:D:43:ALA:CA | 2.31 | 0.60 |
| 1:D:154:LEU:HA | 1:D:157:ARG:HD3 | 1.84 | 0.60 |
| 1:D:342:VAL:HA | 1:D:658:CYS:SG | 2.42 | 0.60 |
| 1:D:609:LYS:HZ3 | 1:D:641:THR:HG21 | 1.64 | 0.60 |
| 1:D:567:TYR:HA | 1:D:572:GLN:HE22 | 1.66 | 0.60 |
| 1:A:12:THR:HG22 | 1:A:44:ALA:HB2 | 1.82 | 0.60 |
| 1:A:564:LEU:HB3 | 1:A:592:VAL:HG11 | 1.84 | 0.60 |
| 1:C:409:ILE:O | 1:C:413:ILE:HG12 | 2.01 | 0.60 |
| 1:D:369:GLU:CG | 1:D:485:VAL:HG23 | 2.30 | 0.60 |
| 1:D:158:MET:HE1 | 1:D:256:LEU:HD13 | 1.84 | 0.60 |
| 1:D:310:ARG:O | 1:D:312:ARG:HG2 | 2.02 | 0.60 |
| 1:D:405:MET:O | 1:D:409:ILE:HD13 | 2.02 | 0.60 |
| 1:C:564:LEU:HB3 | 1:C:592:VAL:HG11 | 1.82 | 0.60 |
| 1:B:535:ARG:O | 1:B:539:LEU:HD12 | 2.01 | 0.60 |
| 1:D:80:PRO:O | 1:D:82:SER:N | 2.35 | 0.60 |
| 1:D:678:ARG:NH2 | 1:D:753:ASP:OD1 | 2.34 | 0.60 |
| 1:B:699:VAL:O | 1:B:703:VAL:HG23 | 2.02 | 0.60 |
| 1:C:561:ILE:HD12 | 1:C:561:ILE:N | 2.17 | 0.60 |
| 1:C:259:VAL:O | 1:C:263:GLN:NE2 | 2.35 | 0.60 |
| 1:C:705:ILE:HG23 | 1:C:711:ILE:HD11 | 1.83 | 0.60 |
| 1:C:284:LYS:N | 1:C:284:LYS:HD2 | 2.17 | 0.60 |
| 1:A:523:VAL:C | 1:A:524:VAL:HG23 | 2.20 | 0.60 |
| 1:B:225:GLN:CD | 1:B:225:GLN:H | 2.05 | 0.60 |
| 1:A:350:ARG:HD3 | 1:A:538:TRP:O | 2.02 | 0.60 |
| 1:A:368:MET:O | 1:A:372:ARG:HB2 | 2.02 | 0.60 |
| 1:B:458:GLY:C | 1:B:460:ALA:H | 2.06 | 0.60 |
| 1:B:361:GLY:O | 1:B:365:GLU:HG3 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:327:SER:O | 1:D:331:VAL:HG23 | 2.02 | 0.60 |
| 1:C:139:ARG:HG3 | 1:C:247:CYS:O | 2.02 | 0.59 |
| 1:A:409:ILE:O | 1:A:413:ILE:HG12 | 2.02 | 0.59 |
| 1:D:747:LEU:HB3 | 1:D:748:PRO:HD3 | 1.84 | 0.59 |
| 1:C:140:LEU:HD23 | 1:C:249:LEU:HB2 | 1.84 | 0.59 |
| 1:A:158:MET:CE | 1:A:256:LEU:HD13 | 2.32 | 0.59 |
| 1:C:36:SER:HB2 | 1:C:312:ARG:O | 2.03 | 0.59 |
| 1:D:217:ARG:HB3 | 1:D:220:ASP:OD2 | 2.00 | 0.59 |
| 1:C:161:THR:OG1 | 1:C:164:ILE:HB | 2.01 | 0.59 |
| 1:B:642:PRO:O | 1:B:644:VAL:N | 2.35 | 0.59 |
| 1:C:693:THR:OG1 | 1:C:722:PHE:HB2 | 2.02 | 0.59 |
| 1:A:567:TYR:HA | 1:A:572:GLN:HE22 | 1.68 | 0.59 |
| 1:D:261:ALA:O | 1:D:264:PHE:HD1 | 1.84 | 0.59 |
| 1:C:612:ALA:O | 1:C:616:VAL:HG23 | 2.02 | 0.59 |
| 1:C:432:MET:HE2 | 1:C:534:ALA:HB1 | 1.84 | 0.59 |
| 1:D:187:ALA:O | 1:D:188:ASN:HB2 | 2.02 | 0.59 |
| 1:C:21:LEU:HD11 | 1:C:110:LEU:HB2 | 1.84 | 0.59 |
| 1:C:171:VAL:HA | 1:C:215:ALA:HB2 | 1.84 | 0.59 |
| 1:B:693:THR:OG1 | 1:B:722:PHE:HB2 | 2.03 | 0.59 |
| 1:A:34:LYS:HB3 | 1:A:45:GLU:HG3 | 1.82 | 0.59 |
| 1:A:523:VAL:HB | 1:A:528:ASP:OD2 | 2.02 | 0.59 |
| 1:A:420:ILE:HD13 | 1:A:569:ARG:NH2 | 2.17 | 0.59 |
| 1:A:458:GLY:C | 1:A:460:ALA:H | 2.06 | 0.59 |
| 1:B:494:ARG:NH1 | 1:B:494:ARG:HG2 | 2.17 | 0.59 |
| 1:B:71:LEU:HD22 | 1:B:262:LEU:CD1 | 2.33 | 0.59 |
| 1:B:448:VAL:HG13 | 1:B:468:LEU:HD23 | 1.84 | 0.59 |
| 1:C:154:LEU:HA | 1:C:157:ARG:HD3 | 1.83 | 0.59 |
| 1:C:14:ARG:HH12 | 1:C:223:ASP:HA | 1.67 | 0.59 |
| 1:C:39:ARG:C | 1:C:41:LEU:H | 2.06 | 0.59 |
| 1:A:256:LEU:O | 1:A:257:ILE:C | 2.41 | 0.59 |
| 1:D:82:SER:O | 1:D:86:ILE:HG13 | 2.02 | 0.59 |
| 1:B:559:PRO:CG | 1:B:599:ILE:HG13 | 2.33 | 0.59 |
| 1:B:599:ILE:HG21 | 1:B:631:PHE:CE1 | 2.38 | 0.59 |
| 1:B:637:GLN:O | 1:B:641:THR:HG23 | 2.02 | 0.59 |
| 1:C:458:GLY:C | 1:C:460:ALA:H | 2.05 | 0.59 |
| 1:B:333:GLN:NE2 | 1:B:672:THR:HB | 2.18 | 0.59 |
| 1:D:144:TYR:CE2 | 1:D:244:PRO:HB3 | 2.38 | 0.59 |
| 1:A:187:ALA:O | 1:A:188:ASN:HB2 | 2.03 | 0.59 |
| 1:D:548:GLN:HE21 | 1:D:548:GLN:HA | 1.67 | 0.59 |
| 1:C:327:SER:O | 1:C:331:VAL:HG23 | 2.02 | 0.59 |
| 1:B:497:PRO:HG2 | 1:B:500:ASP:OD2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:605:SER:CB | 1:C:634:ARG:HH12 | 2.16 | 0.59 |
| 1:C:391:PHE:O | 1:C:392:SER:HB3 | 2.03 | 0.59 |
| 1:D:171:VAL:HA | 1:D:215:ALA:HB2 | 1.84 | 0.59 |
| 1:D:705:ILE:HG23 | 1:D:711:ILE:HD11 | 1.85 | 0.59 |
| 1:D:612:ALA:HB2 | 1:D:703:VAL:HG21 | 1.85 | 0.59 |
| 1:B:94:GLU:HG2 | 1:B:316:GLY:HA3 | 1.84 | 0.59 |
| 1:B:697:PRO:O | 1:B:699:VAL:N | 2.36 | 0.59 |
| 1:C:225:GLN:NE2 | 1:C:225:GLN:H | 2.00 | 0.59 |
| 1:C:217:ARG:HB3 | 1:C:220:ASP:OD2 | 2.02 | 0.58 |
| 1:A:432:MET:HE1 | 1:A:534:ALA:O | 2.03 | 0.58 |
| 1:D:458:GLY:C | 1:D:460:ALA:H | 2.06 | 0.58 |
| 1:C:494:ARG:NH1 | 1:C:494:ARG:HG2 | 2.17 | 0.58 |
| 1:B:473:CYS:HA | 1:B:490:LEU:HD13 | 1.84 | 0.58 |
| 1:A:266:PRO:O | 1:A:270:LYS:HG3 | 2.04 | 0.58 |
| 1:A:80:PRO:O | 1:A:82:SER:N | 2.35 | 0.58 |
| 1:C:310:ARG:O | 1:C:312:ARG:HG2 | 2.03 | 0.58 |
| 1:B:310:ARG:O | 1:B:312:ARG:HG2 | 2.03 | 0.58 |
| 1:A:535:ARG:HH11 | 1:A:535:ARG:HG3 | 1.69 | 0.58 |
| 1:D:564:LEU:HB3 | 1:D:592:VAL:HG11 | 1.84 | 0.58 |
| 1:D:457:MET:O | 1:D:459:GLU:N | 2.36 | 0.58 |
| 1:A:372:ARG:HD2 | 1:A:374:GLU:OE1 | 2.02 | 0.58 |
| 1:D:401:THR:HG22 | 1:D:402:TRP:N | 2.17 | 0.58 |
| 1:A:373:ASN:ND2 | 1:A:401:THR:HG21 | 2.13 | 0.58 |
| 1:C:193:TYR:HE2 | 1:C:241:PHE:HB2 | 1.66 | 0.58 |
| 1:B:82:SER:O | 1:B:86:ILE:HG13 | 2.03 | 0.58 |
| 1:A:253:GLU:O | 1:A:255:ASP:N | 2.35 | 0.58 |
| 1:A:457:MET:O | 1:A:459:GLU:N | 2.36 | 0.58 |
| 1:B:678:ARG:NH2 | 1:B:753:ASP:OD1 | 2.35 | 0.58 |
| 1:C:535:ARG:O | 1:C:539:LEU:HD12 | 2.03 | 0.58 |
| 1:A:445:PRO:HG2 | 1:A:448:VAL:HG23 | 1.85 | 0.58 |
| 1:C:432:MET:HE1 | 1:C:534:ALA:C | 2.23 | 0.58 |
| 1:B:159:VAL:HG23 | 1:B:248:LEU:O | 2.02 | 0.58 |
| 1:C:335:LEU:O | 1:C:411:GLY:HA3 | 2.03 | 0.58 |
| 1:D:139:ARG:HG3 | 1:D:247:CYS:O | 2.03 | 0.58 |
| 1:C:159:VAL:HA | 1:C:250:LEU:HG | 1.86 | 0.58 |
| 1:D:612:ALA:O | 1:D:616:VAL:HG23 | 2.03 | 0.58 |
| 1:D:137:ALA:HB2 | 1:D:251:PRO:HD3 | 1.85 | 0.58 |
| 1:D:225:GLN:CD | 1:D:225:GLN:H | 2.07 | 0.58 |
| 1:D:721:THR:O | 1:D:725:ILE:HG12 | 2.01 | 0.58 |
| 1:B:327:SER:O | 1:B:331:VAL:HG23 | 2.03 | 0.58 |
| 1:A:693:THR:OG1 | 1:A:722:PHE:HB2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:699:VAL:O | 1:A:703:VAL:HG23 | 2.02 | 0.58 |
| 1:C:137:ALA:HB3 | 1:C:248:LEU:HD21 | 1.84 | 0.58 |
| 1:B:284:LYS:N | 1:B:284:LYS:HD2 | 2.18 | 0.58 |
| 1:D:472:ALA:CB | 1:D:477:ILE:HD12 | 2.33 | 0.58 |
| 1:C:310:ARG:O | 1:C:312:ARG:N | 2.37 | 0.58 |
| 1:A:523:VAL:HG13 | 1:D:619:SER:OG | 2.03 | 0.58 |
| 1:A:456:CYS:SG | 1:A:524:VAL:HA | 2.44 | 0.58 |
| 1:C:494:ARG:HH11 | 1:C:494:ARG:HG2 | 1.68 | 0.58 |
| 1:B:213:VAL:O | 1:B:241:PHE:HA | 2.04 | 0.58 |
| 1:C:497:PRO:HG2 | 1:C:500:ASP:OD2 | 2.04 | 0.58 |
| 1:A:154:LEU:HA | 1:A:157:ARG:HD3 | 1.84 | 0.58 |
| 1:B:321:PHE:CD2 | 1:B:325:GLY:HA2 | 2.39 | 0.58 |
| 1:C:114:PRO:O | 1:C:115:LEU:HD23 | 2.03 | 0.58 |
| 1:B:343:LEU:HD13 | 1:B:427:LEU:HD21 | 1.85 | 0.58 |
| 1:D:310:ARG:O | 1:D:312:ARG:N | 2.37 | 0.58 |
| 1:D:527:ILE:N | 1:D:527:ILE:HD12 | 2.19 | 0.58 |
| 1:C:612:ALA:HB2 | 1:C:703:VAL:HG21 | 1.85 | 0.58 |
| 1:C:327:SER:OG | 1:C:329:THR:HB | 2.04 | 0.58 |
| 1:B:360:VAL:O | 1:B:364:VAL:HG23 | 2.04 | 0.58 |
| 1:C:21:LEU:HD13 | 1:C:112:PHE:CE1 | 2.38 | 0.58 |
| 1:C:405:MET:O | 1:C:409:ILE:HD13 | 2.04 | 0.58 |
| 1:C:80:PRO:O | 1:C:82:SER:N | 2.35 | 0.58 |
| 1:B:337:LEU:HD22 | 1:B:673:GLU:HA | 1.84 | 0.58 |
| 1:A:721:THR:O | 1:A:725:ILE:HG12 | 2.03 | 0.58 |
| 1:D:361:GLY:O | 1:D:365:GLU:HG3 | 2.03 | 0.58 |
| 1:A:401:THR:HG22 | 1:A:403:ALA:N | 2.19 | 0.57 |
| 1:B:599:ILE:HG21 | 1:B:631:PHE:HE1 | 1.69 | 0.57 |
| 1:C:125:ARG:NH1 | 1:C:125:ARG:HG2 | 2.18 | 0.57 |
| 1:C:564:LEU:HD23 | 1:C:592:VAL:HG12 | 1.85 | 0.57 |
| 1:B:159:VAL:HG23 | 1:B:248:LEU:C | 2.23 | 0.57 |
| 1:A:327:SER:OG | 1:A:329:THR:HB | 2.04 | 0.57 |
| 1:C:243:PRO:HD2 | 1:C:246:LEU:HD12 | 1.85 | 0.57 |
| 1:A:376:LEU:O | 1:A:380:VAL:HG23 | 2.04 | 0.57 |
| 1:D:161:THR:OG1 | 1:D:164:ILE:HB | 2.04 | 0.57 |
| 1:A:310:ARG:O | 1:A:312:ARG:N | 2.37 | 0.57 |
| 1:C:675:ALA:O | 1:C:679:MET:HG3 | 2.04 | 0.57 |
| 1:B:112:PHE:CG | 1:B:265:LEU:HD22 | 2.40 | 0.57 |
| 1:D:4:LEU:HD21 | 1:D:26:HIS:ND1 | 2.20 | 0.57 |
| 1:B:71:LEU:HD22 | 1:B:262:LEU:HD13 | 1.86 | 0.57 |
| 1:A:298:PHE:CZ | 1:A:331:VAL:HG21 | 2.40 | 0.57 |
| 1:D:372:ARG:HD2 | 1:D:374:GLU:OE1 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:637:GLN:O | 1:A:641:THR:HG23 | 2.05 | 0.57 |
| 1:C:473:CYS:C | 1:C:475:GLN:H | 2.08 | 0.57 |
| 1:D:37:ALA:HB2 | 1:D:43:ALA:CB | 2.35 | 0.57 |
| 1:A:497:PRO:HG2 | 1:A:500:ASP:OD2 | 2.04 | 0.57 |
| 1:C:567:TYR:HA | 1:C:572:GLN:HE22 | 1.69 | 0.57 |
| 1:B:747:LEU:HB3 | 1:B:748:PRO:HD3 | 1.85 | 0.57 |
| 1:D:637:GLN:HA | 1:D:640:LEU:HD12 | 1.85 | 0.57 |
| 1:A:284:LYS:HD2 | 1:A:284:LYS:N | 2.18 | 0.57 |
| 1:A:161:THR:OG1 | 1:A:164:ILE:HB | 2.04 | 0.57 |
| 1:D:227:PRO:HG3 | 1:D:234:ASP:OD2 | 2.05 | 0.57 |
| 1:D:178:GLN:HE21 | 1:D:212:LEU:CD1 | 2.14 | 0.57 |
| 1:A:60:ASP:CG | 1:A:124:LEU:HD13 | 2.24 | 0.57 |
| 1:A:507:LEU:HD22 | 1:A:588:VAL:HG21 | 1.85 | 0.57 |
| 1:D:497:PRO:HG2 | 1:D:500:ASP:OD2 | 2.04 | 0.57 |
| 1:B:251:PRO:HG2 | 1:B:254:PHE:CD1 | 2.40 | 0.57 |
| 1:C:140:LEU:HD12 | 1:C:213:VAL:HG21 | 1.87 | 0.57 |
| 1:B:310:ARG:O | 1:B:312:ARG:N | 2.38 | 0.57 |
| 1:A:470:ASP:O | 1:A:474:GLU:HG2 | 2.04 | 0.57 |
| 1:C:462:ALA:O | 1:C:465:PHE:N | 2.36 | 0.57 |
| 1:A:112:PHE:CD2 | 1:A:265:LEU:HD13 | 2.40 | 0.57 |
| 1:C:721:THR:O | 1:C:725:ILE:HG12 | 2.05 | 0.57 |
| 1:C:33:PHE:CD2 | 1:C:318:ARG:HB2 | 2.40 | 0.57 |
| 1:C:321:PHE:CD2 | 1:C:325:GLY:HA2 | 2.40 | 0.57 |
| 1:D:34:LYS:HB3 | 1:D:45:GLU:HG3 | 1.85 | 0.57 |
| 1:B:60:ASP:CG | 1:B:124:LEU:HD13 | 2.25 | 0.57 |
| 1:B:612:ALA:O | 1:B:616:VAL:HG23 | 2.04 | 0.57 |
| 1:D:37:ALA:HB2 | 1:D:43:ALA:N | 2.20 | 0.56 |
| 1:C:527:ILE:HD12 | 1:C:527:ILE:N | 2.20 | 0.56 |
| 1:B:494:ARG:HH11 | 1:B:494:ARG:HG2 | 1.69 | 0.56 |
| 1:D:145:THR:O | 1:D:147:TYR:N | 2.38 | 0.56 |
| 1:C:708:HIS:HB3 | 1:C:711:ILE:HG21 | 1.87 | 0.56 |
| 1:B:236:ALA:N | 1:B:237:PRO:CD | 2.68 | 0.56 |
| 1:A:225:GLN:CD | 1:A:225:GLN:H | 2.07 | 0.56 |
| 1:A:327:SER:O | 1:A:331:VAL:HG23 | 2.05 | 0.56 |
| 1:C:685:THR:HG22 | 1:D:487:THR:HG21 | 1.87 | 0.56 |
| 1:C:678:ARG:NH2 | 1:C:753:ASP:OD1 | 2.38 | 0.56 |
| 1:C:637:GLN:O | 1:C:641:THR:HG23 | 2.05 | 0.56 |
| 1:A:4:LEU:HD21 | 1:A:26:HIS:ND1 | 2.20 | 0.56 |
| 1:A:97:PHE:HZ | 1:A:301:THR:HA | 1.71 | 0.56 |
| 1:B:14:ARG:HB2 | 1:B:257:ILE:HD12 | 1.87 | 0.56 |
| 1:D:462:ALA:HA | 1:D:498:ALA:HB1 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:112:PHE:CE2 | 1:B:265:LEU:HB3 | 2.41 | 0.56 |
| 1:B:172:LEU:HD12 | 1:B:239:LEU:HD13 | 1.87 | 0.56 |
| 1:C:60:ASP:CG | 1:C:124:LEU:HD13 | 2.25 | 0.56 |
| 1:A:612:ALA:HB2 | 1:A:703:VAL:HG21 | 1.87 | 0.56 |
| 1:C:437:SER:HB3 | 1:C:478:SER:O | 2.06 | 0.56 |
| 1:D:369:GLU:CG | 1:D:482:SER:OG | 2.54 | 0.56 |
| 1:B:711:ILE:O | 1:B:711:ILE:HD12 | 2.06 | 0.56 |
| 1:D:136:ASP:O | 1:D:137:ALA:C | 2.44 | 0.56 |
| 1:D:327:SER:OG | 1:D:329:THR:HB | 2.05 | 0.56 |
| 1:A:321:PHE:CD2 | 1:A:325:GLY:HA2 | 2.41 | 0.56 |
| 1:B:242:LEU:N | 1:B:242:LEU:HD23 | 2.20 | 0.56 |
| 1:D:262:LEU:HD12 | 1:D:262:LEU:O | 2.05 | 0.56 |
| 1:B:527:ILE:HD12 | 1:B:527:ILE:N | 2.19 | 0.56 |
| 1:D:725:ILE:HG22 | 1:D:729:ILE:HD11 | 1.88 | 0.56 |
| 1:A:512:SER:HA | 1:A:517:LEU:HD11 | 1.88 | 0.56 |
| 1:B:680:ARG:HH11 | 1:B:680:ARG:HG3 | 1.71 | 0.56 |
| 1:D:23:LEU:CD2 | 1:D:110:LEU:HB3 | 2.36 | 0.56 |
| 1:B:432:MET:HE1 | 1:B:534:ALA:O | 2.06 | 0.56 |
| 1:C:547:GLU:HG2 | 1:C:548:GLN:N | 2.21 | 0.56 |
| 1:C:432:MET:HA | 1:C:479:VAL:O | 2.06 | 0.56 |
| 1:B:339:GLY:HA3 | 1:B:407:GLU:O | 2.06 | 0.56 |
| 1:D:512:SER:HA | 1:D:517:LEU:HD11 | 1.88 | 0.56 |
| 1:D:369:GLU:HG3 | 1:D:482:SER:HB2 | 1.87 | 0.56 |
| 1:B:80:PRO:O | 1:B:82:SER:N | 2.38 | 0.56 |
| 1:C:262:LEU:C | 1:C:264:PHE:H | 2.10 | 0.56 |
| 1:A:624:ILE:CD1 | 1:A:624:ILE:H | 2.19 | 0.56 |
| 1:B:178:GLN:HE21 | 1:B:212:LEU:CD1 | 2.16 | 0.55 |
| 1:D:143:GLU:O | 1:D:146:ASP:N | 2.39 | 0.55 |
| 1:B:612:ALA:HB2 | 1:B:703:VAL:HG21 | 1.87 | 0.55 |
| 1:B:457:MET:O | 1:B:459:GLU:N | 2.38 | 0.55 |
| 1:D:376:LEU:O | 1:D:380:VAL:HG23 | 2.06 | 0.55 |
| 1:B:394:ASN:HD21 | 1:B:396:VAL:HB | 1.71 | 0.55 |
| 1:D:342:VAL:HG23 | 1:D:343:LEU:N | 2.20 | 0.55 |
| 1:D:711:ILE:O | 1:D:711:ILE:HD12 | 2.05 | 0.55 |
| 1:D:235:LEU:C | 1:D:237:PRO:HD2 | 2.26 | 0.55 |
| 1:B:191:ILE:HG22 | 1:B:192:THR:N | 2.21 | 0.55 |
| 1:C:489:PHE:CZ | 1:C:534:ALA:HA | 2.41 | 0.55 |
| 1:A:464:GLU:O | 1:A:468:LEU:HG | 2.06 | 0.55 |
| 1:B:603:GLU:HA | 1:B:634:ARG:HH22 | 1.70 | 0.55 |
| 1:C:637:GLN:HA | 1:C:640:LEU:HD12 | 1.87 | 0.55 |
| 1:A:361:GLY:O | 1:A:365:GLU:HG3 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:738:ALA:O | 1:B:741:PHE:HB3 | 2.06 | 0.55 |
| 1:D:292:ILE:HD12 | 1:D:292:ILE:C | 2.26 | 0.55 |
| 1:D:360:VAL:O | 1:D:364:VAL:HG23 | 2.06 | 0.55 |
| 1:A:23:LEU:HD21 | 1:A:272:ILE:HD13 | 1.89 | 0.55 |
| 1:D:708:HIS:HB3 | 1:D:711:ILE:HG21 | 1.89 | 0.55 |
| 1:B:171:VAL:HA | 1:B:215:ALA:HB2 | 1.87 | 0.55 |
| 1:A:207:ALA:HB1 | 1:A:210:LEU:HG | 1.88 | 0.55 |
| 1:D:21:LEU:HD13 | 1:D:112:PHE:CE1 | 2.41 | 0.55 |
| 1:D:145:THR:C | 1:D:147:TYR:H | 2.08 | 0.55 |
| 1:B:140:LEU:C | 1:B:142:ASP:H | 2.09 | 0.55 |
| 1:D:207:ALA:HB1 | 1:D:210:LEU:HG | 1.87 | 0.55 |
| 1:C:235:LEU:C | 1:C:237:PRO:CD | 2.75 | 0.55 |
| 1:D:663:HIS:CD2 | 1:D:743:ARG:HB3 | 2.41 | 0.55 |
| 1:D:221:LEU:O | 1:D:222:LYS:C | 2.45 | 0.55 |
| 1:D:242:LEU:N | 1:D:242:LEU:HD23 | 2.21 | 0.55 |
| 1:B:342:VAL:HG12 | 1:B:658:CYS:SG | 2.46 | 0.55 |
| 1:A:527:ILE:N | 1:A:527:ILE:HD12 | 2.22 | 0.55 |
| 1:D:284:LYS:N | 1:D:284:LYS:HD2 | 2.20 | 0.55 |
| 1:C:725:ILE:HG22 | 1:C:729:ILE:HD11 | 1.89 | 0.55 |
| 1:C:457:MET:O | 1:C:459:GLU:N | 2.38 | 0.55 |
| 1:D:471:TYR:CZ | 1:D:475:GLN:HG3 | 2.42 | 0.55 |
| 1:B:114:PRO:O | 1:B:115:LEU:HD23 | 2.06 | 0.55 |
| 1:A:171:VAL:HA | 1:A:215:ALA:HB2 | 1.88 | 0.55 |
| 1:B:708:HIS:HB3 | 1:B:711:ILE:HG21 | 1.88 | 0.55 |
| 1:C:342:VAL:HG23 | 1:C:343:LEU:N | 2.21 | 0.55 |
| 1:D:114:PRO:O | 1:D:115:LEU:HD23 | 2.07 | 0.55 |
| 1:A:725:ILE:HG22 | 1:A:729:ILE:HD11 | 1.89 | 0.55 |
| 1:B:4:LEU:HD21 | 1:B:26:HIS:ND1 | 2.22 | 0.55 |
| 1:B:725:ILE:HG22 | 1:B:729:ILE:HD11 | 1.89 | 0.55 |
| 1:C:697:PRO:O | 1:C:699:VAL:N | 2.39 | 0.55 |
| 1:C:298:PHE:CZ | 1:C:331:VAL:HG21 | 2.42 | 0.55 |
| 1:C:225:GLN:H | 1:C:225:GLN:CD | 2.08 | 0.55 |
| 1:A:298:PHE:HZ | 1:A:331:VAL:HG21 | 1.72 | 0.55 |
| 1:D:375:ALA:O | 1:D:378:TYR:HB3 | 2.06 | 0.55 |
| 1:D:110:LEU:HD13 | 1:D:272:ILE:CD1 | 2.29 | 0.55 |
| 1:D:158:MET:HE1 | 1:D:170:VAL:HB | 1.89 | 0.55 |
| 1:C:42:PRO:HB3 | 1:C:223:ASP:HB3 | 1.88 | 0.55 |
| 1:B:564:LEU:HD23 | 1:B:592:VAL:HG12 | 1.88 | 0.55 |
| 1:A:462:ALA:HB1 | 1:A:498:ALA:HB3 | 1.88 | 0.55 |
| 1:C:306:LEU:HD22 | 1:C:400:LYS:NZ | 2.22 | 0.55 |
| 1:A:178:GLN:HE21 | 1:A:212:LEU:CD1 | 2.15 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:489:PHE:CZ | 1:B:534:ALA:HA | 2.42 | 0.55 |
| 1:B:543:GLY:HA3 | 1:B:561:ILE:O | 2.06 | 0.55 |
| 1:B:562:PRO:HB3 | 1:B:595:LEU:HB2 | 1.89 | 0.55 |
| 1:C:360:VAL:O | 1:C:364:VAL:HG23 | 2.07 | 0.55 |
| 1:B:425:GLU:HG2 | 1:B:429:LYS:HE3 | 1.89 | 0.55 |
| 1:D:191:ILE:HG22 | 1:D:192:THR:N | 2.22 | 0.55 |
| 1:A:437:SER:HB3 | 1:A:478:SER:O | 2.07 | 0.55 |
| 1:D:350:ARG:HD3 | 1:D:538:TRP:O | 2.05 | 0.55 |
| 1:B:179:THR:HG22 | 1:B:181:LEU:H | 1.72 | 0.54 |
| 1:C:305:ARG:HD2 | 1:C:390:GLU:CB | 2.37 | 0.54 |
| 1:D:369:GLU:HG3 | 1:D:482:SER:OG | 2.07 | 0.54 |
| 1:A:637:GLN:HA | 1:A:640:LEU:HD12 | 1.89 | 0.54 |
| 1:B:637:GLN:HA | 1:B:640:LEU:HD12 | 1.89 | 0.54 |
| 1:B:327:SER:OG | 1:B:329:THR:HB | 2.06 | 0.54 |
| 1:B:680:ARG:NH1 | 1:B:680:ARG:HG3 | 2.21 | 0.54 |
| 1:B:161:THR:OG1 | 1:B:164:ILE:HB | 2.06 | 0.54 |
| 1:D:675:ALA:O | 1:D:679:MET:HG3 | 2.07 | 0.54 |
| 1:D:147:TYR:HB3 | 1:D:150:LEU:HB2 | 1.90 | 0.54 |
| 1:A:711:ILE:HD12 | 1:A:711:ILE:O | 2.06 | 0.54 |
| 1:B:428:ALA:HB3 | 1:B:511:PHE:CZ | 2.42 | 0.54 |
| 1:C:663:HIS:CD2 | 1:C:743:ARG:HB3 | 2.42 | 0.54 |
| 1:B:14:ARG:HD3 | 1:B:257:ILE:HD13 | 1.90 | 0.54 |
| 1:B:333:GLN:HE21 | 1:B:673:GLU:CB | 2.21 | 0.54 |
| 1:C:191:ILE:HG22 | 1:C:192:THR:N | 2.22 | 0.54 |
| 1:C:164:ILE:HG22 | 1:C:164:ILE:O | 2.07 | 0.54 |
| 1:C:375:ALA:O | 1:C:378:TYR:HB3 | 2.07 | 0.54 |
| 1:A:738:ALA:O | 1:A:741:PHE:HB3 | 2.07 | 0.54 |
| 1:D:335:LEU:O | 1:D:411:GLY:HA3 | 2.08 | 0.54 |
| 1:C:265:LEU:HB2 | 1:C:266:PRO:HD3 | 1.89 | 0.54 |
| 1:B:663:HIS:CD2 | 1:B:743:ARG:HB3 | 2.43 | 0.54 |
| 1:A:21:LEU:HD21 | 1:A:272:ILE:HD11 | 1.88 | 0.54 |
| 1:A:265:LEU:N | 1:A:266:PRO:CD | 2.70 | 0.54 |
| 1:B:20:LEU:HB2 | 1:B:115:LEU:HD11 | 1.90 | 0.54 |
| 1:D:432:MET:HE1 | 1:D:534:ALA:O | 2.08 | 0.54 |
| 1:D:128:MET:O | 1:D:132:GLN:HG3 | 2.07 | 0.54 |
| 1:D:327:SER:HG | 1:D:329:THR:HB | 1.73 | 0.54 |
| 1:B:567:TYR:HA | 1:B:572:GLN:HE22 | 1.71 | 0.54 |
| 1:C:23:LEU:HD21 | 1:C:272:ILE:HD13 | 1.89 | 0.54 |
| 1:D:170:VAL:HG11 | 1:D:221:LEU:HD22 | 1.87 | 0.54 |
| 1:C:624:ILE:H | 1:C:624:ILE:CD1 | 2.21 | 0.54 |
| 1:D:141:SER:C | 1:D:143:GLU:H | 2.11 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:298:PHE:HZ | 1:C:331:VAL:HG21 | 1.73 | 0.54 |
| 1:D:564:LEU:HD23 | 1:D:592:VAL:HG12 | 1.88 | 0.54 |
| 1:A:697:PRO:O | 1:A:699:VAL:N | 2.40 | 0.54 |
| 1:B:136:ASP:O | 1:B:137:ALA:C | 2.46 | 0.54 |
| 1:C:105:PRO:HG2 | 1:C:106:GLN:H | 1.73 | 0.54 |
| 1:C:596:TYR:CE2 | 1:C:600:LEU:HD11 | 2.42 | 0.54 |
| 1:C:158:MET:HG3 | 1:C:259:VAL:CG2 | 2.37 | 0.54 |
| 1:D:489:PHE:CZ | 1:D:534:ALA:HA | 2.42 | 0.54 |
| 1:C:546:VAL:HB | 1:C:644:VAL:HG13 | 1.89 | 0.54 |
| 1:C:451:ALA:O | 1:C:455:VAL:HG23 | 2.08 | 0.54 |
| 1:A:708:HIS:HB3 | 1:A:711:ILE:HG21 | 1.90 | 0.54 |
| 1:B:230:GLY:HA2 | 1:B:233:ASP:OD2 | 2.07 | 0.54 |
| 1:B:376:LEU:O | 1:B:380:VAL:HG23 | 2.08 | 0.54 |
| 1:B:600:LEU:HD21 | 1:B:631:PHE:HA | 1.89 | 0.54 |
| 1:A:172:LEU:HD12 | 1:A:239:LEU:HD13 | 1.89 | 0.54 |
| 1:B:266:PRO:O | 1:B:270:LYS:HG3 | 2.08 | 0.54 |
| 1:A:159:VAL:HG21 | 1:A:247:CYS:HB3 | 1.90 | 0.54 |
| 1:A:342:VAL:HG23 | 1:A:343:LEU:N | 2.23 | 0.54 |
| 1:A:125:ARG:HG2 | 1:A:125:ARG:NH1 | 2.23 | 0.54 |
| 1:C:4:LEU:HD21 | 1:C:26:HIS:ND1 | 2.22 | 0.54 |
| 1:A:164:ILE:HG22 | 1:A:164:ILE:O | 2.08 | 0.54 |
| 1:D:321:PHE:CD2 | 1:D:325:GLY:HA2 | 2.42 | 0.54 |
| 1:C:535:ARG:HG3 | 1:C:535:ARG:HH11 | 1.73 | 0.54 |
| 1:B:125:ARG:NH1 | 1:B:125:ARG:HG2 | 2.22 | 0.54 |
| 1:A:564:LEU:HD23 | 1:A:592:VAL:HG12 | 1.88 | 0.54 |
| 1:C:242:LEU:HD23 | 1:C:242:LEU:N | 2.23 | 0.54 |
| 1:B:456:CYS:SG | 1:B:524:VAL:HG13 | 2.47 | 0.54 |
| 1:A:680:ARG:HG3 | 1:A:680:ARG:HH11 | 1.73 | 0.54 |
| 1:B:207:ALA:HB1 | 1:B:210:LEU:HG | 1.89 | 0.54 |
| 1:C:12:THR:HG22 | 1:C:44:ALA:HB2 | 1.89 | 0.54 |
| 1:A:221:LEU:O | 1:A:222:LYS:C | 2.47 | 0.54 |
| 1:C:497:PRO:HB2 | 1:C:499:GLU:OE2 | 2.07 | 0.54 |
| 1:C:353:CYS:HB3 | 1:C:541:SER:HB2 | 1.90 | 0.54 |
| 1:C:160:ALA:HB2 | 1:C:168:LEU:CD2 | 2.37 | 0.53 |
| 1:B:23:LEU:HD21 | 1:B:272:ILE:HD13 | 1.90 | 0.53 |
| 1:B:172:LEU:HD12 | 1:B:239:LEU:CD1 | 2.38 | 0.53 |
| 1:B:512:SER:HA | 1:B:517:LEU:HD11 | 1.89 | 0.53 |
| 1:C:207:ALA:HB1 | 1:C:210:LEU:HG | 1.89 | 0.53 |
| 1:C:463:HIS:O | 1:C:464:GLU:C | 2.46 | 0.53 |
| 1:A:369:GLU:CG | 1:A:482:SER:OG | 2.55 | 0.53 |
| 1:C:140:LEU:CD2 | 1:C:249:LEU:HD12 | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:256:LEU:O | 1:B:257:ILE:C | 2.47 | 0.53 |
| 1:A:602:TYR:O | 1:A:634:ARG:NH2 | 2.41 | 0.53 |
| 1:D:220:ASP:HB3 | 1:D:238:LYS:HD3 | 1.90 | 0.53 |
| 1:D:608:SER:C | 1:D:610:HIS:H | 2.11 | 0.53 |
| 1:A:342:VAL:HG12 | 1:A:658:CYS:SG | 2.48 | 0.53 |
| 1:A:375:ALA:O | 1:A:378:TYR:HB3 | 2.07 | 0.53 |
| 1:A:292:ILE:C | 1:A:292:ILE:HD12 | 2.28 | 0.53 |
| 1:C:376:LEU:O | 1:C:380:VAL:HG23 | 2.08 | 0.53 |
| 1:C:390:GLU:O | 1:C:391:PHE:HB3 | 2.07 | 0.53 |
| 1:B:342:VAL:O | 1:B:346:ILE:HG12 | 2.08 | 0.53 |
| 1:A:159:VAL:HG23 | 1:A:248:LEU:C | 2.28 | 0.53 |
| 1:D:125:ARG:NH1 | 1:D:125:ARG:HG2 | 2.23 | 0.53 |
| 1:C:339:GLY:HA3 | 1:C:407:GLU:O | 2.08 | 0.53 |
| 1:C:292:ILE:C | 1:C:292:ILE:HD12 | 2.28 | 0.53 |
| 1:A:342:VAL:O | 1:A:346:ILE:HG12 | 2.07 | 0.53 |
| 1:A:612:ALA:O | 1:A:616:VAL:HG23 | 2.08 | 0.53 |
| 1:A:594:ALA:O | 1:A:598:LYS:HG3 | 2.09 | 0.53 |
| 1:C:391:PHE:CE2 | 1:C:402:TRP:HH2 | 2.27 | 0.53 |
| 1:B:405:MET:O | 1:B:409:ILE:HD13 | 2.07 | 0.53 |
| 1:D:255:ASP:O | 1:D:256:LEU:C | 2.46 | 0.53 |
| 1:C:221:LEU:O | 1:C:222:LYS:C | 2.45 | 0.53 |
| 1:D:546:VAL:HB | 1:D:644:VAL:HG13 | 1.91 | 0.53 |
| 1:A:548:GLN:HA | 1:A:548:GLN:NE2 | 2.23 | 0.53 |
| 1:A:725:ILE:O | 1:A:728:ALA:N | 2.41 | 0.53 |
| 1:B:298:PHE:CZ | 1:B:331:VAL:HG21 | 2.43 | 0.53 |
| 1:B:292:ILE:HD12 | 1:B:292:ILE:C | 2.28 | 0.53 |
| 1:C:562:PRO:HB3 | 1:C:595:LEU:HB2 | 1.89 | 0.53 |
| 1:B:39:ARG:NH2 | 1:B:267:GLU:OE2 | 2.41 | 0.53 |
| 1:A:160:ALA:HB2 | 1:A:168:LEU:CD2 | 2.39 | 0.53 |
| 1:D:262:LEU:HA | 1:D:265:LEU:HD12 | 1.89 | 0.53 |
| 1:C:425:GLU:HG2 | 1:C:429:LYS:HE3 | 1.90 | 0.53 |
| 1:C:90:MET:HE3 | 1:C:318:ARG:HH22 | 1.74 | 0.53 |
| 1:B:375:ALA:O | 1:B:378:TYR:HB3 | 2.08 | 0.53 |
| 1:C:512:SER:HA | 1:C:517:LEU:HD11 | 1.90 | 0.53 |
| 1:A:172:LEU:HD12 | 1:A:239:LEU:CD1 | 2.39 | 0.53 |
| 1:D:697:PRO:O | 1:D:699:VAL:N | 2.41 | 0.53 |
| 1:B:170:VAL:HG11 | 1:B:221:LEU:HD22 | 1.91 | 0.53 |
| 1:B:497:PRO:HB2 | 1:B:499:GLU:OE2 | 2.09 | 0.53 |
| 1:A:437:SER:HB3 | 1:A:478:SER:H | 1.74 | 0.53 |
| 1:A:680:ARG:HG3 | 1:A:680:ARG:NH1 | 2.23 | 0.53 |
| 1:A:675:ALA:O | 1:A:679:MET:HG3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:402:TRP:CE3 | 1:C:405:MET:CE | 2.92 | 0.53 |
| 1:C:42:PRO:HD3 | 1:C:222:LYS:O | 2.08 | 0.53 |
| 1:D:298:PHE:CZ | 1:D:331:VAL:HG21 | 2.44 | 0.53 |
| 1:A:663:HIS:CD2 | 1:A:743:ARG:HB3 | 2.43 | 0.53 |
| 1:B:221:LEU:O | 1:B:222:LYS:C | 2.47 | 0.52 |
| 1:D:290:GLY:HA3 | 1:D:417:PRO:HG2 | 1.90 | 0.52 |
| 1:D:390:GLU:O | 1:D:391:PHE:HB3 | 2.10 | 0.52 |
| 1:A:392:SER:C | 1:A:394:ASN:H | 2.10 | 0.52 |
| 1:C:236:ALA:C | 1:C:238:LYS:H | 2.13 | 0.52 |
| 1:A:369:GLU:HG3 | 1:A:482:SER:CB | 2.40 | 0.52 |
| 1:C:170:VAL:O | 1:C:215:ALA:HB1 | 2.09 | 0.52 |
| 1:A:523:VAL:HG21 | 1:D:618:ARG:NH1 | 2.24 | 0.52 |
| 1:C:614:GLN:O | 1:C:617:SER:HB3 | 2.09 | 0.52 |
| 1:A:497:PRO:HB2 | 1:A:499:GLU:OE2 | 2.09 | 0.52 |
| 1:D:535:ARG:O | 1:D:539:LEU:HD12 | 2.09 | 0.52 |
| 1:C:72:PHE:CG | 1:C:81:ALA:HA | 2.44 | 0.52 |
| 1:A:360:VAL:O | 1:A:364:VAL:HG23 | 2.09 | 0.52 |
| 1:D:451:ALA:O | 1:D:455:VAL:HG23 | 2.08 | 0.52 |
| 1:C:170:VAL:HG11 | 1:C:221:LEU:HD22 | 1.91 | 0.52 |
| 1:C:629:ILE:N | 1:C:630:PRO:HD2 | 2.24 | 0.52 |
| 1:B:353:CYS:HB3 | 1:B:541:SER:HB2 | 1.91 | 0.52 |
| 1:C:738:ALA:O | 1:C:741:PHE:HB3 | 2.09 | 0.52 |
| 1:C:306:LEU:HD22 | 1:C:400:LYS:HZ3 | 1.73 | 0.52 |
| 1:A:179:THR:HG22 | 1:A:181:LEU:H | 1.73 | 0.52 |
| 1:D:172:LEU:CD1 | 1:D:239:LEU:HD13 | 2.39 | 0.52 |
| 1:D:147:TYR:CB | 1:D:150:LEU:HB2 | 2.39 | 0.52 |
| 1:A:99:ARG:NH1 | 1:A:390:GLU:CD | 2.60 | 0.52 |
| 1:B:261:ALA:C | 1:B:263:GLN:H | 2.13 | 0.52 |
| 1:D:425:GLU:HG2 | 1:D:429:LYS:HE3 | 1.91 | 0.52 |
| 1:B:160:ALA:HB2 | 1:B:168:LEU:CD2 | 2.37 | 0.52 |
| 1:B:4:LEU:CD2 | 1:B:26:HIS:HA | 2.40 | 0.52 |
| 1:A:191:ILE:HG22 | 1:A:192:THR:N | 2.24 | 0.52 |
| 1:C:456:CYS:HB2 | 1:C:457:MET:HE2 | 1.92 | 0.52 |
| 1:A:603:GLU:N | 1:A:603:GLU:CD | 2.62 | 0.52 |
| 1:A:562:PRO:HB3 | 1:A:595:LEU:HB2 | 1.90 | 0.52 |
| 1:C:682:SER:HB2 | 1:C:751:VAL:HG12 | 1.91 | 0.52 |
| 1:B:99:ARG:NH1 | 1:B:390:GLU:O | 2.42 | 0.52 |
| 1:A:599:ILE:HG21 | 1:A:631:PHE:HE1 | 1.75 | 0.52 |
| 1:C:160:ALA:CB | 1:C:168:LEU:HD23 | 2.39 | 0.52 |
| 1:C:36:SER:HB3 | 1:C:317:TRP:HE3 | 1.74 | 0.52 |
| 1:B:298:PHE:HZ | 1:B:331:VAL:HG21 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:90:MET:HE1 | 1:D:318:ARG:NH2 | 2.24 | 0.52 |
| 1:A:643:HIS:O | 1:A:646:GLN:HG2 | 2.09 | 0.52 |
| 1:A:259:VAL:O | 1:A:262:LEU:HB3 | 2.09 | 0.52 |
| 1:D:20:LEU:HD23 | 1:D:122:LEU:HD13 | 1.92 | 0.52 |
| 1:D:298:PHE:HZ | 1:D:331:VAL:HG21 | 1.75 | 0.52 |
| 1:D:227:PRO:CB | 1:D:233:ASP:N | 2.73 | 0.52 |
| 1:A:466:ARG:O | 1:A:470:ASP:OD1 | 2.28 | 0.52 |
| 1:B:682:SER:HB2 | 1:B:751:VAL:HG12 | 1.92 | 0.52 |
| 1:B:594:ALA:O | 1:B:598:LYS:HG3 | 2.10 | 0.52 |
| 1:D:562:PRO:HB3 | 1:D:595:LEU:HB2 | 1.91 | 0.52 |
| 1:D:356:PRO:O | 1:D:647:LYS:NZ | 2.43 | 0.52 |
| 1:A:260:GLN:HA | 1:A:263:GLN:HG2 | 1.92 | 0.52 |
| 1:C:307:ASP:OD1 | 1:C:391:PHE:HA | 2.10 | 0.52 |
| 1:D:38:GLY:N | 1:D:41:LEU:HD12 | 2.24 | 0.52 |
| 1:A:379:LEU:HD21 | 1:A:481:CYS:CB | 2.38 | 0.52 |
| 1:D:264:PHE:N | 1:D:264:PHE:CD1 | 2.77 | 0.52 |
| 1:D:624:ILE:H | 1:D:624:ILE:CD1 | 2.20 | 0.52 |
| 1:D:456:CYS:HB2 | 1:D:457:MET:HE2 | 1.92 | 0.52 |
| 1:B:164:ILE:O | 1:B:164:ILE:HG22 | 2.09 | 0.52 |
| 1:D:594:ALA:O | 1:D:598:LYS:HG3 | 2.10 | 0.52 |
| 1:B:258:ARG:C | 1:B:260:GLN:H | 2.13 | 0.52 |
| 1:D:160:ALA:HB2 | 1:D:168:LEU:CD2 | 2.39 | 0.52 |
| 1:C:42:PRO:CB | 1:C:223:ASP:HB3 | 2.40 | 0.52 |
| 1:A:300:ILE:CG2 | 1:A:304:LEU:HD12 | 2.39 | 0.52 |
| 1:B:139:ARG:N | 1:B:142:ASP:OD2 | 2.42 | 0.52 |
| 1:A:729:ILE:HD12 | 1:A:729:ILE:N | 2.25 | 0.52 |
| 1:A:462:ALA:HA | 1:A:498:ALA:HB1 | 1.91 | 0.52 |
| 1:A:35:VAL:O | 1:A:43:ALA:HA | 2.10 | 0.52 |
| 1:B:38:GLY:HA3 | 1:B:41:LEU:HD11 | 1.90 | 0.51 |
| 1:D:300:ILE:CG2 | 1:D:304:LEU:HD12 | 2.38 | 0.51 |
| 1:D:101:ILE:HG23 | 1:D:277:ASN:HD21 | 1.76 | 0.51 |
| 1:C:342:VAL:O | 1:C:346:ILE:HG12 | 2.10 | 0.51 |
| 1:A:606:GLY:HA2 | 1:A:610:HIS:CB | 2.39 | 0.51 |
| 1:D:368:MET:O | 1:D:372:ARG:HB2 | 2.09 | 0.51 |
| 1:D:738:ALA:O | 1:D:741:PHE:HB3 | 2.10 | 0.51 |
| 1:D:72:PHE:CG | 1:D:81:ALA:HA | 2.45 | 0.51 |
| 1:C:18:HIS:O | 1:C:258:ARG:NH2 | 2.43 | 0.51 |
| 1:C:112:PHE:CD2 | 1:C:265:LEU:HD13 | 2.45 | 0.51 |
| 1:C:725:ILE:O | 1:C:728:ALA:N | 2.43 | 0.51 |
| 1:A:395:LEU:O | 1:A:398:LYS:N | 2.43 | 0.51 |
| 1:B:251:PRO:HG2 | 1:B:254:PHE:HD1 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:242:LEU:HD23 | 1:A:242:LEU:N | 2.25 | 0.51 |
| 1:C:236:ALA:N | 1:C:237:PRO:CD | 2.73 | 0.51 |
| 1:A:425:GLU:HG2 | 1:A:429:LYS:HE3 | 1.92 | 0.51 |
| 1:B:624:ILE:H | 1:B:624:ILE:CD1 | 2.21 | 0.51 |
| 1:A:157:ARG:HH21 | 1:A:249:LEU:HD21 | 1.75 | 0.51 |
| 1:C:594:ALA:O | 1:C:598:LYS:HG3 | 2.10 | 0.51 |
| 1:C:357:ASP:OD1 | 1:D:716:LYS:NZ | 2.38 | 0.51 |
| 1:D:172:LEU:HD11 | 1:D:216:VAL:CG2 | 2.40 | 0.51 |
| 1:A:451:ALA:O | 1:A:455:VAL:HG23 | 2.10 | 0.51 |
| 1:B:258:ARG:O | 1:B:260:GLN:N | 2.44 | 0.51 |
| 1:B:1:MET:HG3 | 1:B:55:SER:CB | 2.40 | 0.51 |
| 1:B:72:PHE:CG | 1:B:81:ALA:HA | 2.46 | 0.51 |
| 1:B:507:LEU:HD22 | 1:B:588:VAL:HG21 | 1.92 | 0.51 |
| 1:C:212:LEU:HD13 | 1:C:241:PHE:HB3 | 1.92 | 0.51 |
| 1:D:170:VAL:O | 1:D:215:ALA:HB1 | 2.11 | 0.51 |
| 1:D:401:THR:HG22 | 1:D:402:TRP:H | 1.76 | 0.51 |
| 1:A:587:PRO:HG2 | 1:A:588:VAL:H | 1.76 | 0.51 |
| 1:B:39:ARG:H | 1:B:39:ARG:CD | 2.23 | 0.51 |
| 1:B:559:PRO:HG3 | 1:B:599:ILE:HG13 | 1.92 | 0.51 |
| 1:D:463:HIS:HA | 1:D:466:ARG:HB3 | 1.91 | 0.51 |
| 1:D:614:GLN:O | 1:D:617:SER:HB3 | 2.11 | 0.51 |
| 1:D:251:PRO:O | 1:D:252:ASP:C | 2.48 | 0.51 |
| 1:A:4:LEU:CD2 | 1:A:26:HIS:HA | 2.41 | 0.51 |
| 1:A:698:SER:O | 1:A:702:GLU:HG3 | 2.11 | 0.51 |
| 1:D:535:ARG:HG3 | 1:D:535:ARG:HH11 | 1.75 | 0.51 |
| 1:A:41:LEU:HD13 | 1:A:264:PHE:CE2 | 2.46 | 0.51 |
| 1:D:587:PRO:HG2 | 1:D:588:VAL:H | 1.76 | 0.51 |
| 1:C:366:LEU:O | 1:C:369:GLU:HB3 | 2.10 | 0.51 |
| 1:A:434:PRO:HA | 1:A:527:ILE:HG22 | 1.92 | 0.51 |
| 1:B:368:MET:O | 1:B:372:ARG:HB2 | 2.11 | 0.51 |
| 1:D:373:ASN:HD21 | 1:D:401:THR:HG21 | 1.75 | 0.51 |
| 1:A:614:GLN:O | 1:A:617:SER:HB3 | 2.11 | 0.51 |
| 1:D:456:CYS:HB2 | 1:D:457:MET:CE | 2.41 | 0.51 |
| 1:C:179:THR:HG22 | 1:C:181:LEU:H | 1.75 | 0.50 |
| 1:A:179:THR:HG23 | 1:A:180:SER:N | 2.27 | 0.50 |
| 1:B:614:GLN:O | 1:B:617:SER:HB3 | 2.11 | 0.50 |
| 1:C:434:PRO:HA | 1:C:527:ILE:CG2 | 2.41 | 0.50 |
| 1:D:725:ILE:HG22 | 1:D:729:ILE:CD1 | 2.42 | 0.50 |
| 1:D:497:PRO:HB2 | 1:D:499:GLU:OE2 | 2.11 | 0.50 |
| 1:C:446:ASP:HA | 1:C:449:THR:HB | 1.92 | 0.50 |
| 1:D:366:LEU:O | 1:D:369:GLU:HB3 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:36:SER:HB3 | 1:D:317:TRP:HE3 | 1.75 | 0.50 |
| 1:D:99:ARG:NH1 | 1:D:390:GLU:OE2 | 2.44 | 0.50 |
| 1:A:213:VAL:O | 1:A:241:PHE:HA | 2.11 | 0.50 |
| 1:B:429:LYS:O | 1:B:432:MET:O | 2.29 | 0.50 |
| 1:D:4:LEU:CD2 | 1:D:26:HIS:HA | 2.42 | 0.50 |
| 1:B:105:PRO:HG2 | 1:B:106:GLN:H | 1.76 | 0.50 |
| 1:D:179:THR:HG22 | 1:D:181:LEU:H | 1.76 | 0.50 |
| 1:B:39:ARG:HD2 | 1:B:39:ARG:H | 1.75 | 0.50 |
| 1:B:342:VAL:HG23 | 1:B:343:LEU:N | 2.27 | 0.50 |
| 1:B:629:ILE:N | 1:B:630:PRO:HD2 | 2.27 | 0.50 |
| 1:A:455:VAL:HG21 | 1:A:468:LEU:CD1 | 2.42 | 0.50 |
| 1:B:377:ASN:ND2 | 1:B:395:LEU:HD11 | 2.26 | 0.50 |
| 1:C:172:LEU:HD11 | 1:C:216:VAL:CG2 | 2.39 | 0.50 |
| 1:D:144:TYR:OH | 1:D:213:VAL:HG22 | 2.11 | 0.50 |
| 1:A:21:LEU:HD11 | 1:A:110:LEU:HB2 | 1.93 | 0.50 |
| 1:A:1:MET:HG3 | 1:A:55:SER:CB | 2.41 | 0.50 |
| 1:B:602:TYR:O | 1:B:603:GLU:HB2 | 2.11 | 0.50 |
| 1:D:609:LYS:NZ | 1:D:641:THR:CG2 | 2.74 | 0.50 |
| 1:D:498:ALA:HA | 1:D:501:MET:HE3 | 1.94 | 0.50 |
| 1:D:105:PRO:HG2 | 1:D:106:GLN:H | 1.77 | 0.50 |
| 1:A:682:SER:HB2 | 1:A:751:VAL:HG12 | 1.93 | 0.50 |
| 1:D:632:LEU:HD22 | 1:D:733:CYS:SG | 2.52 | 0.50 |
| 1:D:147:TYR:CD2 | 1:D:150:LEU:HB2 | 2.47 | 0.50 |
| 1:B:160:ALA:CB | 1:B:168:LEU:HD23 | 2.38 | 0.50 |
| 1:C:41:LEU:HD13 | 1:C:264:PHE:CZ | 2.47 | 0.50 |
| 1:B:603:GLU:CA | 1:B:634:ARG:HH22 | 2.24 | 0.50 |
| 1:D:463:HIS:HA | 1:D:466:ARG:CB | 2.42 | 0.50 |
| 1:C:327:SER:HG | 1:C:329:THR:HB | 1.76 | 0.50 |
| 1:A:96:THR:HG21 | 1:A:301:THR:HG23 | 1.94 | 0.50 |
| 1:A:72:PHE:CG | 1:A:81:ALA:HA | 2.47 | 0.50 |
| 1:C:350:ARG:HD2 | 1:C:539:LEU:HA | 1.94 | 0.50 |
| 1:D:261:ALA:O | 1:D:264:PHE:CD1 | 2.62 | 0.50 |
| 1:A:569:ARG:NE | 1:A:735:GLU:OE1 | 2.44 | 0.50 |
| 1:A:434:PRO:HA | 1:A:527:ILE:CG2 | 2.42 | 0.50 |
| 1:D:60:ASP:HA | 1:D:63:ILE:HD12 | 1.93 | 0.50 |
| 1:D:227:PRO:HB2 | 1:D:233:ASP:N | 2.26 | 0.50 |
| 1:B:685:THR:OG1 | 1:B:688:VAL:HG23 | 2.12 | 0.50 |
| 1:A:105:PRO:HG2 | 1:A:106:GLN:H | 1.76 | 0.50 |
| 1:B:179:THR:HG23 | 1:B:180:SER:N | 2.26 | 0.50 |
| 1:C:385:LEU:N | 1:C:386:PRO:CD | 2.75 | 0.50 |
| 1:A:172:LEU:HD11 | 1:A:216:VAL:CG2 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:255:ASP:O | 1:A:258:ARG:HB2 | 2.12 | 0.50 |
| 1:B:603:GLU:CA | 1:B:634:ARG:HH12 | 2.23 | 0.50 |
| 1:B:172:LEU:HD11 | 1:B:216:VAL:CG2 | 2.42 | 0.50 |
| 1:C:4:LEU:CD2 | 1:C:26:HIS:HA | 2.42 | 0.50 |
| 1:B:94:GLU:HG2 | 1:B:316:GLY:HA2 | 1.92 | 0.50 |
| 1:C:114:PRO:CB | 1:C:258:ARG:NH1 | 2.75 | 0.49 |
| 1:B:377:ASN:ND2 | 1:B:395:LEU:HD21 | 2.21 | 0.49 |
| 1:B:258:ARG:C | 1:B:260:GLN:N | 2.65 | 0.49 |
| 1:C:711:ILE:HD12 | 1:C:711:ILE:O | 2.11 | 0.49 |
| 1:B:559:PRO:HG2 | 1:B:599:ILE:HG13 | 1.93 | 0.49 |
| 1:B:486:SER:O | 1:B:489:PHE:HB3 | 2.12 | 0.49 |
| 1:A:561:ILE:CD1 | 1:A:561:ILE:H | 2.24 | 0.49 |
| 1:B:170:VAL:O | 1:B:215:ALA:HB1 | 2.12 | 0.49 |
| 1:C:368:MET:O | 1:C:372:ARG:HB2 | 2.12 | 0.49 |
| 1:C:643:HIS:O | 1:C:646:GLN:HG2 | 2.11 | 0.49 |
| 1:D:564:LEU:C | 1:D:566:ILE:H | 2.15 | 0.49 |
| 1:D:402:TRP:HA | 1:D:402:TRP:CE3 | 2.47 | 0.49 |
| 1:C:456:CYS:HB2 | 1:C:457:MET:CE | 2.42 | 0.49 |
| 1:A:593:LEU:O | 1:A:597:GLU:HG3 | 2.12 | 0.49 |
| 1:B:396:VAL:HG13 | 1:B:396:VAL:O | 2.11 | 0.49 |
| 1:B:39:ARG:NH1 | 1:B:41:LEU:HD21 | 2.27 | 0.49 |
| 1:D:259:VAL:O | 1:D:262:LEU:N | 2.39 | 0.49 |
| 1:A:158:MET:HE3 | 1:A:256:LEU:HB2 | 1.94 | 0.49 |
| 1:A:708:HIS:O | 1:A:711:ILE:HG13 | 2.12 | 0.49 |
| 1:C:333:GLN:HE21 | 1:C:673:GLU:HB3 | 1.76 | 0.49 |
| 1:B:459:GLU:O | 1:B:459:GLU:HG2 | 2.12 | 0.49 |
| 1:C:21:LEU:HD12 | 1:C:22:LEU:N | 2.26 | 0.49 |
| 1:A:366:LEU:O | 1:A:369:GLU:HB3 | 2.12 | 0.49 |
| 1:D:160:ALA:CB | 1:D:168:LEU:HD23 | 2.40 | 0.49 |
| 1:C:14:ARG:NH1 | 1:C:223:ASP:HA | 2.26 | 0.49 |
| 1:D:608:SER:C | 1:D:610:HIS:N | 2.62 | 0.49 |
| 1:C:434:PRO:HA | 1:C:527:ILE:HG22 | 1.94 | 0.49 |
| 1:B:451:ALA:O | 1:B:455:VAL:HG23 | 2.11 | 0.49 |
| 1:A:34:LYS:HA | 1:A:45:GLU:HA | 1.93 | 0.49 |
| 1:C:456:CYS:SG | 1:C:524:VAL:HG13 | 2.52 | 0.49 |
| 1:A:310:ARG:NH2 | 1:A:392:SER:CB | 2.75 | 0.49 |
| 1:B:663:HIS:NE2 | 1:B:743:ARG:HB3 | 2.27 | 0.49 |
| 1:A:369:GLU:HG2 | 1:A:485:VAL:HG23 | 1.93 | 0.49 |
| 1:A:604:SER:N | 1:A:634:ARG:HH12 | 2.10 | 0.49 |
| 1:D:261:ALA:HA | 1:D:264:PHE:CE1 | 2.47 | 0.49 |
| 1:A:87:GLY:O | 1:A:90:MET:HG3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:377:ASN:O | 1:D:381:GLN:HG2 | 2.13 | 0.49 |
| 1:D:164:ILE:O | 1:D:164:ILE:HG22 | 2.11 | 0.49 |
| 1:C:465:PHE:O | 1:C:468:LEU:N | 2.46 | 0.49 |
| 1:D:629:ILE:N | 1:D:630:PRO:HD2 | 2.28 | 0.49 |
| 1:D:401:THR:H | 1:D:404:ASP:CG | 2.15 | 0.49 |
| 1:C:353:CYS:HB3 | 1:C:541:SER:CB | 2.41 | 0.49 |
| 1:C:708:HIS:O | 1:C:711:ILE:HG13 | 2.13 | 0.49 |
| 1:B:535:ARG:HG3 | 1:B:535:ARG:HH11 | 1.77 | 0.49 |
| 1:A:170:VAL:HG11 | 1:A:221:LEU:HD22 | 1.93 | 0.49 |
| 1:A:523:VAL:O | 1:A:524:VAL:HG23 | 2.13 | 0.49 |
| 1:B:703:VAL:O | 1:B:706:GLU:HB3 | 2.13 | 0.49 |
| 1:D:643:HIS:O | 1:D:646:GLN:HG2 | 2.13 | 0.49 |
| 1:B:292:ILE:HD12 | 1:B:292:ILE:O | 2.13 | 0.49 |
| 1:D:110:LEU:N | 1:D:110:LEU:HD23 | 2.28 | 0.49 |
| 1:A:399:SER:CA | 1:B:395:LEU:HD12 | 2.40 | 0.49 |
| 1:C:332:PHE:C | 1:C:332:PHE:CD2 | 2.86 | 0.49 |
| 1:C:172:LEU:HD12 | 1:C:239:LEU:HD13 | 1.93 | 0.49 |
| 1:A:406:TYR:O | 1:A:410:VAL:HG23 | 2.12 | 0.49 |
| 1:C:725:ILE:HG22 | 1:C:729:ILE:CD1 | 2.43 | 0.49 |
| 1:C:698:SER:O | 1:C:702:GLU:HG3 | 2.13 | 0.49 |
| 1:D:725:ILE:O | 1:D:728:ALA:N | 2.44 | 0.49 |
| 1:D:90:MET:CE | 1:D:318:ARG:HH22 | 2.26 | 0.49 |
| 1:C:136:ASP:O | 1:C:138:LYS:HG3 | 2.13 | 0.49 |
| 1:D:38:GLY:H | 1:D:41:LEU:CD1 | 2.23 | 0.49 |
| 1:B:115:LEU:N | 1:B:258:ARG:HH22 | 2.07 | 0.49 |
| 1:B:110:LEU:HD11 | 1:B:269:ALA:HA | 1.95 | 0.49 |
| 1:B:333:GLN:HG2 | 1:B:673:GLU:HB2 | 1.95 | 0.49 |
| 1:C:721:THR:O | 1:C:724:ALA:HB3 | 2.13 | 0.49 |
| 1:B:643:HIS:O | 1:B:646:GLN:HG2 | 2.12 | 0.49 |
| 1:D:472:ALA:HA | 1:D:477:ILE:HD12 | 1.94 | 0.49 |
| 1:C:459:GLU:HG2 | 1:C:459:GLU:O | 2.12 | 0.49 |
| 1:D:682:SER:HB2 | 1:D:751:VAL:HG12 | 1.94 | 0.49 |
| 1:D:336:GLU:HG3 | 1:D:407:GLU:HB2 | 1.95 | 0.49 |
| 1:B:39:ARG:HG3 | 1:B:317:TRP:CE2 | 2.47 | 0.49 |
| 1:D:698:SER:O | 1:D:702:GLU:HG3 | 2.13 | 0.49 |
| 1:D:36:SER:HB2 | 1:D:312:ARG:O | 2.13 | 0.49 |
| 1:C:352:LEU:HD11 | 1:C:650:LEU:HD23 | 1.95 | 0.49 |
| 1:C:466:ARG:NH2 | 1:C:498:ALA:N | 2.59 | 0.49 |
| 1:C:179:THR:HG23 | 1:C:180:SER:N | 2.27 | 0.49 |
| 1:A:110:LEU:HD11 | 1:A:269:ALA:HA | 1.95 | 0.49 |
| 1:C:473:CYS:HA | 1:C:490:LEU:HD13 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:624:ILE:N | 1:A:624:ILE:HD13 | 2.26 | 0.49 |
| 1:D:624:ILE:N | 1:D:624:ILE:HD13 | 2.27 | 0.49 |
| 1:D:138:LYS:CD | 1:D:142:ASP:HB3 | 2.42 | 0.49 |
| 1:C:729:ILE:N | 1:C:729:ILE:HD12 | 2.28 | 0.49 |
| 1:B:546:VAL:HB | 1:B:644:VAL:HG13 | 1.94 | 0.49 |
| 1:D:609:LYS:HZ2 | 1:D:641:THR:HG21 | 1.77 | 0.48 |
| 1:D:461:GLY:H | 1:D:464:GLU:CD | 2.16 | 0.48 |
| 1:B:128:MET:O | 1:B:132:GLN:HG3 | 2.13 | 0.48 |
| 1:D:140:LEU:HB3 | 1:D:144:TYR:CE2 | 2.46 | 0.48 |
| 1:C:703:VAL:O | 1:C:706:GLU:HB3 | 2.13 | 0.48 |
| 1:A:455:VAL:HG21 | 1:A:468:LEU:HD11 | 1.95 | 0.48 |
| 1:D:696:PHE:HB3 | 1:D:700:VAL:HG21 | 1.95 | 0.48 |
| 1:A:471:TYR:O | 1:A:475:GLN:HB2 | 2.13 | 0.48 |
| 1:A:332:PHE:CD2 | 1:A:332:PHE:C | 2.86 | 0.48 |
| 1:C:220:ASP:HB3 | 1:C:238:LYS:HD3 | 1.94 | 0.48 |
| 1:C:708:HIS:HB3 | 1:C:711:ILE:CG2 | 2.43 | 0.48 |
| 1:A:114:PRO:O | 1:A:115:LEU:HD23 | 2.13 | 0.48 |
| 1:B:21:LEU:HD12 | 1:B:22:LEU:N | 2.28 | 0.48 |
| 1:B:725:ILE:HG22 | 1:B:729:ILE:CD1 | 2.43 | 0.48 |
| 1:D:30:LEU:O | 1:D:48:PHE:HB2 | 2.13 | 0.48 |
| 1:A:609:LYS:CD | 1:A:641:THR:HG22 | 2.41 | 0.48 |
| 1:A:599:ILE:HG21 | 1:A:631:PHE:CE1 | 2.47 | 0.48 |
| 1:A:390:GLU:OE1 | 1:A:390:GLU:HA | 2.13 | 0.48 |
| 1:C:446:ASP:O | 1:C:447:ALA:C | 2.51 | 0.48 |
| 1:C:460:ALA:HA | 1:C:464:GLU:HG2 | 1.94 | 0.48 |
| 1:D:179:THR:HG23 | 1:D:180:SER:N | 2.27 | 0.48 |
| 1:C:663:HIS:NE2 | 1:C:743:ARG:HB3 | 2.27 | 0.48 |
| 1:B:675:ALA:O | 1:B:679:MET:HG3 | 2.14 | 0.48 |
| 1:D:599:ILE:HG21 | 1:D:631:PHE:HE1 | 1.78 | 0.48 |
| 1:B:99:ARG:NH2 | 1:B:390:GLU:O | 2.46 | 0.48 |
| 1:D:663:HIS:NE2 | 1:D:743:ARG:HB3 | 2.28 | 0.48 |
| 1:D:39:ARG:C | 1:D:41:LEU:N | 2.66 | 0.48 |
| 1:D:145:THR:C | 1:D:147:TYR:N | 2.67 | 0.48 |
| 1:C:546:VAL:O | 1:C:547:GLU:O | 2.31 | 0.48 |
| 1:D:271:HIS:O | 1:D:275:ILE:HG13 | 2.13 | 0.48 |
| 1:D:159:VAL:HG23 | 1:D:248:LEU:O | 2.13 | 0.48 |
| 1:B:561:ILE:H | 1:B:561:ILE:CD1 | 2.25 | 0.48 |
| 1:C:346:ILE:HD12 | 1:C:424:GLU:HG2 | 1.95 | 0.48 |
| 1:A:459:GLU:O | 1:A:459:GLU:HG2 | 2.12 | 0.48 |
| 1:B:323:PRO:O | 1:B:326:VAL:HG23 | 2.13 | 0.48 |
| 1:A:6:HIS:HB2 | 1:A:21:LEU:HB3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:310:ARG:HH11 | 1:C:310:ARG:CB | 2.27 | 0.48 |
| 1:D:469:VAL:C | 1:D:471:TYR:H | 2.16 | 0.48 |
| 1:A:601:ALA:O | 1:A:603:GLU:OE2 | 2.31 | 0.48 |
| 1:D:680:ARG:HG3 | 1:D:680:ARG:NH1 | 2.29 | 0.48 |
| 1:A:564:LEU:C | 1:A:566:ILE:H | 2.17 | 0.48 |
| 1:D:753:ASP:O | 1:D:754:ALA:C | 2.52 | 0.48 |
| 1:B:12:THR:HG22 | 1:B:44:ALA:HB2 | 1.94 | 0.48 |
| 1:B:472:ALA:O | 1:B:475:GLN:N | 2.41 | 0.48 |
| 1:C:238:LYS:O | 1:C:240:ARG:HG3 | 2.14 | 0.48 |
| 1:A:432:MET:CE | 1:A:534:ALA:HB1 | 2.41 | 0.48 |
| 1:C:168:LEU:HD13 | 1:C:259:VAL:CG1 | 2.42 | 0.48 |
| 1:B:110:LEU:HD23 | 1:B:110:LEU:N | 2.29 | 0.48 |
| 1:C:342:VAL:HG12 | 1:C:658:CYS:SG | 2.54 | 0.48 |
| 1:A:629:ILE:N | 1:A:630:PRO:HD2 | 2.29 | 0.48 |
| 1:A:753:ASP:O | 1:A:754:ALA:C | 2.52 | 0.48 |
| 1:B:725:ILE:O | 1:B:728:ALA:N | 2.47 | 0.48 |
| 1:D:548:GLN:O | 1:D:643:HIS:HB3 | 2.14 | 0.48 |
| 1:D:459:GLU:O | 1:D:459:GLU:HG2 | 2.13 | 0.48 |
| 1:A:356:PRO:CB | 1:A:544:PHE:HA | 2.44 | 0.48 |
| 1:A:377:ASN:O | 1:A:381:GLN:HG2 | 2.13 | 0.48 |
| 1:C:377:ASN:O | 1:C:381:GLN:HG2 | 2.13 | 0.48 |
| 1:C:401:THR:H | 1:C:404:ASP:CG | 2.17 | 0.48 |
| 1:B:366:LEU:O | 1:B:369:GLU:HB3 | 2.14 | 0.48 |
| 1:C:473:CYS:O | 1:C:475:GLN:N | 2.47 | 0.48 |
| 1:B:157:ARG:HH21 | 1:B:249:LEU:HD21 | 1.77 | 0.48 |
| 1:D:708:HIS:HB3 | 1:D:711:ILE:CG2 | 2.44 | 0.48 |
| 1:B:708:HIS:O | 1:B:711:ILE:HG13 | 2.13 | 0.48 |
| 1:C:624:ILE:N | 1:C:624:ILE:HD13 | 2.28 | 0.48 |
| 1:B:420:ILE:HD13 | 1:B:569:ARG:NH2 | 2.28 | 0.48 |
| 1:C:432:MET:HE1 | 1:C:534:ALA:O | 2.13 | 0.48 |
| 1:B:353:CYS:HB3 | 1:B:541:SER:CB | 2.44 | 0.48 |
| 1:D:332:PHE:CD2 | 1:D:332:PHE:C | 2.87 | 0.48 |
| 1:C:680:ARG:NH1 | 1:C:680:ARG:HG3 | 2.29 | 0.48 |
| 1:C:306:LEU:HB2 | 1:C:391:PHE:HB3 | 1.95 | 0.47 |
| 1:D:39:ARG:HE | 1:D:41:LEU:HD21 | 1.79 | 0.47 |
| 1:D:635:LEU:HA | 1:D:638:ILE:HD12 | 1.96 | 0.47 |
| 1:A:67:TYR:CZ | 1:A:114:PRO:HG3 | 2.48 | 0.47 |
| 1:D:67:TYR:CZ | 1:D:114:PRO:HG3 | 2.49 | 0.47 |
| 1:B:729:ILE:HD12 | 1:B:729:ILE:N | 2.28 | 0.47 |
| 1:B:377:ASN:O | 1:B:381:GLN:HG2 | 2.13 | 0.47 |
| 1:C:535:ARG:O | 1:C:538:TRP:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:260:GLN:O | 1:D:264:PHE:CE1 | 2.66 | 0.47 |
| 1:B:708:HIS:HB3 | 1:B:711:ILE:CG2 | 2.44 | 0.47 |
| 1:C:254:PHE:O | 1:C:255:ASP:O | 2.32 | 0.47 |
| 1:A:128:MET:O | 1:A:132:GLN:HG3 | 2.13 | 0.47 |
| 1:D:323:PRO:O | 1:D:326:VAL:HG23 | 2.14 | 0.47 |
| 1:B:332:PHE:CD2 | 1:B:332:PHE:C | 2.88 | 0.47 |
| 1:A:310:ARG:HH11 | 1:A:310:ARG:CB | 2.27 | 0.47 |
| 1:C:139:ARG:HB3 | 1:C:141:SER:H | 1.79 | 0.47 |
| 1:D:602:TYR:O | 1:D:603:GLU:C | 2.53 | 0.47 |
| 1:A:248:LEU:C | 1:A:248:LEU:HD23 | 2.35 | 0.47 |
| 1:D:67:TYR:O | 1:D:70:ILE:HB | 2.15 | 0.47 |
| 1:C:564:LEU:C | 1:C:566:ILE:H | 2.17 | 0.47 |
| 1:B:546:VAL:O | 1:B:547:GLU:C | 2.51 | 0.47 |
| 1:B:248:LEU:HD23 | 1:B:248:LEU:C | 2.35 | 0.47 |
| 1:A:249:LEU:HD23 | 1:A:250:LEU:O | 2.14 | 0.47 |
| 1:C:87:GLY:O | 1:C:90:MET:HG3 | 2.15 | 0.47 |
| 1:D:471:TYR:CE1 | 1:D:475:GLN:HG3 | 2.49 | 0.47 |
| 1:B:96:THR:HG21 | 1:B:301:THR:HG23 | 1.96 | 0.47 |
| 1:C:67:TYR:CZ | 1:C:114:PRO:HG3 | 2.48 | 0.47 |
| 1:D:342:VAL:O | 1:D:346:ILE:HG12 | 2.13 | 0.47 |
| 1:C:406:TYR:O | 1:C:410:VAL:HG23 | 2.15 | 0.47 |
| 1:D:140:LEU:HD21 | 1:D:249:LEU:HD12 | 1.95 | 0.47 |
| 1:A:395:LEU:HD23 | 1:A:395:LEU:H | 1.76 | 0.47 |
| 1:B:632:LEU:HD22 | 1:B:733:CYS:SG | 2.54 | 0.47 |
| 1:A:369:GLU:CG | 1:A:485:VAL:HG23 | 2.45 | 0.47 |
| 1:C:249:LEU:HD23 | 1:C:250:LEU:O | 2.15 | 0.47 |
| 1:D:609:LYS:HD3 | 1:D:641:THR:HG22 | 1.95 | 0.47 |
| 1:B:21:LEU:HD13 | 1:B:112:PHE:CE1 | 2.49 | 0.47 |
| 1:A:395:LEU:CD2 | 1:A:395:LEU:N | 2.78 | 0.47 |
| 1:A:535:ARG:NH1 | 1:A:535:ARG:HG3 | 2.29 | 0.47 |
| 1:D:292:ILE:HD12 | 1:D:292:ILE:O | 2.14 | 0.47 |
| 1:B:593:LEU:O | 1:B:597:GLU:HG3 | 2.15 | 0.47 |
| 1:D:593:LEU:O | 1:D:597:GLU:HG3 | 2.15 | 0.47 |
| 1:C:114:PRO:CA | 1:C:258:ARG:NH1 | 2.69 | 0.47 |
| 1:C:462:ALA:O | 1:C:465:PHE:HB2 | 2.15 | 0.47 |
| 1:A:41:LEU:HD23 | 1:A:263:GLN:HB3 | 1.95 | 0.47 |
| 1:A:486:SER:O | 1:A:489:PHE:HB3 | 2.14 | 0.47 |
| 1:D:596:TYR:CE2 | 1:D:600:LEU:HD11 | 2.49 | 0.47 |
| 1:D:703:VAL:O | 1:D:706:GLU:HB3 | 2.14 | 0.47 |
| 1:D:527:ILE:CD1 | 1:D:527:ILE:H | 2.27 | 0.47 |
| 1:A:445:PRO:HG2 | 1:A:448:VAL:CG2 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:729:ILE:N | 1:D:729:ILE:HD12 | 2.30 | 0.47 |
| 1:C:429:LYS:O | 1:C:432:MET:O | 2.33 | 0.47 |
| 1:D:406:TYR:O | 1:D:410:VAL:HG23 | 2.15 | 0.47 |
| 1:B:259:VAL:O | 1:B:259:VAL:HG12 | 2.15 | 0.47 |
| 1:B:371:VAL:O | 1:B:371:VAL:HG12 | 2.15 | 0.47 |
| 1:A:160:ALA:CB | 1:A:168:LEU:HD23 | 2.40 | 0.47 |
| 1:A:721:THR:O | 1:A:724:ALA:HB3 | 2.14 | 0.47 |
| 1:A:546:VAL:O | 1:A:547:GLU:O | 2.33 | 0.47 |
| 1:C:486:SER:O | 1:C:489:PHE:HB3 | 2.14 | 0.47 |
| 1:D:87:GLY:O | 1:D:90:MET:HG3 | 2.14 | 0.47 |
| 1:C:587:PRO:HG2 | 1:C:588:VAL:H | 1.79 | 0.47 |
| 1:C:6:HIS:HB2 | 1:C:21:LEU:HB3 | 1.97 | 0.47 |
| 1:D:385:LEU:N | 1:D:386:PRO:CD | 2.78 | 0.47 |
| 1:B:4:LEU:HD12 | 1:B:4:LEU:N | 2.29 | 0.47 |
| 1:A:472:ALA:CB | 1:A:477:ILE:HD12 | 2.45 | 0.47 |
| 1:B:406:TYR:O | 1:B:410:VAL:HG23 | 2.15 | 0.47 |
| 1:D:668:HIS:CB | 1:D:671:LEU:HD12 | 2.45 | 0.47 |
| 1:C:461:GLY:O | 1:C:462:ALA:O | 2.33 | 0.47 |
| 1:A:399:SER:HA | 1:B:395:LEU:CD1 | 2.39 | 0.47 |
| 1:B:381:GLN:NE2 | 1:B:402:TRP:HD1 | 2.13 | 0.47 |
| 1:B:38:GLY:HA3 | 1:B:41:LEU:CD1 | 2.45 | 0.47 |
| 1:B:157:ARG:NE | 1:B:249:LEU:HD21 | 2.26 | 0.47 |
| 1:B:721:THR:O | 1:B:724:ALA:HB3 | 2.15 | 0.47 |
| 1:B:456:CYS:HB2 | 1:B:457:MET:CE | 2.45 | 0.47 |
| 1:A:385:LEU:N | 1:A:386:PRO:CD | 2.78 | 0.47 |
| 1:D:6:HIS:HB2 | 1:D:21:LEU:HB3 | 1.97 | 0.46 |
| 1:C:128:MET:O | 1:C:129:VAL:C | 2.53 | 0.46 |
| 1:D:609:LYS:CE | 1:D:637:GLN:HB3 | 2.42 | 0.46 |
| 1:A:137:ALA:HB1 | 1:A:248:LEU:CD2 | 2.45 | 0.46 |
| 1:B:624:ILE:HD13 | 1:B:624:ILE:N | 2.28 | 0.46 |
| 1:D:128:MET:O | 1:D:129:VAL:C | 2.54 | 0.46 |
| 1:A:725:ILE:HG22 | 1:A:729:ILE:CD1 | 2.45 | 0.46 |
| 1:B:698:SER:O | 1:B:702:GLU:HG3 | 2.14 | 0.46 |
| 1:C:35:VAL:HG12 | 1:C:318:ARG:HB3 | 1.98 | 0.46 |
| 1:A:139:ARG:CG | 1:A:245:GLU:O | 2.63 | 0.46 |
| 1:C:696:PHE:HB3 | 1:C:700:VAL:HG21 | 1.96 | 0.46 |
| 1:A:429:LYS:O | 1:A:432:MET:O | 2.33 | 0.46 |
| 1:B:602:TYR:C | 1:B:634:ARG:NH2 | 2.68 | 0.46 |
| 1:D:238:LYS:O | 1:D:240:ARG:HG3 | 2.14 | 0.46 |
| 1:B:465:PHE:HZ | 1:B:505:TYR:CG | 2.33 | 0.46 |
| 1:C:597:GLU:O | 1:C:600:LEU:HB2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:38:GLY:O | 1:A:41:LEU:O | 2.33 | 0.46 |
| 1:C:386:PRO:HB3 | 1:C:402:TRP:NE1 | 2.31 | 0.46 |
| 1:B:238:LYS:O | 1:B:240:ARG:HG3 | 2.14 | 0.46 |
| 1:A:179:THR:HG21 | 1:A:209:ASP:HA | 1.97 | 0.46 |
| 1:A:110:LEU:N | 1:A:110:LEU:HD23 | 2.30 | 0.46 |
| 1:C:300:ILE:CG2 | 1:C:304:LEU:HD12 | 2.43 | 0.46 |
| 1:C:4:LEU:N | 1:C:4:LEU:HD12 | 2.30 | 0.46 |
| 1:A:535:ARG:O | 1:A:538:TRP:HB3 | 2.14 | 0.46 |
| 1:A:632:LEU:HD22 | 1:A:733:CYS:SG | 2.55 | 0.46 |
| 1:C:599:ILE:HG21 | 1:C:631:PHE:HE1 | 1.80 | 0.46 |
| 1:A:402:TRP:CE3 | 1:A:405:MET:CE | 2.98 | 0.46 |
| 1:B:39:ARG:HH22 | 1:B:267:GLU:CD | 2.19 | 0.46 |
| 1:B:300:ILE:CG2 | 1:B:304:LEU:HD12 | 2.40 | 0.46 |
| 1:D:20:LEU:HB2 | 1:D:115:LEU:HD11 | 1.96 | 0.46 |
| 1:A:34:LYS:CB | 1:A:45:GLU:HG3 | 2.46 | 0.46 |
| 1:B:587:PRO:HG2 | 1:B:588:VAL:H | 1.79 | 0.46 |
| 1:A:323:PRO:O | 1:A:326:VAL:HG23 | 2.16 | 0.46 |
| 1:C:465:PHE:CZ | 1:C:502:LEU:HD13 | 2.50 | 0.46 |
| 1:C:82:SER:HB3 | 1:C:85:GLU:HB3 | 1.98 | 0.46 |
| 1:C:153:SER:O | 1:C:157:ARG:HD2 | 2.15 | 0.46 |
| 1:B:6:HIS:HB2 | 1:B:21:LEU:HB3 | 1.96 | 0.46 |
| 1:A:587:PRO:HG2 | 1:A:588:VAL:N | 2.30 | 0.46 |
| 1:D:33:PHE:CD2 | 1:D:318:ARG:HB2 | 2.51 | 0.46 |
| 1:D:21:LEU:HD12 | 1:D:22:LEU:N | 2.31 | 0.46 |
| 1:D:248:LEU:HD23 | 1:D:248:LEU:C | 2.36 | 0.46 |
| 1:A:708:HIS:HB3 | 1:A:711:ILE:CG2 | 2.46 | 0.46 |
| 1:D:142:ASP:O | 1:D:143:GLU:HG3 | 2.16 | 0.46 |
| 1:A:494:ARG:HH11 | 1:A:494:ARG:CG | 2.29 | 0.46 |
| 1:A:90:MET:CE | 1:A:318:ARG:HH22 | 2.29 | 0.46 |
| 1:A:96:THR:CG2 | 1:A:301:THR:HG23 | 2.45 | 0.46 |
| 1:D:680:ARG:HG3 | 1:D:680:ARG:HH11 | 1.80 | 0.46 |
| 1:B:59:THR:O | 1:B:63:ILE:HG13 | 2.16 | 0.46 |
| 1:A:280:CYS:SG | 1:A:280:CYS:O | 2.74 | 0.46 |
| 1:A:663:HIS:NE2 | 1:A:743:ARG:HB3 | 2.30 | 0.46 |
| 1:B:39:ARG:N | 1:B:39:ARG:CD | 2.75 | 0.46 |
| 1:D:153:SER:O | 1:D:157:ARG:HD2 | 2.16 | 0.46 |
| 1:D:352:LEU:CD1 | 1:D:363:LEU:HD13 | 2.45 | 0.46 |
| 1:D:546:VAL:O | 1:D:547:GLU:O | 2.33 | 0.46 |
| 1:A:456:CYS:HB2 | 1:A:457:MET:CE | 2.45 | 0.46 |
| 1:A:4:LEU:N | 1:A:4:LEU:HD12 | 2.31 | 0.46 |
| 1:A:335:LEU:O | 1:A:411:GLY:HA3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:401:THR:HB | 1:A:404:ASP:OD2 | 2.15 | 0.46 |
| 1:D:265:LEU:N | 1:D:266:PRO:CD | 2.79 | 0.46 |
| 1:B:261:ALA:C | 1:B:263:GLN:N | 2.69 | 0.46 |
| 1:D:708:HIS:O | 1:D:711:ILE:HG13 | 2.15 | 0.46 |
| 1:B:564:LEU:C | 1:B:566:ILE:H | 2.18 | 0.46 |
| 1:C:161:THR:CB | 1:C:164:ILE:HB | 2.46 | 0.46 |
| 1:D:708:HIS:CB | 1:D:711:ILE:HG21 | 2.46 | 0.46 |
| 1:C:685:THR:OG1 | 1:C:688:VAL:HG23 | 2.16 | 0.46 |
| 1:A:292:ILE:HD12 | 1:A:292:ILE:O | 2.15 | 0.46 |
| 1:A:685:THR:OG1 | 1:A:688:VAL:HG23 | 2.15 | 0.46 |
| 1:B:493:LEU:HD23 | 1:B:496:ILE:HD12 | 1.98 | 0.46 |
| 1:D:494:ARG:CG | 1:D:494:ARG:HH11 | 2.29 | 0.46 |
| 1:C:90:MET:CE | 1:C:318:ARG:HH22 | 2.28 | 0.46 |
| 1:B:517:LEU:C | 1:B:517:LEU:HD12 | 2.36 | 0.46 |
| 1:B:574:PRO:O | 1:B:575:VAL:C | 2.54 | 0.46 |
| 1:B:7:CYS:HB2 | 1:B:49:GLU:HG3 | 1.96 | 0.46 |
| 1:C:248:LEU:C | 1:C:248:LEU:HD23 | 2.36 | 0.45 |
| 1:D:189:GLU:OE2 | 1:D:191:ILE:HD11 | 2.16 | 0.45 |
| 1:A:189:GLU:OE2 | 1:A:191:ILE:HD11 | 2.16 | 0.45 |
| 1:A:458:GLY:O | 1:A:460:ALA:N | 2.49 | 0.45 |
| 1:D:685:THR:OG1 | 1:D:688:VAL:HG23 | 2.17 | 0.45 |
| 1:D:39:ARG:O | 1:D:41:LEU:N | 2.49 | 0.45 |
| 1:A:604:SER:HB3 | 1:A:634:ARG:NH1 | 2.32 | 0.45 |
| 1:A:170:VAL:O | 1:A:215:ALA:HB1 | 2.15 | 0.45 |
| 1:C:680:ARG:HH11 | 1:C:680:ARG:HG3 | 1.81 | 0.45 |
| 1:D:330:ASP:O | 1:D:334:ARG:HG2 | 2.16 | 0.45 |
| 1:C:632:LEU:HD22 | 1:C:733:CYS:SG | 2.57 | 0.45 |
| 1:D:9:THR:HG23 | 1:D:18:HIS:CE1 | 2.51 | 0.45 |
| 1:A:371:VAL:O | 1:A:371:VAL:HG12 | 2.15 | 0.45 |
| 1:C:593:LEU:O | 1:C:597:GLU:HG3 | 2.17 | 0.45 |
| 1:D:235:LEU:HD23 | 1:D:235:LEU:HA | 1.75 | 0.45 |
| 1:D:4:LEU:N | 1:D:4:LEU:HD12 | 2.32 | 0.45 |
| 1:D:535:ARG:O | 1:D:538:TRP:HB3 | 2.15 | 0.45 |
| 1:D:339:GLY:HA3 | 1:D:407:GLU:O | 2.16 | 0.45 |
| 1:D:332:PHE:CD1 | 1:D:408:GLU:HG3 | 2.51 | 0.45 |
| 1:C:323:PRO:O | 1:C:326:VAL:HG23 | 2.16 | 0.45 |
| 1:B:465:PHE:CZ | 1:B:505:TYR:HB2 | 2.52 | 0.45 |
| 1:C:110:LEU:N | 1:C:110:LEU:HD23 | 2.32 | 0.45 |
| 1:B:67:TYR:CZ | 1:B:114:PRO:HG3 | 2.51 | 0.45 |
| 1:B:154:LEU:HD22 | 1:B:249:LEU:CD1 | 2.47 | 0.45 |
| 1:D:381:GLN:NE2 | 1:D:402:TRP:HD1 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:446:ASP:O | 1:D:447:ALA:C | 2.55 | 0.45 |
| 1:D:371:VAL:HG12 | 1:D:371:VAL:O | 2.16 | 0.45 |
| 1:C:454:ARG:HE | 1:C:464:GLU:CD | 2.20 | 0.45 |
| 1:C:22:LEU:O | 1:C:110:LEU:HA | 2.16 | 0.45 |
| 1:C:279:ILE:HD11 | 1:C:293:GLY:O | 2.17 | 0.45 |
| 1:B:535:ARG:O | 1:B:538:TRP:HB3 | 2.17 | 0.45 |
| 1:B:635:LEU:HA | 1:B:638:ILE:HD12 | 1.97 | 0.45 |
| 1:D:498:ALA:HA | 1:D:501:MET:CE | 2.47 | 0.45 |
| 1:D:429:LYS:O | 1:D:432:MET:O | 2.34 | 0.45 |
| 1:A:524:VAL:O | 1:A:524:VAL:HG12 | 2.16 | 0.45 |
| 1:B:287:PRO:HG2 | 1:B:409:ILE:HG12 | 1.99 | 0.45 |
| 1:D:682:SER:CB | 1:D:751:VAL:HG12 | 2.47 | 0.45 |
| 1:B:96:THR:CG2 | 1:B:301:THR:HG23 | 2.47 | 0.45 |
| 1:D:334:ARG:NH2 | 1:D:669:PRO:HA | 2.32 | 0.45 |
| 1:D:574:PRO:O | 1:D:575:VAL:C | 2.55 | 0.45 |
| 1:D:506:ARG:O | 1:D:510:GLN:HB2 | 2.16 | 0.45 |
| 1:B:385:LEU:N | 1:B:386:PRO:CD | 2.79 | 0.45 |
| 1:C:154:LEU:HD22 | 1:C:249:LEU:HD11 | 1.98 | 0.45 |
| 1:C:137:ALA:HB1 | 1:C:248:LEU:HD21 | 1.98 | 0.45 |
| 1:C:708:HIS:CB | 1:C:711:ILE:HG21 | 2.45 | 0.45 |
| 1:B:153:SER:O | 1:B:157:ARG:HD2 | 2.16 | 0.45 |
| 1:B:602:TYR:C | 1:B:634:ARG:HH22 | 2.20 | 0.45 |
| 1:B:708:HIS:CB | 1:B:711:ILE:HG21 | 2.46 | 0.45 |
| 1:A:90:MET:HE1 | 1:A:318:ARG:NH2 | 2.31 | 0.45 |
| 1:B:753:ASP:O | 1:B:754:ALA:C | 2.55 | 0.45 |
| 1:A:703:VAL:O | 1:A:706:GLU:HB3 | 2.17 | 0.45 |
| 1:A:251:PRO:O | 1:A:252:ASP:C | 2.55 | 0.45 |
| 1:B:178:GLN:NE2 | 1:B:212:LEU:HD12 | 2.23 | 0.45 |
| 1:B:429:LYS:HE2 | 1:B:515:SER:HB3 | 1.99 | 0.45 |
| 1:B:243:PRO:HA | 1:B:244:PRO:HD3 | 1.89 | 0.45 |
| 1:A:682:SER:CB | 1:A:751:VAL:HG12 | 2.47 | 0.45 |
| 1:A:608:SER:O | 1:A:611:ILE:N | 2.50 | 0.45 |
| 1:C:601:ALA:O | 1:C:634:ARG:NH2 | 2.49 | 0.45 |
| 1:B:524:VAL:HG12 | 1:B:524:VAL:O | 2.17 | 0.45 |
| 1:A:74:LEU:HD11 | 1:A:254:PHE:CE2 | 2.52 | 0.45 |
| 1:A:574:PRO:O | 1:A:575:VAL:C | 2.55 | 0.45 |
| 1:D:21:LEU:HD11 | 1:D:110:LEU:HB2 | 1.98 | 0.45 |
| 1:A:21:LEU:HD12 | 1:A:22:LEU:N | 2.32 | 0.45 |
| 1:D:14:ARG:HH12 | 1:D:223:ASP:HA | 1.80 | 0.45 |
| 1:C:222:LYS:O | 1:C:260:GLN:NE2 | 2.50 | 0.45 |
| 1:C:262:LEU:HB3 | 1:C:263:GLN:HE21 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:258:ARG:HA | 1:A:258:ARG:HD3 | 1.78 | 0.45 |
| 1:D:448:VAL:HG13 | 1:D:468:LEU:CD2 | 2.43 | 0.45 |
| 1:D:310:ARG:HH11 | 1:D:310:ARG:CB | 2.29 | 0.45 |
| 1:B:352:LEU:CD1 | 1:B:363:LEU:HD13 | 2.44 | 0.45 |
| 1:B:542:PRO:HA | 1:B:592:VAL:HG22 | 1.98 | 0.45 |
| 1:C:682:SER:CB | 1:C:751:VAL:HG12 | 2.47 | 0.45 |
| 1:C:574:PRO:O | 1:C:575:VAL:C | 2.55 | 0.45 |
| 1:B:696:PHE:HB3 | 1:B:700:VAL:HG21 | 1.99 | 0.45 |
| 1:C:635:LEU:HA | 1:C:638:ILE:HD12 | 1.98 | 0.45 |
| 1:B:401:THR:O | 1:B:404:ASP:CG | 2.55 | 0.45 |
| 1:D:176:SER:C | 1:D:178:GLN:N | 2.69 | 0.45 |
| 1:C:535:ARG:HG3 | 1:C:535:ARG:NH1 | 2.32 | 0.45 |
| 1:A:330:ASP:O | 1:A:334:ARG:HG2 | 2.17 | 0.45 |
| 1:C:330:ASP:O | 1:C:334:ARG:HG2 | 2.17 | 0.45 |
| 1:D:428:ALA:HB3 | 1:D:511:PHE:CZ | 2.52 | 0.45 |
| 1:B:498:ALA:HA | 1:B:501:MET:CE | 2.46 | 0.44 |
| 1:C:179:THR:HG21 | 1:C:209:ASP:HA | 1.98 | 0.44 |
| 1:D:178:GLN:NE2 | 1:D:212:LEU:HD12 | 2.22 | 0.44 |
| 1:A:128:MET:O | 1:A:129:VAL:C | 2.55 | 0.44 |
| 1:B:90:MET:CE | 1:B:318:ARG:NH2 | 2.79 | 0.44 |
| 1:A:368:MET:HG3 | 1:B:368:MET:HG3 | 1.99 | 0.44 |
| 1:B:458:GLY:O | 1:B:460:ALA:N | 2.50 | 0.44 |
| 1:D:524:VAL:O | 1:D:524:VAL:HG12 | 2.17 | 0.44 |
| 1:C:292:ILE:O | 1:C:292:ILE:HD12 | 2.16 | 0.44 |
| 1:D:587:PRO:HG2 | 1:D:588:VAL:N | 2.32 | 0.44 |
| 1:B:330:ASP:O | 1:B:334:ARG:HG2 | 2.16 | 0.44 |
| 1:A:139:ARG:NH2 | 1:A:163:GLU:OE2 | 2.49 | 0.44 |
| 1:D:574:PRO:HA | 1:D:578:GLY:H | 1.83 | 0.44 |
| 1:C:472:ALA:CB | 1:C:477:ILE:HD12 | 2.46 | 0.44 |
| 1:A:312:ARG:HG3 | 1:A:313:GLY:N | 2.32 | 0.44 |
| 1:C:517:LEU:HD12 | 1:C:517:LEU:C | 2.38 | 0.44 |
| 1:D:256:LEU:O | 1:D:257:ILE:C | 2.56 | 0.44 |
| 1:D:243:PRO:HA | 1:D:244:PRO:HD3 | 1.91 | 0.44 |
| 1:B:170:VAL:HG12 | 1:B:216:VAL:O | 2.17 | 0.44 |
| 1:D:402:TRP:HA | 1:D:402:TRP:HE3 | 1.82 | 0.44 |
| 1:C:753:ASP:O | 1:C:754:ALA:C | 2.55 | 0.44 |
| 1:C:609:LYS:HD3 | 1:C:641:THR:HG22 | 1.99 | 0.44 |
| 1:B:14:ARG:HD3 | 1:B:257:ILE:CD1 | 2.48 | 0.44 |
| 1:A:390:GLU:O | 1:A:391:PHE:HB3 | 2.16 | 0.44 |
| 1:A:391:PHE:CE1 | 1:A:393:ASN:HA | 2.52 | 0.44 |
| 1:C:705:ILE:HG12 | 1:C:711:ILE:CD1 | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:312:ARG:HG3 | 1:C:313:GLY:N | 2.32 | 0.44 |
| 1:D:312:ARG:HG3 | 1:D:313:GLY:N | 2.33 | 0.44 |
| 1:B:189:GLU:OE2 | 1:B:191:ILE:HD11 | 2.17 | 0.44 |
| 1:C:566:ILE:HD11 | 1:C:577:TYR:CE2 | 2.53 | 0.44 |
| 1:D:353:CYS:SG | 1:D:563:VAL:HG21 | 2.58 | 0.44 |
| 1:A:238:LYS:O | 1:A:240:ARG:HG3 | 2.17 | 0.44 |
| 1:D:159:VAL:HG21 | 1:D:247:CYS:HB3 | 1.99 | 0.44 |
| 1:B:115:LEU:H | 1:B:258:ARG:NH2 | 2.09 | 0.44 |
| 1:B:67:TYR:O | 1:B:70:ILE:HB | 2.18 | 0.44 |
| 1:C:11:VAL:O | 1:C:44:ALA:HB1 | 2.17 | 0.44 |
| 1:C:458:GLY:O | 1:C:460:ALA:N | 2.50 | 0.44 |
| 1:D:280:CYS:SG | 1:D:280:CYS:O | 2.75 | 0.44 |
| 1:A:21:LEU:HD13 | 1:A:112:PHE:CE1 | 2.52 | 0.44 |
| 1:C:205:LEU:HD22 | 1:C:245:GLU:CD | 2.38 | 0.44 |
| 1:D:599:ILE:HG21 | 1:D:631:PHE:CE1 | 2.52 | 0.44 |
| 1:B:312:ARG:HG3 | 1:B:313:GLY:N | 2.31 | 0.44 |
| 1:D:486:SER:O | 1:D:489:PHE:HB3 | 2.18 | 0.44 |
| 1:C:1:MET:O | 1:C:3:ALA:N | 2.51 | 0.44 |
| 1:C:527:ILE:CD1 | 1:C:527:ILE:H | 2.29 | 0.44 |
| 1:D:517:LEU:HD12 | 1:D:517:LEU:C | 2.38 | 0.44 |
| 1:D:12:THR:HG22 | 1:D:44:ALA:HB2 | 1.98 | 0.44 |
| 1:C:371:VAL:O | 1:C:371:VAL:HG12 | 2.17 | 0.44 |
| 1:D:104:PRO:HG2 | 1:D:107:PHE:CE1 | 2.52 | 0.44 |
| 1:C:512:SER:HG | 1:C:532:HIS:CE1 | 2.36 | 0.44 |
| 1:A:259:VAL:O | 1:A:262:LEU:N | 2.44 | 0.44 |
| 1:A:159:VAL:HG23 | 1:A:248:LEU:O | 2.17 | 0.44 |
| 1:C:189:GLU:OE2 | 1:C:191:ILE:HD11 | 2.17 | 0.44 |
| 1:C:642:PRO:HB2 | 1:C:643:HIS:H | 1.63 | 0.44 |
| 1:B:327:SER:HG | 1:B:329:THR:HB | 1.82 | 0.44 |
| 1:C:480:PHE:C | 1:C:482:SER:H | 2.20 | 0.44 |
| 1:A:9:THR:HG23 | 1:A:18:HIS:CE1 | 2.53 | 0.44 |
| 1:A:668:HIS:CB | 1:A:671:LEU:HD12 | 2.48 | 0.44 |
| 1:D:170:VAL:HG12 | 1:D:216:VAL:O | 2.18 | 0.44 |
| 1:B:1:MET:O | 1:B:3:ALA:N | 2.51 | 0.44 |
| 1:C:39:ARG:C | 1:C:41:LEU:N | 2.71 | 0.44 |
| 1:A:158:MET:HE1 | 1:A:170:VAL:HB | 2.00 | 0.44 |
| 1:A:170:VAL:HG12 | 1:A:216:VAL:O | 2.18 | 0.44 |
| 1:D:465:PHE:O | 1:D:466:ARG:C | 2.55 | 0.44 |
| 1:D:82:SER:HB3 | 1:D:85:GLU:HB3 | 1.99 | 0.44 |
| 1:B:527:ILE:H | 1:B:527:ILE:CD1 | 2.28 | 0.44 |
| 1:B:75:LEU:HD21 | 1:B:262:LEU:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:33:PHE:N | 1:D:321:PHE:CE1 | 2.85 | 0.44 |
| 1:C:446:ASP:O | 1:C:449:THR:HB | 2.18 | 0.44 |
| 1:C:34:LYS:NZ | 1:C:319:THR:HB | 2.32 | 0.44 |
| 1:C:599:ILE:HG21 | 1:C:631:PHE:CE1 | 2.53 | 0.44 |
| 1:C:176:SER:C | 1:C:178:GLN:N | 2.71 | 0.44 |
| 1:D:158:MET:CE | 1:D:170:VAL:HB | 2.47 | 0.44 |
| 1:C:256:LEU:C | 1:C:256:LEU:HD12 | 2.37 | 0.44 |
| 1:B:90:MET:HE1 | 1:B:318:ARG:NH2 | 2.32 | 0.44 |
| 1:A:498:ALA:HA | 1:A:501:MET:CE | 2.47 | 0.44 |
| 1:A:139:ARG:HG3 | 1:A:245:GLU:O | 2.18 | 0.44 |
| 1:A:506:ARG:O | 1:A:510:GLN:HB2 | 2.18 | 0.44 |
| 1:C:465:PHE:O | 1:C:466:ARG:C | 2.56 | 0.44 |
| 1:C:178:GLN:NE2 | 1:C:212:LEU:HD12 | 2.21 | 0.44 |
| 1:B:279:ILE:HD11 | 1:B:293:GLY:O | 2.18 | 0.44 |
| 1:C:473:CYS:C | 1:C:475:GLN:N | 2.70 | 0.44 |
| 1:A:226:ILE:N | 1:A:226:ILE:CD1 | 2.81 | 0.44 |
| 1:A:574:PRO:HA | 1:A:578:GLY:H | 1.83 | 0.44 |
| 1:C:465:PHE:CE1 | 1:C:502:LEU:CB | 2.98 | 0.43 |
| 1:B:179:THR:HG21 | 1:B:209:ASP:HA | 2.00 | 0.43 |
| 1:B:264:PHE:N | 1:B:264:PHE:CD1 | 2.86 | 0.43 |
| 1:B:21:LEU:HD11 | 1:B:110:LEU:HB2 | 1.99 | 0.43 |
| 1:A:527:ILE:H | 1:A:527:ILE:CD1 | 2.29 | 0.43 |
| 1:A:587:PRO:CG | 1:A:588:VAL:H | 2.31 | 0.43 |
| 1:C:428:ALA:HB3 | 1:C:511:PHE:CZ | 2.52 | 0.43 |
| 1:A:38:GLY:O | 1:A:40:GLY:N | 2.51 | 0.43 |
| 1:C:306:LEU:HB3 | 1:C:400:LYS:HZ3 | 1.82 | 0.43 |
| 1:C:280:CYS:O | 1:C:280:CYS:SG | 2.76 | 0.43 |
| 1:A:1:MET:O | 1:A:3:ALA:N | 2.51 | 0.43 |
| 1:B:310:ARG:CB | 1:B:310:ARG:HH11 | 2.29 | 0.43 |
| 1:B:618:ARG:HH11 | 1:B:618:ARG:CB | 2.30 | 0.43 |
| 1:B:698:SER:O | 1:B:699:VAL:C | 2.57 | 0.43 |
| 1:A:461:GLY:H | 1:A:464:GLU:CD | 2.21 | 0.43 |
| 1:B:682:SER:CB | 1:B:751:VAL:HG12 | 2.48 | 0.43 |
| 1:A:696:PHE:HB3 | 1:A:700:VAL:HG21 | 1.99 | 0.43 |
| 1:B:445:PRO:HD2 | 1:B:471:TYR:CE1 | 2.53 | 0.43 |
| 1:D:279:ILE:HD11 | 1:D:293:GLY:O | 2.18 | 0.43 |
| 1:C:158:MET:HE3 | 1:C:256:LEU:CB | 2.42 | 0.43 |
| 1:B:249:LEU:HD23 | 1:B:250:LEU:O | 2.18 | 0.43 |
| 1:A:59:THR:O | 1:A:63:ILE:HG13 | 2.18 | 0.43 |
| 1:A:517:LEU:HD12 | 1:A:517:LEU:C | 2.39 | 0.43 |
| 1:B:97:PHE:HZ | 1:B:301:THR:HA | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:498:ALA:HA | 1:C:501:MET:CE | 2.48 | 0.43 |
| 1:A:402:TRP:HE3 | 1:A:402:TRP:HA | 1.83 | 0.43 |
| 1:B:41:LEU:HB2 | 1:B:42:PRO:HD2 | 1.99 | 0.43 |
| 1:D:39:ARG:O | 1:D:40:GLY:C | 2.55 | 0.43 |
| 1:A:255:ASP:O | 1:A:256:LEU:C | 2.57 | 0.43 |
| 1:C:564:LEU:HD23 | 1:C:592:VAL:CG1 | 2.48 | 0.43 |
| 1:A:402:TRP:CE3 | 1:A:402:TRP:HA | 2.53 | 0.43 |
| 1:A:14:ARG:HH12 | 1:A:223:ASP:HA | 1.83 | 0.43 |
| 1:A:708:HIS:CB | 1:A:711:ILE:HG21 | 2.47 | 0.43 |
| 1:B:87:GLY:O | 1:B:90:MET:HG3 | 2.19 | 0.43 |
| 1:D:179:THR:HG21 | 1:D:209:ASP:HA | 2.00 | 0.43 |
| 1:C:264:PHE:O | 1:C:268:ILE:HG13 | 2.18 | 0.43 |
| 1:D:641:THR:O | 1:D:642:PRO:O | 2.36 | 0.43 |
| 1:B:566:ILE:HD11 | 1:B:577:TYR:CD2 | 2.54 | 0.43 |
| 1:D:566:ILE:HD11 | 1:D:577:TYR:CE2 | 2.54 | 0.43 |
| 1:C:561:ILE:CD1 | 1:C:561:ILE:H | 2.29 | 0.43 |
| 1:A:635:LEU:HA | 1:A:638:ILE:HD12 | 2.01 | 0.43 |
| 1:B:90:MET:HE1 | 1:B:318:ARG:HH22 | 1.83 | 0.43 |
| 1:B:280:CYS:SG | 1:B:280:CYS:O | 2.76 | 0.43 |
| 1:D:721:THR:O | 1:D:724:ALA:HB3 | 2.19 | 0.43 |
| 1:D:161:THR:CB | 1:D:164:ILE:HB | 2.48 | 0.43 |
| 1:D:34:LYS:CB | 1:D:45:GLU:HG3 | 2.48 | 0.43 |
| 1:B:130:THR:HG23 | 1:B:253:GLU:OE1 | 2.19 | 0.43 |
| 1:B:480:PHE:C | 1:B:482:SER:H | 2.22 | 0.43 |
| 1:C:545:TYR:HD1 | 1:C:560:THR:HG1 | 1.64 | 0.43 |
| 1:C:235:LEU:O | 1:C:237:PRO:HD2 | 2.18 | 0.43 |
| 1:C:27:LEU:HA | 1:C:293:GLY:HA3 | 2.00 | 0.43 |
| 1:D:1:MET:CE | 1:D:55:SER:HB3 | 2.48 | 0.43 |
| 1:A:265:LEU:H | 1:A:266:PRO:CD | 2.31 | 0.43 |
| 1:D:463:HIS:O | 1:D:464:GLU:C | 2.56 | 0.43 |
| 1:A:566:ILE:HD11 | 1:A:577:TYR:CD2 | 2.54 | 0.43 |
| 1:D:472:ALA:HB1 | 1:D:477:ILE:HB | 2.00 | 0.43 |
| 1:A:161:THR:CB | 1:A:164:ILE:HB | 2.48 | 0.43 |
| 1:C:326:VAL:HG12 | 1:C:330:ASP:HB2 | 2.01 | 0.43 |
| 1:A:275:ILE:HG23 | 1:A:297:TYR:HB2 | 1.99 | 0.43 |
| 1:A:333:GLN:NE2 | 1:A:672:THR:HB | 2.34 | 0.43 |
| 1:A:178:GLN:NE2 | 1:A:212:LEU:HD12 | 2.23 | 0.43 |
| 1:D:237:PRO:O | 1:D:238:LYS:HG3 | 2.19 | 0.43 |
| 1:D:249:LEU:HD23 | 1:D:250:LEU:O | 2.19 | 0.43 |
| 1:B:228:ALA:HB3 | 1:B:231:SER:HB3 | 2.01 | 0.43 |
| 1:D:59:THR:O | 1:D:63:ILE:HG13 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:566:ILE:HD11 | 1:B:577:TYR:CE2 | 2.54 | 0.43 |
| 1:D:457:MET:C | 1:D:459:GLU:H | 2.20 | 0.43 |
| 1:A:470:ASP:O | 1:A:474:GLU:N | 2.51 | 0.43 |
| 1:D:535:ARG:HG3 | 1:D:535:ARG:NH1 | 2.34 | 0.43 |
| 1:B:178:GLN:NE2 | 1:B:193:TYR:OH | 2.49 | 0.43 |
| 1:A:279:ILE:HD11 | 1:A:293:GLY:O | 2.19 | 0.43 |
| 1:C:140:LEU:CD1 | 1:C:213:VAL:HG21 | 2.48 | 0.43 |
| 1:A:523:VAL:O | 1:A:524:VAL:CB | 2.66 | 0.43 |
| 1:A:60:ASP:HB3 | 1:A:124:LEU:HD13 | 2.00 | 0.43 |
| 1:C:60:ASP:HA | 1:C:63:ILE:HD12 | 1.99 | 0.43 |
| 1:C:698:SER:O | 1:C:699:VAL:C | 2.56 | 0.43 |
| 1:D:564:LEU:HD23 | 1:D:592:VAL:CG1 | 2.49 | 0.43 |
| 1:B:457:MET:C | 1:B:459:GLU:H | 2.22 | 0.43 |
| 1:B:660:LEU:O | 1:B:661:ALA:C | 2.57 | 0.43 |
| 1:B:668:HIS:CB | 1:B:671:LEU:HD12 | 2.49 | 0.43 |
| 1:C:466:ARG:NH1 | 1:C:501:MET:CE | 2.80 | 0.42 |
| 1:D:346:ILE:HG21 | 1:D:427:LEU:HD13 | 2.00 | 0.42 |
| 1:B:559:PRO:HB2 | 1:B:560:THR:H | 1.69 | 0.42 |
| 1:A:352:LEU:CD1 | 1:A:363:LEU:HD13 | 2.43 | 0.42 |
| 1:D:460:ALA:HA | 1:D:464:GLU:OE2 | 2.18 | 0.42 |
| 1:A:137:ALA:HB3 | 1:A:248:LEU:HD21 | 1.99 | 0.42 |
| 1:D:143:GLU:O | 1:D:146:ASP:HB2 | 2.19 | 0.42 |
| 1:B:506:ARG:O | 1:B:510:GLN:HB2 | 2.19 | 0.42 |
| 1:C:465:PHE:HZ | 1:C:502:LEU:HD13 | 1.84 | 0.42 |
| 1:B:381:GLN:HE21 | 1:B:402:TRP:HD1 | 1.66 | 0.42 |
| 1:C:205:LEU:HA | 1:C:245:GLU:OE1 | 2.18 | 0.42 |
| 1:B:256:LEU:O | 1:B:258:ARG:N | 2.53 | 0.42 |
| 1:D:261:ALA:HA | 1:D:264:PHE:CD1 | 2.54 | 0.42 |
| 1:C:624:ILE:HB | 1:C:625:PRO:HD2 | 2.01 | 0.42 |
| 1:C:611:ILE:O | 1:C:615:THR:HG23 | 2.19 | 0.42 |
| 1:A:566:ILE:HD11 | 1:A:577:TYR:CE2 | 2.54 | 0.42 |
| 1:D:566:ILE:HD11 | 1:D:577:TYR:CD2 | 2.54 | 0.42 |
| 1:B:254:PHE:CD1 | 1:B:254:PHE:N | 2.86 | 0.42 |
| 1:A:462:ALA:HB1 | 1:A:498:ALA:CB | 2.47 | 0.42 |
| 1:D:668:HIS:HB3 | 1:D:671:LEU:HD12 | 2.00 | 0.42 |
| 1:C:402:TRP:HA | 1:C:402:TRP:CE3 | 2.55 | 0.42 |
| 1:D:1:MET:O | 1:D:3:ALA:N | 2.52 | 0.42 |
| 1:C:350:ARG:CD | 1:C:539:LEU:HA | 2.50 | 0.42 |
| 1:A:176:SER:C | 1:A:178:GLN:N | 2.70 | 0.42 |
| 1:D:14:ARG:HD3 | 1:D:257:ILE:CD1 | 2.47 | 0.42 |
| 1:D:158:MET:CE | 1:D:256:LEU:HD13 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:41:LEU:HD12 | 1:C:42:PRO:O | 2.20 | 0.42 |
| 1:B:128:MET:O | 1:B:129:VAL:C | 2.57 | 0.42 |
| 1:B:494:ARG:HH11 | 1:B:494:ARG:CG | 2.33 | 0.42 |
| 1:C:33:PHE:HD2 | 1:C:318:ARG:HB2 | 1.84 | 0.42 |
| 1:A:326:VAL:HG12 | 1:A:330:ASP:HB2 | 2.01 | 0.42 |
| 1:D:97:PHE:HZ | 1:D:301:THR:HA | 1.84 | 0.42 |
| 1:B:379:LEU:HD21 | 1:B:481:CYS:HB3 | 2.01 | 0.42 |
| 1:A:747:LEU:N | 1:A:748:PRO:CD | 2.82 | 0.42 |
| 1:B:176:SER:C | 1:B:178:GLN:N | 2.70 | 0.42 |
| 1:D:561:ILE:H | 1:D:561:ILE:CD1 | 2.27 | 0.42 |
| 1:C:170:VAL:HG12 | 1:C:216:VAL:O | 2.19 | 0.42 |
| 1:A:67:TYR:O | 1:A:70:ILE:HB | 2.19 | 0.42 |
| 1:B:603:GLU:N | 1:B:634:ARG:HH22 | 2.17 | 0.42 |
| 1:C:36:SER:CB | 1:C:317:TRP:HE3 | 2.33 | 0.42 |
| 1:D:60:ASP:HB3 | 1:D:124:LEU:HD13 | 2.01 | 0.42 |
| 1:C:494:ARG:HH11 | 1:C:494:ARG:CG | 2.32 | 0.42 |
| 1:A:327:SER:HG | 1:A:329:THR:HB | 1.82 | 0.42 |
| 1:D:587:PRO:CG | 1:D:588:VAL:H | 2.32 | 0.42 |
| 1:C:466:ARG:HD3 | 1:C:466:ARG:HA | 1.84 | 0.42 |
| 1:D:609:LYS:CD | 1:D:641:THR:HG22 | 2.49 | 0.42 |
| 1:B:437:SER:CB | 1:B:478:SER:O | 2.64 | 0.42 |
| 1:B:191:ILE:CG2 | 1:B:195:ARG:HD3 | 2.49 | 0.42 |
| 1:A:236:ALA:N | 1:A:237:PRO:HD3 | 2.34 | 0.42 |
| 1:A:493:LEU:HD23 | 1:A:496:ILE:HD12 | 2.02 | 0.42 |
| 1:C:596:TYR:CD2 | 1:C:600:LEU:HD11 | 2.54 | 0.42 |
| 1:A:217:ARG:HG2 | 1:A:217:ARG:NH1 | 2.34 | 0.42 |
| 1:C:307:ASP:CG | 1:C:391:PHE:HA | 2.39 | 0.42 |
| 1:A:480:PHE:C | 1:A:482:SER:H | 2.21 | 0.42 |
| 1:A:0:ALA:O | 1:A:1:MET:C | 2.55 | 0.42 |
| 1:A:457:MET:C | 1:A:459:GLU:H | 2.21 | 0.42 |
| 1:D:226:ILE:CD1 | 1:D:226:ILE:N | 2.82 | 0.42 |
| 1:A:153:SER:O | 1:A:157:ARG:HD2 | 2.19 | 0.42 |
| 1:B:326:VAL:HG12 | 1:B:330:ASP:HB2 | 2.02 | 0.42 |
| 1:D:96:THR:HG21 | 1:D:301:THR:HG23 | 2.00 | 0.42 |
| 1:B:9:THR:HG23 | 1:B:18:HIS:CE1 | 2.54 | 0.42 |
| 1:B:465:PHE:CD2 | 1:B:501:MET:HB3 | 2.55 | 0.42 |
| 1:A:381:GLN:NE2 | 1:A:402:TRP:CD1 | 2.88 | 0.42 |
| 1:B:82:SER:HB3 | 1:B:85:GLU:HB3 | 2.02 | 0.42 |
| 1:D:259:VAL:O | 1:D:260:GLN:C | 2.56 | 0.42 |
| 1:B:638:ILE:HG13 | 1:B:638:ILE:H | 1.60 | 0.42 |
| 1:C:668:HIS:CB | 1:C:671:LEU:HD12 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:242:LEU:HD12 | 1:D:247:CYS:SG | 2.59 | 0.42 |
| 1:A:458:GLY:C | 1:A:460:ALA:N | 2.72 | 0.42 |
| 1:C:242:LEU:HA | 1:C:243:PRO:HD3 | 1.89 | 0.42 |
| 1:B:161:THR:CB | 1:B:164:ILE:HB | 2.49 | 0.42 |
| 1:C:480:PHE:C | 1:C:482:SER:N | 2.72 | 0.42 |
| 1:C:62:THR:O | 1:C:66:VAL:HG23 | 2.19 | 0.42 |
| 1:B:470:ASP:O | 1:B:474:GLU:HG3 | 2.20 | 0.42 |
| 1:C:20:LEU:HB2 | 1:C:115:LEU:HD11 | 2.02 | 0.42 |
| 1:C:265:LEU:N | 1:C:266:PRO:CD | 2.83 | 0.42 |
| 1:D:602:TYR:CD1 | 1:D:603:GLU:HG2 | 2.55 | 0.42 |
| 1:B:110:LEU:HD11 | 1:B:269:ALA:CB | 2.50 | 0.42 |
| 1:A:548:GLN:NE2 | 1:A:548:GLN:CA | 2.83 | 0.42 |
| 1:D:251:PRO:HG2 | 1:D:254:PHE:HD1 | 1.82 | 0.42 |
| 1:A:342:VAL:CG2 | 1:A:410:VAL:HG12 | 2.49 | 0.42 |
| 1:C:566:ILE:HD11 | 1:C:577:TYR:CD2 | 2.55 | 0.42 |
| 1:B:574:PRO:HA | 1:B:578:GLY:H | 1.83 | 0.42 |
| 1:C:506:ARG:O | 1:C:510:GLN:HB2 | 2.20 | 0.42 |
| 1:D:289:CYS:SG | 1:D:291:ARG:HG3 | 2.60 | 0.42 |
| 1:C:458:GLY:C | 1:C:460:ALA:N | 2.71 | 0.42 |
| 1:A:39:ARG:CD | 1:A:317:TRP:CE2 | 2.97 | 0.42 |
| 1:C:747:LEU:N | 1:C:748:PRO:CD | 2.83 | 0.42 |
| 1:C:401:THR:O | 1:C:404:ASP:N | 2.43 | 0.42 |
| 1:D:162:PRO:HA | 1:D:166:TRP:CD1 | 2.55 | 0.42 |
| 1:D:458:GLY:O | 1:D:460:ALA:N | 2.51 | 0.42 |
| 1:B:265:LEU:N | 1:B:266:PRO:HD3 | 2.35 | 0.42 |
| 1:A:445:PRO:CG | 1:A:448:VAL:HG23 | 2.49 | 0.42 |
| 1:A:698:SER:O | 1:A:699:VAL:C | 2.58 | 0.42 |
| 1:C:493:LEU:HD23 | 1:C:496:ILE:HD12 | 2.01 | 0.42 |
| 1:C:631:PHE:CZ | 1:C:635:LEU:HD11 | 2.55 | 0.41 |
| 1:C:466:ARG:HH21 | 1:C:498:ALA:H | 1.65 | 0.41 |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O | 2.19 | 0.41 |
| 1:A:402:TRP:CE3 | 1:A:405:MET:HE3 | 2.55 | 0.41 |
| 1:B:41:LEU:HD13 | 1:B:42:PRO:O | 2.20 | 0.41 |
| 1:A:110:LEU:HD12 | 1:A:112:PHE:CZ | 2.55 | 0.41 |
| 1:A:480:PHE:C | 1:A:482:SER:N | 2.73 | 0.41 |
| 1:B:432:MET:CE | 1:B:538:TRP:HB2 | 2.50 | 0.41 |
| 1:D:312:ARG:O | 1:D:317:TRP:HA | 2.19 | 0.41 |
| 1:D:67:TYR:CZ | 1:D:114:PRO:CG | 3.03 | 0.41 |
| 1:B:158:MET:HE1 | 1:B:170:VAL:HB | 2.02 | 0.41 |
| 1:D:141:SER:HB3 | 1:D:210:LEU:CD1 | 2.50 | 0.41 |
| 1:A:444:CYS:SG | 1:A:445:PRO:HD2 | 2.60 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:226:ILE:CD1 | 1:B:226:ILE:N | 2.82 | 0.41 |
| 1:C:524:VAL:O | 1:C:524:VAL:HG12 | 2.20 | 0.41 |
| 1:B:587:PRO:HG2 | 1:B:588:VAL:N | 2.35 | 0.41 |
| 1:A:668:HIS:HB3 | 1:A:671:LEU:HD12 | 2.01 | 0.41 |
| 1:C:137:ALA:HB1 | 1:C:248:LEU:CD2 | 2.49 | 0.41 |
| 1:C:158:MET:CE | 1:C:170:VAL:HB | 2.50 | 0.41 |
| 1:D:608:SER:O | 1:D:611:ILE:N | 2.53 | 0.41 |
| 1:B:226:ILE:HA | 1:B:227:PRO:HD3 | 1.97 | 0.41 |
| 1:A:587:PRO:CG | 1:A:588:VAL:N | 2.83 | 0.41 |
| 1:D:23:LEU:HD23 | 1:D:110:LEU:HB3 | 2.02 | 0.41 |
| 1:B:377:ASN:HD21 | 1:B:395:LEU:HD11 | 1.84 | 0.41 |
| 1:D:462:ALA:O | 1:D:464:GLU:N | 2.52 | 0.41 |
| 1:A:97:PHE:CZ | 1:A:301:THR:HA | 2.52 | 0.41 |
| 1:C:210:LEU:HB3 | 1:C:244:PRO:HG2 | 2.02 | 0.41 |
| 1:D:1:MET:HE2 | 1:D:55:SER:HB3 | 2.03 | 0.41 |
| 1:A:23:LEU:HD21 | 1:A:272:ILE:CD1 | 2.49 | 0.41 |
| 1:A:564:LEU:C | 1:A:566:ILE:N | 2.74 | 0.41 |
| 1:C:685:THR:CG2 | 1:D:487:THR:HG21 | 2.50 | 0.41 |
| 1:D:305:ARG:HA | 1:D:305:ARG:HD2 | 1.92 | 0.41 |
| 1:D:142:ASP:C | 1:D:143:GLU:HG3 | 2.40 | 0.41 |
| 1:C:545:TYR:CD1 | 1:C:560:THR:OG1 | 2.73 | 0.41 |
| 1:C:677:THR:O | 1:C:681:GLN:HG3 | 2.21 | 0.41 |
| 1:D:178:GLN:HG3 | 1:D:212:LEU:HD12 | 2.03 | 0.41 |
| 1:B:747:LEU:N | 1:B:748:PRO:CD | 2.83 | 0.41 |
| 1:C:332:PHE:CD1 | 1:C:408:GLU:HG3 | 2.56 | 0.41 |
| 1:B:217:ARG:HG2 | 1:B:217:ARG:NH1 | 2.35 | 0.41 |
| 1:D:480:PHE:C | 1:D:482:SER:H | 2.23 | 0.41 |
| 1:C:262:LEU:C | 1:C:264:PHE:N | 2.73 | 0.41 |
| 1:D:342:VAL:CG1 | 1:D:658:CYS:SG | 3.06 | 0.41 |
| 1:B:162:PRO:HA | 1:B:166:TRP:CD1 | 2.56 | 0.41 |
| 1:C:333:GLN:HE21 | 1:C:673:GLU:CB | 2.34 | 0.41 |
| 1:D:564:LEU:C | 1:D:566:ILE:N | 2.73 | 0.41 |
| 1:B:445:PRO:HD2 | 1:B:471:TYR:CZ | 2.56 | 0.41 |
| 1:B:179:THR:HG23 | 1:B:208:ALA:O | 2.21 | 0.41 |
| 1:D:217:ARG:HG2 | 1:D:217:ARG:NH1 | 2.35 | 0.41 |
| 1:A:243:PRO:HA | 1:A:244:PRO:HD3 | 1.90 | 0.41 |
| 1:C:564:LEU:HD12 | 1:C:564:LEU:C | 2.41 | 0.41 |
| 1:B:331:VAL:O | 1:B:335:LEU:HG | 2.21 | 0.41 |
| 1:B:335:LEU:O | 1:B:411:GLY:HA3 | 2.21 | 0.41 |
| 1:B:480:PHE:C | 1:B:482:SER:N | 2.73 | 0.41 |
| 1:C:227:PRO:HG3 | 1:C:234:ASP:OD2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:275:ILE:HG23 | 1:B:297:TYR:HB2 | 2.02 | 0.41 |
| 1:C:9:THR:HG23 | 1:C:18:HIS:CE1 | 2.56 | 0.41 |
| 1:C:23:LEU:CD2 | 1:C:110:LEU:HB3 | 2.51 | 0.41 |
| 1:B:39:ARG:NH2 | 1:B:267:GLU:CD | 2.74 | 0.41 |
| 1:A:179:THR:HG23 | 1:A:208:ALA:O | 2.21 | 0.41 |
| 1:B:257:ILE:O | 1:B:260:GLN:HB3 | 2.21 | 0.41 |
| 1:C:254:PHE:C | 1:C:255:ASP:O | 2.58 | 0.41 |
| 1:A:158:MET:CE | 1:A:170:VAL:HB | 2.51 | 0.41 |
| 1:B:261:ALA:HA | 1:B:264:PHE:CD1 | 2.55 | 0.41 |
| 1:D:458:GLY:C | 1:D:460:ALA:N | 2.72 | 0.41 |
| 1:A:60:ASP:HA | 1:A:63:ILE:HD12 | 2.03 | 0.41 |
| 1:A:463:HIS:CD2 | 1:A:464:GLU:HG3 | 2.56 | 0.41 |
| 1:B:71:LEU:HD22 | 1:B:262:LEU:HD11 | 2.02 | 0.41 |
| 1:D:456:CYS:SG | 1:D:524:VAL:HG13 | 2.60 | 0.41 |
| 1:D:381:GLN:NE2 | 1:D:402:TRP:CD1 | 2.89 | 0.41 |
| 1:A:319:THR:HA | 1:A:320:PRO:HD3 | 1.84 | 0.41 |
| 1:C:379:LEU:HD21 | 1:C:481:CYS:HB3 | 2.02 | 0.41 |
| 1:B:607:GLY:C | 1:B:609:LYS:H | 2.24 | 0.41 |
| 1:C:67:TYR:O | 1:C:70:ILE:HB | 2.21 | 0.41 |
| 1:C:455:VAL:HA | 1:C:460:ALA:HB3 | 2.03 | 0.41 |
| 1:C:463:HIS:HA | 1:C:466:ARG:HB2 | 2.02 | 0.41 |
| 1:C:455:VAL:HG21 | 1:C:468:LEU:HD11 | 2.03 | 0.41 |
| 1:C:136:ASP:O | 1:C:138:LYS:N | 2.54 | 0.41 |
| 1:A:750:VAL:HG13 | 1:A:750:VAL:O | 2.20 | 0.41 |
| 1:C:380:VAL:HG21 | 1:C:402:TRP:O | 2.21 | 0.41 |
| 1:D:221:LEU:O | 1:D:223:ASP:N | 2.54 | 0.41 |
| 1:B:544:PHE:O | 1:B:560:THR:HG23 | 2.21 | 0.41 |
| 1:B:140:LEU:CD2 | 1:B:249:LEU:HB2 | 2.47 | 0.41 |
| 1:D:698:SER:O | 1:D:699:VAL:C | 2.59 | 0.41 |
| 1:D:461:GLY:O | 1:D:462:ALA:O | 2.39 | 0.41 |
| 1:A:138:LYS:HD3 | 1:A:142:ASP:CB | 2.45 | 0.41 |
| 1:A:469:VAL:O | 1:A:473:CYS:N | 2.53 | 0.41 |
| 1:A:546:VAL:HB | 1:A:644:VAL:HG13 | 2.03 | 0.41 |
| 1:A:455:VAL:HA | 1:A:460:ALA:CB | 2.51 | 0.41 |
| 1:A:465:PHE:O | 1:A:468:LEU:HB2 | 2.20 | 0.41 |
| 1:B:34:LYS:HG3 | 1:B:321:PHE:CD1 | 2.55 | 0.41 |
| 1:A:680:ARG:HG3 | 1:A:681:GLN:N | 2.35 | 0.41 |
| 1:C:587:PRO:HG2 | 1:C:588:VAL:N | 2.35 | 0.41 |
| 1:C:574:PRO:HA | 1:C:578:GLY:H | 1.85 | 0.41 |
| 1:C:34:LYS:HZ3 | 1:C:319:THR:CG2 | 2.33 | 0.41 |
| 1:B:668:HIS:HB3 | 1:B:671:LEU:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:67:TYR:CZ | 1:C:114:PRO:CG | 3.04 | 0.41 |
| 1:C:455:VAL:HA | 1:C:460:ALA:CB | 2.51 | 0.41 |
| 1:D:747:LEU:N | 1:D:748:PRO:CD | 2.84 | 0.41 |
| 1:A:624:ILE:HB | 1:A:625:PRO:HD2 | 2.03 | 0.41 |
| 1:C:352:LEU:CD1 | 1:C:363:LEU:HD13 | 2.50 | 0.41 |
| 1:B:4:LEU:HD21 | 1:B:26:HIS:HA | 2.02 | 0.41 |
| 1:C:191:ILE:CG2 | 1:C:195:ARG:HD3 | 2.48 | 0.41 |
| 1:B:460:ALA:HA | 1:B:464:GLU:HG2 | 2.02 | 0.41 |
| 1:C:115:LEU:N | 1:C:258:ARG:NH2 | 2.50 | 0.40 |
| 1:A:104:PRO:HG2 | 1:A:107:PHE:CE1 | 2.56 | 0.40 |
| 1:B:39:ARG:HH12 | 1:B:41:LEU:HD21 | 1.86 | 0.40 |
| 1:C:128:MET:O | 1:C:132:GLN:HG3 | 2.21 | 0.40 |
| 1:D:631:PHE:CE2 | 1:D:635:LEU:HD11 | 2.56 | 0.40 |
| 1:B:140:LEU:C | 1:B:142:ASP:N | 2.74 | 0.40 |
| 1:A:258:ARG:O | 1:A:259:VAL:O | 2.38 | 0.40 |
| 1:B:434:PRO:CA | 1:B:527:ILE:HG22 | 2.49 | 0.40 |
| 1:D:60:ASP:CB | 1:D:124:LEU:HD13 | 2.52 | 0.40 |
| 1:A:312:ARG:O | 1:A:317:TRP:HA | 2.22 | 0.40 |
| 1:C:235:LEU:HA | 1:C:235:LEU:HD23 | 1.88 | 0.40 |
| 1:B:432:MET:CE | 1:B:534:ALA:HB1 | 2.48 | 0.40 |
| 1:C:1:MET:O | 1:C:2:HIS:C | 2.60 | 0.40 |
| 1:B:455:VAL:HA | 1:B:460:ALA:CB | 2.51 | 0.40 |
| 1:C:609:LYS:CD | 1:C:641:THR:HG22 | 2.52 | 0.40 |
| 1:D:17:SER:OG | 1:D:258:ARG:NH1 | 2.54 | 0.40 |
| 1:B:394:ASN:ND2 | 1:B:396:VAL:HB | 2.34 | 0.40 |
| 1:B:740:ALA:HA | 1:B:743:ARG:HG2 | 2.04 | 0.40 |
| 1:D:1:MET:O | 1:D:2:HIS:C | 2.60 | 0.40 |
| 1:D:150:LEU:HD12 | 1:D:153:SER:OG | 2.20 | 0.40 |
| 1:A:67:TYR:CZ | 1:A:114:PRO:CG | 3.04 | 0.40 |
| 1:B:642:PRO:HB2 | 1:B:643:HIS:H | 1.64 | 0.40 |
| 1:D:469:VAL:C | 1:D:471:TYR:N | 2.75 | 0.40 |
| 1:A:162:PRO:HA | 1:A:166:TRP:CD1 | 2.56 | 0.40 |
| 1:A:581:THR:O | 1:A:585:THR:HG22 | 2.21 | 0.40 |
| 1:C:57:SER:O | 1:C:59:THR:N | 2.54 | 0.40 |
| 1:C:543:GLY:CA | 1:C:561:ILE:O | 2.63 | 0.40 |
| 1:D:480:PHE:C | 1:D:482:SER:N | 2.74 | 0.40 |
| 1:B:157:ARG:NH2 | 1:B:249:LEU:HD21 | 2.36 | 0.40 |
| 1:A:258:ARG:O | 1:A:259:VAL:C | 2.60 | 0.40 |
| 1:D:609:LYS:HZ2 | 1:D:641:THR:CG2 | 2.32 | 0.40 |
| 1:C:36:SER:HB3 | 1:C:317:TRP:CE3 | 2.55 | 0.40 |
| 1:B:564:LEU:HD12 | 1:B:564:LEU:C | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:34:LYS:HA | 1:B:45:GLU:HA | 2.03 | 0.40 |
| 1:C:587:PRO:CG | 1:C:588:VAL:H | 2.35 | 0.40 |
| 1:C:401:THR:O | 1:C:402:TRP:C | 2.59 | 0.40 |
| 1:A:82:SER:HB3 | 1:A:85:GLU:HB3 | 2.04 | 0.40 |
| 1:C:12:THR:OG1 | 1:C:14:ARG:HG3 | 2.22 | 0.40 |
| 1:A:221:LEU:O | 1:A:223:ASP:N | 2.55 | 0.40 |
| 1:C:342:VAL:CG2 | 1:C:410:VAL:HG12 | 2.50 | 0.40 |
| 1:B:158:MET:CE | 1:B:170:VAL:HB | 2.51 | 0.40 |
| 1:A:368:MET:O | 1:A:372:ARG:CB | 2.68 | 0.40 |
| 1:C:210:LEU:HA | 1:C:211:PRO:HD3 | 1.92 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 718/756 (95%) | 593 (83%) | 87 (12%) | 38 (5%) | 2 | 14 |
| 1 | B | 710/756 (94%) | 580 (82%) | 91 (13%) | 39 (6%) | 2 | 13 |
| 1 | C | 700/756 (93%) | 578 (83%) | 87 (12%) | 35 (5%) | 3 | 15 |
| 1 | D | 702/756 (93%) | 578 (82%) | 82 (12%) | 42 (6%) | 2 | 11 |
| All | All | 2830/3024 (94%) | 2329 (82%) | 347 (12%) | 154 (5%) | 2 | 14 |

All (154) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | HIS |
| 1 | A | 39 | ARG |
| 1 | A | 81 | ALA |
| 1 | A | 182 | SER |
| 1 | A | 222 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 259 | VAL |
| 1 | A | 393 | ASN |
| 1 | A | 524 | VAL |
| 1 | A | 547 | GLU |
| 1 | A | 642 | PRO |
| 1 | A | 643 | HIS |
| 1 | A | 698 | SER |
| 1 | B | 2 | HIS |
| 1 | B | 37 | ALA |
| 1 | B | 182 | SER |
| 1 | B | 222 | LYS |
| 1 | B | 234 | ASP |
| 1 | B | 398 | LYS |
| 1 | B | 642 | PRO |
| 1 | B | 643 | HIS |
| 1 | B | 698 | SER |
| 1 | C | 2 | HIS |
| 1 | C | 81 | ALA |
| 1 | C | 138 | LYS |
| 1 | C | 182 | SER |
| 1 | C | 222 | LYS |
| 1 | C | 255 | ASP |
| 1 | C | 462 | ALA |
| 1 | C | 547 | GLU |
| 1 | C | 642 | PRO |
| 1 | C | 643 | HIS |
| 1 | C | 698 | SER |
| 1 | D | 2 | HIS |
| 1 | D | 39 | ARG |
| 1 | D | 81 | ALA |
| 1 | D | 182 | SER |
| 1 | D | 222 | LYS |
| 1 | D | 256 | LEU |
| 1 | D | 445 | PRO |
| 1 | D | 462 | ALA |
| 1 | D | 463 | HIS |
| 1 | D | 547 | GLU |
| 1 | D | 642 | PRO |
| 1 | D | 643 | HIS |
| 1 | D | 698 | SER |
| 1 | A | 229 | PRO |
| 1 | A | 275 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 281 | ALA |
| 1 | A | 311 | GLY |
| 1 | A | 458 | GLY |
| 1 | A | 586 | GLY |
| 1 | A | 606 | GLY |
| 1 | B | 39 | ARG |
| 1 | B | 81 | ALA |
| 1 | B | 275 | ILE |
| 1 | B | 311 | GLY |
| 1 | B | 458 | GLY |
| 1 | B | 586 | GLY |
| 1 | B | 602 | TYR |
| 1 | B | 603 | GLU |
| 1 | B | 605 | SER |
| 1 | C | 40 | GLY |
| 1 | C | 275 | ILE |
| 1 | C | 281 | ALA |
| 1 | C | 311 | GLY |
| 1 | C | 391 | PHE |
| 1 | C | 458 | GLY |
| 1 | C | 474 | GLU |
| 1 | C | 586 | GLY |
| 1 | D | 50 | ALA |
| 1 | D | 146 | ASP |
| 1 | D | 252 | ASP |
| 1 | D | 253 | GLU |
| 1 | D | 257 | ILE |
| 1 | D | 275 | ILE |
| 1 | D | 311 | GLY |
| 1 | D | 447 | ALA |
| 1 | D | 458 | GLY |
| 1 | D | 586 | GLY |
| 1 | A | 50 | ALA |
| 1 | A | 58 | ARG |
| 1 | A | 200 | ALA |
| 1 | A | 237 | PRO |
| 1 | A | 459 | GLU |
| 1 | A | 559 | PRO |
| 1 | A | 587 | PRO |
| 1 | A | 607 | GLY |
| 1 | B | 36 | SER |
| 1 | B | 58 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 108 | ALA |
| 1 | B | 137 | ALA |
| 1 | B | 200 | ALA |
| 1 | B | 229 | PRO |
| 1 | B | 258 | ARG |
| 1 | B | 281 | ALA |
| 1 | B | 397 | ALA |
| 1 | B | 445 | PRO |
| 1 | B | 459 | GLU |
| 1 | B | 559 | PRO |
| 1 | B | 587 | PRO |
| 1 | C | 50 | ALA |
| 1 | C | 58 | ARG |
| 1 | C | 108 | ALA |
| 1 | C | 200 | ALA |
| 1 | C | 459 | GLU |
| 1 | C | 587 | PRO |
| 1 | D | 58 | ARG |
| 1 | D | 108 | ALA |
| 1 | D | 137 | ALA |
| 1 | D | 200 | ALA |
| 1 | D | 258 | ARG |
| 1 | D | 281 | ALA |
| 1 | D | 459 | GLU |
| 1 | D | 464 | GLU |
| 1 | D | 587 | PRO |
| 1 | A | 105 | PRO |
| 1 | A | 108 | ALA |
| 1 | A | 230 | GLY |
| 1 | A | 254 | PHE |
| 1 | B | 50 | ALA |
| 1 | B | 259 | VAL |
| 1 | B | 389 | ALA |
| 1 | C | 473 | CYS |
| 1 | D | 212 | LEU |
| 1 | D | 259 | VAL |
| 1 | A | 673 | GLU |
| 1 | B | 105 | PRO |
| 1 | B | 673 | GLU |
| 1 | C | 105 | PRO |
| 1 | C | 137 | ALA |
| 1 | C | 236 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 257 | ILE |
| 1 | C | 673 | GLU |
| 1 | D | 105 | PRO |
| 1 | D | 238 | LYS |
| 1 | D | 673 | GLU |
| 1 | A | 256 | LEU |
| 1 | A | 257 | ILE |
| 1 | B | 180 | SER |
| 1 | B | 227 | PRO |
| 1 | C | 212 | LEU |
| 1 | D | 82 | SER |
| 1 | A | 227 | PRO |
| 1 | A | 445 | PRO |
| 1 | C | 227 | PRO |
| 1 | D | 227 | PRO |
| 1 | B | 279 | ILE |
| 1 | D | 38 | GLY |
| 1 | C | 279 | ILE |
| 1 | C | 469 | VAL |
| 1 | A | 279 | ILE |
| 1 | A | 575 | VAL |
| 1 | D | 279 | ILE |
| 1 | D | 575 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 611/632 (97%) | 572 (94%) | 39 (6%) | 22 59 |
| 1 | B | 607/632 (96%) | 577 (95%) | 30 (5%) | 31 71 |
| 1 | C | 602/632 (95%) | 574 (95%) | 28 (5%) | 32 72 |
| 1 | D | 605/632 (96%) | 566 (94%) | 39 (6%) | 22 59 |
| All | All | 2425/2528 (96%) | 2289 (94%) | 136 (6%) | 26 65 |

All (136) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | HIS |
| 1 | A | 14 | ARG |
| 1 | A | 35 | VAL |
| 1 | A | 39 | ARG |
| 1 | A | 42 | PRO |
| 1 | A | 68 | GLN |
| 1 | A | 110 | LEU |
| 1 | A | 136 | ASP |
| 1 | A | 139 | ARG |
| 1 | A | 142 | ASP |
| 1 | A | 179 | THR |
| 1 | A | 217 | ARG |
| 1 | A | 222 | LYS |
| 1 | A | 223 | ASP |
| 1 | A | 225 | GLN |
| 1 | A | 242 | LEU |
| 1 | A | 262 | LEU |
| 1 | A | 327 | SER |
| 1 | A | 332 | PHE |
| 1 | A | 357 | ASP |
| 1 | A | 395 | LEU |
| 1 | A | 400 | LYS |
| 1 | A | 402 | TRP |
| 1 | A | 438 | LYS |
| 1 | A | 444 | CYS |
| 1 | A | 457 | MET |
| 1 | A | 467 | SER |
| 1 | A | 488 | MET |
| 1 | A | 491 | GLU |
| 1 | A | 509 | ILE |
| 1 | A | 539 | LEU |
| 1 | A | 546 | VAL |
| 1 | A | 559 | PRO |
| 1 | A | 566 | ILE |
| 1 | A | 581 | THR |
| 1 | A | 618 | ARG |
| 1 | A | 624 | ILE |
| 1 | A | 720 | ASP |
| 1 | A | 753 | ASP |
| 1 | B | 2 | HIS |
| 1 | B | 14 | ARG |
| 1 | B | 39 | ARG |
| 1 | B | 68 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 110 | LEU |
| 1 | B | 179 | THR |
| 1 | B | 217 | ARG |
| 1 | B | 222 | LYS |
| 1 | B | 223 | ASP |
| 1 | B | 225 | GLN |
| 1 | B | 242 | LEU |
| 1 | B | 327 | SER |
| 1 | B | 332 | PHE |
| 1 | B | 352 | LEU |
| 1 | B | 357 | ASP |
| 1 | B | 402 | TRP |
| 1 | B | 438 | LYS |
| 1 | B | 457 | MET |
| 1 | B | 467 | SER |
| 1 | B | 488 | MET |
| 1 | B | 491 | GLU |
| 1 | B | 509 | ILE |
| 1 | B | 539 | LEU |
| 1 | B | 546 | VAL |
| 1 | B | 566 | ILE |
| 1 | B | 581 | THR |
| 1 | B | 608 | SER |
| 1 | B | 618 | ARG |
| 1 | B | 624 | ILE |
| 1 | B | 720 | ASP |
| 1 | C | 2 | HIS |
| 1 | C | 14 | ARG |
| 1 | C | 110 | LEU |
| 1 | C | 179 | THR |
| 1 | C | 217 | ARG |
| 1 | C | 222 | LYS |
| 1 | C | 223 | ASP |
| 1 | C | 225 | GLN |
| 1 | C | 242 | LEU |
| 1 | C | 327 | SER |
| 1 | C | 332 | PHE |
| 1 | C | 357 | ASP |
| 1 | C | 402 | TRP |
| 1 | C | 438 | LYS |
| 1 | C | 444 | CYS |
| 1 | C | 457 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 464 | GLU |
| 1 | C | 475 | GLN |
| 1 | C | 488 | MET |
| 1 | C | 491 | GLU |
| 1 | C | 509 | ILE |
| 1 | C | 539 | LEU |
| 1 | C | 546 | VAL |
| 1 | C | 566 | ILE |
| 1 | C | 581 | THR |
| 1 | C | 618 | ARG |
| 1 | C | 624 | ILE |
| 1 | C | 720 | ASP |
| 1 | D | 2 | HIS |
| 1 | D | 14 | ARG |
| 1 | D | 34 | LYS |
| 1 | D | 35 | VAL |
| 1 | D | 68 | GLN |
| 1 | D | 110 | LEU |
| 1 | D | 139 | ARG |
| 1 | D | 141 | SER |
| 1 | D | 145 | THR |
| 1 | D | 179 | THR |
| 1 | D | 217 | ARG |
| 1 | D | 222 | LYS |
| 1 | D | 223 | ASP |
| 1 | D | 225 | GLN |
| 1 | D | 233 | ASP |
| 1 | D | 242 | LEU |
| 1 | D | 252 | ASP |
| 1 | D | 258 | ARG |
| 1 | D | 264 | PHE |
| 1 | D | 327 | SER |
| 1 | D | 332 | PHE |
| 1 | D | 352 | LEU |
| 1 | D | 357 | ASP |
| 1 | D | 402 | TRP |
| 1 | D | 438 | LYS |
| 1 | D | 457 | MET |
| 1 | D | 463 | HIS |
| 1 | D | 488 | MET |
| 1 | D | 491 | GLU |
| 1 | D | 509 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 539 | LEU |
| 1 | D | 546 | VAL |
| 1 | D | 548 | GLN |
| 1 | D | 566 | ILE |
| 1 | D | 581 | THR |
| 1 | D | 618 | ARG |
| 1 | D | 624 | ILE |
| 1 | D | 720 | ASP |
| 1 | D | 753 | ASP |

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 | 68 | GLN |
| 1 | A | 132 | GLN |
| 1 | A | 178 | GLN |
| 1 | A | 202 | ASN |
| 1 | A | 225 | GLN |
| 1 | A | 260 | GLN |
| 1 | A | 333 | GLN |
| 1 | A | 373 | ASN |
| 1 | A | 418 | ASN |
| 1 | A | 463 | HIS |
| 1 | A | 548 | GLN |
| 1 | A | 572 | GLN |
| 1 | A | 610 | HIS |
| 1 | A | 637 | GLN |
| 1 | A | 745 | HIS |
| 1 | B | 68 | GLN |
| 1 | B | 132 | GLN |
| 1 | B | 178 | GLN |
| 1 | B | 202 | ASN |
| 1 | B | 225 | GLN |
| 1 | B | 333 | GLN |
| 1 | B | 373 | ASN |
| 1 | B | 377 | ASN |
| 1 | B | 381 | GLN |
| 1 | B | 572 | GLN |
| 1 | B | 610 | HIS |
| 1 | B | 745 | HIS |
| 1 | C | 68 | GLN |
| 1 | C | 132 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 178 | GLN |
| 1 | C | 225 | GLN |
| 1 | C | 333 | GLN |
| 1 | C | 373 | ASN |
| 1 | C | 377 | ASN |
| 1 | C | 381 | GLN |
| 1 | C | 418 | ASN |
| 1 | C | 572 | GLN |
| 1 | C | 610 | HIS |
| 1 | C | 614 | GLN |
| 1 | C | 637 | GLN |
| 1 | D | 68 | GLN |
| 1 | D | 132 | GLN |
| 1 | D | 178 | GLN |
| 1 | D | 202 | ASN |
| 1 | D | 225 | GLN |
| 1 | D | 333 | GLN |
| 1 | D | 373 | ASN |
| 1 | D | 377 | ASN |
| 1 | D | 381 | GLN |
| 1 | D | 548 | GLN |
| 1 | D | 572 | GLN |
| 1 | D | 610 | HIS |
| 1 | D | 745 | 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

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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 | 732/756 (96%) | -0.31 | 1 (0%) 95 90 | 19, 36, 65, 92 | 1 (0%) |
| 1 | B | 726/756 (96%) | -0.32 | 0 100 100 | 21, 36, 67, 93 | 1 (0%) |
| 1 | C | 718/756 (94%) | -0.37 | 1 (0%) 95 90 | 18, 36, 66, 92 | 1 (0%) |
| 1 | D | 720/756 (95%) | -0.34 | 4 (0%) 90 73 | 20, 36, 65, 92 | 1 (0%) |
| All | All | 2896/3024 (95%) | -0.33 | 6 (0%) 95 87 | 18, 36, 66, 93 | 4 (0%) |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 187 | ALA | 3.0 |
| 1 | D | 185 | THR | 2.6 |
| 1 | D | 145 | THR | 2.2 |
| 1 | C | 234 | ASP | 2.1 |
| 1 | A | -1 | GLY | 2.1 |
| 1 | D | 188 | ASN | 2.0 |

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 2 | MN | C | 760 | 1/1 | 0.86 | 0.33 | 2.38 | 92,92,92,92 | 0 |
| 2 | MN | B | 758 | 1/1 | 0.83 | 0.23 | 0.61 | 97,97,97,97 | 0 |
| 2 | MN | C | 762 | 1/1 | 0.90 | 0.14 | -1.43 | 93,93,93,93 | 0 |
| 2 | MN | A | 765 | 1/1 | 0.97 | 0.10 | -2.75 | 83,83,83,83 | 0 |
| 2 | MN | C | 755 | 1/1 | 0.94 | 0.06 | -2.75 | 48,48,48,48 | 0 |
| 2 | MN | A | 766 | 1/1 | 0.97 | 0.12 | -2.84 | 76,76,76,76 | 0 |
| 2 | MN | B | 761 | 1/1 | 0.85 | 0.12 | -2.87 | 72,72,72,72 | 0 |
| 2 | MN | B | 755 | 1/1 | 0.99 | 0.03 | -4.97 | 38,38,38,38 | 0 |
| 2 | MN | A | 755 | 1/1 | 0.95 | 0.07 | -6.07 | 32,32,32,32 | 0 |
| 2 | MN | A | 764 | 1/1 | 0.74 | 0.13 | - | 96,96,96,96 | 0 |
| 2 | MN | C | 761 | 1/1 | 0.97 | 0.18 | - | 78,78,78,78 | 0 |
| 2 | MN | D | 758 | 1/1 | 0.90 | 0.16 | - | 99,99,99,99 | 0 |
| 2 | MN | D | 761 | 1/1 | 0.78 | 0.25 | - | 82,82,82,82 | 0 |
| 2 | MN | A | 762 | 1/1 | 0.97 | 0.10 | - | 50,50,50,50 | 0 |
| 2 | MN | B | 763 | 1/1 | 0.94 | 0.10 | - | 48,48,48,48 | 0 |
| 2 | MN | A | 756 | 1/1 | 0.98 | 0.04 | - | 20,20,20,20 | 0 |
| 2 | MN | D | 759 | 1/1 | 0.69 | 0.54 | - | 107,107,107,107 | 0 |
| 2 | MN | C | 759 | 1/1 | 0.55 | 0.26 | - | 113,113,113,113 | 0 |
| 2 | MN | A | 763 | 1/1 | 0.94 | 0.17 | - | 65,65,65,65 | 0 |
| 2 | MN | D | 760 | 1/1 | 0.84 | 0.20 | - | 107,107,107,107 | 0 |
| 2 | MN | C | 758 | 1/1 | 0.75 | 0.20 | - | 85,85,85,85 | 0 |
| 2 | MN | D | 756 | 1/1 | 0.96 | 0.07 | - | 34,34,34,34 | 0 |
| 2 | MN | D | 763 | 1/1 | 0.95 | 0.30 | - | 86,86,86,86 | 0 |
| 2 | MN | D | 757 | 1/1 | 0.88 | 0.24 | - | 70,70,70,70 | 0 |
| 2 | MN | A | 761 | 1/1 | 0.90 | 0.31 | - | 63,63,63,63 | 0 |
| 2 | MN | A | 758 | 1/1 | 0.97 | 0.05 | - | 68,68,68,68 | 0 |
| 2 | MN | B | 760 | 1/1 | 0.93 | 0.18 | - | 49,49,49,49 | 0 |
| 2 | MN | A | 760 | 1/1 | 0.96 | 0.33 | - | 34,34,34,34 | 0 |
| 2 | MN | B | 756 | 1/1 | 0.86 | 0.09 | - | 25,25,25,25 | 0 |
| 2 | MN | D | 762 | 1/1 | 0.57 | 0.26 | - | 114,114,114,114 | 0 |
| 2 | MN | D | 755 | 1/1 | 0.84 | 0.12 | - | 39,39,39,39 | 0 |
| 2 | MN | C | 757 | 1/1 | 0.61 | 0.12 | - | 100,100,100,100 | 0 |
| 2 | MN | B | 757 | 1/1 | 0.95 | 0.34 | - | 79,79,79,79 | 0 |
| 2 | MN | B | 762 | 1/1 | 0.91 | 0.08 | - | 61,61,61,61 | 0 |
| 2 | MN | A | 757 | 1/1 | 0.92 | 0.14 | - | 77,77,77,77 | 0 |
| 2 | MN | C | 756 | 1/1 | 0.96 | 0.08 | - | 39,39,39,39 | 0 |
| 2 | MN | B | 759 | 1/1 | 0.89 | 0.19 | - | 49,49,49,49 | 0 |
| 2 | MN | A | 759 | 1/1 | 0.88 | 0.26 | - | 49,49,49,49 | 0 |
| 2 | MN | C | 763 | 1/1 | 0.66 | 0.31 | - | 114,114,114,114 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.