# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:03 AM EST

| | | |
|---|---|---|
| PDB ID | : | 4K17 |
| Title | : | Crystal Structure of mouse CARMIL residues 1-668 |
| Authors | : | Zwolak, A.; Dominguez, R. |
| Deposited on | : | 2013-04-04 |
| Resolution | : | 2.90 Å(reported) |

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

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

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

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

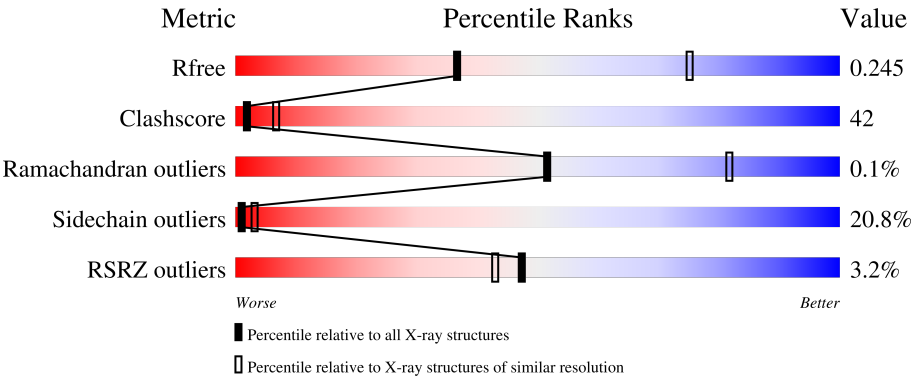
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1957 (2.90-2.90) |
| Clashscore | 141614 | 2172 (2.90-2.90) |
| Ramachandran outliers | 138981 | 2115 (2.90-2.90) |
| Sidechain outliers | 138945 | 2117 (2.90-2.90) |
| RSRZ outliers | 127900 | 1906 (2.90-2.90) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 669 | 2% 47% 41% 10% |
| 1 | B | 669 | 3% 48% 39% 11% |
| 1 | C | 669 | % 42% 46% 10% |
| 1 | D | 669 | 7% 42% 42% 14% |

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 |
|---|---|---|---|---|---|---|---|
| 3 | CL | B | 702 | - | - | X | - |
| 4 | ABU | C | 701 | - | X | - | - |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20371 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.

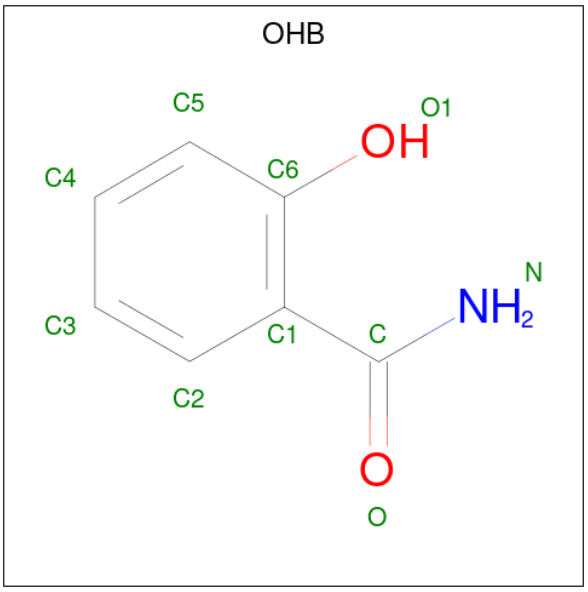
- Molecule 1 is a protein called Leucine-rich repeat-containing protein 16A.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 660 | Total | C | N | O | S | Se | 0 | 2 | 0 |
| | | | 5112 | 3220 | 888 | 969 | 17 | 18 | | | |
| 1 | B | 660 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 5102 | 3211 | 884 | 973 | 16 | 18 | | | |
| 1 | C | 656 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 5073 | 3196 | 880 | 963 | 16 | 18 | | | |
| 1 | D | 655 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 5066 | 3191 | 879 | 962 | 16 | 18 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 0 | SER | - | expression tag | UNP Q6EDY6 |
| B | 0 | SER | - | expression tag | UNP Q6EDY6 |
| C | 0 | SER | - | expression tag | UNP Q6EDY6 |
| D | 0 | SER | - | expression tag | UNP Q6EDY6 |

- Molecule 2 is salicylamide (three-letter code: OHB) (formula: $C_7H_7NO_2$).

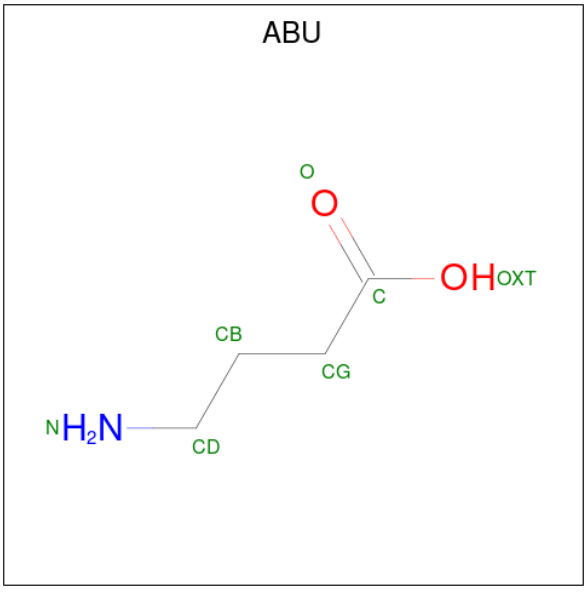



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | B | 1 | Total C N O<br>10 7 1 2 | 0 | 0 |

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | B | 1 | Total Cl<br>1 1 | 0 | 0 |

- Molecule 4 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



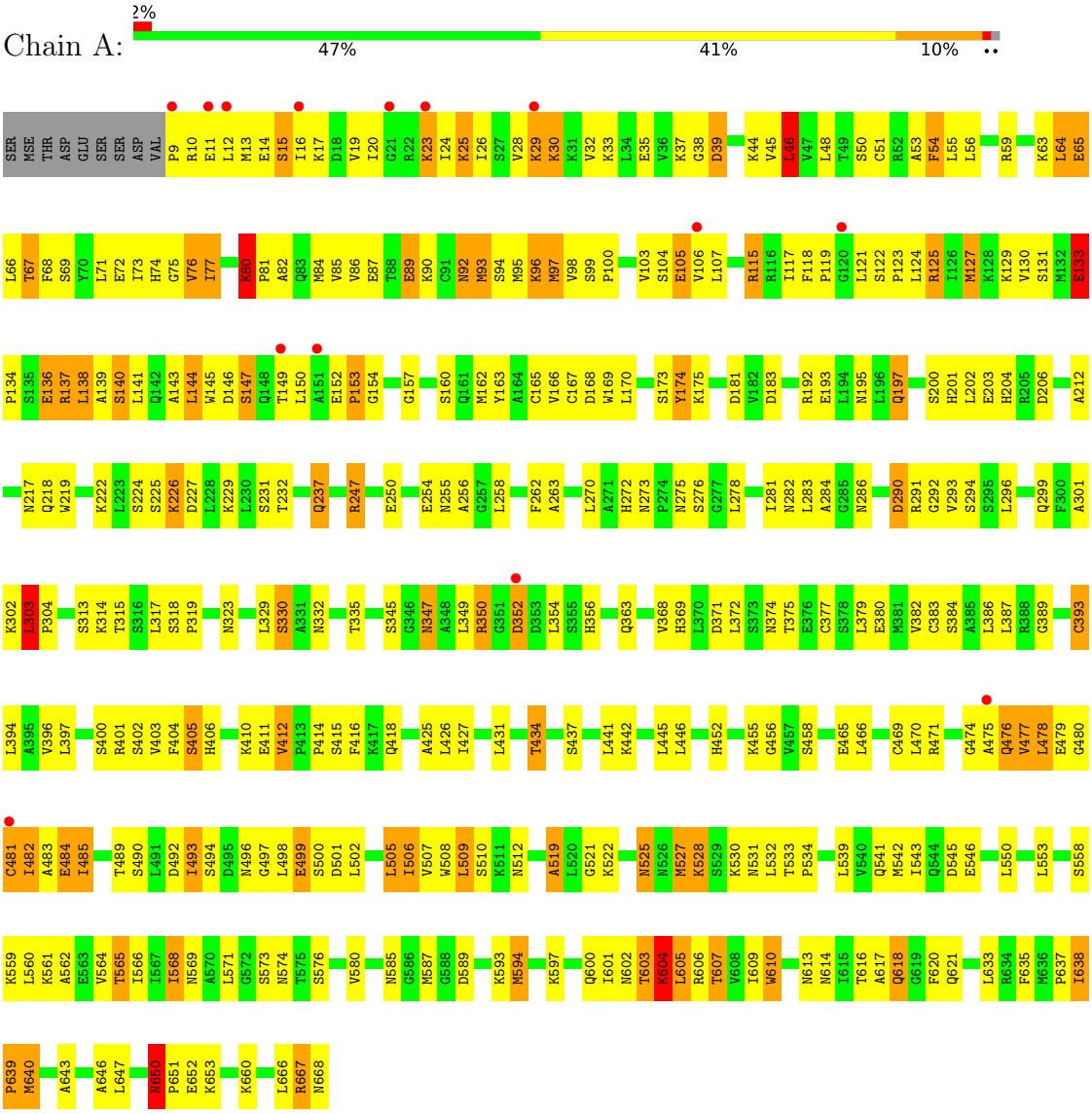
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 7 | 4 | 1 | 2 | | |

# 3 Residue-property plots (i)

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

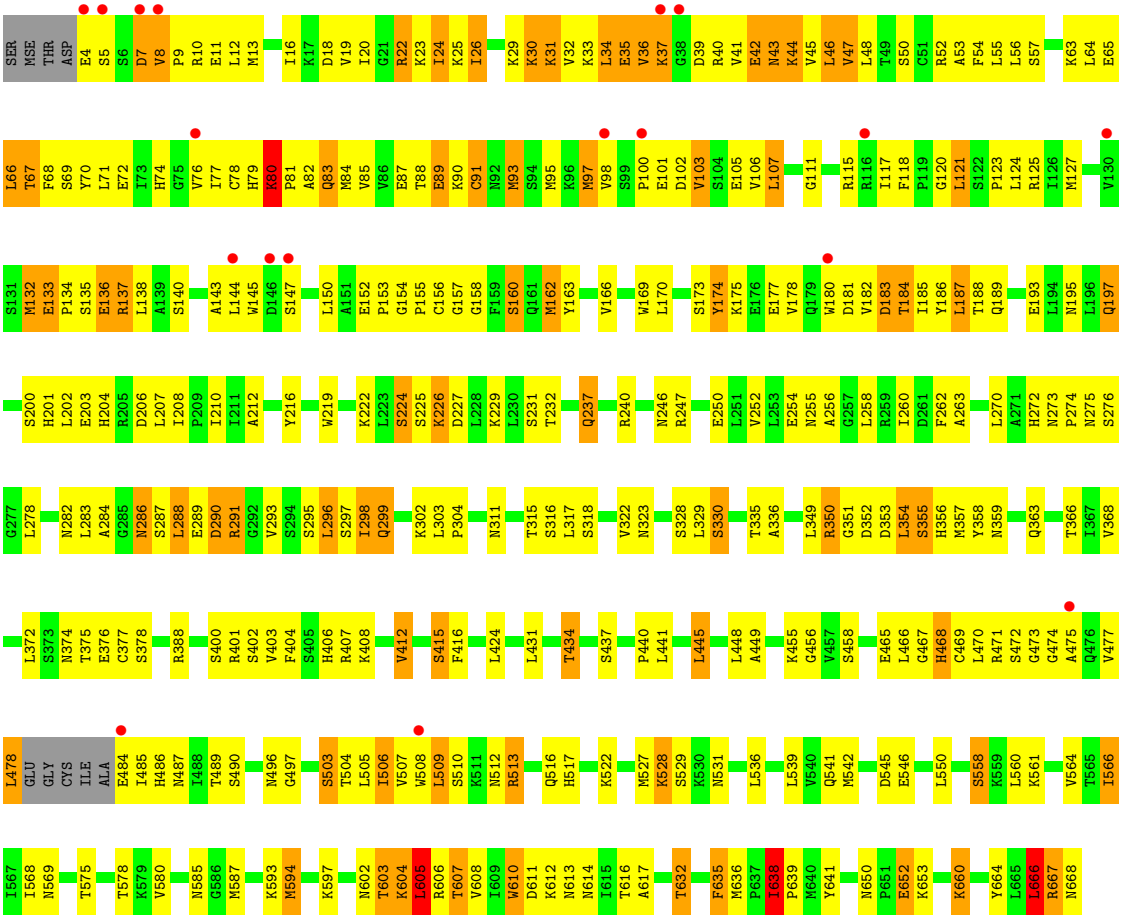
• Molecule 1: Leucine-rich repeat-containing protein 16A

Chain A:



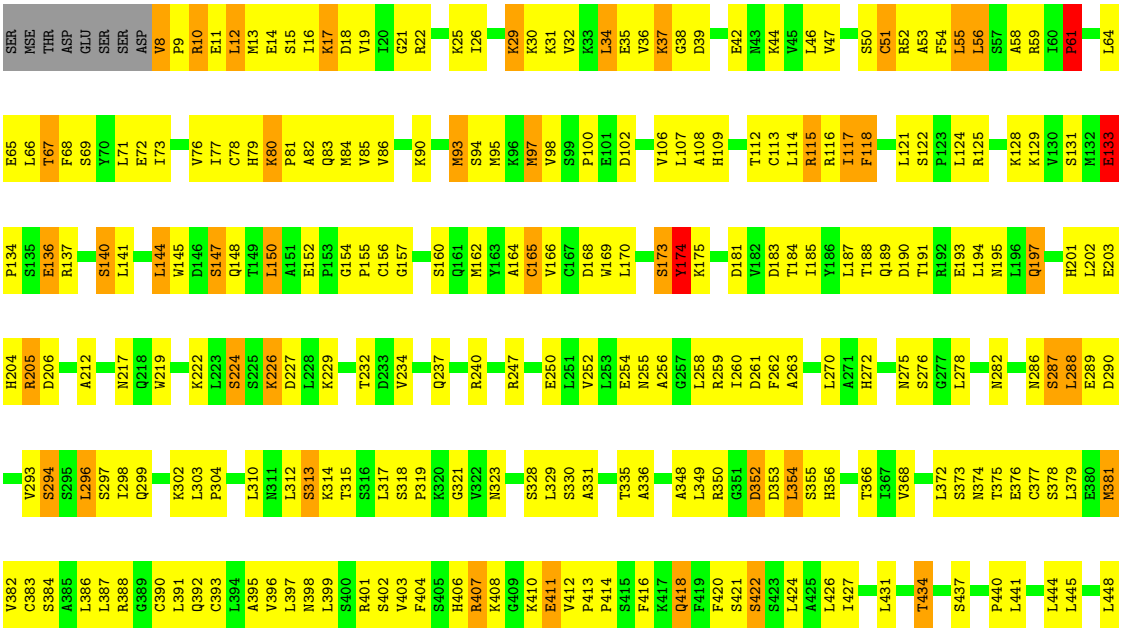

• Molecule 1: Leucine-rich repeat-containing protein 16A

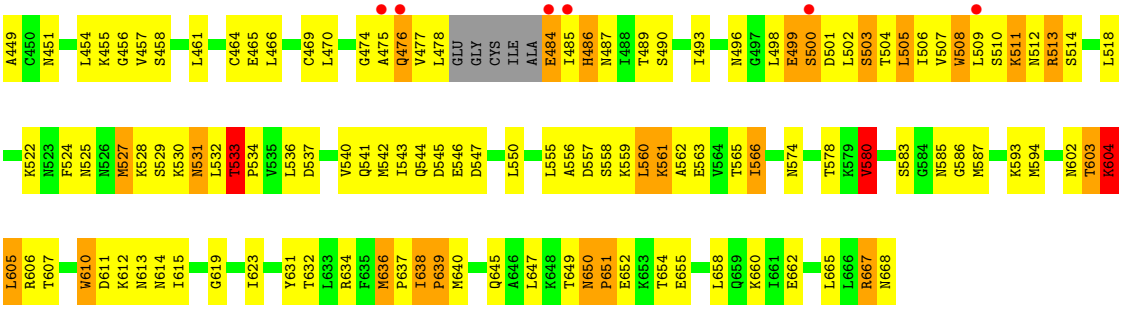
Chain B:



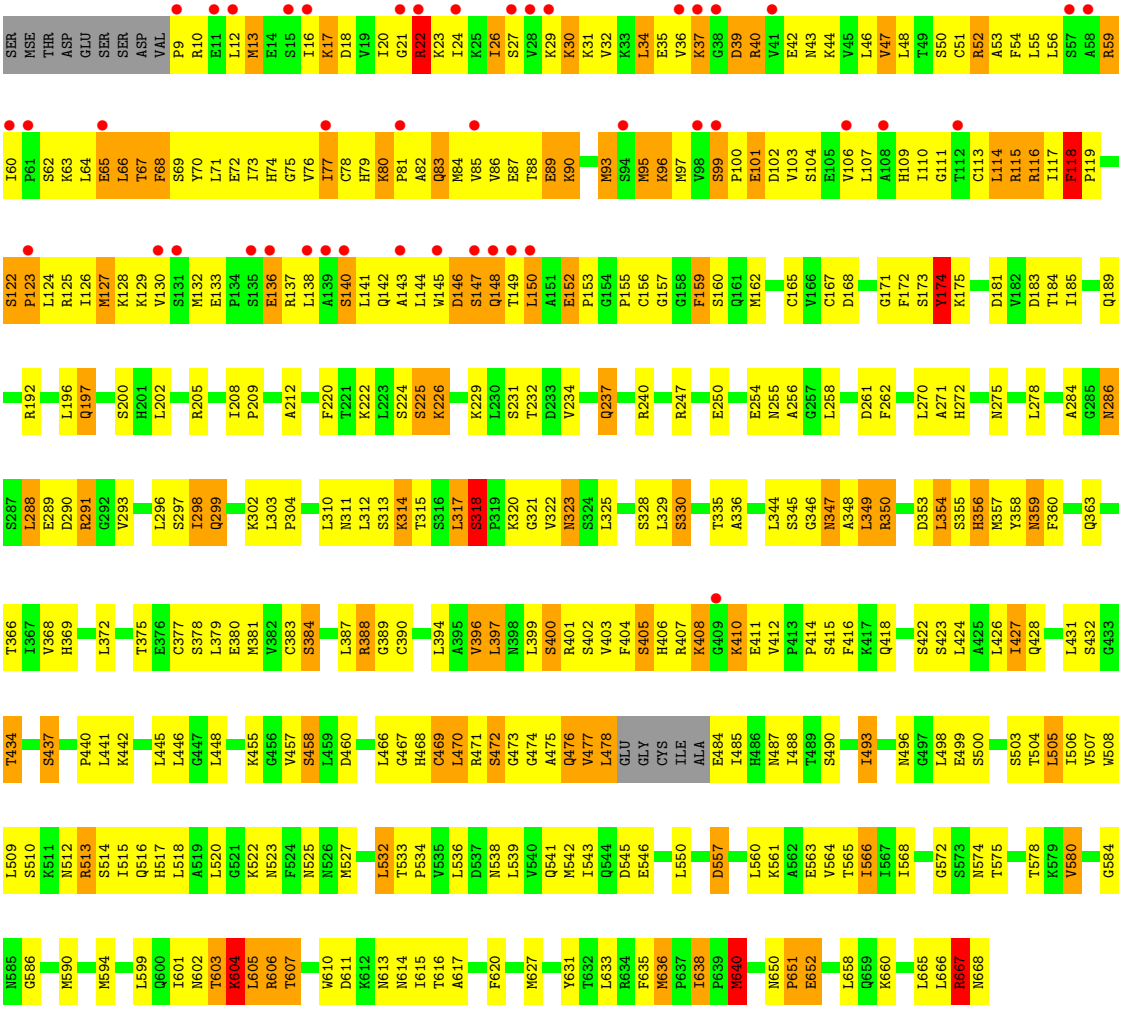
• Molecule 1: Leucine-rich repeat-containing protein 16A

Chain C:



• Molecule 1: Leucine-rich repeat-containing protein 16A

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 57.17Å 67.99Å 212.15Å<br>92.73° 96.95° 110.15° | Depositor |
| Resolution (Å) | 49.76 – 2.90<br>49.76 – 2.90 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 83.4 (49.76-2.90)<br>67.1 (49.76-2.90) | Depositor<br>EDS |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.30 (at 2.91Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.215 , 0.259<br>0.196 , 0.245 | Depositor<br>DCC |
| $R_{free}$ test set | 1583 reflections (3.49%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 34.5 | Xtriage |
| Anisotropy | 0.136 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 53.0 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 20371 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 52.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ABU, OHB

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 1.09 | 5/5179 (0.1%) | 0.99 | 15/6967 (0.2%) |
| 1 | B | 1.03 | 5/5160 (0.1%) | 0.98 | 15/6941 (0.2%) |
| 1 | C | 0.99 | 5/5131 (0.1%) | 0.96 | 12/6902 (0.2%) |
| 1 | D | 0.87 | 5/5124 (0.1%) | 1.08 | 26/6891 (0.4%) |
| All | All | 1.00 | 20/20594 (0.1%) | 1.01 | 68/27701 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 3 |
| 1 | C | 0 | 3 |
| All | All | 0 | 6 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 666 | LEU | CG-CD1 | -6.07 | 1.29 | 1.51 |
| 1 | D | 174 | TYR | CE2-CZ | -5.92 | 1.30 | 1.38 |
| 1 | A | 519 | ALA | CA-CB | -5.77 | 1.40 | 1.52 |
| 1 | B | 605 | LEU | CG-CD1 | -5.72 | 1.30 | 1.51 |
| 1 | A | 237 | GLN | CD-NE2 | -5.55 | 1.19 | 1.32 |
| 1 | C | 580 | VAL | CB-CG2 | -5.51 | 1.41 | 1.52 |
| 1 | C | 61 | PRO | N-CD | 5.40 | 1.55 | 1.47 |
| 1 | C | 165 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | B | 641 | TYR | CE1-CZ | -5.32 | 1.31 | 1.38 |
| 1 | B | 153 | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 1 | A | 639 | PRO | N-CD | 5.29 | 1.55 | 1.47 |
| 1 | D | 167 | CYS | CB-SG | -5.29 | 1.73 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 123 | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 1 | D | 119 | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 1 | D | 651 | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 1 | A | 153 | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 1 | B | 605 | LEU | CG-CD2 | -5.05 | 1.33 | 1.51 |
| 1 | A | 281 | ILE | CA-CB | -5.05 | 1.43 | 1.54 |
| 1 | C | 174 | TYR | CE1-CZ | -5.03 | 1.32 | 1.38 |
| 1 | C | 164 | ALA | CA-CB | -5.03 | 1.41 | 1.52 |

All (68) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 22 | ARG | NE-CZ-NH2 | -23.32 | 108.64 | 120.30 |
| 1 | D | 192 | ARG | NE-CZ-NH1 | -18.59 | 111.01 | 120.30 |
| 1 | D | 192 | ARG | NE-CZ-NH2 | 18.24 | 129.42 | 120.30 |
| 1 | D | 22 | ARG | NE-CZ-NH1 | 16.50 | 128.55 | 120.30 |
| 1 | D | 17 | LYS | CD-CE-NZ | 8.39 | 131.00 | 111.70 |
| 1 | A | 527 | MSE | N-CA-CB | -8.29 | 95.68 | 110.60 |
| 1 | D | 192 | ARG | CD-NE-CZ | 7.83 | 134.56 | 123.60 |
| 1 | D | 640 | MSE | CB-CG-SE | -7.42 | 90.43 | 112.70 |
| 1 | A | 455 | LYS | CD-CE-NZ | 7.38 | 128.67 | 111.70 |
| 1 | D | 23 | LYS | CD-CE-NZ | 6.76 | 127.24 | 111.70 |
| 1 | B | 351 | GLY | N-CA-C | -6.74 | 96.25 | 113.10 |
| 1 | D | 640 | MSE | CB-CA-C | -6.66 | 97.07 | 110.40 |
| 1 | C | 638 | ILE | C-N-CD | 6.25 | 141.53 | 128.40 |
| 1 | D | 240 | ARG | NE-CZ-NH1 | 6.23 | 123.42 | 120.30 |
| 1 | D | 22 | ARG | CD-NE-CZ | 6.19 | 132.27 | 123.60 |
| 1 | D | 640 | MSE | CA-CB-CG | -6.19 | 102.78 | 113.30 |
| 1 | C | 650 | ASN | C-N-CD | 6.17 | 141.35 | 128.40 |
| 1 | A | 133 | GLU | C-N-CD | 6.16 | 141.34 | 128.40 |
| 1 | B | 650 | ASN | C-N-CD | 6.08 | 141.17 | 128.40 |
| 1 | A | 154 | GLY | C-N-CD | 6.06 | 141.12 | 128.40 |
| 1 | B | 80 | LYS | C-N-CD | 6.05 | 141.11 | 128.40 |
| 1 | B | 240 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | C | 8 | VAL | C-N-CD | 6.04 | 141.08 | 128.40 |
| 1 | A | 650 | ASN | C-N-CD | 6.01 | 141.03 | 128.40 |
| 1 | C | 154 | GLY | C-N-CD | 5.99 | 140.98 | 128.40 |
| 1 | B | 154 | GLY | C-N-CD | 5.97 | 140.93 | 128.40 |
| 1 | A | 604 | LYS | N-CA-C | 5.95 | 127.06 | 111.00 |
| 1 | B | 636 | MSE | C-N-CD | 5.93 | 140.86 | 128.40 |
| 1 | D | 318 | SER | C-N-CD | 5.92 | 140.84 | 128.40 |
| 1 | A | 303 | LEU | C-N-CD | 5.91 | 140.82 | 128.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 638 | ILE | C-N-CD | 5.91 | 140.82 | 128.40 |
| 1 | D | 636 | MSE | C-N-CD | 5.89 | 140.76 | 128.40 |
| 1 | C | 636 | MSE | C-N-CD | 5.87 | 140.73 | 128.40 |
| 1 | D | 314 | LYS | CD-CE-NZ | 5.87 | 125.20 | 111.70 |
| 1 | B | 133 | GLU | C-N-CD | 5.86 | 140.71 | 128.40 |
| 1 | A | 80 | LYS | C-N-CD | 5.82 | 140.62 | 128.40 |
| 1 | C | 117 | ILE | CB-CA-C | -5.80 | 100.00 | 111.60 |
| 1 | C | 133 | GLU | C-N-CD | 5.80 | 140.58 | 128.40 |
| 1 | A | 46 | LEU | CA-CB-CG | 5.79 | 128.62 | 115.30 |
| 1 | A | 389 | GLY | N-CA-C | 5.77 | 127.54 | 113.10 |
| 1 | D | 557 | ASP | CB-CG-OD1 | 5.76 | 123.48 | 118.30 |
| 1 | A | 118 | PHE | C-N-CD | 5.74 | 140.45 | 128.40 |
| 1 | D | 122 | SER | C-N-CD | 5.74 | 140.46 | 128.40 |
| 1 | B | 152 | GLU | C-N-CD | 5.74 | 140.45 | 128.40 |
| 1 | B | 132 | MSE | N-CA-C | -5.73 | 95.53 | 111.00 |
| 1 | C | 240 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | C | 118 | PHE | C-N-CD | 5.71 | 140.39 | 128.40 |
| 1 | C | 533 | THR | C-N-CD | 5.70 | 140.36 | 128.40 |
| 1 | B | 8 | VAL | C-N-CD | 5.68 | 140.32 | 128.40 |
| 1 | D | 118 | PHE | C-N-CD | 5.63 | 140.23 | 128.40 |
| 1 | D | 650 | ASN | C-N-CD | 5.62 | 140.20 | 128.40 |
| 1 | B | 473 | GLY | N-CA-C | -5.54 | 99.26 | 113.10 |
| 1 | A | 638 | ILE | C-N-CD | 5.53 | 140.01 | 128.40 |
| 1 | C | 605 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 1 | D | 317 | LEU | CB-CG-CD1 | -5.49 | 101.67 | 111.00 |
| 1 | D | 389 | GLY | N-CA-C | 5.37 | 126.53 | 113.10 |
| 1 | D | 611 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | D | 17 | LYS | CG-CD-CE | 5.31 | 127.84 | 111.90 |
| 1 | D | 60 | ILE | C-N-CD | 5.31 | 139.55 | 128.40 |
| 1 | D | 604 | LYS | CA-CB-CG | 5.23 | 124.91 | 113.40 |
| 1 | B | 296 | LEU | CA-CB-CG | 5.22 | 127.31 | 115.30 |
| 1 | B | 666 | LEU | CD1-CG-CD2 | -5.11 | 95.17 | 110.50 |
| 1 | A | 455 | LYS | CG-CD-CE | 5.08 | 127.13 | 111.90 |
| 1 | C | 38 | GLY | N-CA-C | -5.07 | 100.42 | 113.10 |
| 1 | B | 605 | LEU | CB-CG-CD1 | 5.07 | 119.62 | 111.00 |
| 1 | D | 667 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | A | 605 | LEU | CA-CB-CG | 5.02 | 126.85 | 115.30 |
| 1 | A | 393 | CYS | N-CA-C | 5.01 | 124.54 | 111.00 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 23 | LYS | Peptide |
| 1 | A | 481 | CYS | Peptide |
| 1 | A | 525 | ASN | Peptide |
| 1 | C | 410 | LYS | Peptide |
| 1 | C | 604 | LYS | Mainchain |
| 1 | C | 651 | PRO | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5112 | 0 | 5253 | 411 | 1 |
| 1 | B | 5102 | 0 | 5239 | 368 | 1 |
| 1 | C | 5073 | 0 | 5217 | 458 | 3 |
| 1 | D | 5066 | 0 | 5213 | 515 | 3 |
| 2 | B | 10 | 0 | 7 | 2 | 0 |
| 3 | B | 1 | 0 | 0 | 3 | 1 |
| 4 | C | 7 | 0 | 0 | 0 | 0 |
| All | All | 20371 | 0 | 20929 | 1733 | 5 |

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 42.

All (1733) 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:C:478:LEU:HG | 1:C:508:TRP:CZ2 | 1.28 | 1.59 |
| 1:B:350:ARG:HG3 | 1:B:406:HIS:CE1 | 1.35 | 1.57 |
| 1:D:258:LEU:HD23 | 1:D:262:PHE:CE2 | 1.44 | 1.53 |
| 1:B:54:PHE:CD1 | 1:B:67:THR:HG21 | 1.46 | 1.49 |
| 1:A:474:GLY:HA2 | 1:A:477:VAL:CG1 | 1.43 | 1.46 |
| 1:B:350:ARG:CG | 1:B:406:HIS:CE1 | 1.97 | 1.46 |
| 1:C:478:LEU:CG | 1:C:508:TRP:CZ2 | 1.97 | 1.45 |
| 1:C:350:ARG:HD3 | 1:C:406:HIS:CE1 | 1.53 | 1.41 |
| 1:B:484:GLU:HG2 | 1:B:508:TRP:NE1 | 1.23 | 1.40 |
| 1:C:350:ARG:HD3 | 1:C:406:HIS:ND1 | 1.41 | 1.35 |
| 1:A:319:PRO:HB2 | 1:A:352:ASP:CB | 1.56 | 1.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:319:PRO:CG | 1:A:352:ASP:HB2 | 1.56 | 1.33 |
| 1:C:478:LEU:HG | 1:C:508:TRP:CH2 | 1.62 | 1.33 |
| 1:C:65:GLU:O | 1:C:66:LEU:HD23 | 1.21 | 1.31 |
| 1:D:499:GLU:C | 1:D:527:MSE:CE | 2.01 | 1.28 |
| 1:B:54:PHE:CD1 | 1:B:67:THR:CG2 | 2.15 | 1.28 |
| 1:A:319:PRO:CB | 1:A:352:ASP:HB3 | 1.64 | 1.28 |
| 1:A:374:ASN:OD1 | 1:A:401:ARG:HD2 | 1.34 | 1.27 |
| 1:D:258:LEU:CD2 | 1:D:262:PHE:CE2 | 2.19 | 1.26 |
| 1:C:55:LEU:HD11 | 1:C:95:MSE:CE | 1.66 | 1.25 |
| 1:D:145:TRP:HA | 1:D:148:GLN:OE1 | 1.37 | 1.24 |
| 1:A:319:PRO:CB | 1:A:352:ASP:CB | 2.14 | 1.24 |
| 1:B:484:GLU:HG2 | 1:B:508:TRP:CD1 | 1.70 | 1.24 |
| 1:C:484:GLU:OE2 | 1:C:511:LYS:HB3 | 1.38 | 1.23 |
| 1:A:9:PRO:CB | 1:A:12:LEU:HD21 | 1.68 | 1.22 |
| 1:C:44:LYS:NZ | 1:C:65:GLU:CD | 1.92 | 1.22 |
| 1:A:402:SER:O | 1:A:434:THR:CG2 | 1.86 | 1.22 |
| 1:A:474:GLY:CA | 1:A:477:VAL:HG12 | 1.69 | 1.22 |
| 1:C:477:VAL:O | 1:C:508:TRP:CZ3 | 1.90 | 1.21 |
| 1:C:374:ASN:OD1 | 1:C:401:ARG:HG3 | 1.36 | 1.21 |
| 1:C:448:LEU:O | 1:C:487:ASN:ND2 | 1.70 | 1.21 |
| 1:D:258:LEU:HD23 | 1:D:262:PHE:CD2 | 1.75 | 1.21 |
| 1:C:478:LEU:CB | 1:C:508:TRP:CZ2 | 2.19 | 1.20 |
| 1:C:504:THR:O | 1:C:507:VAL:HG22 | 1.41 | 1.20 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:O | 1.57 | 1.19 |
| 1:C:350:ARG:CD | 1:C:406:HIS:CE1 | 2.22 | 1.19 |
| 1:C:484:GLU:OE2 | 1:C:511:LYS:CB | 1.88 | 1.19 |
| 1:B:484:GLU:CG | 1:B:508:TRP:NE1 | 2.07 | 1.18 |
| 1:B:36:VAL:HG21 | 1:B:42:GLU:CG | 1.72 | 1.17 |
| 1:A:9:PRO:HB2 | 1:A:12:LEU:HD21 | 1.17 | 1.17 |
| 1:A:349:LEU:HG | 1:A:375:THR:OG1 | 1.44 | 1.16 |
| 1:A:484:GLU:HG3 | 1:A:508:TRP:NE1 | 1.59 | 1.16 |
| 1:D:136:GLU:O | 1:D:140:SER:OG | 1.63 | 1.16 |
| 1:C:478:LEU:CG | 1:C:508:TRP:HZ2 | 1.46 | 1.14 |
| 1:D:349:LEU:CD1 | 1:D:357:MSE:HE1 | 1.76 | 1.13 |
| 1:D:499:GLU:HA | 1:D:527:MSE:HE3 | 1.28 | 1.13 |
| 1:D:118:PHE:CD2 | 1:D:126:ILE:CD1 | 2.32 | 1.12 |
| 1:B:24:ILE:HD12 | 1:B:25:LYS:H | 1.14 | 1.12 |
| 1:A:402:SER:O | 1:A:434:THR:HG23 | 1.43 | 1.12 |
| 1:D:349:LEU:HB3 | 1:D:354:LEU:HD21 | 1.33 | 1.11 |
| 1:A:484:GLU:CG | 1:A:508:TRP:HE1 | 1.62 | 1.11 |
| 1:A:485:ILE:HG22 | 1:A:512:ASN:HD22 | 1.12 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:493:ILE:O | 1:A:496:ASN:ND2 | 1.83 | 1.10 |
| 1:A:374:ASN:OD1 | 1:A:401:ARG:CD | 1.99 | 1.09 |
| 1:A:484:GLU:HG3 | 1:A:508:TRP:HE1 | 0.95 | 1.09 |
| 1:D:144:LEU:O | 1:D:148:GLN:OE1 | 1.71 | 1.09 |
| 1:C:474:GLY:HA2 | 1:C:475:ALA:CB | 1.82 | 1.09 |
| 1:D:474:GLY:HA2 | 1:D:475:ALA:HB3 | 1.29 | 1.09 |
| 1:C:349:LEU:HG | 1:C:375:THR:OG1 | 1.50 | 1.09 |
| 1:B:323:ASN:ND2 | 1:B:356:HIS:ND1 | 2.01 | 1.08 |
| 1:C:36:VAL:HG12 | 1:C:37:LYS:HD2 | 1.32 | 1.08 |
| 1:A:652:GLU:HG2 | 1:A:653:LYS:H | 1.17 | 1.08 |
| 1:D:118:PHE:HD2 | 1:D:126:ILE:CD1 | 1.67 | 1.08 |
| 1:A:485:ILE:CG2 | 1:A:512:ASN:ND2 | 2.18 | 1.07 |
| 1:D:499:GLU:C | 1:D:527:MSE:HE1 | 1.75 | 1.07 |
| 1:C:44:LYS:NZ | 1:C:65:GLU:OE1 | 1.85 | 1.06 |
| 1:B:36:VAL:HG21 | 1:B:42:GLU:HG3 | 1.07 | 1.06 |
| 1:B:354:LEU:HB3 | 1:B:358:TYR:CE2 | 1.90 | 1.06 |
| 1:A:498:LEU:HD12 | 1:A:502:LEU:HD13 | 1.32 | 1.06 |
| 1:B:54:PHE:HD1 | 1:B:67:THR:CG2 | 1.58 | 1.06 |
| 1:C:68:PHE:CD2 | 1:C:93:MSE:CE | 2.39 | 1.06 |
| 1:D:411:GLU:OE2 | 1:D:412:VAL:N | 1.88 | 1.06 |
| 1:A:485:ILE:HG22 | 1:A:512:ASN:ND2 | 1.69 | 1.06 |
| 1:B:448:LEU:O | 1:B:487:ASN:ND2 | 1.89 | 1.06 |
| 1:D:322:VAL:HG11 | 1:D:357:MSE:HE3 | 1.37 | 1.06 |
| 1:B:182:VAL:O | 1:B:186:TYR:HB2 | 1.55 | 1.05 |
| 1:D:145:TRP:CA | 1:D:148:GLN:OE1 | 2.04 | 1.05 |
| 1:A:638:ILE:HD12 | 1:B:638:ILE:HG12 | 1.34 | 1.05 |
| 1:D:349:LEU:HD11 | 1:D:357:MSE:HE1 | 1.34 | 1.05 |
| 1:B:374:ASN:OD1 | 1:B:401:ARG:HD3 | 1.55 | 1.05 |
| 1:D:513:ARG:HH21 | 1:D:513:ARG:HG3 | 1.22 | 1.05 |
| 1:B:350:ARG:HG2 | 1:B:406:HIS:CE1 | 1.87 | 1.05 |
| 1:C:44:LYS:NZ | 1:C:65:GLU:OE2 | 1.89 | 1.04 |
| 1:C:562:ALA:O | 1:C:565:THR:OG1 | 1.76 | 1.04 |
| 1:C:610:TRP:CE2 | 1:C:636:MSE:HE2 | 1.91 | 1.04 |
| 1:C:68:PHE:CD2 | 1:C:93:MSE:HE2 | 1.93 | 1.04 |
| 1:C:474:GLY:HA3 | 1:C:476:GLN:H | 1.21 | 1.04 |
| 1:B:74:HIS:CE1 | 1:B:89:GLU:HB2 | 1.93 | 1.04 |
| 1:C:474:GLY:CA | 1:C:475:ALA:HB3 | 1.87 | 1.03 |
| 1:B:349:LEU:HG | 1:B:375:THR:OG1 | 1.57 | 1.03 |
| 1:C:478:LEU:HB2 | 1:C:508:TRP:CZ2 | 1.90 | 1.02 |
| 1:C:113:CYS:O | 1:C:117:ILE:HD12 | 1.59 | 1.02 |
| 1:B:177:GLU:OE1 | 1:B:177:GLU:N | 1.91 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:36:VAL:CG1 | 1:C:37:LYS:HD2 | 1.89 | 1.02 |
| 1:C:44:LYS:HZ2 | 1:C:65:GLU:CD | 1.52 | 1.02 |
| 1:B:402:SER:O | 1:B:434:THR:HB | 1.58 | 1.01 |
| 1:C:36:VAL:HG12 | 1:C:37:LYS:H | 1.20 | 1.01 |
| 1:B:78:CYS:HB2 | 1:B:132:MSE:HA | 1.43 | 1.01 |
| 1:C:350:ARG:HG2 | 1:C:406:HIS:HE1 | 1.26 | 1.01 |
| 1:C:402:SER:O | 1:C:434:THR:HB | 1.60 | 1.01 |
| 1:D:499:GLU:CA | 1:D:527:MSE:HE3 | 1.89 | 1.01 |
| 1:A:303:LEU:HD23 | 1:A:304:PRO:HD2 | 1.39 | 1.00 |
| 1:B:484:GLU:CG | 1:B:508:TRP:CD1 | 2.41 | 1.00 |
| 1:C:478:LEU:CB | 1:C:508:TRP:HZ2 | 1.67 | 0.99 |
| 1:B:88:THR:HG23 | 1:B:91:CYS:H | 1.23 | 0.99 |
| 1:C:399:LEU:O | 1:C:402:SER:OG | 1.81 | 0.99 |
| 1:B:80:LYS:CE | 1:B:81:PRO:HD2 | 1.92 | 0.99 |
| 1:C:350:ARG:CG | 1:C:406:HIS:HE1 | 1.76 | 0.99 |
| 1:C:474:GLY:HA2 | 1:C:475:ALA:HB3 | 1.02 | 0.99 |
| 1:A:24:ILE:HD12 | 1:A:25:LYS:H | 1.24 | 0.98 |
| 1:C:477:VAL:O | 1:C:508:TRP:HZ3 | 1.03 | 0.98 |
| 1:D:37:LYS:HA | 1:D:39:ASP:H | 1.25 | 0.98 |
| 1:C:114:LEU:O | 1:C:117:ILE:O | 1.81 | 0.98 |
| 1:D:291:ARG:HB3 | 1:D:291:ARG:HH21 | 1.29 | 0.98 |
| 1:D:118:PHE:CD2 | 1:D:126:ILE:HD13 | 1.98 | 0.97 |
| 1:C:474:GLY:CA | 1:C:476:GLN:H | 1.77 | 0.97 |
| 1:A:652:GLU:HG2 | 1:A:653:LYS:N | 1.71 | 0.97 |
| 1:C:478:LEU:CG | 1:C:508:TRP:CH2 | 2.23 | 0.97 |
| 1:D:322:VAL:CG1 | 1:D:357:MSE:HE3 | 1.94 | 0.97 |
| 1:B:484:GLU:CD | 1:B:508:TRP:O | 2.02 | 0.97 |
| 1:A:369:HIS:CD2 | 1:A:396:VAL:HG21 | 2.00 | 0.96 |
| 1:A:319:PRO:CB | 1:A:352:ASP:HB2 | 1.87 | 0.96 |
| 1:D:26:ILE:HD12 | 1:D:47:VAL:CG2 | 1.94 | 0.96 |
| 1:A:319:PRO:CG | 1:A:352:ASP:CB | 2.41 | 0.96 |
| 1:C:353:ASP:OD1 | 1:C:355:SER:OG | 1.83 | 0.96 |
| 1:D:78:CYS:SG | 1:D:103:VAL:HG11 | 2.04 | 0.96 |
| 1:C:431:LEU:O | 1:C:434:THR:HG23 | 1.66 | 0.96 |
| 1:D:638:ILE:H | 1:D:638:ILE:HD12 | 1.28 | 0.96 |
| 1:A:319:PRO:HG2 | 1:A:352:ASP:HB2 | 0.99 | 0.96 |
| 1:B:66:LEU:HD12 | 1:B:93:MSE:HE1 | 1.46 | 0.95 |
| 1:B:456:GLY:HA2 | 1:B:489:THR:HG23 | 1.48 | 0.95 |
| 1:B:36:VAL:CG2 | 1:B:42:GLU:HG3 | 1.95 | 0.95 |
| 1:C:68:PHE:CE2 | 1:C:93:MSE:HE2 | 2.01 | 0.95 |
| 1:A:290:ASP:O | 1:A:294:SER:N | 1.99 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:55:LEU:HD21 | 1:C:95:MSE:HE2 | 1.47 | 0.95 |
| 1:D:13:MSE:HE1 | 1:D:26:ILE:HD11 | 1.46 | 0.95 |
| 1:B:66:LEU:CD1 | 1:B:93:MSE:HE1 | 1.97 | 0.95 |
| 1:A:474:GLY:CA | 1:A:477:VAL:CG1 | 2.36 | 0.95 |
| 1:A:293:VAL:HG21 | 1:A:317:LEU:HD11 | 1.46 | 0.94 |
| 1:A:9:PRO:CB | 1:A:12:LEU:CD2 | 2.46 | 0.94 |
| 1:D:507:VAL:O | 1:D:510:SER:OG | 1.85 | 0.94 |
| 1:B:611:ASP:OD1 | 1:B:612:LYS:N | 2.00 | 0.94 |
| 1:D:258:LEU:HD23 | 1:D:262:PHE:HE2 | 1.32 | 0.94 |
| 1:C:350:ARG:CD | 1:C:406:HIS:ND1 | 2.30 | 0.94 |
| 1:D:467:GLY:CA | 1:D:498:LEU:HD23 | 1.98 | 0.94 |
| 1:C:543:ILE:CG2 | 1:C:574:ASN:ND2 | 2.31 | 0.93 |
| 1:D:18:ASP:OD1 | 1:D:22:ARG:NH2 | 2.02 | 0.93 |
| 1:A:9:PRO:HB2 | 1:A:12:LEU:CD2 | 1.98 | 0.93 |
| 1:D:344:LEU:O | 1:D:347:ASN:ND2 | 2.00 | 0.93 |
| 2:B:701:OHB:O | 3:B:702:CL:CL | 2.24 | 0.93 |
| 1:B:88:THR:HG23 | 1:B:91:CYS:N | 1.84 | 0.93 |
| 1:B:54:PHE:CE1 | 1:B:67:THR:HG21 | 2.04 | 0.92 |
| 1:C:68:PHE:CE2 | 1:C:93:MSE:CE | 2.52 | 0.92 |
| 1:D:512:ASN:OD1 | 1:D:515:ILE:HG13 | 1.68 | 0.92 |
| 1:B:80:LYS:HE3 | 1:B:81:PRO:HD2 | 1.48 | 0.92 |
| 1:C:381:MSE:HA | 1:C:381:MSE:HE3 | 1.51 | 0.92 |
| 1:B:178:VAL:O | 1:B:182:VAL:HG23 | 1.68 | 0.92 |
| 1:C:610:TRP:NE1 | 1:C:636:MSE:HE2 | 1.84 | 0.91 |
| 1:A:319:PRO:HG2 | 1:A:352:ASP:CB | 1.96 | 0.91 |
| 1:C:256:ALA:HB3 | 1:C:258:LEU:HD13 | 1.51 | 0.91 |
| 1:B:180:TRP:O | 1:B:184:THR:OG1 | 1.88 | 0.91 |
| 1:B:185:ILE:O | 1:B:189:GLN:HG3 | 1.71 | 0.91 |
| 1:C:55:LEU:HD11 | 1:C:95:MSE:HE3 | 1.53 | 0.90 |
| 1:C:350:ARG:HG2 | 1:C:406:HIS:CE1 | 2.05 | 0.90 |
| 1:D:13:MSE:CE | 1:D:26:ILE:HD11 | 2.01 | 0.90 |
| 1:C:68:PHE:HD2 | 1:C:93:MSE:HE1 | 1.33 | 0.90 |
| 1:D:322:VAL:HG11 | 1:D:357:MSE:CE | 2.01 | 0.90 |
| 1:C:506:ILE:HG23 | 1:C:542:MSE:CE | 2.03 | 0.89 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:CD1 | 2.26 | 0.89 |
| 1:D:34:LEU:CD2 | 1:D:42:GLU:HB2 | 2.02 | 0.89 |
| 1:C:350:ARG:CG | 1:C:406:HIS:CE1 | 2.54 | 0.89 |
| 1:C:509:LEU:CD2 | 1:C:518:LEU:HD22 | 2.03 | 0.89 |
| 1:C:528:LYS:O | 1:C:531:ASN:ND2 | 2.04 | 0.89 |
| 1:C:484:GLU:OE1 | 1:C:484:GLU:N | 2.06 | 0.89 |
| 1:D:64:LEU:HD23 | 1:D:65:GLU:N | 1.88 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:449:ALA:O | 1:B:486:HIS:HE1 | 1.56 | 0.89 |
| 1:D:499:GLU:O | 1:D:527:MSE:HE1 | 1.71 | 0.89 |
| 1:B:7:ASP:O | 1:B:31:LYS:HG3 | 1.72 | 0.89 |
| 1:C:134:PRO:HD2 | 1:C:137:ARG:HH21 | 1.37 | 0.88 |
| 1:D:431:LEU:O | 1:D:434:THR:HG23 | 1.73 | 0.88 |
| 1:C:55:LEU:HD11 | 1:C:95:MSE:HE1 | 1.54 | 0.88 |
| 1:C:8:VAL:HG12 | 1:C:9:PRO:CD | 2.04 | 0.88 |
| 1:D:423:SER:OG | 1:D:426:LEU:HD13 | 1.73 | 0.88 |
| 1:A:605:LEU:O | 1:A:633:LEU:HD12 | 1.74 | 0.88 |
| 1:C:117:ILE:HB | 1:C:118:PHE:CD2 | 2.09 | 0.88 |
| 1:C:115:ARG:HB3 | 1:C:115:ARG:HH21 | 1.36 | 0.88 |
| 1:A:319:PRO:HB2 | 1:A:352:ASP:HB3 | 0.87 | 0.87 |
| 1:C:115:ARG:HH21 | 1:C:115:ARG:CB | 1.88 | 0.87 |
| 1:A:349:LEU:HG | 1:A:375:THR:HG1 | 1.39 | 0.87 |
| 1:D:350:ARG:H | 1:D:350:ARG:HD3 | 1.37 | 0.87 |
| 1:A:402:SER:O | 1:A:434:THR:HG22 | 1.75 | 0.86 |
| 1:B:24:ILE:HD12 | 1:B:25:LYS:N | 1.88 | 0.86 |
| 1:B:350:ARG:HG2 | 1:B:406:HIS:NE2 | 1.90 | 0.86 |
| 1:D:543:ILE:HG22 | 1:D:574:ASN:ND2 | 1.90 | 0.86 |
| 1:A:374:ASN:HD21 | 1:A:401:ARG:HH21 | 1.20 | 0.86 |
| 1:C:193:GLU:HG3 | 1:C:222:LYS:HD3 | 1.54 | 0.86 |
| 1:C:531:ASN:O | 1:C:534:PRO:HD2 | 1.76 | 0.86 |
| 1:D:32:VAL:HG23 | 1:D:96:LYS:O | 1.76 | 0.86 |
| 1:D:143:ALA:O | 1:D:147:SER:OG | 1.93 | 0.86 |
| 1:A:24:ILE:HD12 | 1:A:25:LYS:N | 1.91 | 0.85 |
| 1:A:138:LEU:HD23 | 1:A:139:ALA:N | 1.91 | 0.85 |
| 1:C:68:PHE:CD2 | 1:C:93:MSE:HE1 | 2.08 | 0.85 |
| 1:C:543:ILE:CG2 | 1:C:574:ASN:HD22 | 1.90 | 0.85 |
| 1:C:12:LEU:HD12 | 1:C:12:LEU:O | 1.77 | 0.85 |
| 1:C:113:CYS:O | 1:C:117:ILE:CD1 | 2.24 | 0.85 |
| 1:A:258:LEU:HD23 | 1:A:262:PHE:CE2 | 2.12 | 0.85 |
| 1:A:372:LEU:O | 1:A:375:THR:CG2 | 2.25 | 0.85 |
| 1:A:562:ALA:O | 1:A:565:THR:OG1 | 1.95 | 0.85 |
| 1:B:484:GLU:HG2 | 1:B:508:TRP:HE1 | 1.04 | 0.84 |
| 1:C:484:GLU:OE1 | 1:C:508:TRP:CD1 | 2.30 | 0.84 |
| 1:C:504:THR:O | 1:C:507:VAL:CG2 | 2.24 | 0.84 |
| 1:D:26:ILE:HD12 | 1:D:47:VAL:HG21 | 1.58 | 0.84 |
| 1:A:258:LEU:HD23 | 1:A:262:PHE:CD2 | 2.13 | 0.84 |
| 1:C:555:LEU:O | 1:C:558:SER:OG | 1.94 | 0.84 |
| 1:D:467:GLY:HA2 | 1:D:498:LEU:CD2 | 2.08 | 0.84 |
| 1:D:499:GLU:C | 1:D:527:MSE:HE3 | 1.93 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:162:MSE:O | 1:B:166:VAL:HG23 | 1.78 | 0.84 |
| 1:D:46:LEU:HD13 | 1:D:95:MSE:HE1 | 1.60 | 0.84 |
| 1:B:431:LEU:O | 1:B:434:THR:HG23 | 1.78 | 0.83 |
| 1:A:117:ILE:CD1 | 1:A:165:CYS:SG | 2.66 | 0.83 |
| 1:A:121:LEU:HD22 | 1:A:125:ARG:NH1 | 1.92 | 0.83 |
| 1:D:118:PHE:CD2 | 1:D:126:ILE:HD11 | 2.10 | 0.83 |
| 1:D:496:ASN:O | 1:D:523:ASN:OD1 | 1.94 | 0.83 |
| 1:A:9:PRO:HB3 | 1:A:12:LEU:HD21 | 1.56 | 0.83 |
| 1:A:474:GLY:HA2 | 1:A:477:VAL:HG11 | 1.54 | 0.83 |
| 1:A:474:GLY:HA2 | 1:A:477:VAL:HG12 | 0.84 | 0.83 |
| 1:B:74:HIS:ND1 | 1:B:89:GLU:HB2 | 1.93 | 0.83 |
| 1:C:8:VAL:HG12 | 1:C:9:PRO:HD2 | 1.59 | 0.83 |
| 1:A:256:ALA:HB3 | 1:A:258:LEU:HD13 | 1.61 | 0.83 |
| 1:B:484:GLU:CD | 1:B:508:TRP:CD1 | 2.51 | 0.83 |
| 1:D:117:ILE:HD13 | 1:D:165:CYS:SG | 2.18 | 0.83 |
| 1:C:26:ILE:HG23 | 1:C:47:VAL:CG1 | 2.08 | 0.83 |
| 1:D:610:TRP:CZ3 | 1:D:615:ILE:HD12 | 2.14 | 0.82 |
| 1:C:374:ASN:OD1 | 1:C:401:ARG:CG | 2.23 | 0.82 |
| 1:C:65:GLU:O | 1:C:66:LEU:CD2 | 2.17 | 0.82 |
| 1:A:44:LYS:NZ | 1:A:65:GLU:OE2 | 2.12 | 0.82 |
| 1:A:372:LEU:O | 1:A:375:THR:HG22 | 1.78 | 0.82 |
| 1:D:325:LEU:HD12 | 1:D:325:LEU:O | 1.79 | 0.82 |
| 1:A:68:PHE:CD1 | 1:A:93:MSE:CE | 2.62 | 0.82 |
| 1:D:404:PHE:CE1 | 1:D:440:PRO:HB3 | 2.14 | 0.82 |
| 1:A:374:ASN:HD21 | 1:A:401:ARG:NH2 | 1.76 | 0.81 |
| 1:C:353:ASP:OD1 | 1:C:355:SER:N | 2.12 | 0.81 |
| 1:D:610:TRP:CZ3 | 1:D:615:ILE:CD1 | 2.62 | 0.81 |
| 1:C:407:ARG:HH21 | 1:C:407:ARG:HG3 | 1.43 | 0.81 |
| 1:D:318:SER:O | 1:D:322:VAL:HG23 | 1.79 | 0.81 |
| 1:D:504:THR:O | 1:D:507:VAL:HG22 | 1.81 | 0.81 |
| 1:C:65:GLU:C | 1:C:66:LEU:HD23 | 1.99 | 0.81 |
| 1:C:373:SER:HB3 | 1:C:398:ASN:OD1 | 1.80 | 0.81 |
| 1:D:467:GLY:HA3 | 1:D:498:LEU:HD23 | 1.63 | 0.81 |
| 1:C:505:LEU:O | 1:C:509:LEU:HD12 | 1.81 | 0.81 |
| 1:D:117:ILE:CD1 | 1:D:165:CYS:SG | 2.68 | 0.81 |
| 1:D:318:SER:OG | 1:D:320:LYS:N | 2.14 | 0.81 |
| 1:D:467:GLY:CA | 1:D:498:LEU:CD2 | 2.58 | 0.81 |
| 1:A:485:ILE:HG23 | 1:A:512:ASN:ND2 | 1.94 | 0.81 |
| 1:B:65:GLU:O | 1:B:66:LEU:HD23 | 1.79 | 0.80 |
| 1:D:474:GLY:HA2 | 1:D:475:ALA:CB | 2.11 | 0.80 |
| 1:C:474:GLY:O | 1:C:477:VAL:HG12 | 1.81 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:172:PHE:CD2 | 1:D:209:PRO:HD3 | 2.16 | 0.80 |
| 1:A:485:ILE:HG23 | 1:A:512:ASN:HD21 | 1.44 | 0.80 |
| 1:B:124:LEU:O | 1:B:127:MSE:O | 2.00 | 0.80 |
| 1:D:34:LEU:HD22 | 1:D:42:GLU:HB2 | 1.62 | 0.80 |
| 1:A:484:GLU:CG | 1:A:508:TRP:NE1 | 2.30 | 0.80 |
| 1:B:456:GLY:HA2 | 1:B:489:THR:CG2 | 2.11 | 0.80 |
| 1:C:258:LEU:HD23 | 1:C:262:PHE:CE2 | 2.17 | 0.80 |
| 1:D:37:LYS:HA | 1:D:39:ASP:N | 1.96 | 0.80 |
| 1:B:256:ALA:HB3 | 1:B:258:LEU:HD13 | 1.62 | 0.80 |
| 1:D:349:LEU:HD13 | 1:D:357:MSE:HE1 | 1.63 | 0.80 |
| 1:B:54:PHE:HD1 | 1:B:67:THR:HG21 | 0.97 | 0.79 |
| 1:D:44:LYS:NZ | 1:D:65:GLU:OE2 | 2.13 | 0.79 |
| 1:D:499:GLU:CA | 1:D:527:MSE:CE | 2.55 | 0.79 |
| 1:D:500:SER:N | 1:D:527:MSE:CE | 2.45 | 0.79 |
| 1:B:258:LEU:HD23 | 1:B:262:PHE:CE2 | 2.18 | 0.79 |
| 1:D:142:GLN:O | 1:D:146:ASP:OD1 | 2.00 | 0.79 |
| 1:D:99:SER:HB2 | 1:D:101:GLU:HG3 | 1.63 | 0.78 |
| 1:D:500:SER:N | 1:D:527:MSE:HE2 | 1.98 | 0.78 |
| 1:D:36:VAL:HG12 | 1:D:37:LYS:O | 1.83 | 0.78 |
| 1:A:283:LEU:O | 1:A:286:ASN:ND2 | 2.16 | 0.78 |
| 1:D:117:ILE:HG22 | 1:D:118:PHE:CD1 | 2.18 | 0.78 |
| 1:A:638:ILE:HD13 | 1:A:640:MSE:HE1 | 1.64 | 0.78 |
| 1:B:283:LEU:O | 1:B:286:ASN:ND2 | 2.15 | 0.78 |
| 1:C:51:CYS:HB3 | 1:C:165:CYS:SG | 2.24 | 0.78 |
| 1:A:16:ILE:O | 1:A:19:VAL:HG12 | 1.83 | 0.78 |
| 1:C:509:LEU:CD2 | 1:C:518:LEU:CD2 | 2.62 | 0.78 |
| 1:C:418:GLN:O | 1:C:422:SER:OG | 2.02 | 0.77 |
| 1:D:116:ARG:HH21 | 1:D:116:ARG:HB2 | 1.49 | 0.77 |
| 1:D:468:HIS:O | 1:D:472:SER:HB3 | 1.84 | 0.77 |
| 1:A:638:ILE:HD13 | 1:A:640:MSE:CE | 2.13 | 0.77 |
| 1:A:13:MSE:SE | 1:A:29:LYS:HD2 | 2.34 | 0.77 |
| 1:A:484:GLU:HG3 | 1:A:508:TRP:CE2 | 2.19 | 0.77 |
| 1:A:638:ILE:CD1 | 1:B:638:ILE:HG12 | 2.14 | 0.77 |
| 1:B:7:ASP:O | 1:B:31:LYS:CG | 2.31 | 0.77 |
| 1:D:256:ALA:HB3 | 1:D:258:LEU:HD13 | 1.64 | 0.77 |
| 1:D:610:TRP:CE2 | 1:D:636:MSE:HE2 | 2.19 | 0.77 |
| 1:B:350:ARG:CG | 1:B:406:HIS:NE2 | 2.47 | 0.77 |
| 1:A:374:ASN:ND2 | 1:A:401:ARG:HH21 | 1.81 | 0.77 |
| 1:D:26:ILE:HD12 | 1:D:47:VAL:HG23 | 1.67 | 0.77 |
| 1:A:666:LEU:HD22 | 1:B:666:LEU:CD1 | 2.15 | 0.77 |
| 1:B:258:LEU:HD23 | 1:B:262:PHE:CD2 | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:478:LEU:HB3 | 1:D:508:TRP:NE1 | 1.98 | 0.77 |
| 1:B:115:ARG:NH2 | 1:B:150:LEU:HD11 | 1.99 | 0.77 |
| 1:B:65:GLU:C | 1:B:66:LEU:HD23 | 2.04 | 0.76 |
| 1:C:476:GLN:N | 1:C:476:GLN:HE21 | 1.82 | 0.76 |
| 1:A:160:SER:OG | 1:A:183:ASP:OD1 | 2.02 | 0.76 |
| 1:B:183:ASP:O | 1:B:187:LEU:HB3 | 1.86 | 0.76 |
| 1:B:354:LEU:CB | 1:B:358:TYR:CE2 | 2.66 | 0.76 |
| 1:C:77:ILE:HB | 1:C:85:VAL:HG22 | 1.67 | 0.76 |
| 1:C:372:LEU:O | 1:C:375:THR:CG2 | 2.34 | 0.76 |
| 1:C:407:ARG:HG3 | 1:C:407:ARG:NH2 | 2.00 | 0.76 |
| 1:B:350:ARG:HG3 | 1:B:406:HIS:HE1 | 0.93 | 0.76 |
| 1:D:288:LEU:HD12 | 1:D:288:LEU:O | 1.86 | 0.76 |
| 1:B:372:LEU:O | 1:B:375:THR:CG2 | 2.33 | 0.76 |
| 1:B:353:ASP:OD1 | 1:B:355:SER:OG | 2.02 | 0.76 |
| 1:C:379:LEU:HD13 | 1:C:402:SER:CB | 2.16 | 0.76 |
| 1:A:23:LYS:HA | 1:A:23:LYS:HE3 | 1.68 | 0.76 |
| 1:C:543:ILE:HG23 | 1:C:574:ASN:ND2 | 2.00 | 0.75 |
| 1:A:143:ALA:O | 1:A:147:SER:N | 2.19 | 0.75 |
| 1:C:350:ARG:CD | 1:C:406:HIS:HE1 | 1.90 | 0.75 |
| 1:C:474:GLY:HA3 | 1:C:476:GLN:HG2 | 1.67 | 0.75 |
| 1:A:498:LEU:CD1 | 1:A:502:LEU:HD13 | 2.15 | 0.75 |
| 1:B:136:GLU:N | 1:B:136:GLU:OE2 | 2.20 | 0.75 |
| 1:C:411:GLU:HA | 1:C:411:GLU:OE2 | 1.87 | 0.75 |
| 1:C:610:TRP:CE2 | 1:C:636:MSE:CE | 2.70 | 0.75 |
| 1:D:114:LEU:HD23 | 1:D:123:PRO:HB3 | 1.69 | 0.75 |
| 1:C:485:ILE:HG22 | 1:C:487:ASN:HB2 | 1.68 | 0.74 |
| 1:B:32:VAL:HG21 | 1:B:95:MSE:HB3 | 1.70 | 0.74 |
| 1:B:513:ARG:CB | 1:B:513:ARG:HH11 | 2.00 | 0.74 |
| 1:D:372:LEU:O | 1:D:375:THR:CG2 | 2.36 | 0.74 |
| 1:A:73:ILE:HG21 | 1:A:127:MSE:HE2 | 1.68 | 0.74 |
| 1:B:54:PHE:HA | 1:B:67:THR:HG22 | 1.67 | 0.74 |
| 1:C:456:GLY:HA2 | 1:C:489:THR:HG23 | 1.68 | 0.74 |
| 1:D:258:LEU:HD21 | 1:D:262:PHE:CE2 | 2.22 | 0.74 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:C | 2.26 | 0.74 |
| 1:B:484:GLU:OE1 | 1:B:508:TRP:O | 2.04 | 0.74 |
| 1:C:475:ALA:C | 1:C:476:GLN:HE21 | 1.90 | 0.74 |
| 1:C:640:MSE:SE | 1:D:640:MSE:HG3 | 2.38 | 0.74 |
| 1:D:54:PHE:CD1 | 1:D:67:THR:HG23 | 2.22 | 0.74 |
| 1:A:13:MSE:HG3 | 1:A:17:LYS:CE | 2.18 | 0.74 |
| 1:A:121:LEU:CD2 | 1:A:125:ARG:NH1 | 2.49 | 0.74 |
| 1:C:420:PHE:CZ | 1:C:444:LEU:HD13 | 2.23 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:66:LEU:HD12 | 1:B:93:MSE:CE | 2.18 | 0.74 |
| 1:B:449:ALA:O | 1:B:486:HIS:CE1 | 2.40 | 0.74 |
| 1:B:604:LYS:HG3 | 1:B:604:LYS:O | 1.88 | 0.74 |
| 1:D:63:LYS:HG3 | 1:D:63:LYS:O | 1.88 | 0.74 |
| 1:D:82:ALA:HB1 | 1:D:97:MSE:O | 1.85 | 0.74 |
| 1:C:26:ILE:HG23 | 1:C:47:VAL:HG12 | 1.69 | 0.73 |
| 1:D:564:VAL:HG13 | 1:D:568:ILE:HD12 | 1.69 | 0.73 |
| 1:A:104:SER:OG | 1:A:137:ARG:NH1 | 2.20 | 0.73 |
| 1:C:133:GLU:HA | 1:C:133:GLU:OE1 | 1.87 | 0.73 |
| 1:A:76:VAL:HG23 | 1:A:130:VAL:HG12 | 1.71 | 0.73 |
| 1:B:115:ARG:HG3 | 1:B:123:PRO:HG3 | 1.69 | 0.73 |
| 1:B:134:PRO:HD2 | 1:B:137:ARG:HH21 | 1.53 | 0.73 |
| 1:C:509:LEU:HD22 | 1:C:518:LEU:CD2 | 2.18 | 0.73 |
| 1:D:13:MSE:HE1 | 1:D:26:ILE:CD1 | 2.19 | 0.73 |
| 1:A:498:LEU:HD12 | 1:A:502:LEU:CD1 | 2.15 | 0.73 |
| 1:B:115:ARG:CZ | 1:B:150:LEU:HD11 | 2.17 | 0.73 |
| 1:D:323:ASN:ND2 | 1:D:356:HIS:HB2 | 2.03 | 0.73 |
| 1:D:349:LEU:N | 1:D:349:LEU:HD23 | 2.04 | 0.73 |
| 1:D:315:THR:OG1 | 1:D:317:LEU:CD1 | 2.36 | 0.73 |
| 1:C:604:LYS:O | 1:C:604:LYS:HG3 | 1.89 | 0.73 |
| 1:D:68:PHE:CE2 | 1:D:86:VAL:HG11 | 2.24 | 0.73 |
| 1:A:68:PHE:CD1 | 1:A:93:MSE:HE2 | 2.24 | 0.73 |
| 1:B:638:ILE:HD12 | 1:B:638:ILE:N | 2.03 | 0.73 |
| 1:B:293:VAL:HG21 | 1:B:317:LEU:HD11 | 1.71 | 0.73 |
| 1:A:369:HIS:CD2 | 1:A:396:VAL:CG2 | 2.72 | 0.73 |
| 1:D:485:ILE:O | 1:D:512:ASN:ND2 | 2.21 | 0.73 |
| 1:A:638:ILE:CG2 | 1:A:640:MSE:HE3 | 2.19 | 0.72 |
| 1:D:114:LEU:O | 1:D:117:ILE:O | 2.06 | 0.72 |
| 1:B:134:PRO:HB2 | 1:B:137:ARG:HB2 | 1.71 | 0.72 |
| 1:B:80:LYS:HG2 | 1:B:81:PRO:CD | 2.19 | 0.72 |
| 1:B:132:MSE:SE | 1:B:138:LEU:HD13 | 2.39 | 0.72 |
| 1:C:509:LEU:HD23 | 1:C:518:LEU:HD22 | 1.71 | 0.72 |
| 1:D:349:LEU:HG | 1:D:375:THR:OG1 | 1.89 | 0.72 |
| 1:D:474:GLY:HA3 | 1:D:476:GLN:CG | 2.20 | 0.72 |
| 1:D:604:LYS:HG3 | 1:D:604:LYS:O | 1.89 | 0.72 |
| 1:B:115:ARG:HG3 | 1:B:123:PRO:CG | 2.19 | 0.72 |
| 1:C:498:LEU:HD13 | 1:C:505:LEU:HD12 | 1.71 | 0.72 |
| 1:B:64:LEU:HD11 | 1:B:66:LEU:O | 1.90 | 0.72 |
| 1:B:66:LEU:CD1 | 1:B:93:MSE:CE | 2.68 | 0.72 |
| 1:D:478:LEU:HB3 | 1:D:508:TRP:HE1 | 1.52 | 0.72 |
| 1:A:13:MSE:HG3 | 1:A:17:LYS:HE2 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:329:LEU:HD23 | 1:D:335:THR:HG21 | 1.71 | 0.72 |
| 1:C:503:SER:O | 1:C:506:ILE:HB | 1.90 | 0.71 |
| 1:D:118:PHE:CE2 | 1:D:126:ILE:HD13 | 2.24 | 0.71 |
| 1:C:505:LEU:O | 1:C:509:LEU:CD1 | 2.38 | 0.71 |
| 1:D:77:ILE:O | 1:D:85:VAL:HG12 | 1.90 | 0.71 |
| 1:B:177:GLU:O | 1:B:181:ASP:HB2 | 1.90 | 0.71 |
| 1:C:498:LEU:HD11 | 1:C:505:LEU:HD13 | 1.72 | 0.71 |
| 1:D:64:LEU:HD23 | 1:D:65:GLU:H | 1.53 | 0.71 |
| 1:B:484:GLU:CG | 1:B:508:TRP:HE1 | 1.86 | 0.71 |
| 1:C:395:ALA:O | 1:C:427:ILE:HG22 | 1.90 | 0.71 |
| 1:A:124:LEU:HD22 | 1:A:130:VAL:HG21 | 1.72 | 0.71 |
| 1:C:77:ILE:HB | 1:C:85:VAL:CG2 | 2.20 | 0.71 |
| 1:D:54:PHE:CD1 | 1:D:67:THR:CG2 | 2.74 | 0.71 |
| 1:D:580:VAL:CG1 | 1:D:605:LEU:HD21 | 2.21 | 0.71 |
| 1:D:507:VAL:HG23 | 1:D:508:TRP:N | 2.05 | 0.71 |
| 1:C:352:ASP:N | 1:C:352:ASP:OD1 | 2.20 | 0.71 |
| 1:B:32:VAL:CG2 | 1:B:95:MSE:HB3 | 2.21 | 0.71 |
| 1:C:506:ILE:HG23 | 1:C:542:MSE:HE1 | 1.72 | 0.71 |
| 1:C:543:ILE:HG23 | 1:C:574:ASN:HD21 | 1.56 | 0.71 |
| 1:C:478:LEU:HB2 | 1:C:508:TRP:HZ2 | 1.39 | 0.70 |
| 1:D:34:LEU:HD21 | 1:D:42:GLU:OE2 | 1.91 | 0.70 |
| 1:A:73:ILE:HD13 | 1:A:127:MSE:CE | 2.21 | 0.70 |
| 1:A:479:GLU:HA | 1:A:481:CYS:SG | 2.31 | 0.70 |
| 1:C:543:ILE:HG22 | 1:C:574:ASN:ND2 | 2.04 | 0.70 |
| 1:C:117:ILE:HB | 1:C:118:PHE:HD2 | 1.55 | 0.70 |
| 1:A:480:GLY:N | 1:A:481:CYS:HA | 2.06 | 0.70 |
| 1:D:349:LEU:CB | 1:D:354:LEU:HD21 | 2.16 | 0.70 |
| 1:A:134:PRO:O | 1:A:137:ARG:HG3 | 1.92 | 0.70 |
| 1:B:54:PHE:CD1 | 1:B:67:THR:HG22 | 2.24 | 0.70 |
| 1:B:80:LYS:CD | 1:B:81:PRO:HD2 | 2.22 | 0.70 |
| 1:B:652:GLU:HG2 | 1:B:653:LYS:N | 2.05 | 0.70 |
| 1:D:99:SER:HB3 | 1:D:100:PRO:HD2 | 1.73 | 0.70 |
| 1:C:502:LEU:HD12 | 1:C:502:LEU:O | 1.91 | 0.70 |
| 1:D:291:ARG:HB3 | 1:D:291:ARG:NH2 | 2.05 | 0.70 |
| 1:A:76:VAL:HG13 | 1:A:86:VAL:HG22 | 1.74 | 0.70 |
| 1:C:256:ALA:HB3 | 1:C:258:LEU:CD1 | 2.19 | 0.70 |
| 1:C:610:TRP:CZ3 | 1:C:615:ILE:HD13 | 2.26 | 0.70 |
| 1:A:323:ASN:OD1 | 1:A:354:LEU:HA | 1.91 | 0.70 |
| 1:C:543:ILE:HG22 | 1:C:574:ASN:HD22 | 1.54 | 0.70 |
| 1:D:616:THR:HG22 | 1:D:617:ALA:N | 2.07 | 0.70 |
| 1:A:618:GLN:HE21 | 1:A:618:GLN:C | 1.95 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:499:GLU:C | 1:D:527:MSE:HE2 | 2.07 | 0.69 |
| 1:B:36:VAL:HG21 | 1:B:42:GLU:HG2 | 1.71 | 0.69 |
| 1:C:484:GLU:OE2 | 1:C:511:LYS:CG | 2.39 | 0.69 |
| 1:D:77:ILE:HD12 | 1:D:85:VAL:HG11 | 1.73 | 0.69 |
| 1:D:513:ARG:HG3 | 1:D:513:ARG:NH2 | 1.94 | 0.69 |
| 1:B:4:GLU:HG2 | 1:B:5:SER:N | 2.07 | 0.69 |
| 1:C:55:LEU:CD1 | 1:C:95:MSE:CE | 2.59 | 0.69 |
| 1:C:530:LYS:O | 1:C:534:PRO:HD3 | 1.91 | 0.69 |
| 1:D:258:LEU:CD2 | 1:D:262:PHE:CD2 | 2.61 | 0.69 |
| 1:A:568:ILE:O | 1:A:571:LEU:HB2 | 1.93 | 0.69 |
| 1:B:80:LYS:HG2 | 1:B:81:PRO:HD3 | 1.74 | 0.69 |
| 1:C:603:THR:O | 1:C:603:THR:OG1 | 2.10 | 0.69 |
| 1:A:9:PRO:O | 1:A:12:LEU:HG | 1.92 | 0.69 |
| 1:B:323:ASN:ND2 | 1:B:356:HIS:CG | 2.61 | 0.69 |
| 1:A:77:ILE:O | 1:A:85:VAL:HG12 | 1.92 | 0.69 |
| 1:B:156:CYS:HA | 1:B:219:TRP:CD1 | 2.28 | 0.69 |
| 1:C:610:TRP:NE1 | 1:C:636:MSE:CE | 2.56 | 0.69 |
| 1:D:377:CYS:O | 1:D:403:VAL:HG22 | 1.92 | 0.69 |
| 1:B:36:VAL:HB | 1:B:41:VAL:HA | 1.74 | 0.69 |
| 1:C:379:LEU:HD13 | 1:C:402:SER:HB3 | 1.74 | 0.69 |
| 1:A:470:LEU:CD2 | 1:A:477:VAL:HG11 | 2.23 | 0.69 |
| 1:D:30:LYS:HE3 | 1:D:102:ASP:OD1 | 1.93 | 0.69 |
| 1:D:53:ALA:HB3 | 1:D:68:PHE:CE1 | 2.28 | 0.69 |
| 1:D:506:ILE:HG21 | 1:D:538:ASN:HB3 | 1.74 | 0.69 |
| 1:A:414:PRO:O | 1:A:418:GLN:HB2 | 1.93 | 0.68 |
| 1:B:8:VAL:HA | 1:B:31:LYS:HD2 | 1.75 | 0.68 |
| 1:B:135:SER:HB3 | 1:B:136:GLU:OE2 | 1.93 | 0.68 |
| 1:C:290:ASP:OD2 | 1:C:321:GLY:N | 2.26 | 0.68 |
| 1:A:117:ILE:HD13 | 1:A:165:CYS:SG | 2.33 | 0.68 |
| 1:A:618:GLN:O | 1:A:618:GLN:NE2 | 2.15 | 0.68 |
| 1:D:43:ASN:O | 1:D:44:LYS:CE | 2.41 | 0.68 |
| 1:A:12:LEU:C | 1:A:12:LEU:HD12 | 2.14 | 0.68 |
| 1:A:73:ILE:CD1 | 1:A:127:MSE:HE3 | 2.23 | 0.68 |
| 1:A:638:ILE:HG21 | 1:A:640:MSE:HE3 | 1.75 | 0.68 |
| 1:D:507:VAL:HG23 | 1:D:508:TRP:H | 1.58 | 0.68 |
| 1:B:78:CYS:HB2 | 1:B:132:MSE:CA | 2.21 | 0.68 |
| 1:C:98:VAL:HG22 | 1:C:102:ASP:OD2 | 1.94 | 0.68 |
| 1:D:651:PRO:HG2 | 1:D:652:GLU:N | 2.09 | 0.68 |
| 1:B:54:PHE:HA | 1:B:67:THR:CG2 | 2.23 | 0.68 |
| 1:D:638:ILE:HD12 | 1:D:638:ILE:N | 2.04 | 0.68 |
| 1:A:73:ILE:HG21 | 1:A:127:MSE:CE | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:36:VAL:HB | 1:B:40:ARG:O | 1.93 | 0.68 |
| 1:D:144:LEU:C | 1:D:148:GLN:OE1 | 2.31 | 0.68 |
| 1:A:374:ASN:OD1 | 1:A:401:ARG:HD3 | 1.89 | 0.67 |
| 1:B:513:ARG:HH11 | 1:B:513:ARG:CG | 2.07 | 0.67 |
| 1:C:256:ALA:CB | 1:C:258:LEU:HD13 | 2.24 | 0.67 |
| 1:D:34:LEU:HD21 | 1:D:36:VAL:HG21 | 1.75 | 0.67 |
| 1:C:36:VAL:HG12 | 1:C:37:LYS:CD | 2.18 | 0.67 |
| 1:D:543:ILE:CG2 | 1:D:574:ASN:ND2 | 2.57 | 0.67 |
| 1:A:95:MSE:HB2 | 1:A:97:MSE:CE | 2.25 | 0.67 |
| 1:A:452:HIS:H | 1:A:452:HIS:CD2 | 2.11 | 0.67 |
| 1:B:56:LEU:HD23 | 1:B:64:LEU:HB2 | 1.76 | 0.67 |
| 1:C:478:LEU:CD2 | 1:C:508:TRP:CH2 | 2.77 | 0.67 |
| 1:C:563:GLU:O | 1:C:566:ILE:HG23 | 1.94 | 0.67 |
| 1:C:578:THR:HG22 | 1:C:604:LYS:HD2 | 1.75 | 0.67 |
| 1:D:46:LEU:CD1 | 1:D:95:MSE:HE1 | 2.25 | 0.67 |
| 1:D:80:LYS:HD2 | 1:D:81:PRO:HD2 | 1.77 | 0.67 |
| 1:A:80:LYS:HD2 | 1:A:81:PRO:N | 2.10 | 0.67 |
| 1:D:610:TRP:CE3 | 1:D:615:ILE:HD12 | 2.29 | 0.67 |
| 1:A:141:LEU:HD23 | 1:A:144:LEU:HD23 | 1.77 | 0.67 |
| 1:A:143:ALA:HA | 1:A:146:ASP:HB2 | 1.77 | 0.67 |
| 1:B:143:ALA:O | 1:B:147:SER:HB3 | 1.95 | 0.67 |
| 1:C:185:ILE:HA | 1:D:601:ILE:HD11 | 1.76 | 0.67 |
| 1:C:217:ASN:OD1 | 1:C:219:TRP:N | 2.19 | 0.67 |
| 1:D:349:LEU:CD1 | 1:D:357:MSE:CE | 2.64 | 0.67 |
| 1:B:52:ARG:HD3 | 1:B:67:THR:HB | 1.76 | 0.66 |
| 1:C:378:SER:O | 1:C:382:VAL:HG23 | 1.95 | 0.66 |
| 1:A:98:VAL:HG23 | 1:A:99:SER:N | 2.09 | 0.66 |
| 1:C:478:LEU:HD23 | 1:C:508:TRP:HH2 | 1.58 | 0.66 |
| 1:D:46:LEU:HD13 | 1:D:95:MSE:CE | 2.24 | 0.66 |
| 1:B:18:ASP:OD1 | 1:B:22:ARG:NH2 | 2.29 | 0.66 |
| 1:B:372:LEU:O | 1:B:375:THR:HG22 | 1.94 | 0.66 |
| 1:C:134:PRO:CD | 1:C:137:ARG:HH21 | 2.07 | 0.66 |
| 1:A:597:LYS:HE3 | 1:B:201:HIS:CE1 | 2.31 | 0.66 |
| 1:B:212:ALA:HB2 | 1:B:237:GLN:CG | 2.25 | 0.66 |
| 1:B:478:LEU:HB3 | 1:B:508:TRP:CZ3 | 2.31 | 0.66 |
| 1:C:372:LEU:O | 1:C:375:THR:HG22 | 1.94 | 0.66 |
| 1:C:527:MSE:CE | 1:C:532:LEU:HG | 2.25 | 0.66 |
| 1:D:100:PRO:CD | 1:D:101:GLU:H | 2.08 | 0.66 |
| 1:C:636:MSE:HB3 | 1:C:665:LEU:HD11 | 1.78 | 0.66 |
| 1:D:46:LEU:HD22 | 1:D:95:MSE:CE | 2.25 | 0.66 |
| 1:A:13:MSE:CE | 1:A:26:ILE:CD1 | 2.73 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:485:ILE:HG22 | 1:B:512:ASN:ND2 | 2.10 | 0.66 |
| 1:D:99:SER:CB | 1:D:100:PRO:HD2 | 2.26 | 0.66 |
| 1:D:474:GLY:CA | 1:D:475:ALA:HB3 | 2.16 | 0.66 |
| 1:B:7:ASP:N | 1:B:7:ASP:OD1 | 2.28 | 0.66 |
| 1:C:115:ARG:NH2 | 1:C:150:LEU:HD21 | 2.09 | 0.66 |
| 1:C:484:GLU:OE2 | 1:C:511:LYS:HB2 | 1.89 | 0.66 |
| 1:D:318:SER:HG | 1:D:320:LYS:HG3 | 1.61 | 0.66 |
| 1:A:35:GLU:HB2 | 1:A:94:SER:HB3 | 1.78 | 0.66 |
| 1:D:160:SER:OG | 1:D:183:ASP:OD1 | 2.13 | 0.66 |
| 1:D:427:ILE:O | 1:D:427:ILE:HD13 | 1.94 | 0.66 |
| 1:A:13:MSE:CE | 1:A:26:ILE:HD12 | 2.25 | 0.65 |
| 1:A:97:MSE:SE | 1:A:103:VAL:HG12 | 2.46 | 0.65 |
| 1:B:355:SER:O | 1:B:359:ASN:HB2 | 1.97 | 0.65 |
| 1:C:478:LEU:CD2 | 1:C:508:TRP:HH2 | 2.09 | 0.65 |
| 1:C:478:LEU:CD1 | 1:C:508:TRP:HZ2 | 2.09 | 0.65 |
| 1:B:478:LEU:HB3 | 1:B:508:TRP:CE3 | 2.32 | 0.65 |
| 1:C:193:GLU:CG | 1:C:222:LYS:HD3 | 2.27 | 0.65 |
| 1:D:117:ILE:HG22 | 1:D:118:PHE:CE1 | 2.31 | 0.65 |
| 1:D:563:GLU:O | 1:D:564:VAL:C | 2.30 | 0.65 |
| 1:C:256:ALA:CB | 1:C:258:LEU:CD1 | 2.74 | 0.65 |
| 1:C:315:THR:OG1 | 1:C:317:LEU:HD13 | 1.95 | 0.65 |
| 1:A:89:GLU:HA | 1:A:89:GLU:OE2 | 1.96 | 0.65 |
| 1:D:478:LEU:CB | 1:D:508:TRP:HE1 | 2.10 | 0.65 |
| 1:A:119:PRO:HG2 | 1:A:153:PRO:HB3 | 1.79 | 0.65 |
| 1:C:503:SER:HA | 1:C:506:ILE:HG13 | 1.77 | 0.65 |
| 1:D:172:PHE:CE2 | 1:D:209:PRO:HD3 | 2.32 | 0.65 |
| 1:D:117:ILE:HD11 | 1:D:165:CYS:SG | 2.37 | 0.65 |
| 1:D:448:LEU:O | 1:D:487:ASN:ND2 | 2.30 | 0.65 |
| 1:D:474:GLY:HA3 | 1:D:476:GLN:HG2 | 1.79 | 0.65 |
| 1:D:499:GLU:HA | 1:D:527:MSE:CE | 2.16 | 0.65 |
| 1:A:138:LEU:HD23 | 1:A:138:LEU:C | 2.16 | 0.65 |
| 1:D:34:LEU:O | 1:D:36:VAL:HG23 | 1.97 | 0.65 |
| 1:D:84:MSE:SE | 1:D:107:LEU:CD1 | 2.95 | 0.65 |
| 1:C:474:GLY:CA | 1:C:476:GLN:N | 2.57 | 0.65 |
| 1:A:138:LEU:HD23 | 1:A:139:ALA:CA | 2.27 | 0.64 |
| 1:B:52:ARG:HG3 | 1:B:68:PHE:O | 1.97 | 0.64 |
| 1:C:160:SER:OG | 1:C:183:ASP:OD1 | 2.13 | 0.64 |
| 1:A:394:LEU:HD21 | 1:A:397:LEU:HD13 | 1.78 | 0.64 |
| 1:C:349:LEU:HG | 1:C:375:THR:HG1 | 1.62 | 0.64 |
| 1:D:437:SER:O | 1:D:440:PRO:HD2 | 1.98 | 0.64 |
| 1:D:610:TRP:CE3 | 1:D:615:ILE:CD1 | 2.81 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:146:ASP:OD1 | 1:D:146:ASP:N | 2.31 | 0.64 |
| 1:B:256:ALA:HB3 | 1:B:258:LEU:CD1 | 2.27 | 0.64 |
| 1:D:113:CYS:O | 1:D:116:ARG:HB3 | 1.98 | 0.64 |
| 1:D:40:ARG:HH21 | 1:D:40:ARG:CG | 2.10 | 0.64 |
| 1:D:76:VAL:O | 1:D:130:VAL:HA | 1.98 | 0.64 |
| 1:A:23:LYS:N | 1:A:23:LYS:HD2 | 2.12 | 0.64 |
| 1:D:78:CYS:SG | 1:D:103:VAL:CG1 | 2.83 | 0.64 |
| 1:D:110:ILE:HG21 | 1:D:127:MSE:HE1 | 1.80 | 0.64 |
| 1:A:593:LYS:HE2 | 1:B:200:SER:OG | 1.98 | 0.64 |
| 1:D:37:LYS:CA | 1:D:39:ASP:H | 2.06 | 0.64 |
| 1:D:408:LYS:HE3 | 1:D:408:LYS:HA | 1.79 | 0.64 |
| 1:A:258:LEU:CD2 | 1:A:262:PHE:CE2 | 2.81 | 0.64 |
| 1:B:8:VAL:HG22 | 1:B:31:LYS:HG2 | 1.80 | 0.64 |
| 1:C:193:GLU:HG3 | 1:C:222:LYS:CD | 2.28 | 0.64 |
| 1:C:381:MSE:HA | 1:C:381:MSE:CE | 2.27 | 0.64 |
| 1:B:32:VAL:CG2 | 1:B:95:MSE:HG2 | 2.28 | 0.63 |
| 1:A:84:MSE:HE1 | 1:A:106:VAL:HG11 | 1.80 | 0.63 |
| 1:C:290:ASP:O | 1:C:294:SER:OG | 2.16 | 0.63 |
| 1:C:484:GLU:N | 1:C:508:TRP:HE1 | 1.96 | 0.63 |
| 1:D:53:ALA:O | 1:D:67:THR:HG22 | 1.99 | 0.63 |
| 1:D:115:ARG:HH11 | 1:D:115:ARG:HG3 | 1.62 | 0.63 |
| 1:C:602:ASN:ND2 | 1:C:605:LEU:HD23 | 2.13 | 0.63 |
| 1:A:601:ILE:HD11 | 1:B:184:THR:O | 1.97 | 0.63 |
| 1:C:404:PHE:CE1 | 1:C:440:PRO:HB3 | 2.32 | 0.63 |
| 1:C:449:ALA:HA | 1:C:485:ILE:HG23 | 1.80 | 0.63 |
| 1:D:36:VAL:O | 1:D:39:ASP:N | 2.32 | 0.63 |
| 1:A:117:ILE:HD11 | 1:A:165:CYS:SG | 2.37 | 0.63 |
| 1:D:70:TYR:CD1 | 1:D:110:ILE:HG23 | 2.32 | 0.63 |
| 1:A:543:ILE:CG2 | 1:A:574:ASN:ND2 | 2.61 | 0.63 |
| 1:C:611:ASP:OD1 | 1:C:612:LYS:N | 2.31 | 0.63 |
| 1:A:143:ALA:O | 1:A:146:ASP:HB2 | 1.98 | 0.63 |
| 1:A:290:ASP:HA | 1:A:293:VAL:HB | 1.81 | 0.63 |
| 1:A:638:ILE:CD1 | 1:A:640:MSE:HE1 | 2.27 | 0.63 |
| 1:B:288:LEU:O | 1:B:289:GLU:HB2 | 1.97 | 0.63 |
| 1:C:55:LEU:CD2 | 1:C:95:MSE:HE2 | 2.27 | 0.63 |
| 1:B:115:ARG:HG3 | 1:B:123:PRO:CD | 2.29 | 0.63 |
| 1:B:580:VAL:HG12 | 1:B:608:VAL:HG22 | 1.81 | 0.63 |
| 1:C:134:PRO:HD2 | 1:C:137:ARG:HD3 | 1.81 | 0.63 |
| 1:C:441:LEU:HD11 | 1:C:445:LEU:HD11 | 1.81 | 0.63 |
| 1:B:8:VAL:HG21 | 1:B:45:VAL:HG13 | 1.81 | 0.62 |
| 1:B:115:ARG:HG3 | 1:B:123:PRO:HD3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:12:LEU:HD12 | 1:C:12:LEU:C | 2.19 | 0.62 |
| 1:D:48:LEU:HD11 | 1:D:106:VAL:HG13 | 1.80 | 0.62 |
| 1:D:144:LEU:C | 1:D:144:LEU:HD13 | 2.20 | 0.62 |
| 1:B:80:LYS:HB3 | 1:B:83:GLN:HB3 | 1.82 | 0.62 |
| 1:C:470:LEU:HD11 | 1:C:505:LEU:HD11 | 1.81 | 0.62 |
| 1:B:474:GLY:O | 1:B:475:ALA:HB3 | 2.00 | 0.62 |
| 1:C:36:VAL:HG12 | 1:C:37:LYS:N | 2.01 | 0.62 |
| 1:D:43:ASN:O | 1:D:44:LYS:HE2 | 1.97 | 0.62 |
| 1:A:301:ALA:O | 1:A:332:ASN:HB2 | 1.99 | 0.62 |
| 1:B:513:ARG:HH11 | 1:B:513:ARG:CA | 2.12 | 0.62 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:CA | 2.48 | 0.62 |
| 1:C:474:GLY:HA3 | 1:C:476:GLN:N | 2.05 | 0.62 |
| 1:A:617:ALA:O | 1:A:621:GLN:HG3 | 2.00 | 0.62 |
| 1:C:532:LEU:CD2 | 1:C:536:LEU:HG | 2.29 | 0.62 |
| 1:D:379:LEU:HD13 | 1:D:402:SER:OG | 2.00 | 0.62 |
| 1:A:68:PHE:CD1 | 1:A:93:MSE:HE1 | 2.34 | 0.62 |
| 1:C:484:GLU:CD | 1:C:511:LYS:HB3 | 2.16 | 0.62 |
| 1:C:509:LEU:HD22 | 1:C:518:LEU:HD22 | 1.77 | 0.62 |
| 1:A:133:GLU:OE1 | 1:A:133:GLU:HA | 1.98 | 0.61 |
| 1:B:349:LEU:HG | 1:B:375:THR:HG1 | 1.63 | 0.61 |
| 1:B:496:ASN:O | 1:B:497:GLY:C | 2.37 | 0.61 |
| 1:B:638:ILE:HD12 | 1:B:638:ILE:H | 1.65 | 0.61 |
| 1:D:43:ASN:O | 1:D:44:LYS:CD | 2.48 | 0.61 |
| 1:D:378:SER:HB2 | 1:D:406:HIS:CD2 | 2.35 | 0.61 |
| 1:D:26:ILE:CD1 | 1:D:47:VAL:HG21 | 2.29 | 0.61 |
| 1:D:256:ALA:HB3 | 1:D:258:LEU:CD1 | 2.30 | 0.61 |
| 1:D:470:LEU:O | 1:D:473:GLY:O | 2.18 | 0.61 |
| 1:A:349:LEU:CG | 1:A:375:THR:OG1 | 2.35 | 0.61 |
| 1:A:589:ASP:OD1 | 1:A:616:THR:OG1 | 2.18 | 0.61 |
| 1:D:348:ALA:C | 1:D:349:LEU:HD23 | 2.20 | 0.61 |
| 1:D:313:SER:HA | 1:D:345:SER:O | 2.01 | 0.61 |
| 1:B:115:ARG:NH1 | 1:B:150:LEU:HD11 | 2.16 | 0.61 |
| 1:B:157:GLY:O | 1:B:162:MSE:HE3 | 2.00 | 0.61 |
| 1:B:477:VAL:HG23 | 1:B:478:LEU:HG | 1.81 | 0.61 |
| 1:C:477:VAL:O | 1:C:477:VAL:HG13 | 2.00 | 0.61 |
| 1:D:477:VAL:O | 1:D:478:LEU:HD23 | 2.00 | 0.61 |
| 1:A:482:ILE:HG23 | 1:A:483:ALA:N | 2.15 | 0.61 |
| 1:B:298:ILE:HG22 | 1:B:299:GLN:N | 2.15 | 0.61 |
| 1:C:387:LEU:O | 1:C:391:LEU:HD21 | 2.01 | 0.61 |
| 1:D:39:ASP:N | 1:D:39:ASP:OD1 | 2.29 | 0.61 |
| 1:D:372:LEU:O | 1:D:375:THR:HB | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:54:PHE:CD1 | 1:C:67:THR:HG23 | 2.35 | 0.61 |
| 1:C:498:LEU:CD1 | 1:C:505:LEU:CD1 | 2.79 | 0.61 |
| 1:A:76:VAL:HG12 | 1:A:85:VAL:O | 2.01 | 0.61 |
| 1:A:479:GLU:C | 1:A:481:CYS:HB2 | 2.21 | 0.61 |
| 1:C:80:LYS:HG2 | 1:C:81:PRO:HD2 | 1.82 | 0.61 |
| 1:D:318:SER:OG | 1:D:320:LYS:HG3 | 2.01 | 0.61 |
| 1:D:34:LEU:O | 1:D:34:LEU:HD23 | 2.00 | 0.61 |
| 1:D:82:ALA:O | 1:D:97:MSE:N | 2.25 | 0.61 |
| 1:D:322:VAL:HG12 | 1:D:357:MSE:HE3 | 1.83 | 0.61 |
| 1:A:478:LEU:HD13 | 1:A:508:TRP:CB | 2.31 | 0.60 |
| 1:A:602:ASN:ND2 | 1:A:605:LEU:HD23 | 2.16 | 0.60 |
| 1:D:54:PHE:CE1 | 1:D:67:THR:HG21 | 2.36 | 0.60 |
| 1:D:284:ALA:HB1 | 1:D:313:SER:HB3 | 1.84 | 0.60 |
| 1:B:349:LEU:CG | 1:B:375:THR:OG1 | 2.44 | 0.60 |
| 1:D:97:MSE:HE2 | 1:D:103:VAL:HA | 1.83 | 0.60 |
| 1:D:474:GLY:HA3 | 1:D:476:GLN:HG3 | 1.83 | 0.60 |
| 1:B:36:VAL:CG2 | 1:B:42:GLU:CG | 2.65 | 0.60 |
| 1:A:65:GLU:O | 1:A:66:LEU:HD23 | 2.02 | 0.60 |
| 1:A:666:LEU:HD22 | 1:B:666:LEU:HD11 | 1.83 | 0.60 |
| 1:C:185:ILE:O | 1:C:189:GLN:HG3 | 2.01 | 0.60 |
| 1:C:509:LEU:HD22 | 1:C:518:LEU:HD21 | 1.84 | 0.60 |
| 1:C:650:ASN:O | 1:C:652:GLU:HB3 | 2.00 | 0.60 |
| 1:D:325:LEU:HD11 | 1:D:329:LEU:HD11 | 1.84 | 0.60 |
| 1:D:355:SER:O | 1:D:359:ASN:N | 2.30 | 0.60 |
| 1:B:182:VAL:O | 1:B:186:TYR:CB | 2.43 | 0.60 |
| 1:A:431:LEU:O | 1:A:434:THR:OG1 | 2.18 | 0.60 |
| 1:C:115:ARG:HH21 | 1:C:115:ARG:CG | 2.14 | 0.60 |
| 1:D:586:GLY:HA2 | 1:D:614:ASN:HD22 | 1.65 | 0.60 |
| 1:A:263:ALA:CB | 1:A:292:GLY:HA3 | 2.32 | 0.60 |
| 1:A:254:GLU:O | 1:A:255:ASN:C | 2.38 | 0.60 |
| 1:D:115:ARG:HH11 | 1:D:115:ARG:CG | 2.14 | 0.60 |
| 1:D:638:ILE:H | 1:D:638:ILE:CD1 | 1.99 | 0.60 |
| 1:A:303:LEU:HD23 | 1:A:304:PRO:CD | 2.23 | 0.59 |
| 1:A:506:ILE:HG23 | 1:A:542:MSE:HE3 | 1.83 | 0.59 |
| 1:C:122:SER:O | 1:C:125:ARG:N | 2.35 | 0.59 |
| 1:C:169:TRP:CZ3 | 1:C:170:LEU:HD21 | 2.36 | 0.59 |
| 1:A:256:ALA:HB3 | 1:A:258:LEU:CD1 | 2.29 | 0.59 |
| 1:A:483:ALA:O | 1:A:484:GLU:HB3 | 2.02 | 0.59 |
| 1:B:66:LEU:HD13 | 1:B:93:MSE:HE1 | 1.81 | 0.59 |
| 1:C:350:ARG:HG3 | 1:C:376:GLU:HG2 | 1.83 | 0.59 |
| 1:D:314:LYS:HG3 | 1:D:346:GLY:HA3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:56:LEU:HD23 | 1:A:63:LYS:O | 2.01 | 0.59 |
| 1:B:84:MSE:HE1 | 1:B:106:VAL:HB | 1.84 | 0.59 |
| 1:B:136:GLU:H | 1:B:136:GLU:CD | 2.04 | 0.59 |
| 1:C:117:ILE:CG2 | 1:C:118:PHE:CE2 | 2.85 | 0.59 |
| 1:C:651:PRO:N | 1:C:652:GLU:HB2 | 2.16 | 0.59 |
| 1:A:9:PRO:HB3 | 1:A:12:LEU:CD2 | 2.26 | 0.59 |
| 1:A:162:MSE:O | 1:A:166:VAL:HG23 | 2.02 | 0.59 |
| 1:A:506:ILE:HG23 | 1:A:542:MSE:CE | 2.32 | 0.59 |
| 1:B:374:ASN:OD1 | 1:B:401:ARG:CD | 2.43 | 0.59 |
| 1:D:117:ILE:HG22 | 1:D:118:PHE:CG | 2.38 | 0.59 |
| 1:D:142:GLN:OE1 | 1:D:146:ASP:OD1 | 2.20 | 0.59 |
| 1:B:44:LYS:HB3 | 1:B:56:LEU:O | 2.02 | 0.59 |
| 1:C:414:PRO:O | 1:C:418:GLN:HB2 | 2.02 | 0.59 |
| 1:A:652:GLU:CG | 1:A:653:LYS:H | 2.05 | 0.59 |
| 1:B:354:LEU:HD23 | 1:B:358:TYR:OH | 2.03 | 0.59 |
| 1:D:16:ILE:HG23 | 1:D:56:LEU:HD13 | 1.83 | 0.59 |
| 1:A:32:VAL:HG21 | 1:A:95:MSE:HB3 | 1.85 | 0.59 |
| 1:A:528:LYS:O | 1:A:531:ASN:HB2 | 2.02 | 0.59 |
| 1:A:574:ASN:OD1 | 1:A:576:SER:N | 2.31 | 0.59 |
| 1:D:34:LEU:HD21 | 1:D:36:VAL:CG2 | 2.33 | 0.59 |
| 1:D:422:SER:O | 1:D:424:LEU:CD1 | 2.51 | 0.59 |
| 1:D:620:PHE:CD1 | 1:D:658:LEU:HD21 | 2.38 | 0.59 |
| 1:B:76:VAL:HG11 | 1:B:107:LEU:HD21 | 1.85 | 0.59 |
| 1:C:36:VAL:HG21 | 1:C:42:GLU:HG3 | 1.85 | 0.59 |
| 1:D:616:THR:CG2 | 1:D:617:ALA:N | 2.66 | 0.59 |
| 1:A:28:VAL:HB | 1:A:48:LEU:HB2 | 1.85 | 0.59 |
| 1:A:121:LEU:HD22 | 1:A:125:ARG:HH11 | 1.66 | 0.59 |
| 1:B:56:LEU:CD2 | 1:B:64:LEU:HB2 | 2.33 | 0.59 |
| 1:D:372:LEU:O | 1:D:375:THR:HG22 | 2.01 | 0.59 |
| 1:B:174:TYR:CD1 | 1:B:174:TYR:C | 2.76 | 0.58 |
| 1:B:558:SER:HB2 | 1:B:560:LEU:HG | 1.84 | 0.58 |
| 1:D:64:LEU:CD2 | 1:D:65:GLU:N | 2.64 | 0.58 |
| 1:B:564:VAL:O | 1:B:564:VAL:HG22 | 2.03 | 0.58 |
| 1:D:144:LEU:O | 1:D:148:GLN:CD | 2.40 | 0.58 |
| 1:C:498:LEU:CD1 | 1:C:505:LEU:HD13 | 2.33 | 0.58 |
| 1:C:536:LEU:O | 1:C:540:VAL:HG23 | 2.02 | 0.58 |
| 1:D:117:ILE:CG2 | 1:D:118:PHE:CE1 | 2.86 | 0.58 |
| 1:A:403:VAL:HG23 | 1:A:403:VAL:O | 2.04 | 0.58 |
| 1:A:470:LEU:CD2 | 1:A:477:VAL:CG1 | 2.81 | 0.58 |
| 1:B:54:PHE:CA | 1:B:67:THR:HG22 | 2.34 | 0.58 |
| 1:C:53:ALA:O | 1:C:67:THR:HG22 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:387:LEU:O | 1:C:391:LEU:HD11 | 2.03 | 0.58 |
| 1:C:509:LEU:HD12 | 1:C:509:LEU:H | 1.68 | 0.58 |
| 1:C:647:LEU:HD23 | 1:C:654:THR:HB | 1.83 | 0.58 |
| 1:A:13:MSE:O | 1:A:16:ILE:HB | 2.02 | 0.58 |
| 1:A:610:TRP:O | 1:A:613:ASN:ND2 | 2.28 | 0.58 |
| 1:A:667:ARG:HG3 | 1:A:668:ASN:N | 2.19 | 0.58 |
| 1:D:397:LEU:HD11 | 1:D:399:LEU:HD11 | 1.84 | 0.58 |
| 1:D:504:THR:O | 1:D:507:VAL:CG2 | 2.51 | 0.58 |
| 1:A:543:ILE:HG22 | 1:A:574:ASN:ND2 | 2.19 | 0.58 |
| 1:C:16:ILE:HA | 1:C:19:VAL:HG12 | 1.86 | 0.58 |
| 1:D:208:ILE:HG23 | 1:D:237:GLN:HE21 | 1.68 | 0.58 |
| 1:D:563:GLU:O | 1:D:566:ILE:HG23 | 2.04 | 0.58 |
| 1:A:222:LYS:HG3 | 1:A:250:GLU:HB2 | 1.84 | 0.58 |
| 1:B:53:ALA:O | 1:B:67:THR:HG22 | 2.04 | 0.58 |
| 1:C:117:ILE:CB | 1:C:118:PHE:CD2 | 2.85 | 0.58 |
| 1:D:336:ALA:O | 1:D:366:THR:HG22 | 2.03 | 0.58 |
| 1:B:80:LYS:HD3 | 1:B:82:ALA:H | 1.68 | 0.58 |
| 1:B:270:LEU:HD21 | 1:B:278:LEU:HD12 | 1.85 | 0.58 |
| 1:B:322:VAL:HG21 | 1:B:349:LEU:HD21 | 1.86 | 0.58 |
| 1:C:476:GLN:HE21 | 1:C:476:GLN:CA | 2.16 | 0.58 |
| 1:D:80:LYS:HD2 | 1:D:81:PRO:CD | 2.34 | 0.58 |
| 1:D:115:ARG:NH2 | 1:D:150:LEU:HD22 | 2.18 | 0.58 |
| 1:D:477:VAL:C | 1:D:478:LEU:HG | 2.23 | 0.58 |
| 1:D:610:TRP:HZ3 | 1:D:615:ILE:CD1 | 2.17 | 0.58 |
| 1:A:23:LYS:HE3 | 1:A:23:LYS:CA | 2.34 | 0.57 |
| 1:A:603:THR:O | 1:A:603:THR:OG1 | 2.21 | 0.57 |
| 1:D:174:TYR:HD1 | 1:D:174:TYR:C | 2.08 | 0.57 |
| 1:B:258:LEU:CD2 | 1:B:262:PHE:CE2 | 2.86 | 0.57 |
| 1:D:56:LEU:HD23 | 1:D:64:LEU:HA | 1.85 | 0.57 |
| 1:B:503:SER:O | 1:B:504:THR:C | 2.42 | 0.57 |
| 1:C:69:SER:N | 1:C:72:GLU:OE1 | 2.34 | 0.57 |
| 1:C:493:ILE:O | 1:C:496:ASN:ND2 | 2.34 | 0.57 |
| 1:D:97:MSE:HG3 | 1:D:103:VAL:HG22 | 1.87 | 0.57 |
| 1:D:110:ILE:HG21 | 1:D:127:MSE:CE | 2.34 | 0.57 |
| 1:D:110:ILE:CG2 | 1:D:127:MSE:HE1 | 2.34 | 0.57 |
| 1:D:174:TYR:C | 1:D:174:TYR:CD1 | 2.76 | 0.57 |
| 1:A:212:ALA:HB2 | 1:A:237:GLN:CG | 2.35 | 0.57 |
| 1:B:132:MSE:SE | 1:B:138:LEU:CD1 | 3.02 | 0.57 |
| 1:C:510:SER:O | 1:C:513:ARG:NH1 | 2.37 | 0.57 |
| 1:D:37:LYS:CD | 1:D:37:LYS:H | 2.18 | 0.57 |
| 1:A:99:SER:OG | 1:A:100:PRO:HD2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:407:ARG:HH21 | 1:C:407:ARG:CG | 2.15 | 0.57 |
| 1:A:19:VAL:HG13 | 1:A:20:ILE:HG23 | 1.86 | 0.57 |
| 1:A:589:ASP:OD2 | 1:A:616:THR:OG1 | 2.22 | 0.57 |
| 1:A:638:ILE:HG23 | 1:A:640:MSE:CE | 2.35 | 0.57 |
| 1:A:650:ASN:HB3 | 1:A:652:GLU:OE2 | 2.05 | 0.57 |
| 1:D:70:TYR:CE1 | 1:D:110:ILE:HG12 | 2.39 | 0.57 |
| 1:D:212:ALA:HB2 | 1:D:237:GLN:CG | 2.35 | 0.57 |
| 1:D:290:ASP:OD2 | 1:D:321:GLY:N | 2.38 | 0.57 |
| 1:A:290:ASP:OD1 | 1:A:317:LEU:HA | 2.04 | 0.57 |
| 1:A:380:GLU:CD | 1:A:405:SER:OG | 2.43 | 0.57 |
| 1:D:499:GLU:HA | 1:D:499:GLU:OE2 | 2.04 | 0.57 |
| 1:C:26:ILE:CG2 | 1:C:47:VAL:CG1 | 2.81 | 0.57 |
| 1:C:486:HIS:HA | 1:C:514:SER:HB3 | 1.87 | 0.57 |
| 1:D:114:LEU:HB3 | 1:D:123:PRO:HG3 | 1.87 | 0.57 |
| 1:A:13:MSE:HG3 | 1:A:17:LYS:HE3 | 1.86 | 0.57 |
| 1:C:524:PHE:N | 1:C:524:PHE:CD1 | 2.73 | 0.57 |
| 1:D:196:LEU:HB2 | 1:D:225:SER:HB2 | 1.87 | 0.57 |
| 1:A:604:LYS:HG3 | 1:A:604:LYS:O | 2.05 | 0.57 |
| 1:B:315:THR:OG1 | 1:B:317:LEU:HD13 | 2.05 | 0.57 |
| 1:B:485:ILE:HG22 | 1:B:512:ASN:HD22 | 1.70 | 0.57 |
| 1:C:610:TRP:CD1 | 1:C:636:MSE:HE3 | 2.40 | 0.57 |
| 1:D:66:LEU:HD13 | 1:D:93:MSE:HE2 | 1.87 | 0.57 |
| 1:A:471:ARG:HG3 | 1:A:471:ARG:NH2 | 2.19 | 0.56 |
| 1:B:468:HIS:O | 1:B:472:SER:HB3 | 2.05 | 0.56 |
| 1:C:381:MSE:HE3 | 1:C:381:MSE:CA | 2.27 | 0.56 |
| 1:C:420:PHE:CZ | 1:C:444:LEU:CD1 | 2.87 | 0.56 |
| 1:C:461:LEU:O | 1:C:464:CYS:SG | 2.62 | 0.56 |
| 1:C:587:MSE:HG2 | 1:C:613:ASN:CG | 2.25 | 0.56 |
| 1:C:613:ASN:O | 1:C:614:ASN:HB2 | 2.03 | 0.56 |
| 1:C:34:LEU:HD23 | 1:C:36:VAL:HG22 | 1.87 | 0.56 |
| 1:D:27:SER:HB2 | 1:D:109:HIS:HE1 | 1.70 | 0.56 |
| 1:D:466:LEU:O | 1:D:469:CYS:HB3 | 2.06 | 0.56 |
| 1:A:323:ASN:ND2 | 1:A:356:HIS:HB2 | 2.20 | 0.56 |
| 1:B:46:LEU:HA | 1:B:55:LEU:HD23 | 1.88 | 0.56 |
| 1:D:159:PHE:O | 1:D:159:PHE:HD1 | 1.88 | 0.56 |
| 1:D:325:LEU:HD12 | 1:D:325:LEU:C | 2.26 | 0.56 |
| 1:D:516:GLN:C | 1:D:517:HIS:CD2 | 2.78 | 0.56 |
| 1:C:68:PHE:HD2 | 1:C:93:MSE:CE | 1.92 | 0.56 |
| 1:A:479:GLU:CA | 1:A:481:CYS:SG | 2.93 | 0.56 |
| 1:C:545:ASP:OD1 | 1:C:546:GLU:N | 2.38 | 0.56 |
| 1:D:506:ILE:HG23 | 1:D:542:MSE:HE3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:369:HIS:CG | 1:A:396:VAL:CG2 | 2.89 | 0.56 |
| 1:C:116:ARG:HH11 | 1:C:116:ARG:HG3 | 1.71 | 0.56 |
| 1:A:13:MSE:HE2 | 1:A:26:ILE:HD11 | 1.87 | 0.56 |
| 1:A:652:GLU:HG2 | 1:A:653:LYS:HG3 | 1.88 | 0.56 |
| 1:C:498:LEU:HD13 | 1:C:505:LEU:CD1 | 2.35 | 0.56 |
| 1:D:375:THR:HG23 | 1:D:377:CYS:HB3 | 1.88 | 0.56 |
| 1:A:46:LEU:HD23 | 1:A:55:LEU:HD23 | 1.86 | 0.56 |
| 1:A:558:SER:HB2 | 1:A:585:ASN:OD1 | 2.06 | 0.56 |
| 1:B:88:THR:HG23 | 1:B:91:CYS:CA | 2.36 | 0.56 |
| 1:B:323:ASN:ND2 | 1:B:356:HIS:HB2 | 2.21 | 0.56 |
| 1:C:602:ASN:HD21 | 1:C:605:LEU:HD23 | 1.70 | 0.56 |
| 1:D:563:GLU:O | 1:D:565:THR:N | 2.39 | 0.56 |
| 1:A:13:MSE:HE2 | 1:A:26:ILE:CD1 | 2.36 | 0.56 |
| 1:A:369:HIS:HA | 1:A:396:VAL:HG22 | 1.88 | 0.56 |
| 1:B:284:ALA:HB2 | 1:B:311:ASN:OD1 | 2.05 | 0.56 |
| 1:C:29:LYS:O | 1:C:30:LYS:HD2 | 2.05 | 0.56 |
| 1:A:119:PRO:HG2 | 1:A:153:PRO:CB | 2.36 | 0.56 |
| 1:B:183:ASP:OD1 | 1:B:183:ASP:N | 2.38 | 0.56 |
| 1:D:512:ASN:OD1 | 1:D:514:SER:OG | 2.24 | 0.56 |
| 1:A:115:ARG:NH2 | 1:A:145:TRP:O | 2.39 | 0.55 |
| 1:C:586:GLY:N | 1:C:613:ASN:OD1 | 2.38 | 0.55 |
| 1:A:587:MSE:HG2 | 1:A:613:ASN:OD1 | 2.06 | 0.55 |
| 1:B:32:VAL:HG21 | 1:B:95:MSE:CG | 2.37 | 0.55 |
| 1:B:32:VAL:HG22 | 1:B:95:MSE:HG2 | 1.88 | 0.55 |
| 1:C:323:ASN:ND2 | 1:C:356:HIS:ND1 | 2.54 | 0.55 |
| 1:D:390:CYS:HB3 | 1:D:394:LEU:HB2 | 1.87 | 0.55 |
| 1:A:601:ILE:HD11 | 1:B:184:THR:C | 2.27 | 0.55 |
| 1:B:77:ILE:HG23 | 1:B:79:HIS:CE1 | 2.40 | 0.55 |
| 1:D:159:PHE:HD2 | 1:D:220:PHE:CE2 | 2.24 | 0.55 |
| 1:A:284:ALA:HB1 | 1:A:313:SER:HB3 | 1.88 | 0.55 |
| 1:A:471:ARG:HH21 | 1:A:471:ARG:CG | 2.18 | 0.55 |
| 1:C:36:VAL:CG1 | 1:C:37:LYS:H | 2.05 | 0.55 |
| 1:C:270:LEU:HD21 | 1:C:278:LEU:HD12 | 1.88 | 0.55 |
| 1:C:368:VAL:O | 1:C:368:VAL:HG12 | 2.04 | 0.55 |
| 1:B:84:MSE:HE3 | 1:B:103:VAL:HB | 1.87 | 0.55 |
| 1:B:117:ILE:HG22 | 1:B:118:PHE:CD2 | 2.42 | 0.55 |
| 1:B:375:THR:HG23 | 1:B:377:CYS:H | 1.71 | 0.55 |
| 1:D:100:PRO:HD2 | 1:D:101:GLU:H | 1.71 | 0.55 |
| 1:C:84:MSE:HE1 | 1:C:106:VAL:HG11 | 1.88 | 0.55 |
| 1:D:16:ILE:HG23 | 1:D:56:LEU:CD1 | 2.36 | 0.55 |
| 1:B:174:TYR:HD1 | 1:B:175:LYS:N | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:174:TYR:HD1 | 1:C:175:LYS:N | 2.05 | 0.55 |
| 1:C:197:GLN:OE1 | 1:C:226:LYS:N | 2.32 | 0.55 |
| 1:C:561:LYS:O | 1:C:562:ALA:HB3 | 2.07 | 0.55 |
| 1:B:561:LYS:O | 1:B:564:VAL:HG12 | 2.06 | 0.55 |
| 1:D:651:PRO:HG2 | 1:D:652:GLU:H | 1.71 | 0.55 |
| 1:A:32:VAL:HG23 | 1:A:96:LYS:O | 2.05 | 0.55 |
| 1:C:55:LEU:HD11 | 1:C:95:MSE:HE2 | 1.79 | 0.55 |
| 1:C:422:SER:O | 1:C:424:LEU:CD1 | 2.55 | 0.55 |
| 1:C:502:LEU:O | 1:C:506:ILE:HG12 | 2.07 | 0.55 |
| 1:A:218:GLN:HA | 1:A:247:ARG:HG3 | 1.89 | 0.55 |
| 1:A:456:GLY:HA2 | 1:A:489:THR:HG23 | 1.89 | 0.55 |
| 1:A:494:SER:HB2 | 1:A:521:GLY:O | 2.07 | 0.55 |
| 1:C:474:GLY:C | 1:C:476:GLN:H | 2.10 | 0.55 |
| 1:D:408:LYS:CA | 1:D:408:LYS:CE | 2.85 | 0.55 |
| 1:B:88:THR:CG2 | 1:B:91:CYS:CB | 2.86 | 0.54 |
| 1:D:84:MSE:SE | 1:D:107:LEU:HD11 | 2.57 | 0.54 |
| 1:D:99:SER:CB | 1:D:101:GLU:HG3 | 2.36 | 0.54 |
| 1:D:290:ASP:OD2 | 1:D:318:SER:HB3 | 2.08 | 0.54 |
| 1:B:513:ARG:HH11 | 1:B:513:ARG:HA | 1.71 | 0.54 |
| 1:C:14:GLU:OE1 | 1:C:14:GLU:HA | 2.06 | 0.54 |
| 1:C:531:ASN:ND2 | 1:C:531:ASN:H | 2.05 | 0.54 |
| 1:D:34:LEU:CD2 | 1:D:36:VAL:CG2 | 2.85 | 0.54 |
| 1:D:372:LEU:O | 1:D:375:THR:CB | 2.55 | 0.54 |
| 1:B:134:PRO:CD | 1:B:137:ARG:HH21 | 2.19 | 0.54 |
| 1:C:8:VAL:HG11 | 1:C:13:MSE:HE3 | 1.88 | 0.54 |
| 1:C:372:LEU:O | 1:C:375:THR:HB | 2.08 | 0.54 |
| 1:A:174:TYR:C | 1:A:174:TYR:CD1 | 2.81 | 0.54 |
| 1:C:287:SER:O | 1:C:287:SER:OG | 2.26 | 0.54 |
| 1:C:610:TRP:CE3 | 1:C:615:ILE:CD1 | 2.90 | 0.54 |
| 1:D:118:PHE:HD2 | 1:D:126:ILE:HD12 | 1.66 | 0.54 |
| 1:D:603:THR:O | 1:D:603:THR:OG1 | 2.26 | 0.54 |
| 1:A:394:LEU:O | 1:A:425:ALA:HB3 | 2.06 | 0.54 |
| 1:A:471:ARG:NH1 | 1:A:497:GLY:O | 2.41 | 0.54 |
| 1:B:9:PRO:HG2 | 1:B:12:LEU:HB3 | 1.90 | 0.54 |
| 1:B:80:LYS:CG | 1:B:81:PRO:CD | 2.86 | 0.54 |
| 1:D:43:ASN:O | 1:D:44:LYS:HD3 | 2.08 | 0.54 |
| 1:D:408:LYS:HE3 | 1:D:408:LYS:CA | 2.37 | 0.54 |
| 1:A:104:SER:HG | 1:A:137:ARG:HH11 | 1.54 | 0.54 |
| 1:A:478:LEU:HD13 | 1:A:508:TRP:HB2 | 1.90 | 0.54 |
| 1:A:600:GLN:OE1 | 1:B:185:ILE:HD13 | 2.07 | 0.54 |
| 1:B:404:PHE:CE1 | 1:B:440:PRO:HB3 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:212:ALA:HB2 | 1:C:237:GLN:CG | 2.38 | 0.54 |
| 1:C:484:GLU:OE1 | 1:C:508:TRP:HD1 | 1.89 | 0.54 |
| 1:D:314:LYS:N | 1:D:345:SER:O | 2.41 | 0.54 |
| 1:A:98:VAL:CG2 | 1:A:99:SER:N | 2.71 | 0.54 |
| 1:A:200:SER:OG | 1:B:593:LYS:HE2 | 2.08 | 0.54 |
| 1:A:290:ASP:OD1 | 1:A:290:ASP:N | 2.40 | 0.54 |
| 1:B:174:TYR:C | 1:B:174:TYR:HD1 | 2.10 | 0.54 |
| 1:B:415:SER:OG | 3:B:702:CL:CL | 2.60 | 0.54 |
| 1:B:477:VAL:HG23 | 1:B:478:LEU:N | 2.22 | 0.54 |
| 1:C:381:MSE:CE | 1:C:381:MSE:CA | 2.85 | 0.54 |
| 1:D:315:THR:OG1 | 1:D:317:LEU:HD12 | 2.07 | 0.54 |
| 1:D:172:PHE:HE2 | 1:D:208:ILE:HB | 1.72 | 0.54 |
| 1:D:222:LYS:HG3 | 1:D:250:GLU:HB2 | 1.90 | 0.54 |
| 1:D:289:GLU:O | 1:D:293:VAL:HG23 | 2.06 | 0.54 |
| 1:B:24:ILE:CD1 | 1:B:25:LYS:N | 2.68 | 0.54 |
| 1:C:54:PHE:CD1 | 1:C:67:THR:CG2 | 2.91 | 0.54 |
| 1:C:141:LEU:O | 1:C:144:LEU:N | 2.41 | 0.54 |
| 1:C:386:LEU:HD23 | 1:C:390:CYS:SG | 2.47 | 0.54 |
| 1:C:639:PRO:O | 1:C:639:PRO:HG2 | 2.07 | 0.54 |
| 1:A:485:ILE:CG2 | 1:A:512:ASN:HD22 | 1.90 | 0.53 |
| 1:B:607:THR:HB | 1:B:635:PHE:HD2 | 1.73 | 0.53 |
| 1:C:329:LEU:HD23 | 1:C:335:THR:HG21 | 1.91 | 0.53 |
| 1:A:319:PRO:HD2 | 1:A:352:ASP:OD2 | 2.07 | 0.53 |
| 1:C:162:MSE:HE1 | 1:C:217:ASN:HA | 1.91 | 0.53 |
| 1:D:442:LYS:HG3 | 1:D:477:VAL:HG13 | 1.91 | 0.53 |
| 1:D:578:THR:HG22 | 1:D:604:LYS:HD2 | 1.90 | 0.53 |
| 1:A:601:ILE:CD1 | 1:B:184:THR:O | 2.57 | 0.53 |
| 1:B:80:LYS:CD | 1:B:81:PRO:CD | 2.85 | 0.53 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:HA | 2.08 | 0.53 |
| 1:B:506:ILE:CD1 | 1:B:539:LEU:HD13 | 2.38 | 0.53 |
| 1:C:162:MSE:O | 1:C:166:VAL:HG23 | 2.09 | 0.53 |
| 1:D:46:LEU:HD22 | 1:D:95:MSE:HE1 | 1.91 | 0.53 |
| 1:D:610:TRP:HZ3 | 1:D:615:ILE:HD13 | 1.74 | 0.53 |
| 1:A:638:ILE:CG2 | 1:A:640:MSE:CE | 2.85 | 0.53 |
| 1:D:80:LYS:HE2 | 1:D:82:ALA:HB3 | 1.90 | 0.53 |
| 1:D:408:LYS:HA | 1:D:408:LYS:CE | 2.38 | 0.53 |
| 1:A:76:VAL:HG13 | 1:A:86:VAL:CG2 | 2.38 | 0.53 |
| 1:A:474:GLY:O | 1:A:475:ALA:HB3 | 2.07 | 0.53 |
| 1:A:474:GLY:C | 1:A:477:VAL:HG12 | 2.29 | 0.53 |
| 1:B:32:VAL:HG21 | 1:B:95:MSE:CB | 2.36 | 0.53 |
| 1:B:197:GLN:OE1 | 1:B:226:LYS:N | 2.36 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:336:ALA:O | 1:B:366:THR:HG22 | 2.09 | 0.53 |
| 1:D:261:ASP:OD1 | 1:D:262:PHE:N | 2.42 | 0.53 |
| 1:B:484:GLU:OE2 | 1:B:508:TRP:CG | 2.62 | 0.53 |
| 1:D:99:SER:CB | 1:D:100:PRO:CD | 2.87 | 0.53 |
| 1:D:516:GLN:HB2 | 1:D:517:HIS:CD2 | 2.44 | 0.53 |
| 1:A:607:THR:HB | 1:A:635:PHE:HB2 | 1.90 | 0.53 |
| 1:B:16:ILE:O | 1:B:19:VAL:HG12 | 2.09 | 0.53 |
| 1:B:117:ILE:CG2 | 1:B:118:PHE:CD2 | 2.92 | 0.53 |
| 1:C:107:LEU:O | 1:C:108:ALA:C | 2.42 | 0.53 |
| 1:C:498:LEU:HD11 | 1:C:505:LEU:CD1 | 2.39 | 0.53 |
| 1:C:71:LEU:HD12 | 1:C:71:LEU:N | 2.23 | 0.53 |
| 1:C:195:ASN:OD1 | 1:C:197:GLN:HG2 | 2.08 | 0.53 |
| 1:C:466:LEU:HA | 1:C:469:CYS:HB3 | 1.91 | 0.53 |
| 1:D:74:HIS:N | 1:D:87:GLU:O | 2.42 | 0.53 |
| 1:A:543:ILE:HG22 | 1:A:574:ASN:HD22 | 1.74 | 0.53 |
| 1:B:74:HIS:CE1 | 1:B:89:GLU:CB | 2.81 | 0.53 |
| 1:B:77:ILE:O | 1:B:85:VAL:HG12 | 2.09 | 0.53 |
| 1:B:297:SER:HB2 | 1:B:328:SER:HB2 | 1.90 | 0.53 |
| 1:D:68:PHE:CE2 | 1:D:86:VAL:CG1 | 2.91 | 0.53 |
| 1:D:172:PHE:CE2 | 1:D:208:ILE:HB | 2.44 | 0.53 |
| 1:D:256:ALA:N | 1:D:286:ASN:OD1 | 2.42 | 0.53 |
| 1:B:46:LEU:HG | 1:B:55:LEU:HD21 | 1.90 | 0.52 |
| 1:C:116:ARG:HG3 | 1:C:116:ARG:NH1 | 2.24 | 0.52 |
| 1:C:610:TRP:CD1 | 1:C:636:MSE:CE | 2.92 | 0.52 |
| 1:D:51:CYS:C | 1:D:70:TYR:CE2 | 2.82 | 0.52 |
| 1:D:145:TRP:C | 1:D:148:GLN:OE1 | 2.47 | 0.52 |
| 1:A:169:TRP:CZ3 | 1:A:170:LEU:HD21 | 2.44 | 0.52 |
| 1:A:382:VAL:O | 1:A:386:LEU:HG | 2.08 | 0.52 |
| 1:C:456:GLY:HA2 | 1:C:489:THR:CG2 | 2.38 | 0.52 |
| 1:D:72:GLU:OE2 | 1:D:90:LYS:HE3 | 2.09 | 0.52 |
| 1:D:408:LYS:HE2 | 1:D:408:LYS:O | 2.08 | 0.52 |
| 1:A:73:ILE:HD12 | 1:A:127:MSE:HE3 | 1.90 | 0.52 |
| 1:A:368:VAL:O | 1:A:368:VAL:HG12 | 2.09 | 0.52 |
| 1:D:111:GLY:O | 1:D:115:ARG:N | 2.36 | 0.52 |
| 1:D:298:ILE:HG22 | 1:D:299:GLN:HE21 | 1.75 | 0.52 |
| 1:A:602:ASN:HD21 | 1:A:605:LEU:CD2 | 2.23 | 0.52 |
| 1:B:604:LYS:O | 1:B:604:LYS:CG | 2.57 | 0.52 |
| 1:C:411:GLU:O | 1:C:413:PRO:HD3 | 2.10 | 0.52 |
| 1:D:71:LEU:N | 1:D:71:LEU:HD12 | 2.24 | 0.52 |
| 1:A:647:LEU:HD23 | 1:A:651:PRO:HA | 1.92 | 0.52 |
| 1:B:71:LEU:HD21 | 1:B:118:PHE:CZ | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:79:HIS:HA | 1:D:133:GLU:HB2 | 1.91 | 0.52 |
| 1:D:349:LEU:HD13 | 1:D:357:MSE:CE | 2.33 | 0.52 |
| 1:A:480:GLY:N | 1:A:481:CYS:CA | 2.72 | 0.52 |
| 1:A:485:ILE:O | 1:A:512:ASN:ND2 | 2.42 | 0.52 |
| 1:A:558:SER:O | 1:A:559:LYS:HB2 | 2.10 | 0.52 |
| 1:A:640:MSE:HE2 | 1:A:640:MSE:HA | 1.92 | 0.52 |
| 1:B:513:ARG:CG | 1:B:513:ARG:NH1 | 2.72 | 0.52 |
| 1:C:16:ILE:O | 1:C:19:VAL:HG12 | 2.10 | 0.52 |
| 1:C:117:ILE:HG21 | 1:C:118:PHE:CE2 | 2.45 | 0.52 |
| 1:C:155:PRO:HB3 | 1:C:187:LEU:HD13 | 1.91 | 0.52 |
| 1:C:478:LEU:CD1 | 1:C:508:TRP:CZ2 | 2.87 | 0.52 |
| 1:C:556:ALA:HA | 1:C:583:SER:O | 2.09 | 0.52 |
| 1:C:558:SER:HB2 | 1:C:585:ASN:OD1 | 2.09 | 0.52 |
| 1:C:610:TRP:CH2 | 1:C:623:ILE:HG13 | 2.45 | 0.52 |
| 1:D:72:GLU:HG2 | 1:D:89:GLU:CG | 2.40 | 0.52 |
| 1:D:152:GLU:HG2 | 1:D:153:PRO:CD | 2.40 | 0.52 |
| 1:B:195:ASN:OD1 | 1:B:197:GLN:HG2 | 2.10 | 0.52 |
| 1:D:52:ARG:N | 1:D:70:TYR:CE2 | 2.78 | 0.52 |
| 1:D:424:LEU:CD1 | 1:D:424:LEU:N | 2.72 | 0.52 |
| 1:A:330:SER:HB3 | 1:A:363:GLN:OE1 | 2.09 | 0.52 |
| 1:A:380:GLU:OE2 | 1:A:405:SER:OG | 2.28 | 0.52 |
| 1:B:16:ILE:HG23 | 1:B:56:LEU:HD13 | 1.90 | 0.52 |
| 1:B:158:GLY:O | 1:B:162:MSE:HG3 | 2.09 | 0.52 |
| 1:B:158:GLY:O | 1:B:162:MSE:CG | 2.58 | 0.52 |
| 1:C:655:GLU:HA | 1:D:640:MSE:HE1 | 1.91 | 0.52 |
| 1:D:13:MSE:CE | 1:D:26:ILE:CD1 | 2.82 | 0.52 |
| 1:D:85:VAL:HG13 | 1:D:85:VAL:O | 2.09 | 0.52 |
| 1:D:384:SER:HA | 1:D:415:SER:HB3 | 1.92 | 0.52 |
| 1:B:36:VAL:CG1 | 1:B:37:LYS:N | 2.73 | 0.52 |
| 1:C:98:VAL:CG2 | 1:C:102:ASP:OD2 | 2.58 | 0.52 |
| 1:C:441:LEU:HD22 | 1:C:466:LEU:HD22 | 1.92 | 0.52 |
| 1:D:474:GLY:CA | 1:D:475:ALA:CB | 2.85 | 0.52 |
| 1:A:174:TYR:C | 1:A:174:TYR:HD1 | 2.13 | 0.52 |
| 1:C:115:ARG:NH1 | 1:C:145:TRP:O | 2.42 | 0.52 |
| 1:C:645:GLN:OE1 | 1:C:645:GLN:HA | 2.10 | 0.52 |
| 1:D:100:PRO:CG | 1:D:101:GLU:N | 2.73 | 0.52 |
| 1:D:150:LEU:N | 1:D:150:LEU:HD23 | 2.24 | 0.52 |
| 1:D:208:ILE:CG2 | 1:D:237:GLN:HE21 | 2.23 | 0.52 |
| 1:D:397:LEU:HD11 | 1:D:399:LEU:CD1 | 2.40 | 0.52 |
| 1:A:323:ASN:OD1 | 1:A:354:LEU:CA | 2.58 | 0.51 |
| 1:B:36:VAL:HG13 | 1:B:37:LYS:H | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:543:ILE:HG22 | 1:D:574:ASN:HD22 | 1.71 | 0.51 |
| 1:C:169:TRP:CE3 | 1:C:170:LEU:HD21 | 2.45 | 0.51 |
| 1:D:30:LYS:CE | 1:D:102:ASP:OD1 | 2.57 | 0.51 |
| 1:D:54:PHE:CD1 | 1:D:67:THR:HG21 | 2.45 | 0.51 |
| 1:B:16:ILE:HD11 | 1:B:45:VAL:HG21 | 1.92 | 0.51 |
| 1:B:34:LEU:HD12 | 1:B:35:GLU:O | 2.10 | 0.51 |
| 1:B:212:ALA:HB2 | 1:B:237:GLN:HG2 | 1.93 | 0.51 |
| 1:C:8:VAL:HG11 | 1:C:13:MSE:CE | 2.39 | 0.51 |
| 1:C:503:SER:HA | 1:C:506:ILE:CG1 | 2.40 | 0.51 |
| 1:C:513:ARG:HH21 | 1:C:547:ASP:HB3 | 1.76 | 0.51 |
| 1:C:662:GLU:OE1 | 1:D:638:ILE:HD11 | 2.09 | 0.51 |
| 1:A:54:PHE:CD2 | 1:A:67:THR:CG2 | 2.93 | 0.51 |
| 1:D:616:THR:CG2 | 1:D:617:ALA:H | 2.22 | 0.51 |
| 1:A:13:MSE:HE2 | 1:A:29:LYS:HD3 | 1.93 | 0.51 |
| 1:A:270:LEU:HD21 | 1:A:278:LEU:HD12 | 1.93 | 0.51 |
| 1:D:115:ARG:CG | 1:D:115:ARG:NH1 | 2.73 | 0.51 |
| 1:D:355:SER:O | 1:D:359:ASN:HB2 | 2.11 | 0.51 |
| 1:A:138:LEU:HD23 | 1:A:139:ALA:HA | 1.92 | 0.51 |
| 1:A:352:ASP:O | 1:A:354:LEU:HG | 2.10 | 0.51 |
| 1:B:184:THR:O | 1:B:188:THR:OG1 | 2.16 | 0.51 |
| 1:C:174:TYR:C | 1:C:174:TYR:CD1 | 2.84 | 0.51 |
| 1:C:293:VAL:HG21 | 1:C:317:LEU:HD11 | 1.91 | 0.51 |
| 1:C:476:GLN:CA | 1:C:476:GLN:NE2 | 2.73 | 0.51 |
| 1:D:80:LYS:HD2 | 1:D:81:PRO:N | 2.26 | 0.51 |
| 1:D:375:THR:CG2 | 1:D:377:CYS:HB3 | 2.41 | 0.51 |
| 1:A:470:LEU:HD23 | 1:A:477:VAL:HG11 | 1.93 | 0.51 |
| 1:A:478:LEU:HD13 | 1:A:508:TRP:CG | 2.46 | 0.51 |
| 1:A:484:GLU:HG3 | 1:A:508:TRP:CZ2 | 2.45 | 0.51 |
| 1:A:638:ILE:HG23 | 1:A:640:MSE:HE3 | 1.89 | 0.51 |
| 1:C:512:ASN:OD1 | 1:C:514:SER:N | 2.43 | 0.51 |
| 1:D:40:ARG:CG | 1:D:40:ARG:NH2 | 2.72 | 0.51 |
| 1:B:32:VAL:HG21 | 1:B:95:MSE:HG2 | 1.91 | 0.51 |
| 1:B:484:GLU:OE1 | 1:B:512:ASN:HB2 | 2.10 | 0.51 |
| 1:C:144:LEU:O | 1:C:147:SER:OG | 2.28 | 0.51 |
| 1:C:203:GLU:O | 1:C:206:ASP:HB2 | 2.11 | 0.51 |
| 1:C:310:LEU:HD11 | 1:C:312:LEU:HD11 | 1.93 | 0.51 |
| 1:D:72:GLU:CD | 1:D:90:LYS:HE3 | 2.31 | 0.51 |
| 1:D:115:ARG:CB | 1:D:115:ARG:CZ | 2.89 | 0.51 |
| 1:D:507:VAL:CG2 | 1:D:508:TRP:N | 2.73 | 0.51 |
| 1:D:667:ARG:HG3 | 1:D:668:ASN:N | 2.24 | 0.51 |
| 1:C:391:LEU:HD22 | 1:C:422:SER:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:64:LEU:HD21 | 1:D:66:LEU:O | 2.10 | 0.51 |
| 1:C:636:MSE:HB3 | 1:C:665:LEU:CD1 | 2.41 | 0.51 |
| 1:D:99:SER:HB3 | 1:D:100:PRO:CD | 2.40 | 0.51 |
| 1:D:197:GLN:OE1 | 1:D:226:LYS:N | 2.42 | 0.51 |
| 1:D:383:CYS:O | 1:D:384:SER:C | 2.47 | 0.51 |
| 1:D:475:ALA:C | 1:D:476:GLN:HG2 | 2.31 | 0.51 |
| 1:A:23:LYS:N | 1:A:23:LYS:CD | 2.73 | 0.50 |
| 1:A:484:GLU:CD | 1:A:508:TRP:HE1 | 2.11 | 0.50 |
| 1:B:375:THR:HG23 | 1:B:377:CYS:N | 2.27 | 0.50 |
| 1:B:478:LEU:HB2 | 1:B:508:TRP:CD2 | 2.46 | 0.50 |
| 1:B:652:GLU:HG2 | 1:B:653:LYS:H | 1.74 | 0.50 |
| 1:D:506:ILE:CD1 | 1:D:539:LEU:HD13 | 2.41 | 0.50 |
| 1:A:589:ASP:CG | 1:A:616:THR:OG1 | 2.50 | 0.50 |
| 1:B:366:THR:OG1 | 1:B:366:THR:O | 2.26 | 0.50 |
| 1:C:68:PHE:HE1 | 1:C:73:ILE:HD11 | 1.75 | 0.50 |
| 1:B:93:MSE:HG3 | 1:B:95:MSE:HE2 | 1.93 | 0.50 |
| 1:B:222:LYS:HG3 | 1:B:250:GLU:HB2 | 1.93 | 0.50 |
| 1:C:531:ASN:C | 1:C:534:PRO:HD2 | 2.32 | 0.50 |
| 1:A:478:LEU:O | 1:A:480:GLY:N | 2.41 | 0.50 |
| 1:C:258:LEU:HD23 | 1:C:262:PHE:CD2 | 2.45 | 0.50 |
| 1:A:143:ALA:O | 1:A:146:ASP:N | 2.45 | 0.50 |
| 1:B:78:CYS:CB | 1:B:132:MSE:HA | 2.28 | 0.50 |
| 1:C:478:LEU:HD23 | 1:C:508:TRP:CH2 | 2.42 | 0.50 |
| 1:D:68:PHE:CD1 | 1:D:68:PHE:N | 2.80 | 0.50 |
| 1:D:355:SER:HA | 1:D:358:TYR:CD2 | 2.46 | 0.50 |
| 1:D:355:SER:HA | 1:D:358:TYR:HD2 | 1.76 | 0.50 |
| 1:B:561:LYS:HA | 1:B:585:ASN:O | 2.11 | 0.50 |
| 1:C:80:LYS:C | 1:C:80:LYS:HD3 | 2.32 | 0.50 |
| 1:C:115:ARG:HB3 | 1:C:115:ARG:NH2 | 2.17 | 0.50 |
| 1:D:350:ARG:HD3 | 1:D:350:ARG:N | 2.07 | 0.50 |
| 1:A:192:ARG:NH1 | 1:A:219:TRP:CZ3 | 2.80 | 0.50 |
| 1:B:506:ILE:HG23 | 1:B:542:MSE:CE | 2.42 | 0.50 |
| 1:C:498:LEU:CD1 | 1:C:505:LEU:HD12 | 2.41 | 0.50 |
| 1:C:667:ARG:HG3 | 1:C:668:ASN:N | 2.25 | 0.50 |
| 1:D:208:ILE:N | 1:D:209:PRO:HD2 | 2.26 | 0.50 |
| 1:A:23:LYS:N | 1:A:24:ILE:O | 2.45 | 0.50 |
| 1:A:53:ALA:HB3 | 1:A:68:PHE:CE1 | 2.47 | 0.50 |
| 1:A:92:ASN:OD1 | 1:A:92:ASN:N | 2.44 | 0.50 |
| 1:D:115:ARG:NH1 | 1:D:115:ARG:HB2 | 2.27 | 0.50 |
| 1:D:174:TYR:HD1 | 1:D:175:LYS:N | 2.10 | 0.50 |
| 1:A:638:ILE:HD13 | 1:A:640:MSE:HE3 | 1.91 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:7:ASP:O | 1:B:31:LYS:CD | 2.60 | 0.50 |
| 1:B:507:VAL:HG23 | 1:B:508:TRP:N | 2.27 | 0.50 |
| 1:C:86:VAL:HB | 1:C:93:MSE:HG3 | 1.94 | 0.50 |
| 1:C:117:ILE:CG2 | 1:C:118:PHE:CD2 | 2.95 | 0.50 |
| 1:D:55:LEU:O | 1:D:64:LEU:HD23 | 2.12 | 0.50 |
| 1:A:602:ASN:HD21 | 1:A:605:LEU:HD23 | 1.76 | 0.49 |
| 1:D:613:ASN:O | 1:D:614:ASN:HB2 | 2.12 | 0.49 |
| 1:D:631:TYR:O | 1:D:668:ASN:CG | 2.50 | 0.49 |
| 1:B:569:ASN:OD1 | 1:B:594:MSE:HG3 | 2.12 | 0.49 |
| 1:C:372:LEU:O | 1:C:375:THR:CB | 2.60 | 0.49 |
| 1:C:503:SER:O | 1:C:506:ILE:CB | 2.59 | 0.49 |
| 1:C:611:ASP:O | 1:C:612:LYS:HB2 | 2.11 | 0.49 |
| 1:B:52:ARG:CG | 1:B:53:ALA:N | 2.75 | 0.49 |
| 1:B:484:GLU:CB | 1:B:508:TRP:NE1 | 2.73 | 0.49 |
| 1:C:386:LEU:CD2 | 1:C:390:CYS:SG | 3.00 | 0.49 |
| 1:A:73:ILE:HD13 | 1:A:127:MSE:HE1 | 1.94 | 0.49 |
| 1:A:212:ALA:HB2 | 1:A:237:GLN:HG2 | 1.94 | 0.49 |
| 1:A:493:ILE:C | 1:A:496:ASN:ND2 | 2.58 | 0.49 |
| 1:A:506:ILE:CD1 | 1:A:539:LEU:HD13 | 2.43 | 0.49 |
| 1:B:610:TRP:N | 1:B:610:TRP:CD1 | 2.80 | 0.49 |
| 1:C:379:LEU:CD1 | 1:C:402:SER:CB | 2.88 | 0.49 |
| 1:A:602:ASN:ND2 | 1:A:605:LEU:CD2 | 2.76 | 0.49 |
| 1:B:667:ARG:HG3 | 1:B:668:ASN:N | 2.27 | 0.49 |
| 1:C:387:LEU:O | 1:C:387:LEU:HD12 | 2.13 | 0.49 |
| 1:C:536:LEU:CB | 1:C:566:ILE:HD11 | 2.42 | 0.49 |
| 1:D:54:PHE:HD1 | 1:D:64:LEU:HD11 | 1.78 | 0.49 |
| 1:D:323:ASN:ND2 | 1:D:356:HIS:CB | 2.75 | 0.49 |
| 1:A:197:GLN:OE1 | 1:A:226:LYS:N | 2.39 | 0.49 |
| 1:A:506:ILE:HD13 | 1:A:539:LEU:HD13 | 1.95 | 0.49 |
| 1:B:69:SER:O | 1:B:72:GLU:N | 2.46 | 0.49 |
| 1:B:134:PRO:HD2 | 1:B:137:ARG:HD3 | 1.94 | 0.49 |
| 1:B:416:PHE:HE2 | 1:B:440:PRO:O | 1.96 | 0.49 |
| 1:C:282:ASN:C | 1:C:282:ASN:OD1 | 2.51 | 0.49 |
| 1:C:647:LEU:O | 1:C:651:PRO:HB3 | 2.12 | 0.49 |
| 1:D:72:GLU:HG2 | 1:D:89:GLU:HG3 | 1.93 | 0.49 |
| 1:D:231:SER:OG | 1:D:234:VAL:HG23 | 2.12 | 0.49 |
| 1:D:394:LEU:O | 1:D:426:LEU:HD12 | 2.12 | 0.49 |
| 1:B:160:SER:O | 1:B:163:TYR:HB3 | 2.11 | 0.49 |
| 1:C:69:SER:O | 1:C:72:GLU:HB2 | 2.12 | 0.49 |
| 1:C:174:TYR:HD1 | 1:C:174:TYR:C | 2.15 | 0.49 |
| 1:C:604:LYS:O | 1:C:604:LYS:CG | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:159:PHE:HD1 | 1:D:159:PHE:C | 2.16 | 0.49 |
| 1:D:412:VAL:O | 1:D:412:VAL:HG23 | 2.12 | 0.49 |
| 1:D:636:MSE:HB3 | 1:D:665:LEU:HD11 | 1.92 | 0.49 |
| 1:A:12:LEU:O | 1:A:16:ILE:HG13 | 2.11 | 0.49 |
| 1:A:618:GLN:NE2 | 1:A:618:GLN:CA | 2.76 | 0.49 |
| 1:C:379:LEU:HD13 | 1:C:402:SER:HB2 | 1.92 | 0.49 |
| 1:C:16:ILE:HG12 | 1:C:56:LEU:HD13 | 1.94 | 0.49 |
| 1:C:260:ILE:O | 1:C:263:ALA:HB3 | 2.12 | 0.49 |
| 1:C:474:GLY:C | 1:C:476:GLN:N | 2.66 | 0.49 |
| 1:D:97:MSE:HG3 | 1:D:103:VAL:CG2 | 2.43 | 0.49 |
| 1:A:484:GLU:CG | 1:A:508:TRP:CE2 | 2.89 | 0.49 |
| 1:A:640:MSE:CE | 1:A:640:MSE:HA | 2.40 | 0.49 |
| 1:B:290:ASP:N | 1:B:290:ASP:OD1 | 2.43 | 0.49 |
| 1:C:348:ALA:C | 1:C:349:LEU:HD23 | 2.33 | 0.49 |
| 1:C:431:LEU:O | 1:C:434:THR:CG2 | 2.50 | 0.49 |
| 1:D:68:PHE:CZ | 1:D:86:VAL:HG11 | 2.47 | 0.49 |
| 1:D:80:LYS:HG3 | 1:D:83:GLN:H | 1.77 | 0.49 |
| 1:D:145:TRP:N | 1:D:148:GLN:OE1 | 2.46 | 0.49 |
| 1:D:297:SER:HB2 | 1:D:328:SER:HB2 | 1.95 | 0.49 |
| 1:D:303:LEU:HD23 | 1:D:304:PRO:HD2 | 1.95 | 0.49 |
| 1:D:26:ILE:CD1 | 1:D:47:VAL:CG2 | 2.80 | 0.48 |
| 1:A:68:PHE:HD1 | 1:A:93:MSE:HE1 | 1.78 | 0.48 |
| 1:A:174:TYR:HD1 | 1:A:175:LYS:N | 2.11 | 0.48 |
| 1:C:224:SER:HB2 | 1:C:252:VAL:HB | 1.95 | 0.48 |
| 1:C:397:LEU:HD11 | 1:C:399:LEU:HD11 | 1.95 | 0.48 |
| 1:C:647:LEU:CD2 | 1:C:654:THR:HB | 2.43 | 0.48 |
| 1:D:310:LEU:HD11 | 1:D:312:LEU:CD1 | 2.43 | 0.48 |
| 1:B:115:ARG:HH22 | 1:B:150:LEU:HD11 | 1.75 | 0.48 |
| 1:B:124:LEU:HD13 | 1:B:145:TRP:HZ3 | 1.78 | 0.48 |
| 1:B:506:ILE:HG23 | 1:B:542:MSE:HE3 | 1.94 | 0.48 |
| 1:D:354:LEU:O | 1:D:357:MSE:HB3 | 2.13 | 0.48 |
| 1:D:507:VAL:CG2 | 1:D:508:TRP:H | 2.23 | 0.48 |
| 1:A:14:GLU:O | 1:A:16:ILE:N | 2.46 | 0.48 |
| 1:A:80:LYS:HD2 | 1:A:80:LYS:C | 2.33 | 0.48 |
| 1:B:474:GLY:HA2 | 1:B:477:VAL:HG13 | 1.95 | 0.48 |
| 1:C:610:TRP:CZ3 | 1:C:623:ILE:HG13 | 2.48 | 0.48 |
| 1:D:64:LEU:CD2 | 1:D:66:LEU:N | 2.76 | 0.48 |
| 1:D:185:ILE:O | 1:D:189:GLN:HG3 | 2.13 | 0.48 |
| 1:A:12:LEU:HD12 | 1:A:13:MSE:N | 2.28 | 0.48 |
| 1:A:201:HIS:CE1 | 1:B:597:LYS:HE3 | 2.49 | 0.48 |
| 1:B:97:MSE:CG | 1:B:103:VAL:HG12 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:330:SER:HB3 | 1:D:363:GLN:OE1 | 2.14 | 0.48 |
| 1:A:441:LEU:HD22 | 1:A:466:LEU:HD22 | 1.96 | 0.48 |
| 1:B:12:LEU:HD12 | 1:B:12:LEU:O | 2.13 | 0.48 |
| 1:C:638:ILE:HG23 | 1:C:638:ILE:O | 2.13 | 0.48 |
| 1:D:159:PHE:C | 1:D:159:PHE:CD1 | 2.86 | 0.48 |
| 1:D:516:GLN:HB2 | 1:D:517:HIS:HD2 | 1.79 | 0.48 |
| 1:B:254:GLU:O | 1:B:255:ASN:C | 2.51 | 0.48 |
| 1:D:322:VAL:HG21 | 1:D:349:LEU:HD22 | 1.95 | 0.48 |
| 1:D:586:GLY:HA2 | 1:D:614:ASN:ND2 | 2.28 | 0.48 |
| 1:D:73:ILE:CD1 | 1:D:127:MSE:HE2 | 2.43 | 0.48 |
| 1:D:310:LEU:HD11 | 1:D:312:LEU:HD11 | 1.96 | 0.48 |
| 1:D:478:LEU:CB | 1:D:508:TRP:NE1 | 2.73 | 0.48 |
| 1:D:478:LEU:HA | 1:D:508:TRP:CZ2 | 2.49 | 0.48 |
| 1:D:602:ASN:HD21 | 1:D:605:LEU:HD12 | 1.79 | 0.48 |
| 1:C:602:ASN:HD21 | 1:C:605:LEU:CD2 | 2.26 | 0.48 |
| 1:D:79:HIS:O | 1:D:133:GLU:HB3 | 2.13 | 0.48 |
| 1:A:56:LEU:HD23 | 1:A:64:LEU:HA | 1.96 | 0.48 |
| 1:B:528:LYS:O | 1:B:531:ASN:HB2 | 2.14 | 0.48 |
| 1:A:558:SER:HB3 | 1:A:560:LEU:HG | 1.96 | 0.47 |
| 1:B:26:ILE:HG12 | 1:B:26:ILE:O | 2.14 | 0.47 |
| 1:B:118:PHE:CD1 | 1:B:216:TYR:HB2 | 2.49 | 0.47 |
| 1:B:368:VAL:O | 1:B:368:VAL:HG12 | 2.13 | 0.47 |
| 1:C:81:PRO:O | 1:C:100:PRO:HB3 | 2.13 | 0.47 |
| 1:C:375:THR:HG23 | 1:C:377:CYS:HB3 | 1.95 | 0.47 |
| 1:C:449:ALA:CA | 1:C:485:ILE:HG23 | 2.43 | 0.47 |
| 1:D:111:GLY:O | 1:D:115:ARG:CG | 2.61 | 0.47 |
| 1:D:312:LEU:C | 1:D:315:THR:HG23 | 2.34 | 0.47 |
| 1:D:323:ASN:HD21 | 1:D:356:HIS:HB2 | 1.74 | 0.47 |
| 1:D:369:HIS:CD2 | 1:D:396:VAL:HG21 | 2.49 | 0.47 |
| 1:C:212:ALA:HB2 | 1:C:237:GLN:HE21 | 1.79 | 0.47 |
| 1:C:513:ARG:NH2 | 1:C:547:ASP:HB3 | 2.28 | 0.47 |
| 1:C:610:TRP:CZ3 | 1:C:615:ILE:CD1 | 2.97 | 0.47 |
| 1:A:141:LEU:CD2 | 1:A:144:LEU:HD23 | 2.44 | 0.47 |
| 1:A:666:LEU:HD22 | 1:B:666:LEU:HD13 | 1.94 | 0.47 |
| 1:B:474:GLY:O | 1:B:475:ALA:CB | 2.62 | 0.47 |
| 1:B:528:LYS:HE3 | 1:B:529:SER:H | 1.80 | 0.47 |
| 1:B:580:VAL:CG1 | 1:B:608:VAL:HG22 | 2.44 | 0.47 |
| 1:C:68:PHE:HE2 | 1:C:93:MSE:CE | 2.21 | 0.47 |
| 1:D:532:LEU:O | 1:D:532:LEU:HD23 | 2.14 | 0.47 |
| 1:D:100:PRO:CG | 1:D:101:GLU:H | 2.26 | 0.47 |
| 1:D:506:ILE:HG21 | 1:D:538:ASN:CB | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:506:ILE:CG2 | 1:A:542:MSE:HE3 | 2.43 | 0.47 |
| 1:D:616:THR:HG22 | 1:D:617:ALA:H | 1.77 | 0.47 |
| 1:A:103:VAL:CG2 | 1:A:104:SER:N | 2.78 | 0.47 |
| 1:B:36:VAL:HG13 | 1:B:37:LYS:N | 2.30 | 0.47 |
| 1:C:58:ALA:C | 1:C:59:ARG:HG3 | 2.34 | 0.47 |
| 1:C:297:SER:HB2 | 1:C:328:SER:HB2 | 1.95 | 0.47 |
| 1:C:353:ASP:OD1 | 1:C:355:SER:CB | 2.62 | 0.47 |
| 1:C:441:LEU:HD11 | 1:C:445:LEU:CD1 | 2.44 | 0.47 |
| 1:D:152:GLU:HG2 | 1:D:153:PRO:HD3 | 1.97 | 0.47 |
| 1:A:9:PRO:C | 1:A:12:LEU:HG | 2.33 | 0.47 |
| 1:A:383:CYS:HG | 1:A:416:PHE:HD1 | 1.56 | 0.47 |
| 1:B:32:VAL:CG2 | 1:B:95:MSE:CB | 2.92 | 0.47 |
| 1:B:120:GLY:O | 1:B:121:LEU:HD23 | 2.14 | 0.47 |
| 1:C:61:PRO:HG2 | 1:C:61:PRO:O | 2.14 | 0.47 |
| 1:C:157:GLY:O | 1:C:162:MSE:HE3 | 2.14 | 0.47 |
| 1:C:484:GLU:N | 1:C:508:TRP:NE1 | 2.63 | 0.47 |
| 1:D:298:ILE:HG22 | 1:D:299:GLN:N | 2.29 | 0.47 |
| 1:D:384:SER:O | 1:D:387:LEU:HB3 | 2.15 | 0.47 |
| 1:D:414:PRO:O | 1:D:418:GLN:HB2 | 2.14 | 0.47 |
| 1:A:80:LYS:CD | 1:A:81:PRO:N | 2.78 | 0.47 |
| 1:A:195:ASN:OD1 | 1:A:197:GLN:HG2 | 2.14 | 0.47 |
| 1:A:498:LEU:CD1 | 1:A:502:LEU:CD1 | 2.84 | 0.47 |
| 1:B:613:ASN:O | 1:B:614:ASN:HB2 | 2.13 | 0.47 |
| 1:C:634:ARG:O | 1:D:666:LEU:HD11 | 2.14 | 0.47 |
| 1:A:93:MSE:HG3 | 1:A:95:MSE:HE3 | 1.97 | 0.47 |
| 1:A:384:SER:HA | 1:A:415:SER:HB3 | 1.97 | 0.47 |
| 1:B:401:ARG:N | 1:B:434:THR:HG22 | 2.30 | 0.47 |
| 1:B:513:ARG:HA | 1:B:513:ARG:NH1 | 2.30 | 0.47 |
| 1:D:442:LYS:HE2 | 1:D:446:LEU:CD1 | 2.45 | 0.47 |
| 1:A:144:LEU:HD12 | 1:A:144:LEU:O | 2.15 | 0.47 |
| 1:B:10:ARG:O | 1:B:13:MSE:HB2 | 2.15 | 0.47 |
| 1:D:115:ARG:NH1 | 1:D:115:ARG:CB | 2.78 | 0.47 |
| 1:A:14:GLU:O | 1:A:15:SER:C | 2.54 | 0.46 |
| 1:A:69:SER:HB3 | 1:A:169:TRP:CD1 | 2.49 | 0.46 |
| 1:A:643:ALA:O | 1:A:646:ALA:N | 2.48 | 0.46 |
| 1:B:57:SER:HB3 | 1:B:65:GLU:OE2 | 2.15 | 0.46 |
| 1:B:71:LEU:HD11 | 1:B:118:PHE:HZ | 1.80 | 0.46 |
| 1:B:660:LYS:O | 1:B:664:TYR:CD2 | 2.67 | 0.46 |
| 1:C:128:LYS:CD | 1:C:128:LYS:N | 2.78 | 0.46 |
| 1:C:128:LYS:N | 1:C:128:LYS:HD2 | 2.30 | 0.46 |
| 1:C:261:ASP:OD1 | 1:C:262:PHE:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:103:VAL:HG23 | 1:A:104:SER:N | 2.28 | 0.46 |
| 1:A:602:ASN:CG | 1:A:605:LEU:HD23 | 2.35 | 0.46 |
| 1:B:330:SER:HB3 | 1:B:363:GLN:OE1 | 2.14 | 0.46 |
| 1:B:568:ILE:HD11 | 1:B:587:MSE:SE | 2.65 | 0.46 |
| 1:D:78:CYS:HB2 | 1:D:132:MSE:HG2 | 1.97 | 0.46 |
| 1:D:401:ARG:N | 1:D:434:THR:HG22 | 2.31 | 0.46 |
| 1:B:118:PHE:HD1 | 1:B:216:TYR:CB | 2.27 | 0.46 |
| 1:B:226:LYS:O | 1:B:227:ASP:HB2 | 2.14 | 0.46 |
| 1:D:545:ASP:OD1 | 1:D:546:GLU:N | 2.48 | 0.46 |
| 1:A:122:SER:HA | 1:A:123:PRO:HD3 | 1.82 | 0.46 |
| 1:A:427:ILE:O | 1:A:427:ILE:HG12 | 2.14 | 0.46 |
| 1:B:354:LEU:HB3 | 1:B:358:TYR:CD2 | 2.45 | 0.46 |
| 1:D:44:LYS:NZ | 1:D:65:GLU:CD | 2.68 | 0.46 |
| 1:D:100:PRO:CD | 1:D:101:GLU:N | 2.73 | 0.46 |
| 1:D:258:LEU:CD2 | 1:D:262:PHE:HE2 | 1.99 | 0.46 |
| 1:B:610:TRP:HD1 | 1:B:610:TRP:H | 1.63 | 0.46 |
| 1:C:155:PRO:O | 1:C:156:CYS:HB2 | 2.16 | 0.46 |
| 1:C:336:ALA:O | 1:C:366:THR:HG22 | 2.15 | 0.46 |
| 1:D:26:ILE:HB | 1:D:47:VAL:CG2 | 2.46 | 0.46 |
| 1:D:30:LYS:HA | 1:D:30:LYS:HD2 | 1.69 | 0.46 |
| 1:D:100:PRO:HG2 | 1:D:101:GLU:N | 2.30 | 0.46 |
| 1:D:111:GLY:HA2 | 1:D:114:LEU:HB2 | 1.97 | 0.46 |
| 1:D:144:LEU:HA | 1:D:147:SER:OG | 2.15 | 0.46 |
| 1:D:254:GLU:HG3 | 1:D:284:ALA:O | 2.15 | 0.46 |
| 1:D:284:ALA:CB | 1:D:313:SER:HB3 | 2.44 | 0.46 |
| 1:D:325:LEU:CD1 | 1:D:329:LEU:CD1 | 2.93 | 0.46 |
| 1:D:441:LEU:HD11 | 1:D:445:LEU:HD11 | 1.97 | 0.46 |
| 1:B:88:THR:CG2 | 1:B:91:CYS:CA | 2.93 | 0.46 |
| 1:B:117:ILE:HB | 1:B:118:PHE:CD2 | 2.51 | 0.46 |
| 1:C:15:SER:O | 1:C:18:ASP:HB2 | 2.16 | 0.46 |
| 1:C:112:THR:HG23 | 1:C:148:GLN:OE1 | 2.15 | 0.46 |
| 1:C:534:PRO:O | 1:C:537:ASP:HB2 | 2.16 | 0.46 |
| 1:D:599:LEU:HD22 | 1:D:633:LEU:HD22 | 1.97 | 0.46 |
| 1:A:138:LEU:O | 1:A:141:LEU:HB2 | 2.16 | 0.46 |
| 1:B:98:VAL:HG22 | 1:B:102:ASP:OD2 | 2.14 | 0.46 |
| 1:B:207:LEU:HA | 1:B:210:ILE:HD12 | 1.98 | 0.46 |
| 1:C:662:GLU:OE1 | 1:D:638:ILE:CD1 | 2.64 | 0.46 |
| 1:D:12:LEU:HD12 | 1:D:12:LEU:O | 2.16 | 0.46 |
| 1:D:22:ARG:HA | 1:D:22:ARG:HD3 | 1.49 | 0.46 |
| 1:D:27:SER:CB | 1:D:109:HIS:CE1 | 2.98 | 0.46 |
| 1:D:493:ILE:HD11 | 1:D:520:LEU:CD2 | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:575:THR:O | 1:D:604:LYS:HG2 | 2.16 | 0.46 |
| 1:A:441:LEU:HD11 | 1:A:445:LEU:HD11 | 1.97 | 0.46 |
| 1:A:561:LYS:O | 1:A:564:VAL:HG12 | 2.15 | 0.46 |
| 2:B:701:OHB:C | 3:B:702:CL:CL | 3.00 | 0.46 |
| 1:D:437:SER:C | 1:D:440:PRO:HD2 | 2.36 | 0.46 |
| 1:D:516:GLN:CB | 1:D:517:HIS:CD2 | 2.99 | 0.46 |
| 1:D:517:HIS:CD2 | 1:D:517:HIS:N | 2.83 | 0.46 |
| 1:B:375:THR:HG23 | 1:B:377:CYS:HB3 | 1.98 | 0.46 |
| 1:C:477:VAL:CG2 | 1:C:478:LEU:HD23 | 2.46 | 0.46 |
| 1:D:312:LEU:O | 1:D:315:THR:HG23 | 2.15 | 0.46 |
| 1:D:377:CYS:O | 1:D:403:VAL:CG2 | 2.62 | 0.46 |
| 1:D:379:LEU:HB2 | 1:D:404:PHE:HA | 1.97 | 0.46 |
| 1:D:513:ARG:HH21 | 1:D:513:ARG:CG | 2.07 | 0.46 |
| 1:D:563:GLU:C | 1:D:565:THR:N | 2.64 | 0.46 |
| 1:A:74:HIS:CE1 | 1:A:89:GLU:HG2 | 2.51 | 0.46 |
| 1:A:315:THR:OG1 | 1:A:317:LEU:HD13 | 2.15 | 0.46 |
| 1:A:329:LEU:HD23 | 1:A:335:THR:HG21 | 1.97 | 0.46 |
| 1:B:52:ARG:HG2 | 1:B:53:ALA:N | 2.30 | 0.46 |
| 1:B:80:LYS:HE3 | 1:B:81:PRO:CD | 2.34 | 0.46 |
| 1:B:117:ILE:HG22 | 1:B:118:PHE:N | 2.31 | 0.46 |
| 1:B:208:ILE:HG23 | 1:B:237:GLN:HE21 | 1.81 | 0.46 |
| 1:B:260:ILE:HD11 | 1:B:291:ARG:HB3 | 1.98 | 0.46 |
| 1:B:513:ARG:HH11 | 1:B:513:ARG:HG2 | 1.80 | 0.46 |
| 1:C:226:LYS:O | 1:C:227:ASP:HB2 | 2.16 | 0.46 |
| 1:D:77:ILE:HB | 1:D:85:VAL:CG1 | 2.44 | 0.46 |
| 1:D:369:HIS:CD2 | 1:D:396:VAL:CG2 | 2.98 | 0.46 |
| 1:D:503:SER:O | 1:D:504:THR:C | 2.53 | 0.46 |
| 1:A:256:ALA:CB | 1:A:258:LEU:CD1 | 2.93 | 0.45 |
| 1:C:222:LYS:HG3 | 1:C:250:GLU:HB2 | 1.98 | 0.45 |
| 1:D:66:LEU:CD1 | 1:D:93:MSE:HE2 | 2.45 | 0.45 |
| 1:D:323:ASN:CG | 1:D:356:HIS:HB2 | 2.36 | 0.45 |
| 1:D:604:LYS:O | 1:D:604:LYS:CG | 2.58 | 0.45 |
| 1:D:605:LEU:O | 1:D:633:LEU:HD12 | 2.16 | 0.45 |
| 1:A:485:ILE:HG23 | 1:A:485:ILE:O | 2.16 | 0.45 |
| 1:A:528:LYS:HB2 | 1:A:531:ASN:ND2 | 2.31 | 0.45 |
| 1:B:372:LEU:O | 1:B:375:THR:HB | 2.16 | 0.45 |
| 1:D:68:PHE:N | 1:D:68:PHE:HD1 | 2.13 | 0.45 |
| 1:D:205:ARG:O | 1:D:208:ILE:HG13 | 2.16 | 0.45 |
| 1:A:68:PHE:HE2 | 1:A:73:ILE:HD11 | 1.82 | 0.45 |
| 1:C:193:GLU:HG3 | 1:C:222:LYS:CG | 2.46 | 0.45 |
| 1:C:403:VAL:HG23 | 1:C:403:VAL:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:454:LEU:HD13 | 1:C:457:VAL:HG21 | 1.99 | 0.45 |
| 1:D:40:ARG:NH2 | 1:D:40:ARG:HG2 | 2.31 | 0.45 |
| 1:A:543:ILE:CG2 | 1:A:574:ASN:HD22 | 2.28 | 0.45 |
| 1:A:618:GLN:HE21 | 1:A:618:GLN:CA | 2.29 | 0.45 |
| 1:A:620:PHE:CE1 | 1:A:639:PRO:HG3 | 2.52 | 0.45 |
| 1:B:507:VAL:CG2 | 1:B:508:TRP:N | 2.79 | 0.45 |
| 1:C:610:TRP:CZ2 | 1:C:636:MSE:HE2 | 2.46 | 0.45 |
| 1:D:65:GLU:C | 1:D:66:LEU:HG | 2.37 | 0.45 |
| 1:D:172:PHE:CD2 | 1:D:209:PRO:CD | 2.96 | 0.45 |
| 1:D:607:THR:HB | 1:D:635:PHE:HB2 | 1.98 | 0.45 |
| 1:A:32:VAL:CG2 | 1:A:95:MSE:HB3 | 2.45 | 0.45 |
| 1:A:157:GLY:O | 1:A:162:MSE:HE3 | 2.17 | 0.45 |
| 1:A:484:GLU:CG | 1:A:508:TRP:CZ2 | 2.99 | 0.45 |
| 1:C:144:LEU:HA | 1:C:147:SER:OG | 2.17 | 0.45 |
| 1:C:201:HIS:HB2 | 1:D:590:MSE:HE1 | 1.99 | 0.45 |
| 1:C:258:LEU:HD12 | 1:C:258:LEU:N | 2.32 | 0.45 |
| 1:C:650:ASN:C | 1:C:652:GLU:CB | 2.85 | 0.45 |
| 1:D:477:VAL:C | 1:D:478:LEU:CG | 2.85 | 0.45 |
| 1:A:80:LYS:C | 1:A:80:LYS:CD | 2.85 | 0.45 |
| 1:A:137:ARG:HE | 1:A:137:ARG:HB3 | 1.63 | 0.45 |
| 1:B:181:ASP:OD2 | 1:B:185:ILE:HD12 | 2.16 | 0.45 |
| 1:B:329:LEU:HD23 | 1:B:335:THR:HG21 | 1.99 | 0.45 |
| 1:B:527:MSE:CE | 1:B:531:ASN:HB3 | 2.46 | 0.45 |
| 1:B:639:PRO:O | 1:B:639:PRO:HG2 | 2.16 | 0.45 |
| 1:B:652:GLU:CG | 1:B:653:LYS:N | 2.79 | 0.45 |
| 1:C:26:ILE:CG2 | 1:C:47:VAL:HG13 | 2.46 | 0.45 |
| 1:C:461:LEU:C | 1:C:464:CYS:HG | 2.19 | 0.45 |
| 1:A:143:ALA:CA | 1:A:146:ASP:HB2 | 2.45 | 0.45 |
| 1:A:204:HIS:CD2 | 1:A:231:SER:HB3 | 2.52 | 0.45 |
| 1:A:609:ILE:HG13 | 1:A:637:PRO:HG2 | 1.99 | 0.45 |
| 1:B:315:THR:O | 1:B:316:SER:HB2 | 2.17 | 0.45 |
| 1:C:375:THR:HG23 | 1:C:377:CYS:H | 1.82 | 0.45 |
| 1:D:20:ILE:HG13 | 1:D:21:GLY:N | 2.31 | 0.45 |
| 1:D:54:PHE:HA | 1:D:67:THR:HG23 | 1.99 | 0.45 |
| 1:D:71:LEU:HD12 | 1:D:71:LEU:H | 1.81 | 0.45 |
| 1:D:313:SER:O | 1:D:314:LYS:C | 2.53 | 0.45 |
| 1:D:410:LYS:H | 1:D:410:LYS:HG2 | 1.56 | 0.45 |
| 1:A:313:SER:O | 1:A:314:LYS:C | 2.54 | 0.45 |
| 1:A:466:LEU:HA | 1:A:469:CYS:HB3 | 1.99 | 0.45 |
| 1:A:493:ILE:C | 1:A:496:ASN:HD21 | 2.19 | 0.45 |
| 1:A:528:LYS:HD3 | 1:A:528:LYS:HA | 1.61 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:13:MSE:O | 1:C:17:LYS:HG2 | 2.17 | 0.45 |
| 1:C:26:ILE:HG23 | 1:C:47:VAL:HG13 | 1.97 | 0.45 |
| 1:C:117:ILE:HB | 1:C:118:PHE:CE2 | 2.51 | 0.45 |
| 1:C:173:SER:O | 1:C:174:TYR:C | 2.56 | 0.45 |
| 1:C:319:PRO:HB3 | 1:C:354:LEU:HD13 | 1.98 | 0.45 |
| 1:D:34:LEU:CD2 | 1:D:36:VAL:HG23 | 2.47 | 0.45 |
| 1:D:52:ARG:HG3 | 1:D:68:PHE:O | 2.17 | 0.45 |
| 1:D:397:LEU:HD11 | 1:D:399:LEU:CG | 2.47 | 0.45 |
| 1:A:263:ALA:HB3 | 1:A:292:GLY:HA3 | 1.99 | 0.45 |
| 1:B:603:THR:O | 1:B:603:THR:OG1 | 2.34 | 0.45 |
| 1:C:54:PHE:CE1 | 1:C:67:THR:HG21 | 2.52 | 0.45 |
| 1:D:536:LEU:CB | 1:D:566:ILE:HD11 | 2.47 | 0.45 |
| 1:A:545:ASP:OD1 | 1:A:546:GLU:N | 2.50 | 0.45 |
| 1:B:77:ILE:CG2 | 1:B:79:HIS:CE1 | 3.00 | 0.45 |
| 1:B:408:LYS:HE2 | 1:B:408:LYS:HB3 | 1.61 | 0.45 |
| 1:C:288:LEU:H | 1:C:288:LEU:HG | 1.55 | 0.45 |
| 1:C:303:LEU:HD23 | 1:C:304:PRO:HD2 | 1.99 | 0.45 |
| 1:D:171:GLY:C | 1:D:172:PHE:HD1 | 2.20 | 0.45 |
| 1:A:525:ASN:N | 1:A:525:ASN:HD22 | 2.15 | 0.44 |
| 1:B:375:THR:CG2 | 1:B:377:CYS:HB3 | 2.46 | 0.44 |
| 1:C:563:GLU:C | 1:C:565:THR:H | 2.21 | 0.44 |
| 1:D:111:GLY:O | 1:D:115:ARG:HG3 | 2.17 | 0.44 |
| 1:B:115:ARG:NH1 | 1:B:150:LEU:CD1 | 2.79 | 0.44 |
| 1:B:219:TRP:O | 1:B:219:TRP:CG | 2.70 | 0.44 |
| 1:B:323:ASN:ND2 | 1:B:356:HIS:CB | 2.81 | 0.44 |
| 1:B:603:THR:O | 1:B:632:THR:HG21 | 2.17 | 0.44 |
| 1:C:9:PRO:HG2 | 1:C:12:LEU:HB3 | 2.00 | 0.44 |
| 1:C:115:ARG:NH2 | 1:C:115:ARG:CG | 2.73 | 0.44 |
| 1:C:137:ARG:HA | 1:C:140:SER:OG | 2.17 | 0.44 |
| 1:C:286:ASN:O | 1:C:315:THR:HA | 2.17 | 0.44 |
| 1:C:587:MSE:HG2 | 1:C:613:ASN:ND2 | 2.31 | 0.44 |
| 1:D:360:PHE:CD1 | 1:D:360:PHE:O | 2.70 | 0.44 |
| 1:A:13:MSE:CE | 1:A:26:ILE:HD11 | 2.44 | 0.44 |
| 1:B:48:LEU:HB3 | 1:B:70:TYR:OH | 2.18 | 0.44 |
| 1:B:111:GLY:HA3 | 1:B:145:TRP:CZ2 | 2.51 | 0.44 |
| 1:C:395:ALA:O | 1:C:427:ILE:CG2 | 2.63 | 0.44 |
| 1:A:30:LYS:HE2 | 1:A:105:GLU:OE2 | 2.18 | 0.44 |
| 1:A:163:TYR:CE1 | 1:A:167:CYS:SG | 3.10 | 0.44 |
| 1:A:482:ILE:CG2 | 1:A:483:ALA:N | 2.80 | 0.44 |
| 1:A:500:SER:C | 1:A:502:LEU:H | 2.21 | 0.44 |
| 1:B:513:ARG:NH1 | 1:B:513:ARG:HG2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:378:SER:HB2 | 1:C:406:HIS:CD2 | 2.52 | 0.44 |
| 1:D:34:LEU:CD2 | 1:D:42:GLU:CB | 2.85 | 0.44 |
| 1:D:408:LYS:O | 1:D:408:LYS:HD3 | 2.18 | 0.44 |
| 1:A:46:LEU:HD23 | 1:A:55:LEU:CD2 | 2.47 | 0.44 |
| 1:A:80:LYS:HD3 | 1:A:81:PRO:CD | 2.48 | 0.44 |
| 1:A:136:GLU:CD | 1:A:136:GLU:H | 2.19 | 0.44 |
| 1:A:169:TRP:CE3 | 1:A:170:LEU:HD21 | 2.52 | 0.44 |
| 1:C:328:SER:O | 1:C:331:ALA:HB3 | 2.18 | 0.44 |
| 1:D:26:ILE:HB | 1:D:47:VAL:HG23 | 2.00 | 0.44 |
| 1:A:387:LEU:HD21 | 1:A:418:GLN:OE1 | 2.18 | 0.44 |
| 1:C:310:LEU:HD11 | 1:C:312:LEU:CD1 | 2.47 | 0.44 |
| 1:C:375:THR:CG2 | 1:C:377:CYS:HB3 | 2.48 | 0.44 |
| 1:C:387:LEU:HA | 1:C:391:LEU:HD21 | 1.99 | 0.44 |
| 1:D:142:GLN:O | 1:D:146:ASP:CG | 2.56 | 0.44 |
| 1:D:212:ALA:HB2 | 1:D:237:GLN:HG2 | 2.00 | 0.44 |
| 1:D:380:GLU:OE2 | 1:D:405:SER:OG | 2.35 | 0.44 |
| 1:A:456:GLY:HA2 | 1:A:489:THR:CG2 | 2.47 | 0.44 |
| 1:A:509:LEU:O | 1:A:512:ASN:HB3 | 2.18 | 0.44 |
| 1:A:543:ILE:HG23 | 1:A:574:ASN:ND2 | 2.33 | 0.44 |
| 1:B:478:LEU:CB | 1:B:508:TRP:CD2 | 3.01 | 0.44 |
| 1:C:416:PHE:CE1 | 1:C:420:PHE:HE2 | 2.35 | 0.44 |
| 1:C:650:ASN:C | 1:C:652:GLU:HB3 | 2.38 | 0.44 |
| 1:D:605:LEU:O | 1:D:633:LEU:CD1 | 2.66 | 0.44 |
| 1:A:77:ILE:HD12 | 1:A:85:VAL:HG11 | 1.99 | 0.44 |
| 1:A:374:ASN:ND2 | 1:A:401:ARG:NH2 | 2.50 | 0.44 |
| 1:B:64:LEU:HD11 | 1:B:67:THR:HG23 | 1.99 | 0.44 |
| 1:C:189:GLN:O | 1:C:190:ASP:C | 2.53 | 0.44 |
| 1:C:383:CYS:HA | 1:C:386:LEU:HB2 | 2.00 | 0.44 |
| 1:C:470:LEU:HD23 | 1:C:470:LEU:HA | 1.83 | 0.44 |
| 1:C:513:ARG:NH2 | 1:C:547:ASP:CB | 2.81 | 0.44 |
| 1:C:610:TRP:HZ3 | 1:C:615:ILE:HD13 | 1.80 | 0.44 |
| 1:D:73:ILE:HD13 | 1:D:127:MSE:HE2 | 1.99 | 0.44 |
| 1:A:26:ILE:O | 1:A:26:ILE:HG13 | 2.17 | 0.44 |
| 1:A:412:VAL:O | 1:A:412:VAL:HG22 | 2.18 | 0.44 |
| 1:A:471:ARG:HG3 | 1:A:471:ARG:HH21 | 1.82 | 0.44 |
| 1:A:500:SER:C | 1:A:502:LEU:N | 2.71 | 0.44 |
| 1:C:533:THR:N | 1:C:534:PRO:CD | 2.81 | 0.44 |
| 1:D:64:LEU:CD2 | 1:D:64:LEU:C | 2.86 | 0.44 |
| 1:D:80:LYS:HG3 | 1:D:83:GLN:N | 2.33 | 0.44 |
| 1:D:424:LEU:N | 1:D:424:LEU:HD12 | 2.32 | 0.44 |
| 1:B:354:LEU:HB3 | 1:B:358:TYR:CZ | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:97:MSE:HE3 | 1:D:97:MSE:HB3 | 1.78 | 0.43 |
| 1:D:602:ASN:ND2 | 1:D:605:LEU:CD1 | 2.81 | 0.43 |
| 1:A:93:MSE:HG3 | 1:A:95:MSE:CE | 2.47 | 0.43 |
| 1:A:192:ARG:NH1 | 1:A:219:TRP:CE3 | 2.86 | 0.43 |
| 1:A:479:GLU:O | 1:A:481:CYS:HB2 | 2.18 | 0.43 |
| 1:B:602:ASN:ND2 | 1:B:605:LEU:HD22 | 2.33 | 0.43 |
| 1:C:474:GLY:CA | 1:C:476:GLN:HG2 | 2.43 | 0.43 |
| 1:D:460:ASP:OD1 | 1:D:460:ASP:C | 2.57 | 0.43 |
| 1:B:666:LEU:HD12 | 1:B:666:LEU:HA | 1.63 | 0.43 |
| 1:C:124:LEU:HD21 | 1:C:145:TRP:CZ3 | 2.53 | 0.43 |
| 1:C:150:LEU:N | 1:C:150:LEU:HD12 | 2.33 | 0.43 |
| 1:C:536:LEU:HB3 | 1:C:566:ILE:HD11 | 1.99 | 0.43 |
| 1:C:563:GLU:C | 1:C:565:THR:N | 2.72 | 0.43 |
| 1:D:533:THR:HB | 1:D:534:PRO:HD3 | 1.98 | 0.43 |
| 1:A:38:GLY:O | 1:A:39:ASP:C | 2.57 | 0.43 |
| 1:A:479:GLU:C | 1:A:481:CYS:CB | 2.85 | 0.43 |
| 1:A:533:THR:HB | 1:A:534:PRO:HD3 | 2.01 | 0.43 |
| 1:C:136:GLU:O | 1:C:140:SER:OG | 2.36 | 0.43 |
| 1:C:258:LEU:CD1 | 1:C:258:LEU:N | 2.81 | 0.43 |
| 1:C:259:ARG:HA | 1:C:259:ARG:HD3 | 1.80 | 0.43 |
| 1:C:485:ILE:CG2 | 1:C:487:ASN:HB2 | 2.45 | 0.43 |
| 1:C:543:ILE:CG2 | 1:C:574:ASN:HD21 | 2.15 | 0.43 |
| 1:D:40:ARG:HH21 | 1:D:40:ARG:HG3 | 1.82 | 0.43 |
| 1:D:69:SER:O | 1:D:72:GLU:HB2 | 2.18 | 0.43 |
| 1:D:271:ALA:HB2 | 1:D:299:GLN:OE1 | 2.19 | 0.43 |
| 1:A:226:LYS:O | 1:A:227:ASP:HB2 | 2.17 | 0.43 |
| 1:A:452:HIS:CD2 | 1:A:452:HIS:N | 2.84 | 0.43 |
| 1:A:470:LEU:HD22 | 1:A:477:VAL:CG1 | 2.49 | 0.43 |
| 1:B:203:GLU:O | 1:B:206:ASP:HB2 | 2.19 | 0.43 |
| 1:C:8:VAL:CG1 | 1:C:9:PRO:CD | 2.86 | 0.43 |
| 1:D:51:CYS:C | 1:D:70:TYR:CD2 | 2.92 | 0.43 |
| 1:D:77:ILE:HB | 1:D:85:VAL:HG11 | 2.00 | 0.43 |
| 1:D:379:LEU:CD1 | 1:D:402:SER:OG | 2.67 | 0.43 |
| 1:A:273:ASN:OD1 | 1:A:273:ASN:C | 2.57 | 0.43 |
| 1:A:442:LYS:HE2 | 1:A:446:LEU:CD1 | 2.49 | 0.43 |
| 1:B:297:SER:HB2 | 1:B:328:SER:CB | 2.49 | 0.43 |
| 1:C:254:GLU:O | 1:C:255:ASN:C | 2.54 | 0.43 |
| 1:C:376:GLU:HG2 | 1:C:376:GLU:O | 2.19 | 0.43 |
| 1:C:498:LEU:HD12 | 1:C:502:LEU:HD13 | 2.01 | 0.43 |
| 1:D:40:ARG:HH21 | 1:D:40:ARG:HG2 | 1.83 | 0.43 |
| 1:A:14:GLU:C | 1:A:16:ILE:N | 2.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:483:ALA:O | 1:A:484:GLU:CB | 2.66 | 0.43 |
| 1:B:441:LEU:CD1 | 1:B:445:LEU:CD1 | 2.96 | 0.43 |
| 1:B:539:LEU:HA | 1:B:539:LEU:HD12 | 1.81 | 0.43 |
| 1:C:109:HIS:CE1 | 1:C:113:CYS:SG | 3.12 | 0.43 |
| 1:D:16:ILE:CG2 | 1:D:56:LEU:HD13 | 2.46 | 0.43 |
| 1:D:325:LEU:HD11 | 1:D:329:LEU:CD1 | 2.47 | 0.43 |
| 1:D:404:PHE:CZ | 1:D:440:PRO:HB3 | 2.51 | 0.43 |
| 1:A:383:CYS:SG | 1:A:416:PHE:HD1 | 2.41 | 0.43 |
| 1:A:505:LEU:HD13 | 1:A:505:LEU:HA | 1.85 | 0.43 |
| 1:C:375:THR:HG23 | 1:C:377:CYS:N | 2.32 | 0.43 |
| 1:C:638:ILE:HD11 | 1:C:658:LEU:HB3 | 2.01 | 0.43 |
| 1:D:93:MSE:O | 1:D:93:MSE:HG3 | 2.19 | 0.43 |
| 1:D:403:VAL:O | 1:D:403:VAL:HG23 | 2.19 | 0.43 |
| 1:A:613:ASN:O | 1:A:614:ASN:HB2 | 2.17 | 0.43 |
| 1:B:355:SER:O | 1:B:359:ASN:CB | 2.65 | 0.43 |
| 1:B:376:GLU:O | 1:B:376:GLU:HG2 | 2.19 | 0.43 |
| 1:C:560:LEU:H | 1:C:560:LEU:HG | 1.68 | 0.43 |
| 1:C:631:TYR:N | 1:C:631:TYR:CD1 | 2.87 | 0.43 |
| 1:D:46:LEU:CD2 | 1:D:95:MSE:HE1 | 2.49 | 0.43 |
| 1:D:403:VAL:HG21 | 1:D:406:HIS:CE1 | 2.53 | 0.43 |
| 1:A:80:LYS:HD2 | 1:A:82:ALA:H | 1.84 | 0.43 |
| 1:A:84:MSE:HE2 | 1:A:97:MSE:HE1 | 2.00 | 0.43 |
| 1:A:638:ILE:HG23 | 1:A:638:ILE:O | 2.18 | 0.43 |
| 1:B:32:VAL:CG2 | 1:B:95:MSE:CG | 2.95 | 0.43 |
| 1:B:372:LEU:O | 1:B:375:THR:CB | 2.66 | 0.43 |
| 1:C:76:VAL:HG11 | 1:C:107:LEU:HD11 | 2.01 | 0.43 |
| 1:C:256:ALA:CB | 1:C:258:LEU:HD11 | 2.48 | 0.43 |
| 1:D:514:SER:HG | 1:D:515:ILE:N | 2.17 | 0.43 |
| 1:A:9:PRO:HB2 | 1:A:12:LEU:CG | 2.47 | 0.42 |
| 1:A:282:ASN:OD1 | 1:A:282:ASN:C | 2.57 | 0.42 |
| 1:A:347:ASN:ND2 | 1:A:347:ASN:N | 2.67 | 0.42 |
| 1:A:396:VAL:O | 1:A:396:VAL:HG23 | 2.18 | 0.42 |
| 1:B:349:LEU:HD13 | 1:B:357:MSE:SE | 2.69 | 0.42 |
| 1:B:561:LYS:N | 1:B:585:ASN:O | 2.52 | 0.42 |
| 1:C:117:ILE:C | 1:C:118:PHE:CD2 | 2.92 | 0.42 |
| 1:C:212:ALA:HB2 | 1:C:237:GLN:HG2 | 2.01 | 0.42 |
| 1:C:499:GLU:HB3 | 1:C:500:SER:H | 1.67 | 0.42 |
| 1:D:185:ILE:HG22 | 1:D:189:GLN:HE21 | 1.84 | 0.42 |
| 1:A:203:GLU:O | 1:A:206:ASP:HB2 | 2.19 | 0.42 |
| 1:A:476:GLN:CD | 1:A:476:GLN:N | 2.72 | 0.42 |
| 1:A:647:LEU:HD23 | 1:A:647:LEU:HA | 1.77 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:17:LYS:O | 1:C:21:GLY:N | 2.52 | 0.42 |
| 1:C:296:LEU:O | 1:C:299:GLN:N | 2.50 | 0.42 |
| 1:C:297:SER:HB2 | 1:C:328:SER:CB | 2.49 | 0.42 |
| 1:C:602:ASN:CG | 1:C:605:LEU:HD23 | 2.39 | 0.42 |
| 1:D:59:ARG:H | 1:D:59:ARG:HD2 | 1.84 | 0.42 |
| 1:D:651:PRO:CG | 1:D:652:GLU:N | 2.76 | 0.42 |
| 1:A:138:LEU:CD2 | 1:A:139:ALA:N | 2.73 | 0.42 |
| 1:A:569:ASN:OD1 | 1:A:594:MSE:HG3 | 2.19 | 0.42 |
| 1:B:88:THR:HG22 | 1:B:91:CYS:O | 2.19 | 0.42 |
| 1:B:117:ILE:CG2 | 1:B:118:PHE:CE2 | 3.02 | 0.42 |
| 1:B:193:GLU:CG | 1:B:222:LYS:HD3 | 2.50 | 0.42 |
| 1:B:262:PHE:O | 1:B:263:ALA:C | 2.57 | 0.42 |
| 1:B:478:LEU:CB | 1:B:508:TRP:CE3 | 3.01 | 0.42 |
| 1:C:189:GLN:HB2 | 1:C:191:THR:HG23 | 2.00 | 0.42 |
| 1:C:256:ALA:O | 1:C:258:LEU:HD12 | 2.18 | 0.42 |
| 1:C:416:PHE:CE1 | 1:C:420:PHE:CE2 | 3.07 | 0.42 |
| 1:C:602:ASN:ND2 | 1:C:605:LEU:CD2 | 2.81 | 0.42 |
| 1:D:350:ARG:NE | 1:D:350:ARG:O | 2.52 | 0.42 |
| 1:D:602:ASN:HD21 | 1:D:605:LEU:CD1 | 2.31 | 0.42 |
| 1:A:46:LEU:HD23 | 1:A:54:PHE:O | 2.20 | 0.42 |
| 1:A:124:LEU:HD21 | 1:A:145:TRP:HZ3 | 1.83 | 0.42 |
| 1:A:481:CYS:SG | 1:A:481:CYS:O | 2.78 | 0.42 |
| 1:A:652:GLU:CG | 1:A:653:LYS:HG3 | 2.48 | 0.42 |
| 1:B:81:PRO:O | 1:B:100:PRO:HB3 | 2.20 | 0.42 |
| 1:B:516:GLN:HB2 | 1:B:517:HIS:CD2 | 2.54 | 0.42 |
| 1:C:80:LYS:CE | 1:C:82:ALA:H | 2.33 | 0.42 |
| 1:C:540:VAL:O | 1:C:544:GLN:HG2 | 2.18 | 0.42 |
| 1:D:271:ALA:HA | 1:D:299:GLN:OE1 | 2.19 | 0.42 |
| 1:D:368:VAL:O | 1:D:368:VAL:HG12 | 2.18 | 0.42 |
| 1:D:375:THR:HG23 | 1:D:377:CYS:N | 2.35 | 0.42 |
| 1:A:54:PHE:CD1 | 1:A:54:PHE:N | 2.87 | 0.42 |
| 1:A:568:ILE:HD11 | 1:A:587:MSE:SE | 2.70 | 0.42 |
| 1:B:224:SER:HB2 | 1:B:252:VAL:HB | 2.00 | 0.42 |
| 1:B:536:LEU:CB | 1:B:566:ILE:HD11 | 2.50 | 0.42 |
| 1:D:270:LEU:HD21 | 1:D:278:LEU:HD12 | 2.02 | 0.42 |
| 1:D:297:SER:HB2 | 1:D:328:SER:CB | 2.49 | 0.42 |
| 1:D:580:VAL:CG1 | 1:D:605:LEU:CD2 | 2.96 | 0.42 |
| 1:A:73:ILE:HD13 | 1:A:127:MSE:HE3 | 1.87 | 0.42 |
| 1:A:263:ALA:CB | 1:A:292:GLY:CA | 2.97 | 0.42 |
| 1:C:561:LYS:H | 1:C:561:LYS:HG3 | 1.54 | 0.42 |
| 1:D:64:LEU:HD22 | 1:D:66:LEU:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:474:GLY:CA | 1:A:477:VAL:HG11 | 2.26 | 0.42 |
| 1:B:88:THR:CG2 | 1:B:91:CYS:HB3 | 2.49 | 0.42 |
| 1:C:34:LEU:O | 1:C:36:VAL:HG23 | 2.19 | 0.42 |
| 1:C:507:VAL:HA | 1:C:510:SER:OG | 2.20 | 0.42 |
| 1:A:604:LYS:O | 1:A:604:LYS:CG | 2.68 | 0.42 |
| 1:A:620:PHE:HE1 | 1:A:639:PRO:HG3 | 1.84 | 0.42 |
| 1:D:312:LEU:N | 1:D:312:LEU:HD12 | 2.35 | 0.42 |
| 1:D:315:THR:OG1 | 1:D:317:LEU:HD11 | 2.17 | 0.42 |
| 1:D:493:ILE:O | 1:D:496:ASN:ND2 | 2.53 | 0.42 |
| 1:D:543:ILE:HG22 | 1:D:574:ASN:HD21 | 1.77 | 0.42 |
| 1:B:155:PRO:O | 1:B:156:CYS:HB2 | 2.19 | 0.42 |
| 1:D:322:VAL:CG1 | 1:D:357:MSE:CE | 2.76 | 0.42 |
| 1:D:354:LEU:HB2 | 1:D:358:TYR:CZ | 2.55 | 0.42 |
| 1:D:606:ARG:HD3 | 1:D:606:ARG:HA | 1.83 | 0.42 |
| 1:A:75:GLY:H | 1:A:87:GLU:HG3 | 1.85 | 0.42 |
| 1:A:375:THR:HG23 | 1:A:377:CYS:HB3 | 2.02 | 0.42 |
| 1:A:402:SER:H | 1:A:434:THR:HG23 | 1.84 | 0.42 |
| 1:A:568:ILE:CD1 | 1:A:587:MSE:SE | 3.17 | 0.42 |
| 1:B:282:ASN:OD1 | 1:B:282:ASN:C | 2.59 | 0.42 |
| 1:B:477:VAL:CG2 | 1:B:478:LEU:HG | 2.49 | 0.42 |
| 1:C:256:ALA:HB1 | 1:C:258:LEU:HD11 | 2.02 | 0.42 |
| 1:C:529:SER:O | 1:C:533:THR:OG1 | 2.37 | 0.42 |
| 1:D:127:MSE:O | 1:D:128:LYS:HB2 | 2.20 | 0.42 |
| 1:D:311:ASN:OD1 | 1:D:311:ASN:C | 2.57 | 0.42 |
| 1:D:518:LEU:HD21 | 1:D:520:LEU:HD21 | 2.01 | 0.42 |
| 1:A:84:MSE:HB3 | 1:A:97:MSE:HE3 | 2.01 | 0.41 |
| 1:A:136:GLU:O | 1:A:140:SER:OG | 2.38 | 0.41 |
| 1:A:507:VAL:CG2 | 1:A:508:TRP:N | 2.83 | 0.41 |
| 1:A:638:ILE:HG23 | 1:A:640:MSE:HE2 | 2.02 | 0.41 |
| 1:B:30:LYS:HE2 | 1:B:105:GLU:OE2 | 2.19 | 0.41 |
| 1:C:36:VAL:CG1 | 1:C:37:LYS:N | 2.73 | 0.41 |
| 1:D:380:GLU:CD | 1:D:405:SER:OG | 2.58 | 0.41 |
| 1:D:572:GLY:O | 1:D:601:ILE:HG22 | 2.20 | 0.41 |
| 1:A:71:LEU:N | 1:A:71:LEU:HD12 | 2.34 | 0.41 |
| 1:A:374:ASN:CG | 1:A:401:ARG:HH21 | 2.22 | 0.41 |
| 1:B:39:ASP:O | 1:B:41:VAL:HG13 | 2.20 | 0.41 |
| 1:B:117:ILE:HG21 | 1:B:118:PHE:CE2 | 2.54 | 0.41 |
| 1:B:412:VAL:O | 1:B:412:VAL:HG22 | 2.20 | 0.41 |
| 1:C:368:VAL:O | 1:C:368:VAL:CG1 | 2.67 | 0.41 |
| 1:D:122:SER:O | 1:D:125:ARG:HB2 | 2.20 | 0.41 |
| 1:D:560:LEU:HD23 | 1:D:560:LEU:HA | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:345:SER:HB3 | 1:A:371:ASP:OD1 | 2.19 | 0.41 |
| 1:A:476:GLN:NE2 | 1:A:476:GLN:C | 2.73 | 0.41 |
| 1:A:499:GLU:HB3 | 1:A:500:SER:H | 1.59 | 0.41 |
| 1:B:273:ASN:HA | 1:B:274:PRO:HD2 | 1.92 | 0.41 |
| 1:B:545:ASP:OD1 | 1:B:546:GLU:N | 2.53 | 0.41 |
| 1:B:568:ILE:CD1 | 1:B:587:MSE:SE | 3.18 | 0.41 |
| 1:C:35:GLU:C | 1:C:36:VAL:HG23 | 2.40 | 0.41 |
| 1:C:58:ALA:O | 1:C:59:ARG:HG3 | 2.20 | 0.41 |
| 1:C:386:LEU:HD23 | 1:C:386:LEU:HA | 1.71 | 0.41 |
| 1:C:532:LEU:HD22 | 1:C:536:LEU:CD1 | 2.50 | 0.41 |
| 1:D:99:SER:O | 1:D:102:ASP:N | 2.54 | 0.41 |
| 1:A:77:ILE:O | 1:A:85:VAL:CG1 | 2.63 | 0.41 |
| 1:A:350:ARG:HG2 | 1:A:406:HIS:CE1 | 2.56 | 0.41 |
| 1:C:556:ALA:O | 1:C:557:ASP:HB2 | 2.20 | 0.41 |
| 1:D:317:LEU:HB2 | 1:D:347:ASN:HB3 | 2.02 | 0.41 |
| 1:D:565:THR:O | 1:D:565:THR:HG22 | 2.21 | 0.41 |
| 1:A:500:SER:O | 1:A:502:LEU:N | 2.53 | 0.41 |
| 1:B:26:ILE:HB | 1:B:47:VAL:HG12 | 2.01 | 0.41 |
| 1:C:42:GLU:HB2 | 1:C:44:LYS:HE2 | 2.02 | 0.41 |
| 1:C:77:ILE:O | 1:C:85:VAL:HG22 | 2.20 | 0.41 |
| 1:C:169:TRP:CE3 | 1:C:170:LEU:CD2 | 3.03 | 0.41 |
| 1:D:9:PRO:HG2 | 1:D:10:ARG:H | 1.86 | 0.41 |
| 1:D:27:SER:HB2 | 1:D:109:HIS:CE1 | 2.52 | 0.41 |
| 1:D:114:LEU:HD12 | 1:D:114:LEU:HA | 1.76 | 0.41 |
| 1:D:560:LEU:O | 1:D:561:LYS:HB2 | 2.20 | 0.41 |
| 1:C:509:LEU:HD21 | 1:C:518:LEU:CD1 | 2.51 | 0.41 |
| 1:C:593:LYS:HE2 | 1:D:200:SER:OG | 2.21 | 0.41 |
| 1:D:30:LYS:HE3 | 1:D:102:ASP:CG | 2.41 | 0.41 |
| 1:D:75:GLY:HA2 | 1:D:129:LYS:O | 2.21 | 0.41 |
| 1:D:298:ILE:HG22 | 1:D:299:GLN:NE2 | 2.36 | 0.41 |
| 1:D:400:SER:HB3 | 1:D:432:SER:OG | 2.21 | 0.41 |
| 1:A:258:LEU:CD2 | 1:A:262:PHE:CD2 | 2.95 | 0.41 |
| 1:B:441:LEU:HD22 | 1:B:466:LEU:HD22 | 2.01 | 0.41 |
| 1:C:150:LEU:HD12 | 1:C:150:LEU:H | 1.85 | 0.41 |
| 1:C:532:LEU:HD23 | 1:C:536:LEU:HG | 2.02 | 0.41 |
| 1:D:37:LYS:H | 1:D:37:LYS:HD3 | 1.85 | 0.41 |
| 1:D:51:CYS:O | 1:D:70:TYR:CD2 | 2.74 | 0.41 |
| 1:D:172:PHE:HD2 | 1:D:209:PRO:HD3 | 1.79 | 0.41 |
| 1:D:311:ASN:C | 1:D:312:LEU:HD12 | 2.41 | 0.41 |
| 1:D:557:ASP:HA | 1:D:584:GLY:O | 2.21 | 0.41 |
| 1:A:410:LYS:C | 1:A:411:GLU:O | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:602:ASN:OD1 | 1:A:605:LEU:HD23 | 2.20 | 0.41 |
| 1:B:19:VAL:HG13 | 1:B:20:ILE:HG23 | 2.03 | 0.41 |
| 1:B:256:ALA:CB | 1:B:258:LEU:CD1 | 2.98 | 0.41 |
| 1:B:470:LEU:HA | 1:B:470:LEU:HD12 | 1.80 | 0.41 |
| 1:C:10:ARG:O | 1:C:12:LEU:N | 2.54 | 0.41 |
| 1:C:448:LEU:C | 1:C:487:ASN:HD22 | 2.11 | 0.41 |
| 1:C:470:LEU:CD1 | 1:C:505:LEU:HD11 | 2.47 | 0.41 |
| 1:D:68:PHE:CD2 | 1:D:88:THR:HG21 | 2.55 | 0.41 |
| 1:D:539:LEU:HA | 1:D:539:LEU:HD12 | 1.81 | 0.41 |
| 1:A:10:ARG:O | 1:A:13:MSE:N | 2.38 | 0.41 |
| 1:A:217:ASN:OD1 | 1:A:219:TRP:N | 2.46 | 0.41 |
| 1:A:379:LEU:HB2 | 1:A:404:PHE:HA | 2.02 | 0.41 |
| 1:A:492:ASP:HA | 1:A:519:ALA:HB3 | 2.03 | 0.41 |
| 1:B:43:ASN:OD1 | 1:B:43:ASN:N | 2.54 | 0.41 |
| 1:B:65:GLU:H | 1:B:65:GLU:HG2 | 1.63 | 0.41 |
| 1:B:193:GLU:CD | 1:B:222:LYS:HD3 | 2.41 | 0.41 |
| 1:B:374:ASN:HD21 | 1:B:401:ARG:NH1 | 2.19 | 0.41 |
| 1:B:587:MSE:HG2 | 1:B:613:ASN:OD1 | 2.21 | 0.41 |
| 1:C:205:ARG:HB2 | 1:C:205:ARG:HH11 | 1.86 | 0.41 |
| 1:D:141:LEU:HD12 | 1:D:141:LEU:HA | 1.77 | 0.41 |
| 1:D:155:PRO:O | 1:D:156:CYS:HB2 | 2.20 | 0.41 |
| 1:D:254:GLU:O | 1:D:255:ASN:C | 2.58 | 0.41 |
| 1:D:387:LEU:HD23 | 1:D:388:ARG:CZ | 2.51 | 0.41 |
| 1:A:193:GLU:CG | 1:A:222:LYS:HD3 | 2.50 | 0.41 |
| 1:A:533:THR:N | 1:A:534:PRO:CD | 2.83 | 0.41 |
| 1:A:543:ILE:HD13 | 1:A:543:ILE:HG21 | 1.88 | 0.41 |
| 1:B:43:ASN:C | 1:B:44:LYS:HG2 | 2.42 | 0.41 |
| 1:B:138:LEU:HD12 | 1:B:138:LEU:HA | 1.80 | 0.41 |
| 1:B:169:TRP:CZ3 | 1:B:170:LEU:HD21 | 2.56 | 0.41 |
| 1:C:10:ARG:C | 1:C:12:LEU:N | 2.73 | 0.41 |
| 1:C:116:ARG:HH11 | 1:C:116:ARG:CG | 2.34 | 0.41 |
| 1:C:374:ASN:OD1 | 1:C:401:ARG:CD | 2.69 | 0.41 |
| 1:C:524:PHE:CG | 1:C:560:LEU:HD21 | 2.55 | 0.41 |
| 1:C:527:MSE:HE1 | 1:C:532:LEU:HG | 2.01 | 0.41 |
| 1:C:580:VAL:CG1 | 1:C:605:LEU:HD11 | 2.51 | 0.41 |
| 1:D:512:ASN:ND2 | 1:D:514:SER:OG | 2.54 | 0.41 |
| 1:A:32:VAL:CG2 | 1:A:33:LYS:N | 2.84 | 0.40 |
| 1:B:374:ASN:HD21 | 1:B:401:ARG:HH11 | 1.69 | 0.40 |
| 1:D:34:LEU:HG | 1:D:36:VAL:CG2 | 2.51 | 0.40 |
| 1:A:476:GLN:CD | 1:A:476:GLN:H | 2.24 | 0.40 |
| 1:B:378:SER:HB2 | 1:B:406:HIS:CD2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:441:LEU:HD11 | 1:B:445:LEU:CD1 | 2.51 | 0.40 |
| 1:C:97:MSE:HE3 | 1:C:97:MSE:HB3 | 2.01 | 0.40 |
| 1:C:441:LEU:CD1 | 1:C:445:LEU:CD1 | 3.00 | 0.40 |
| 1:C:615:ILE:HG23 | 1:C:619:GLY:HA3 | 2.03 | 0.40 |
| 1:D:270:LEU:HD21 | 1:D:278:LEU:CD1 | 2.51 | 0.40 |
| 1:A:138:LEU:C | 1:A:138:LEU:CD2 | 2.85 | 0.40 |
| 1:A:263:ALA:HB1 | 1:A:292:GLY:CA | 2.51 | 0.40 |
| 1:A:507:VAL:HG23 | 1:A:508:TRP:N | 2.35 | 0.40 |
| 1:B:204:HIS:CD2 | 1:B:231:SER:HB3 | 2.57 | 0.40 |
| 1:B:616:THR:O | 1:B:617:ALA:C | 2.59 | 0.40 |
| 1:C:313:SER:O | 1:C:314:LYS:C | 2.60 | 0.40 |
| 1:C:509:LEU:CD2 | 1:C:518:LEU:HD21 | 2.44 | 0.40 |
| 1:D:157:GLY:O | 1:D:162:MSE:HE3 | 2.20 | 0.40 |
| 1:D:208:ILE:N | 1:D:209:PRO:CD | 2.84 | 0.40 |
| 1:D:359:ASN:O | 1:D:363:GLN:HG3 | 2.21 | 0.40 |
| 1:D:457:VAL:HG12 | 1:D:458:SER:N | 2.37 | 0.40 |
| 1:D:485:ILE:HD13 | 1:D:488:ILE:HD12 | 2.04 | 0.40 |
| 1:A:130:VAL:O | 1:A:130:VAL:HG23 | 2.22 | 0.40 |
| 1:A:484:GLU:HA | 1:A:485:ILE:HA | 1.68 | 0.40 |
| 1:A:638:ILE:CD1 | 1:A:640:MSE:CE | 2.88 | 0.40 |
| 1:B:74:HIS:HE1 | 1:B:89:GLU:HB2 | 1.71 | 0.40 |
| 1:B:258:LEU:CD2 | 1:B:262:PHE:CD2 | 2.99 | 0.40 |
| 1:B:303:LEU:HD23 | 1:B:304:PRO:HD2 | 2.03 | 0.40 |
| 1:B:467:GLY:O | 1:B:471:ARG:HG3 | 2.22 | 0.40 |
| 1:B:509:LEU:O | 1:B:512:ASN:HB3 | 2.21 | 0.40 |
| 1:B:587:MSE:HG2 | 1:B:613:ASN:CG | 2.42 | 0.40 |
| 1:C:121:LEU:HD23 | 1:C:121:LEU:HA | 1.80 | 0.40 |
| 1:C:204:HIS:CE1 | 1:C:234:VAL:HG21 | 2.57 | 0.40 |
| 1:D:383:CYS:HG | 1:D:416:PHE:HE1 | 1.67 | 0.40 |
| 1:D:397:LEU:HD11 | 1:D:399:LEU:HG | 2.03 | 0.40 |
| 1:D:627:MSE:HE1 | 1:D:633:LEU:HB3 | 2.02 | 0.40 |
| 1:A:150:LEU:HD23 | 1:A:150:LEU:HA | 1.86 | 0.40 |
| 1:A:543:ILE:HD11 | 1:A:553:LEU:HD22 | 2.03 | 0.40 |
| 1:B:78:CYS:HB2 | 1:B:132:MSE:CB | 2.51 | 0.40 |
| 1:B:401:ARG:H | 1:B:434:THR:HG22 | 1.87 | 0.40 |
| 1:B:578:THR:HG22 | 1:B:604:LYS:HD2 | 2.02 | 0.40 |
| 1:B:638:ILE:H | 1:B:638:ILE:CD1 | 2.27 | 0.40 |
| 1:C:16:ILE:O | 1:C:19:VAL:CG1 | 2.70 | 0.40 |
| 1:C:379:LEU:CD1 | 1:C:402:SER:HB3 | 2.47 | 0.40 |
| 1:C:477:VAL:HA | 1:C:478:LEU:HA | 1.73 | 0.40 |
| 1:D:505:LEU:HA | 1:D:505:LEU:HD13 | 1.81 | 0.40 |

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:392:GLN:O | 1:C:649:THR:OG1[1_655] | 1.32 | 0.88 |
| 1:C:289:GLU:OE1 | 1:D:513:ARG:CG[1_545] | 1.55 | 0.65 |
| 1:C:289:GLU:OE2 | 1:D:513:ARG:NH2[1_545] | 1.64 | 0.56 |
| 1:A:415:SER:OG | 3:B:702:CL:CL[1_465] | 1.74 | 0.46 |
| 1:B:35:GLU:OE2 | 1:D:476:GLN:NE2[1_545] | 1.90 | 0.30 |

## 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 | 660/669 (99%) | 628 (95%) | 31 (5%) | 1 (0%) | 47 78 |
| 1 | B | 656/669 (98%) | 635 (97%) | 21 (3%) | 0 | 100 100 |
| 1 | C | 652/669 (98%) | 631 (97%) | 20 (3%) | 1 (0%) | 47 78 |
| 1 | D | 651/669 (97%) | 628 (96%) | 23 (4%) | 0 | 100 100 |
| All | All | 2619/2676 (98%) | 2522 (96%) | 95 (4%) | 2 (0%) | 51 82 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 15 | SER |
| 1 | C | 11 | GLU |

### 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 | 585/573 (102%) | 472 (81%) | 113 (19%) | 1 4 |
| 1 | B | 585/573 (102%) | 464 (79%) | 121 (21%) | 1 3 |
| 1 | C | 581/573 (101%) | 460 (79%) | 121 (21%) | 1 3 |
| 1 | D | 580/573 (101%) | 450 (78%) | 130 (22%) | 1 2 |
| All | All | 2331/2292 (102%) | 1846 (79%) | 485 (21%) | 1 3 |

All (485) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 11 | GLU |
| 1 | A | 25 | LYS |
| 1 | A | 29 | LYS |
| 1 | A | 30 | LYS |
| 1 | A | 37 | LYS |
| 1 | A | 39 | ASP |
| 1 | A | 45 | VAL |
| 1 | A | 46 | LEU |
| 1 | A | 50 | SER |
| 1 | A | 51 | CYS |
| 1 | A | 54 | PHE |
| 1 | A | 59 | ARG |
| 1 | A | 64 | LEU |
| 1 | A | 65 | GLU |
| 1 | A | 67 | THR |
| 1 | A | 72 | GLU |
| 1 | A | 76 | VAL |
| 1 | A | 77 | ILE |
| 1 | A | 80 | LYS |
| 1 | A | 89 | GLU |
| 1 | A | 90 | LYS |
| 1 | A | 92 | ASN |
| 1 | A | 93 | MSE |
| 1 | A | 96 | LYS |
| 1 | A | 97 | MSE |
| 1 | A | 105 | GLU |
| 1 | A | 107 | LEU |
| 1 | A | 115 | ARG |
| 1 | A | 125 | ARG |
| 1 | A | 127 | MSE |
| 1 | A | 129 | LYS |
| 1 | A | 131 | SER |
| 1 | A | 133 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 136 | GLU |
| 1 | A | 137 | ARG |
| 1 | A | 138 | LEU |
| 1 | A | 140 | SER |
| 1 | A | 144 | LEU |
| 1 | A | 147 | SER |
| 1 | A | 149 | THR |
| 1 | A | 152 | GLU |
| 1 | A | 168 | ASP |
| 1 | A | 173 | SER |
| 1 | A | 174 | TYR |
| 1 | A | 181 | ASP |
| 1 | A | 197 | GLN |
| 1 | A | 202 | LEU |
| 1 | A | 224 | SER |
| 1 | A | 225 | SER |
| 1 | A | 226 | LYS |
| 1 | A | 229 | LYS |
| 1 | A | 232 | THR |
| 1 | A | 247 | ARG |
| 1 | A | 272 | HIS |
| 1 | A | 275 | ASN |
| 1 | A | 276 | SER |
| 1 | A | 290 | ASP |
| 1 | A | 291 | ARG |
| 1 | A | 296 | LEU |
| 1 | A | 299 | GLN |
| 1 | A | 302 | LYS |
| 1 | A | 303 | LEU |
| 1 | A | 318 | SER |
| 1 | A | 330 | SER |
| 1 | A | 347 | ASN |
| 1 | A | 350 | ARG |
| 1 | A | 352 | ASP |
| 1 | A | 393 | CYS |
| 1 | A | 400 | SER |
| 1 | A | 405 | SER |
| 1 | A | 412 | VAL |
| 1 | A | 426 | LEU |
| 1 | A | 434 | THR |
| 1 | A | 437 | SER |
| 1 | A | 458 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 465 | GLU |
| 1 | A | 476 | GLN |
| 1 | A | 477 | VAL |
| 1 | A | 478 | LEU |
| 1 | A | 482 | ILE |
| 1 | A | 484 | GLU |
| 1 | A | 485 | ILE |
| 1 | A | 490 | SER |
| 1 | A | 493 | ILE |
| 1 | A | 499 | GLU |
| 1 | A | 501 | ASP |
| 1 | A | 505 | LEU |
| 1 | A | 506 | ILE |
| 1 | A | 509 | LEU |
| 1 | A | 510 | SER |
| 1 | A | 522 | LYS |
| 1 | A | 527 | MSE |
| 1 | A | 528 | LYS |
| 1 | A | 530 | LYS |
| 1 | A | 532 | LEU |
| 1 | A | 541 | GLN |
| 1 | A | 550 | LEU |
| 1 | A | 565 | THR |
| 1 | A | 566 | ILE |
| 1 | A | 568 | ILE |
| 1 | A | 573 | SER |
| 1 | A | 580 | VAL |
| 1 | A | 594 | MSE |
| 1 | A | 603 | THR |
| 1 | A | 604 | LYS |
| 1 | A | 606 | ARG |
| 1 | A | 607 | THR |
| 1 | A | 610 | TRP |
| 1 | A | 618 | GLN |
| 1 | A | 640 | MSE |
| 1 | A | 650 | ASN |
| 1 | A | 660 | LYS |
| 1 | A | 667 | ARG |
| 1 | B | 7 | ASP |
| 1 | B | 11 | GLU |
| 1 | B | 22 | ARG |
| 1 | B | 23 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 24 | ILE |
| 1 | B | 26 | ILE |
| 1 | B | 29 | LYS |
| 1 | B | 30 | LYS |
| 1 | B | 31 | LYS |
| 1 | B | 33 | LYS |
| 1 | B | 34 | LEU |
| 1 | B | 35 | GLU |
| 1 | B | 36 | VAL |
| 1 | B | 37 | LYS |
| 1 | B | 42 | GLU |
| 1 | B | 43 | ASN |
| 1 | B | 44 | LYS |
| 1 | B | 46 | LEU |
| 1 | B | 47 | VAL |
| 1 | B | 50 | SER |
| 1 | B | 63 | LYS |
| 1 | B | 66 | LEU |
| 1 | B | 67 | THR |
| 1 | B | 80 | LYS |
| 1 | B | 83 | GLN |
| 1 | B | 87 | GLU |
| 1 | B | 89 | GLU |
| 1 | B | 90 | LYS |
| 1 | B | 91 | CYS |
| 1 | B | 93 | MSE |
| 1 | B | 97 | MSE |
| 1 | B | 101 | GLU |
| 1 | B | 103 | VAL |
| 1 | B | 107 | LEU |
| 1 | B | 121 | LEU |
| 1 | B | 125 | ARG |
| 1 | B | 133 | GLU |
| 1 | B | 136 | GLU |
| 1 | B | 137 | ARG |
| 1 | B | 140 | SER |
| 1 | B | 144 | LEU |
| 1 | B | 160 | SER |
| 1 | B | 162 | MSE |
| 1 | B | 173 | SER |
| 1 | B | 174 | TYR |
| 1 | B | 183 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 184 | THR |
| 1 | B | 187 | LEU |
| 1 | B | 197 | GLN |
| 1 | B | 202 | LEU |
| 1 | B | 224 | SER |
| 1 | B | 225 | SER |
| 1 | B | 226 | LYS |
| 1 | B | 229 | LYS |
| 1 | B | 232 | THR |
| 1 | B | 237 | GLN |
| 1 | B | 246 | ASN |
| 1 | B | 247 | ARG |
| 1 | B | 272 | HIS |
| 1 | B | 275 | ASN |
| 1 | B | 276 | SER |
| 1 | B | 286 | ASN |
| 1 | B | 287 | SER |
| 1 | B | 288 | LEU |
| 1 | B | 290 | ASP |
| 1 | B | 291 | ARG |
| 1 | B | 295 | SER |
| 1 | B | 296 | LEU |
| 1 | B | 298 | ILE |
| 1 | B | 299 | GLN |
| 1 | B | 302 | LYS |
| 1 | B | 318 | SER |
| 1 | B | 330 | SER |
| 1 | B | 350 | ARG |
| 1 | B | 352 | ASP |
| 1 | B | 354 | LEU |
| 1 | B | 355 | SER |
| 1 | B | 388 | ARG |
| 1 | B | 400 | SER |
| 1 | B | 403 | VAL |
| 1 | B | 407 | ARG |
| 1 | B | 412 | VAL |
| 1 | B | 415 | SER |
| 1 | B | 424 | LEU |
| 1 | B | 434 | THR |
| 1 | B | 437 | SER |
| 1 | B | 445 | LEU |
| 1 | B | 455 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 458 | SER |
| 1 | B | 465 | GLU |
| 1 | B | 468 | HIS |
| 1 | B | 469 | CYS |
| 1 | B | 478 | LEU |
| 1 | B | 490 | SER |
| 1 | B | 503 | SER |
| 1 | B | 505 | LEU |
| 1 | B | 506 | ILE |
| 1 | B | 509 | LEU |
| 1 | B | 510 | SER |
| 1 | B | 513 | ARG |
| 1 | B | 522 | LYS |
| 1 | B | 528 | LYS |
| 1 | B | 541 | GLN |
| 1 | B | 550 | LEU |
| 1 | B | 558 | SER |
| 1 | B | 566 | ILE |
| 1 | B | 575 | THR |
| 1 | B | 594 | MSE |
| 1 | B | 603 | THR |
| 1 | B | 604 | LYS |
| 1 | B | 605 | LEU |
| 1 | B | 606 | ARG |
| 1 | B | 607 | THR |
| 1 | B | 610 | TRP |
| 1 | B | 632 | THR |
| 1 | B | 635 | PHE |
| 1 | B | 638 | ILE |
| 1 | B | 652 | GLU |
| 1 | B | 660 | LYS |
| 1 | B | 666 | LEU |
| 1 | B | 667 | ARG |
| 1 | C | 10 | ARG |
| 1 | C | 12 | LEU |
| 1 | C | 17 | LYS |
| 1 | C | 22 | ARG |
| 1 | C | 25 | LYS |
| 1 | C | 29 | LYS |
| 1 | C | 31 | LYS |
| 1 | C | 32 | VAL |
| 1 | C | 34 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 37 | LYS |
| 1 | C | 39 | ASP |
| 1 | C | 46 | LEU |
| 1 | C | 50 | SER |
| 1 | C | 51 | CYS |
| 1 | C | 52 | ARG |
| 1 | C | 55 | LEU |
| 1 | C | 56 | LEU |
| 1 | C | 61 | PRO |
| 1 | C | 64 | LEU |
| 1 | C | 67 | THR |
| 1 | C | 78 | CYS |
| 1 | C | 79 | HIS |
| 1 | C | 80 | LYS |
| 1 | C | 83 | GLN |
| 1 | C | 90 | LYS |
| 1 | C | 93 | MSE |
| 1 | C | 94 | SER |
| 1 | C | 97 | MSE |
| 1 | C | 115 | ARG |
| 1 | C | 129 | LYS |
| 1 | C | 131 | SER |
| 1 | C | 133 | GLU |
| 1 | C | 136 | GLU |
| 1 | C | 140 | SER |
| 1 | C | 144 | LEU |
| 1 | C | 147 | SER |
| 1 | C | 150 | LEU |
| 1 | C | 152 | GLU |
| 1 | C | 168 | ASP |
| 1 | C | 173 | SER |
| 1 | C | 174 | TYR |
| 1 | C | 181 | ASP |
| 1 | C | 184 | THR |
| 1 | C | 188 | THR |
| 1 | C | 194 | LEU |
| 1 | C | 197 | GLN |
| 1 | C | 202 | LEU |
| 1 | C | 205 | ARG |
| 1 | C | 224 | SER |
| 1 | C | 226 | LYS |
| 1 | C | 229 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 232 | THR |
| 1 | C | 247 | ARG |
| 1 | C | 272 | HIS |
| 1 | C | 275 | ASN |
| 1 | C | 276 | SER |
| 1 | C | 287 | SER |
| 1 | C | 288 | LEU |
| 1 | C | 294 | SER |
| 1 | C | 296 | LEU |
| 1 | C | 298 | ILE |
| 1 | C | 302 | LYS |
| 1 | C | 313 | SER |
| 1 | C | 318 | SER |
| 1 | C | 330 | SER |
| 1 | C | 352 | ASP |
| 1 | C | 354 | LEU |
| 1 | C | 381 | MSE |
| 1 | C | 384 | SER |
| 1 | C | 388 | ARG |
| 1 | C | 393 | CYS |
| 1 | C | 396 | VAL |
| 1 | C | 407 | ARG |
| 1 | C | 408 | LYS |
| 1 | C | 411 | GLU |
| 1 | C | 412 | VAL |
| 1 | C | 418 | GLN |
| 1 | C | 421 | SER |
| 1 | C | 422 | SER |
| 1 | C | 426 | LEU |
| 1 | C | 434 | THR |
| 1 | C | 437 | SER |
| 1 | C | 451 | ASN |
| 1 | C | 455 | LYS |
| 1 | C | 458 | SER |
| 1 | C | 465 | GLU |
| 1 | C | 476 | GLN |
| 1 | C | 484 | GLU |
| 1 | C | 486 | HIS |
| 1 | C | 490 | SER |
| 1 | C | 499 | GLU |
| 1 | C | 500 | SER |
| 1 | C | 501 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 503 | SER |
| 1 | C | 505 | LEU |
| 1 | C | 508 | TRP |
| 1 | C | 511 | LYS |
| 1 | C | 513 | ARG |
| 1 | C | 522 | LYS |
| 1 | C | 525 | ASN |
| 1 | C | 527 | MSE |
| 1 | C | 531 | ASN |
| 1 | C | 533 | THR |
| 1 | C | 541 | GLN |
| 1 | C | 550 | LEU |
| 1 | C | 559 | LYS |
| 1 | C | 560 | LEU |
| 1 | C | 561 | LYS |
| 1 | C | 566 | ILE |
| 1 | C | 580 | VAL |
| 1 | C | 594 | MSE |
| 1 | C | 603 | THR |
| 1 | C | 604 | LYS |
| 1 | C | 606 | ARG |
| 1 | C | 607 | THR |
| 1 | C | 610 | TRP |
| 1 | C | 632 | THR |
| 1 | C | 637 | PRO |
| 1 | C | 639 | PRO |
| 1 | C | 660 | LYS |
| 1 | C | 667 | ARG |
| 1 | D | 13 | MSE |
| 1 | D | 17 | LYS |
| 1 | D | 22 | ARG |
| 1 | D | 24 | ILE |
| 1 | D | 26 | ILE |
| 1 | D | 29 | LYS |
| 1 | D | 30 | LYS |
| 1 | D | 31 | LYS |
| 1 | D | 34 | LEU |
| 1 | D | 35 | GLU |
| 1 | D | 37 | LYS |
| 1 | D | 39 | ASP |
| 1 | D | 40 | ARG |
| 1 | D | 47 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 50 | SER |
| 1 | D | 52 | ARG |
| 1 | D | 59 | ARG |
| 1 | D | 62 | SER |
| 1 | D | 65 | GLU |
| 1 | D | 66 | LEU |
| 1 | D | 67 | THR |
| 1 | D | 68 | PHE |
| 1 | D | 77 | ILE |
| 1 | D | 80 | LYS |
| 1 | D | 83 | GLN |
| 1 | D | 89 | GLU |
| 1 | D | 90 | LYS |
| 1 | D | 93 | MSE |
| 1 | D | 95 | MSE |
| 1 | D | 96 | LYS |
| 1 | D | 99 | SER |
| 1 | D | 101 | GLU |
| 1 | D | 104 | SER |
| 1 | D | 114 | LEU |
| 1 | D | 115 | ARG |
| 1 | D | 116 | ARG |
| 1 | D | 118 | PHE |
| 1 | D | 124 | LEU |
| 1 | D | 127 | MSE |
| 1 | D | 136 | GLU |
| 1 | D | 137 | ARG |
| 1 | D | 138 | LEU |
| 1 | D | 140 | SER |
| 1 | D | 146 | ASP |
| 1 | D | 147 | SER |
| 1 | D | 148 | GLN |
| 1 | D | 149 | THR |
| 1 | D | 150 | LEU |
| 1 | D | 152 | GLU |
| 1 | D | 159 | PHE |
| 1 | D | 168 | ASP |
| 1 | D | 173 | SER |
| 1 | D | 174 | TYR |
| 1 | D | 181 | ASP |
| 1 | D | 184 | THR |
| 1 | D | 197 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 202 | LEU |
| 1 | D | 224 | SER |
| 1 | D | 225 | SER |
| 1 | D | 226 | LYS |
| 1 | D | 229 | LYS |
| 1 | D | 232 | THR |
| 1 | D | 237 | GLN |
| 1 | D | 247 | ARG |
| 1 | D | 272 | HIS |
| 1 | D | 275 | ASN |
| 1 | D | 286 | ASN |
| 1 | D | 288 | LEU |
| 1 | D | 291 | ARG |
| 1 | D | 296 | LEU |
| 1 | D | 298 | ILE |
| 1 | D | 299 | GLN |
| 1 | D | 302 | LYS |
| 1 | D | 318 | SER |
| 1 | D | 323 | ASN |
| 1 | D | 330 | SER |
| 1 | D | 347 | ASN |
| 1 | D | 349 | LEU |
| 1 | D | 350 | ARG |
| 1 | D | 353 | ASP |
| 1 | D | 354 | LEU |
| 1 | D | 356 | HIS |
| 1 | D | 359 | ASN |
| 1 | D | 381 | MSE |
| 1 | D | 384 | SER |
| 1 | D | 388 | ARG |
| 1 | D | 396 | VAL |
| 1 | D | 397 | LEU |
| 1 | D | 400 | SER |
| 1 | D | 405 | SER |
| 1 | D | 407 | ARG |
| 1 | D | 408 | LYS |
| 1 | D | 410 | LYS |
| 1 | D | 427 | ILE |
| 1 | D | 428 | GLN |
| 1 | D | 434 | THR |
| 1 | D | 437 | SER |
| 1 | D | 455 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 458 | SER |
| 1 | D | 469 | CYS |
| 1 | D | 470 | LEU |
| 1 | D | 471 | ARG |
| 1 | D | 472 | SER |
| 1 | D | 476 | GLN |
| 1 | D | 477 | VAL |
| 1 | D | 478 | LEU |
| 1 | D | 484 | GLU |
| 1 | D | 490 | SER |
| 1 | D | 493 | ILE |
| 1 | D | 505 | LEU |
| 1 | D | 509 | LEU |
| 1 | D | 513 | ARG |
| 1 | D | 522 | LYS |
| 1 | D | 525 | ASN |
| 1 | D | 532 | LEU |
| 1 | D | 541 | GLN |
| 1 | D | 550 | LEU |
| 1 | D | 566 | ILE |
| 1 | D | 580 | VAL |
| 1 | D | 594 | MSE |
| 1 | D | 603 | THR |
| 1 | D | 604 | LYS |
| 1 | D | 605 | LEU |
| 1 | D | 606 | ARG |
| 1 | D | 607 | THR |
| 1 | D | 638 | ILE |
| 1 | D | 640 | MSE |
| 1 | D | 652 | GLU |
| 1 | D | 660 | LYS |
| 1 | D | 667 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 74 | HIS |
| 1 | A | 369 | HIS |
| 1 | A | 452 | HIS |
| 1 | A | 463 | ASN |
| 1 | A | 476 | GLN |
| 1 | A | 512 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 525 | ASN |
| 1 | A | 618 | GLN |
| 1 | A | 650 | ASN |
| 1 | B | 79 | HIS |
| 1 | B | 83 | GLN |
| 1 | B | 148 | GLN |
| 1 | B | 201 | HIS |
| 1 | B | 323 | ASN |
| 1 | B | 486 | HIS |
| 1 | B | 525 | ASN |
| 1 | B | 645 | GLN |
| 1 | C | 109 | HIS |
| 1 | C | 189 | GLN |
| 1 | C | 246 | ASN |
| 1 | C | 323 | ASN |
| 1 | C | 369 | HIS |
| 1 | C | 406 | HIS |
| 1 | C | 476 | GLN |
| 1 | D | 109 | HIS |
| 1 | D | 189 | GLN |
| 1 | D | 237 | GLN |
| 1 | D | 323 | ASN |
| 1 | D | 369 | HIS |
| 1 | D | 406 | HIS |
| 1 | D | 512 | ASN |
| 1 | D | 517 | HIS |
| 1 | D | 614 | ASN |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | OHB | B | 701 | - | 10,10,10 | 1.85 | 1 (10%) | 13,13,13 | 2.32 | 2 (15%) |
| 4 | ABU | C | 701 | - | 6,6,6 | 1.28 | 2 (33%) | 6,6,6 | 2.42 | 4 (66%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | OHB | B | 701 | - | - | 1/4/4/4 | 0/1/1/1 |
| 4 | ABU | C | 701 | - | - | 1/4/4/4 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 701 | OHB | C-N | 5.39 | 1.43 | 1.33 |
| 4 | C | 701 | ABU | CG-C | 2.18 | 1.55 | 1.50 |
| 4 | C | 701 | ABU | O-C | 2.16 | 1.29 | 1.22 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 701 | OHB | C6-C1-C | 7.00 | 123.62 | 119.18 |
| 4 | C | 701 | ABU | CB-CG-C | 4.10 | 124.81 | 114.47 |
| 2 | B | 701 | OHB | O-C-C1 | 2.73 | 123.46 | 120.24 |
| 4 | C | 701 | ABU | CD-CB-CG | 2.51 | 120.29 | 112.84 |
| 4 | C | 701 | ABU | OXT-C-O | -2.49 | 117.09 | 123.30 |
| 4 | C | 701 | ABU | OXT-C-CG | 2.01 | 120.48 | 114.03 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | C | 701 | ABU | CD-CB-CG-C |
| 2 | B | 701 | OHB | N-C-C1-C2 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 701 | OHB | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 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 | 642/669 (95%) | -0.29 | 14 (2%) | 62 | 59 | 8, 38, 107, 159 | 0 |
| 1 | B | 642/669 (95%) | -0.22 | 18 (2%) | 53 | 49 | 8, 41, 113, 176 | 0 |
| 1 | C | 638/669 (95%) | -0.36 | 6 (0%) | 84 | 84 | 13, 43, 89, 142 | 0 |
| 1 | D | 637/669 (95%) | 0.14 | 44 (6%) | 16 | 13 | 20, 52, 120, 175 | 0 |
| All | All | 2559/2676 (95%) | -0.18 | 82 (3%) | 47 | 43 | 8, 45, 109, 176 | 0 |

All (82) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 8 | VAL | 5.8 |
| 1 | D | 140 | SER | 5.7 |
| 1 | D | 131 | SER | 5.2 |
| 1 | D | 143 | ALA | 5.0 |
| 1 | D | 61 | PRO | 4.9 |
| 1 | A | 352 | ASP | 4.4 |
| 1 | D | 22 | ARG | 4.2 |
| 1 | D | 37 | LYS | 4.1 |
| 1 | D | 136 | GLU | 4.1 |
| 1 | A | 12 | LEU | 4.1 |
| 1 | D | 60 | ILE | 4.0 |
| 1 | A | 9 | PRO | 4.0 |
| 1 | B | 100 | PRO | 3.8 |
| 1 | D | 139 | ALA | 3.7 |
| 1 | C | 476 | GLN | 3.7 |
| 1 | D | 150 | LEU | 3.7 |
| 1 | A | 481 | CYS | 3.7 |
| 1 | C | 485 | ILE | 3.6 |
| 1 | D | 21 | GLY | 3.6 |
| 1 | B | 484 | GLU | 3.5 |
| 1 | B | 130 | VAL | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 76 | VAL | 3.4 |
| 1 | D | 85 | VAL | 3.4 |
| 1 | D | 11 | GLU | 3.4 |
| 1 | B | 7 | ASP | 3.3 |
| 1 | B | 38 | GLY | 3.2 |
| 1 | D | 138 | LEU | 3.2 |
| 1 | A | 23 | LYS | 3.2 |
| 1 | D | 27 | SER | 3.2 |
| 1 | B | 37 | LYS | 3.1 |
| 1 | A | 16 | ILE | 3.0 |
| 1 | D | 24 | ILE | 2.9 |
| 1 | D | 16 | ILE | 2.8 |
| 1 | C | 500 | SER | 2.8 |
| 1 | D | 9 | PRO | 2.8 |
| 1 | D | 36 | VAL | 2.7 |
| 1 | D | 149 | THR | 2.7 |
| 1 | A | 149 | THR | 2.7 |
| 1 | A | 475 | ALA | 2.7 |
| 1 | B | 98 | VAL | 2.7 |
| 1 | A | 151 | ALA | 2.7 |
| 1 | D | 409 | GLY | 2.7 |
| 1 | B | 5 | SER | 2.7 |
| 1 | D | 81 | PRO | 2.6 |
| 1 | D | 94 | SER | 2.6 |
| 1 | D | 65 | GLU | 2.6 |
| 1 | D | 58 | ALA | 2.6 |
| 1 | D | 12 | LEU | 2.6 |
| 1 | B | 4 | GLU | 2.5 |
| 1 | A | 21 | GLY | 2.5 |
| 1 | D | 38 | GLY | 2.4 |
| 1 | D | 41 | VAL | 2.4 |
| 1 | D | 147 | SER | 2.4 |
| 1 | C | 475 | ALA | 2.4 |
| 1 | A | 29 | LYS | 2.4 |
| 1 | B | 146 | ASP | 2.3 |
| 1 | D | 98 | VAL | 2.3 |
| 1 | D | 130 | VAL | 2.3 |
| 1 | B | 180 | TRP | 2.3 |
| 1 | A | 106 | VAL | 2.2 |
| 1 | D | 29 | LYS | 2.2 |
| 1 | D | 15 | SER | 2.2 |
| 1 | D | 57 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 112 | THR | 2.2 |
| 1 | B | 475 | ALA | 2.2 |
| 1 | C | 509 | LEU | 2.2 |
| 1 | A | 120 | GLY | 2.2 |
| 1 | B | 508 | TRP | 2.2 |
| 1 | D | 99 | SER | 2.2 |
| 1 | B | 116 | ARG | 2.2 |
| 1 | A | 11 | GLU | 2.2 |
| 1 | D | 123 | PRO | 2.1 |
| 1 | B | 147 | SER | 2.1 |
| 1 | D | 135 | SER | 2.1 |
| 1 | D | 148 | GLN | 2.1 |
| 1 | C | 484 | GLU | 2.1 |
| 1 | D | 77 | ILE | 2.1 |
| 1 | B | 144 | LEU | 2.1 |
| 1 | D | 108 | ALA | 2.1 |
| 1 | D | 28 | VAL | 2.1 |
| 1 | D | 145 | TRP | 2.0 |
| 1 | D | 106 | VAL | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | ABU | C | 701 | 7/7 | 0.89 | 0.27 | 31,54,83,85 | 0 |
| 2 | OHB | B | 701 | 10/10 | 0.95 | 0.20 | 10,42,92,98 | 0 |
| 3 | CL | B | 702 | 1/1 | 0.98 | 0.14 | 2,2,2,2 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.