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

Jan 31, 2016 – 09:53 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1R0B |
| Title | : | Aspartate Transcarbamylase (ATCase) of Escherichia coli: A New Crystalline R State Bound to PALA, or to Product Analogues Phosphate and Citrate |
| Authors | : | Huang, J.; Lipscomb, W.N. |
| Deposited on | : | 2003-09-19 |
| 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

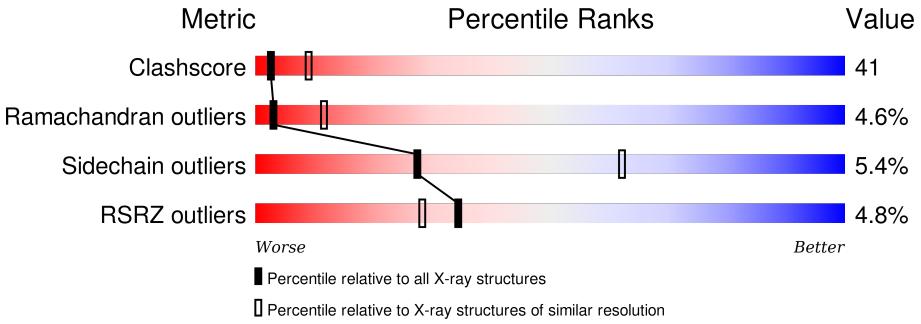
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)) |
|---|---|---|
| Clashscore | 102246 | 1668 (2.90-2.90) |
| Ramachandran outliers | 100387 | 1630 (2.90-2.90) |
| Sidechain outliers | 100360 | 1632 (2.90-2.90) |
| RSRZ outliers | 91569 | 1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 310 | 52% 43% 5% |
| 1 | B | 310 | % 50% 45% |
| 1 | C | 310 | 50% 43% 7% |
| 1 | D | 310 | % 50% 45% |
| 1 | E | 310 | % 53% 43% |
| 1 | F | 310 | 2% 49% 46% |
| 2 | G | 153 | 14% 21% 69% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | H | 153 | 6% 28% 60% 11% |
| 2 | I | 153 | 15% 27% 66% 6% |
| 2 | J | 153 | 10% 33% 58% 9% |
| 2 | K | 153 | 8% 29% 61% 9% |
| 2 | L | 153 | 22% 29% 58% 12% |

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 | FLC | A | 2001 | - | - | X | - |
| 3 | FLC | B | 2002 | - | - | X | - |
| 3 | FLC | C | 2003 | - | - | X | - |
| 3 | FLC | D | 2004 | - | - | X | - |
| 3 | FLC | E | 2005 | - | - | X | - |
| 5 | PO4 | A | 3001 | - | - | X | - |
| 5 | PO4 | F | 3006 | - | - | X | - |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22698 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.

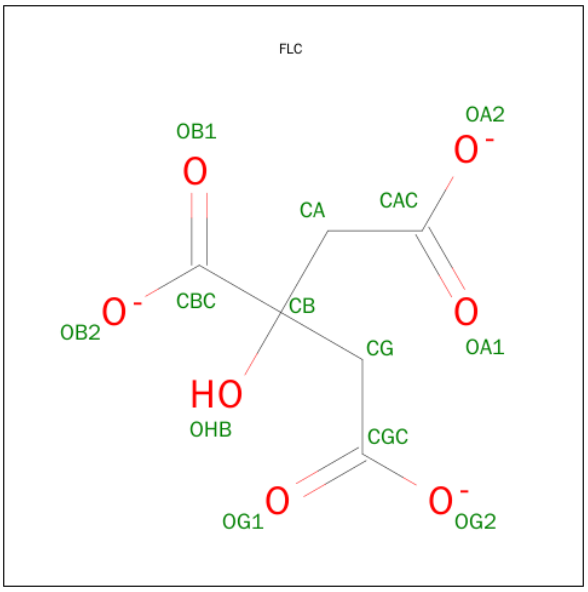
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |
| 1 | B | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |
| 1 | C | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |
| 1 | D | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |
| 1 | E | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |
| 1 | F | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2415 | 1527 | 423 | 456 | 9 | | | |

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | G | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |
| 2 | H | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |
| 2 | I | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |
| 2 | J | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |
| 2 | K | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |
| 2 | L | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1201 | 752 | 213 | 230 | 6 | | | |

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

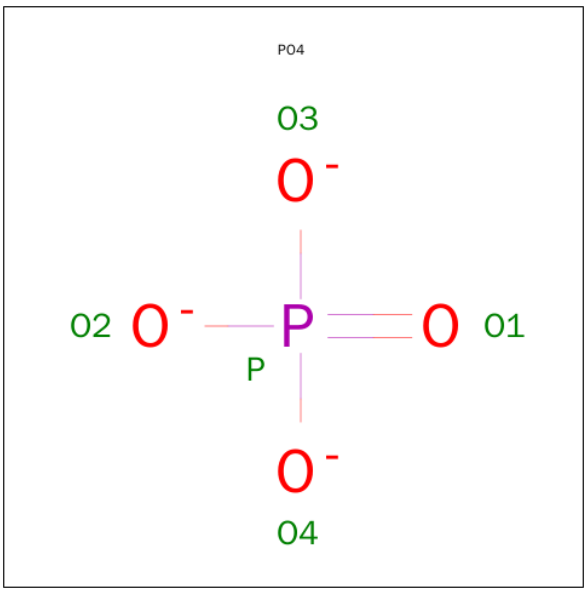



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C O<br>13 6 7 | 0 | 0 |
| 3 | B | 1 | Total C O<br>13 6 7 | 0 | 0 |
| 3 | C | 1 | Total C O<br>13 6 7 | 0 | 0 |
| 3 | D | 1 | Total C O<br>13 6 7 | 0 | 0 |
| 3 | E | 1 | Total C O<br>13 6 7 | 0 | 0 |
| 3 | F | 1 | Total C O<br>13 6 7 | 0 | 0 |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | G | 1 | Total Zn<br>1 1 | 0 | 0 |
| 4 | J | 1 | Total Zn<br>1 1 | 0 | 0 |
| 4 | K | 1 | Total Zn<br>1 1 | 0 | 0 |
| 4 | H | 1 | Total Zn<br>1 1 | 0 | 0 |
| 4 | I | 1 | Total Zn<br>1 1 | 0 | 0 |
| 4 | L | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: $O_4P$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 1 | Total O P<br>5 4 1 | 0 | 0 |
| 5 | B | 1 | Total O P<br>5 4 1 | 0 | 0 |
| 5 | C | 1 | Total O P<br>5 4 1 | 0 | 0 |
| 5 | D | 1 | Total O P<br>5 4 1 | 0 | 0 |
| 5 | E | 1 | Total O P<br>5 4 1 | 0 | 0 |
| 5 | F | 1 | Total O P<br>5 4 1 | 0 | 0 |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | A | 84 | Total O<br>84 84 | 0 | 0 |
| 6 | B | 95 | Total O<br>95 95 | 0 | 0 |
| 6 | C | 113 | Total O<br>113 113 | 0 | 0 |
| 6 | D | 102 | Total O<br>102 102 | 0 | 0 |
| 6 | E | 86 | Total O<br>86 86 | 0 | 0 |

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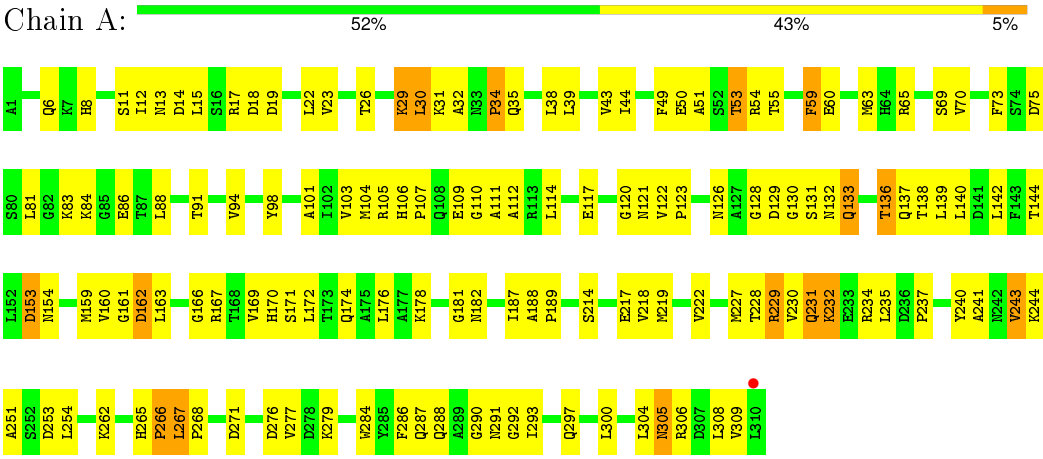
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | F | 82 | Total O<br>82 82 | 0 | 0 |
| 6 | G | 65 | Total O<br>65 65 | 0 | 0 |
| 6 | H | 59 | Total O<br>59 59 | 0 | 0 |
| 6 | I | 45 | Total O<br>45 45 | 0 | 0 |
| 6 | J | 51 | Total O<br>51 51 | 0 | 0 |
| 6 | K | 51 | Total O<br>51 51 | 0 | 0 |
| 6 | L | 55 | Total O<br>55 55 | 0 | 0 |

# 3 Residue-property plots (i)

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

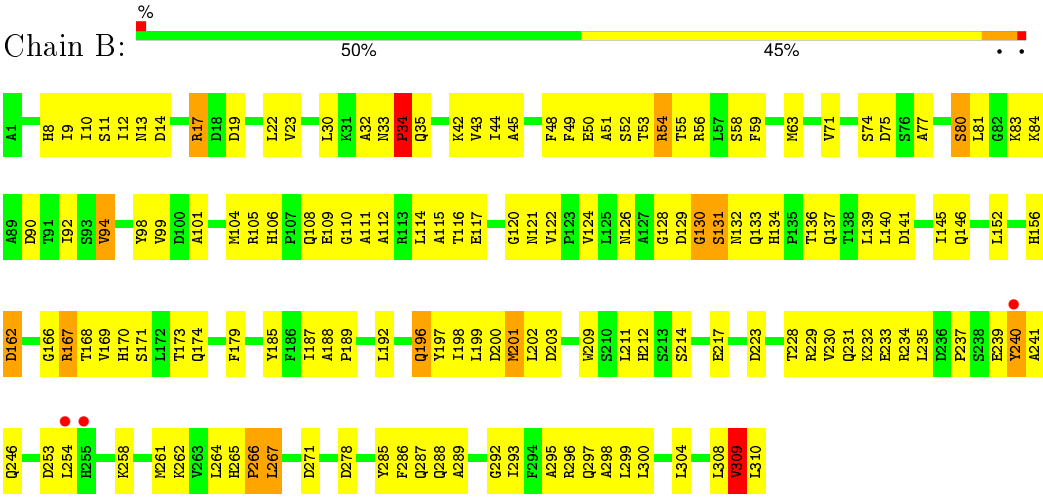
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A:



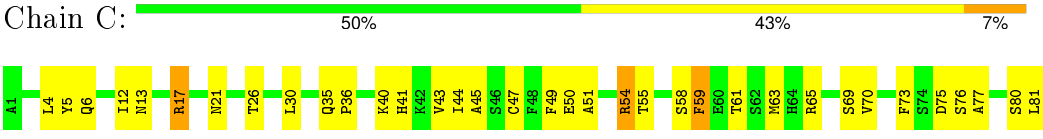

- Molecule 1: Aspartate carbamoyltransferase catalytic chain

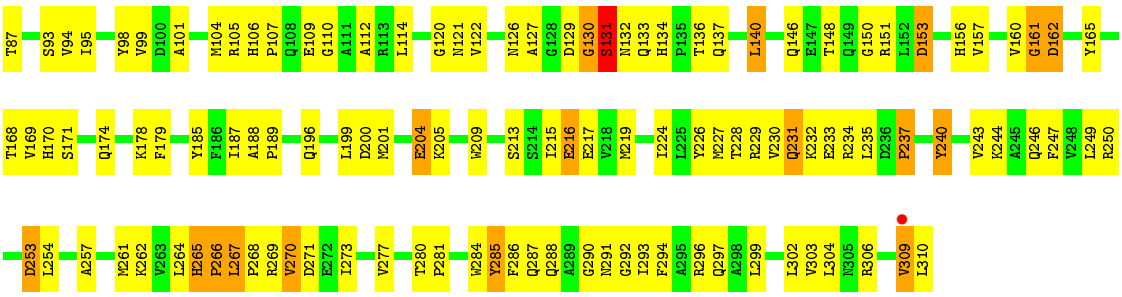
Chain B:




- Molecule 1: Aspartate carbamoyltransferase catalytic chain

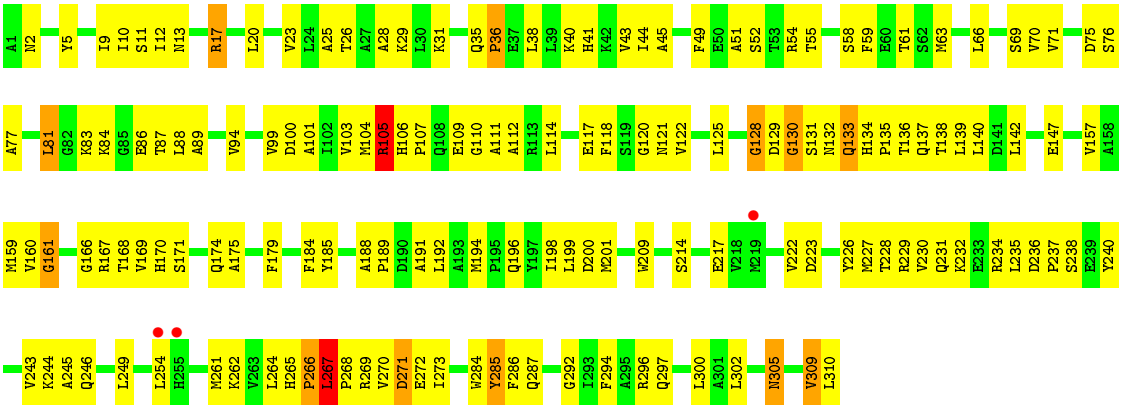
Chain C:





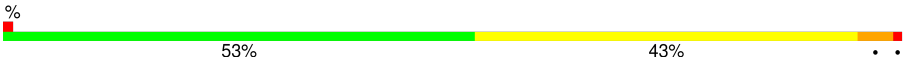
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

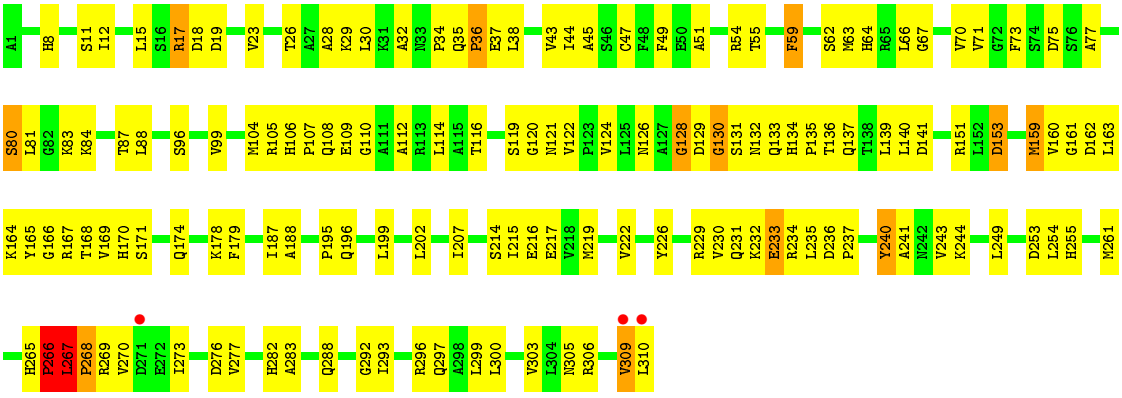
Chain D:

• Molecule 1: Aspartate carbamoyltransferase catalytic chain

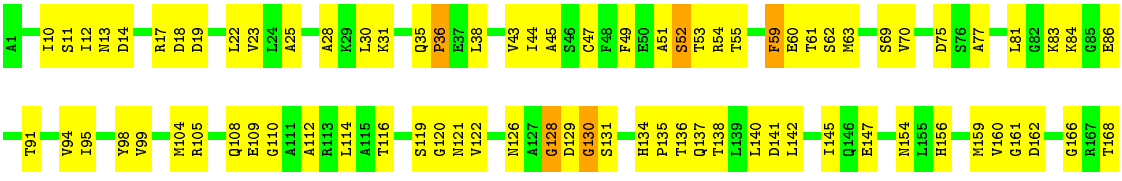
Chain E:

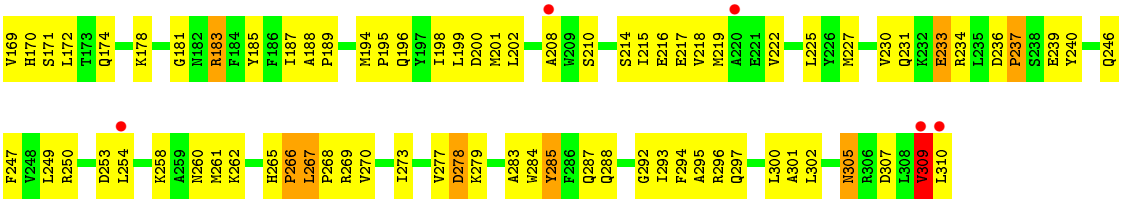


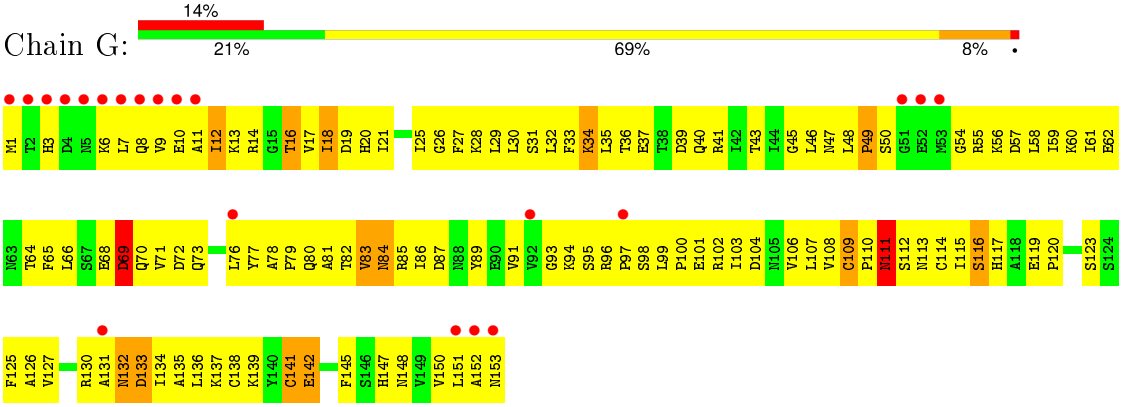
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain F:

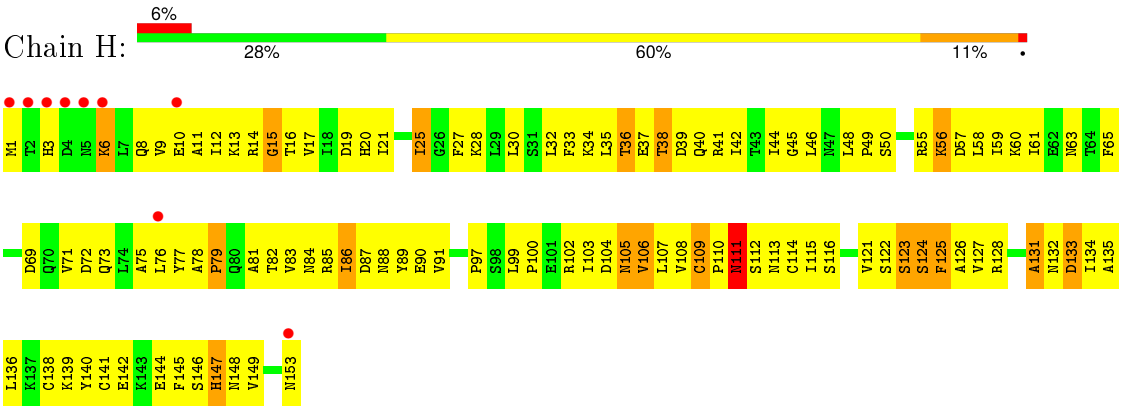





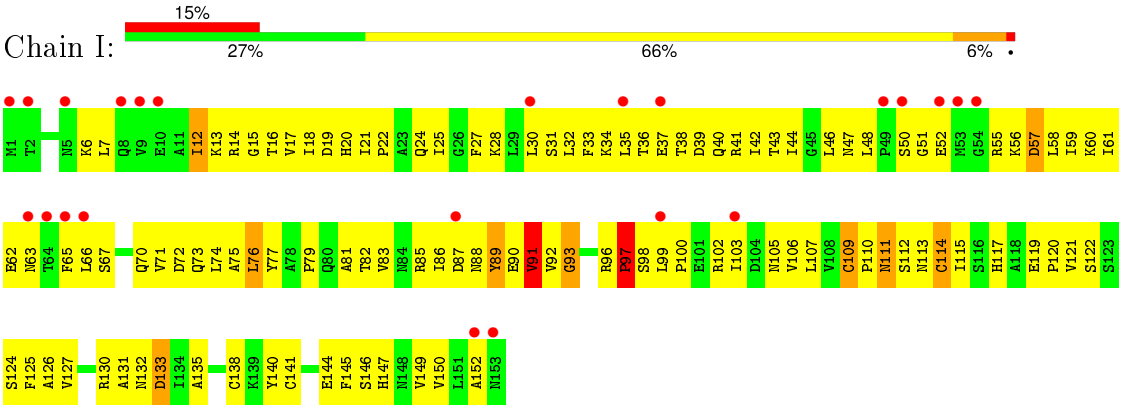

• Molecule 2: Aspartate carbamoyltransferase regulatory chain



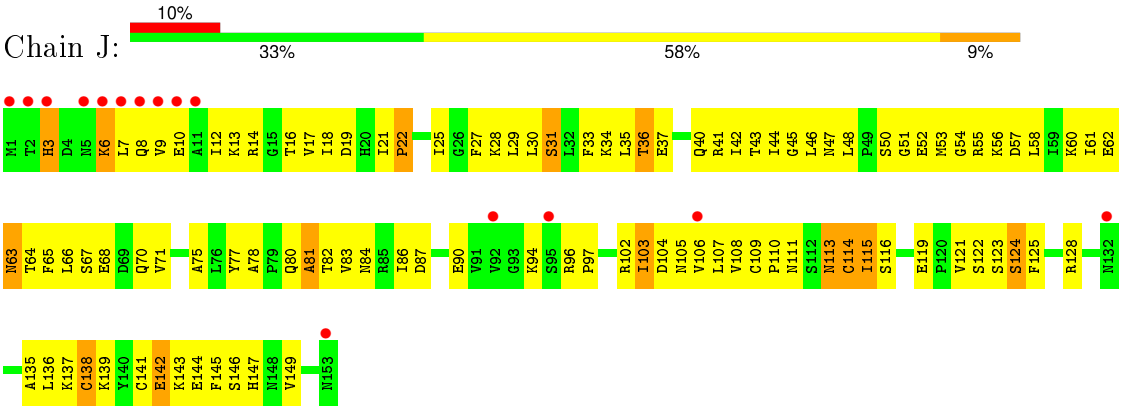

• Molecule 2: Aspartate carbamoyltransferase regulatory chain



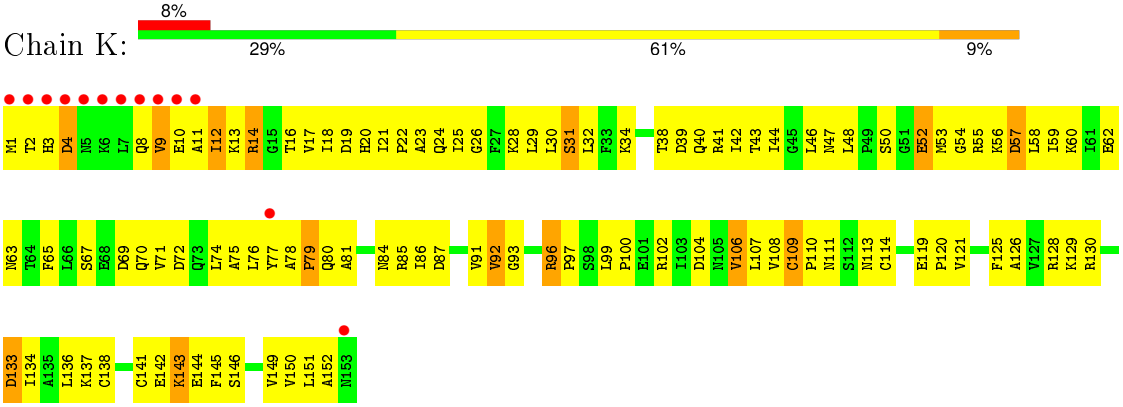

• Molecule 2: Aspartate carbamoyltransferase regulatory chain



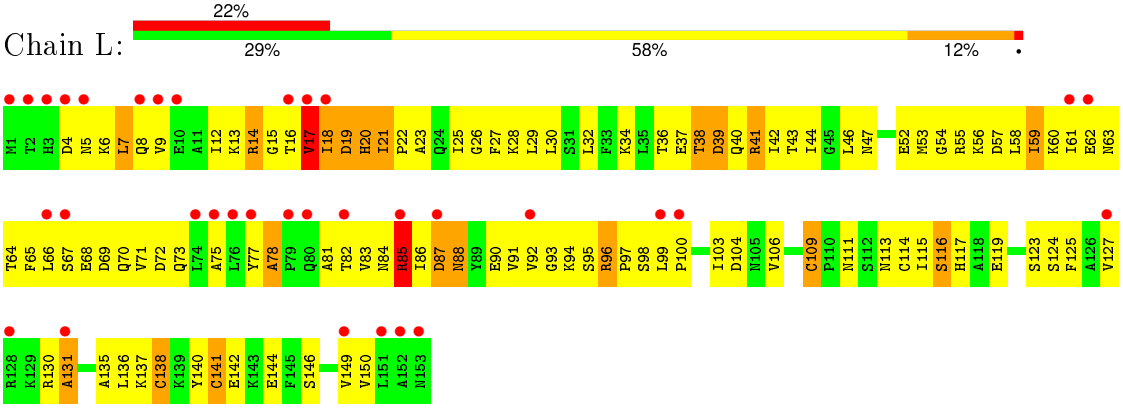

• Molecule 2: Aspartate carbamoyltransferase regulatory chain




• Molecule 2: Aspartate carbamoyltransferase regulatory chain




• Molecule 2: Aspartate carbamoyltransferase regulatory chain



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 120.69Å 155.40Å 194.96Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.90<br>42.82 – 2.86 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 72.5 (50.00-2.90)<br>70.5 (42.82-2.86) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.93 (at 2.86Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, $R_{free}$ | 0.240 , 0.300<br>0.238 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | DCC |
| Wilson B-factor (Å$^2$) | 57.4 | Xtriage |
| Anisotropy | 0.405 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.25 , 45.2 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Outliers | 0 of 61065 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 22698 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 66.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FLC, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.41 | 0/2461 | 0.75 | 3/3339 (0.1%) |
| 1 | B | 0.38 | 0/2461 | 0.75 | 4/3339 (0.1%) |
| 1 | C | 0.39 | 0/2461 | 0.72 | 4/3339 (0.1%) |
| 1 | D | 0.37 | 0/2461 | 0.69 | 3/3339 (0.1%) |
| 1 | E | 0.37 | 0/2461 | 0.69 | 3/3339 (0.1%) |
| 1 | F | 0.34 | 0/2461 | 0.67 | 4/3339 (0.1%) |
| 2 | G | 0.37 | 0/1219 | 0.66 | 0/1647 |
| 2 | H | 0.43 | 0/1219 | 0.79 | 0/1647 |
| 2 | I | 0.39 | 0/1219 | 0.70 | 0/1647 |
| 2 | J | 0.37 | 0/1219 | 0.73 | 1/1647 (0.1%) |
| 2 | K | 0.39 | 0/1219 | 0.70 | 0/1647 |
| 2 | L | 0.39 | 0/1219 | 0.83 | 2/1647 (0.1%) |
| All | All | 0.38 | 0/22080 | 0.72 | 24/29916 (0.1%) |

There are no bond length outliers.

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 267 | LEU | N-CA-C | 9.60 | 136.91 | 111.00 |
| 1 | F | 267 | LEU | N-CA-C | 9.08 | 135.52 | 111.00 |
| 1 | A | 267 | LEU | N-CA-C | 9.05 | 135.44 | 111.00 |
| 1 | B | 267 | LEU | N-CA-C | 8.47 | 133.88 | 111.00 |
| 1 | C | 266 | PRO | N-CA-C | -8.28 | 90.57 | 112.10 |
| 1 | B | 267 | LEU | CA-CB-CG | -8.00 | 96.91 | 115.30 |
| 1 | A | 266 | PRO | N-CA-C | -7.76 | 91.93 | 112.10 |
| 1 | F | 267 | LEU | C-N-CD | 7.29 | 143.70 | 128.40 |
| 1 | D | 267 | LEU | N-CA-C | 7.10 | 130.16 | 111.00 |
| 1 | B | 266 | PRO | N-CA-C | -6.96 | 94.01 | 112.10 |
| 1 | F | 267 | LEU | CA-CB-CG | -6.76 | 99.75 | 115.30 |
| 1 | B | 254 | LEU | N-CA-C | 6.71 | 129.11 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 3 | HIS | N-CA-C | -6.60 | 93.18 | 111.00 |
| 1 | F | 266 | PRO | N-CA-C | -6.44 | 95.36 | 112.10 |
| 2 | L | 141 | CYS | CA-CB-SG | -6.29 | 102.69 | 114.00 |
| 1 | C | 267 | LEU | C-N-CD | 6.18 | 141.39 | 128.40 |
| 1 | A | 267 | LEU | C-N-CD | 6.11 | 141.24 | 128.40 |
| 1 | E | 266 | PRO | C-N-CA | -5.88 | 107.01 | 121.70 |
| 2 | L | 21 | ILE | CB-CA-C | -5.50 | 100.60 | 111.60 |
| 1 | E | 267 | LEU | CA-CB-CG | -5.18 | 103.38 | 115.30 |
| 1 | D | 266 | PRO | N-CA-C | -5.16 | 98.69 | 112.10 |
| 1 | E | 266 | PRO | N-CA-C | -5.13 | 98.76 | 112.10 |
| 1 | D | 105 | ARG | NE-CZ-NH2 | -5.10 | 117.75 | 120.30 |
| 1 | C | 140 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2415 | 0 | 2422 | 155 | 0 |
| 1 | B | 2415 | 0 | 2422 | 162 | 0 |
| 1 | C | 2415 | 0 | 2422 | 166 | 0 |
| 1 | D | 2415 | 0 | 2422 | 175 | 0 |
| 1 | E | 2415 | 0 | 2422 | 150 | 0 |
| 1 | F | 2415 | 0 | 2422 | 167 | 0 |
| 2 | G | 1201 | 0 | 1219 | 159 | 0 |
| 2 | H | 1201 | 0 | 1219 | 143 | 0 |
| 2 | I | 1201 | 0 | 1219 | 161 | 0 |
| 2 | J | 1201 | 0 | 1219 | 141 | 0 |
| 2 | K | 1201 | 0 | 1219 | 135 | 0 |
| 2 | L | 1201 | 0 | 1219 | 216 | 0 |
| 3 | A | 13 | 0 | 5 | 7 | 0 |
| 3 | B | 13 | 0 | 5 | 4 | 0 |
| 3 | C | 13 | 0 | 5 | 4 | 0 |
| 3 | D | 13 | 0 | 5 | 7 | 0 |
| 3 | E | 13 | 0 | 5 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | F | 13 | 0 | 5 | 1 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | I | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | K | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 5 | 0 | 0 | 5 | 0 |
| 5 | B | 5 | 0 | 0 | 1 | 0 |
| 5 | C | 5 | 0 | 0 | 0 | 0 |
| 5 | D | 5 | 0 | 0 | 1 | 0 |
| 5 | E | 5 | 0 | 0 | 1 | 0 |
| 5 | F | 5 | 0 | 0 | 2 | 0 |
| 6 | A | 84 | 0 | 0 | 1 | 0 |
| 6 | B | 95 | 0 | 0 | 3 | 0 |
| 6 | C | 113 | 0 | 0 | 4 | 0 |
| 6 | D | 102 | 0 | 0 | 2 | 0 |
| 6 | E | 86 | 0 | 0 | 3 | 0 |
| 6 | F | 82 | 0 | 0 | 8 | 0 |
| 6 | G | 65 | 0 | 0 | 5 | 0 |
| 6 | H | 59 | 0 | 0 | 4 | 0 |
| 6 | I | 45 | 0 | 0 | 5 | 0 |
| 6 | J | 51 | 0 | 0 | 0 | 0 |
| 6 | K | 51 | 0 | 0 | 4 | 0 |
| 6 | L | 55 | 0 | 0 | 2 | 0 |
| All | All | 22698 | 0 | 21876 | 1795 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1795) 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) |
|---|---|---|---|
| 2:J:109:CYS:HB3 | 2:J:138:CYS:SG | 1.64 | 1.36 |
| 1:F:114:LEU:HD22 | 2:L:115:ILE:CD1 | 1.62 | 1.28 |
| 2:L:21:ILE:O | 2:L:21:ILE:HD12 | 1.35 | 1.25 |
| 2:J:114:CYS:SG | 2:J:116:SER:HB3 | 1.81 | 1.20 |
| 2:L:21:ILE:HG22 | 2:L:56:LYS:HD3 | 1.25 | 1.19 |
| 2:K:12:ILE:HG22 | 2:K:13:LYS:H | 1.01 | 1.14 |
| 1:F:140:LEU:HD22 | 1:F:292:GLY:HA2 | 1.29 | 1.14 |
| 2:L:22:PRO:HD2 | 2:L:57:ASP:HB3 | 1.25 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:140:LEU:HD22 | 1:C:292:GLY:HA2 | 1.30 | 1.11 |
| 2:L:14:ARG:HG2 | 2:L:88:ASN:HA | 1.29 | 1.11 |
| 2:J:6:LYS:HB2 | 2:J:9:VAL:HB | 1.30 | 1.11 |
| 2:I:109:CYS:SG | 2:I:114:CYS:CB | 2.39 | 1.11 |
| 2:G:34:LYS:HB3 | 2:G:37:GLU:HG3 | 1.30 | 1.10 |
| 1:F:114:LEU:CD2 | 2:L:115:ILE:HD11 | 1.82 | 1.09 |
| 1:F:114:LEU:HD22 | 2:L:115:ILE:HD13 | 1.28 | 1.09 |
| 2:J:109:CYS:CB | 2:J:138:CYS:SG | 2.29 | 1.09 |
| 2:K:72:ASP:HB3 | 2:K:100:PRO:HG3 | 1.33 | 1.09 |
| 1:A:94:VAL:HG11 | 1:C:54:ARG:HH12 | 1.08 | 1.08 |
| 2:L:82:THR:HG22 | 2:L:83:VAL:H | 0.93 | 1.08 |
| 2:L:72:ASP:HB3 | 2:L:100:PRO:HG2 | 1.33 | 1.07 |
| 2:L:83:VAL:HG11 | 2:L:94:LYS:HB2 | 1.31 | 1.07 |
| 2:K:12:ILE:HG23 | 2:K:62:GLU:HG2 | 1.37 | 1.06 |
| 1:F:114:LEU:CD2 | 2:L:115:ILE:CD1 | 2.33 | 1.06 |
| 2:G:12:ILE:HG22 | 2:G:13:LYS:H | 1.13 | 1.06 |
| 2:J:104:ASP:HB3 | 2:J:124:SER:HA | 1.38 | 1.05 |
| 2:J:114:CYS:SG | 2:J:116:SER:CB | 2.45 | 1.05 |
| 1:C:243:VAL:HG13 | 1:C:244:LYS:HD2 | 1.40 | 1.04 |
| 2:G:76:LEU:HD11 | 2:G:103:ILE:HG21 | 1.39 | 1.03 |
| 1:A:44:ILE:HD12 | 1:A:63:MET:HG2 | 1.40 | 1.03 |
| 2:L:82:THR:HG22 | 2:L:83:VAL:N | 1.75 | 1.02 |
| 1:A:94:VAL:HG11 | 1:C:54:ARG:NH1 | 1.72 | 1.02 |
| 2:L:82:THR:CG2 | 2:L:83:VAL:H | 1.72 | 1.00 |
| 2:G:103:ILE:HD12 | 2:G:107:LEU:HD11 | 1.44 | 1.00 |
| 1:B:243:VAL:HG13 | 1:B:244:LYS:HD2 | 1.42 | 1.00 |
| 2:K:30:LEU:HD21 | 2:K:44:ILE:HG12 | 1.46 | 0.98 |
| 2:K:14:ARG:H | 2:K:87:ASP:HA | 1.26 | 0.98 |
| 2:K:38:THR:HG22 | 2:K:40:GLN:H | 1.24 | 0.98 |
| 1:F:114:LEU:HD22 | 2:L:115:ILE:HD11 | 1.41 | 0.97 |
| 2:L:83:VAL:HG13 | 2:L:95:SER:H | 1.24 | 0.96 |
| 1:F:265:HIS:H | 1:F:288:GLN:HE22 | 1.09 | 0.96 |
| 1:B:109:GLU:HG3 | 1:B:130:GLY:O | 1.66 | 0.96 |
| 2:L:21:ILE:CD1 | 2:L:21:ILE:O | 2.14 | 0.95 |
| 1:C:104:MET:HE1 | 1:C:112:ALA:HA | 1.49 | 0.94 |
| 2:I:109:CYS:HB2 | 2:I:138:CYS:SG | 2.04 | 0.94 |
| 2:L:42:ILE:HG22 | 2:L:44:ILE:HG13 | 1.48 | 0.94 |
| 2:I:13:LYS:HB2 | 2:I:89:TYR:CE1 | 2.02 | 0.94 |
| 2:K:12:ILE:HG22 | 2:K:13:LYS:N | 1.82 | 0.94 |
| 2:L:16:THR:HB | 2:L:60:LYS:HB3 | 1.46 | 0.94 |
| 1:E:243:VAL:HG13 | 1:E:244:LYS:HD2 | 1.50 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:105:ASN:H | 2:J:123:SER:HB3 | 1.34 | 0.93 |
| 1:C:257:ALA:HB1 | 1:C:261:MET:CE | 1.98 | 0.93 |
| 1:D:243:VAL:HG13 | 1:D:244:LYS:HD2 | 1.48 | 0.93 |
| 2:G:34:LYS:HB3 | 2:G:37:GLU:CG | 1.99 | 0.92 |
| 2:H:138:CYS:HB2 | 2:H:141:CYS:SG | 2.09 | 0.92 |
| 1:D:140:LEU:HD22 | 1:D:292:GLY:HA2 | 1.50 | 0.91 |
| 2:G:12:ILE:H | 2:G:60:LYS:HZ3 | 1.18 | 0.91 |
| 2:H:17:VAL:HG22 | 2:H:60:LYS:HG2 | 1.50 | 0.91 |
| 2:H:138:CYS:CB | 2:H:141:CYS:SG | 2.59 | 0.91 |
| 2:L:96:ARG:O | 2:L:96:ARG:HG2 | 1.70 | 0.90 |
| 2:G:68:GLU:HA | 2:G:71:VAL:HG12 | 1.54 | 0.90 |
| 2:I:109:CYS:SG | 2:I:111:ASN:HB3 | 2.11 | 0.90 |
| 2:L:70:GLN:HA | 2:L:73:GLN:NE2 | 1.85 | 0.90 |
| 2:I:42:ILE:HD11 | 2:L:46:LEU:HD12 | 1.54 | 0.90 |
| 1:F:44:ILE:HD12 | 1:F:63:MET:HG2 | 1.52 | 0.90 |
| 2:G:111:ASN:ND2 | 2:G:113:ASN:H | 1.71 | 0.89 |
| 2:G:13:LYS:HD3 | 2:G:89:TYR:CE1 | 2.07 | 0.89 |
| 1:B:108:GLN:HB2 | 2:H:115:ILE:HG13 | 1.53 | 0.89 |
| 2:H:114:CYS:SG | 2:H:140:TYR:HB2 | 2.12 | 0.89 |
| 1:C:30:LEU:HD21 | 1:C:309:VAL:HG21 | 1.55 | 0.88 |
| 1:A:170:HIS:O | 1:A:174:GLN:HG3 | 1.73 | 0.88 |
| 1:D:54:ARG:HD3 | 1:D:267:LEU:HB2 | 1.54 | 0.88 |
| 2:L:21:ILE:CG2 | 2:L:56:LYS:HD3 | 2.03 | 0.88 |
| 2:L:14:ARG:HD3 | 2:L:65:PHE:HZ | 1.38 | 0.88 |
| 2:L:78:ALA:HB1 | 2:L:81:ALA:HB2 | 1.54 | 0.88 |
| 1:A:59:PHE:HE1 | 1:A:136:THR:HG21 | 1.37 | 0.88 |
| 2:G:54:GLY:HA2 | 6:G:1026:HOH:O | 1.72 | 0.87 |
| 2:H:41:ARG:CZ | 2:K:8:GLN:HE21 | 1.86 | 0.87 |
| 1:A:109:GLU:HG3 | 1:A:130:GLY:O | 1.73 | 0.87 |
| 2:G:48:LEU:HD23 | 2:J:41:ARG:HD2 | 1.57 | 0.86 |
| 2:L:21:ILE:HG22 | 2:L:56:LYS:CD | 2.05 | 0.86 |
| 2:G:114:CYS:SG | 2:G:116:SER:OG | 2.34 | 0.86 |
| 2:K:14:ARG:HH11 | 2:K:14:ARG:HB3 | 1.41 | 0.85 |
| 2:G:152:ALA:HB3 | 6:G:1058:HOH:O | 1.76 | 0.85 |
| 1:B:35:GLN:HE22 | 1:B:309:VAL:HG23 | 1.40 | 0.85 |
| 2:L:25:ILE:HG22 | 2:L:29:LEU:HG | 1.55 | 0.85 |
| 2:G:17:VAL:HG22 | 2:G:60:LYS:HE3 | 1.58 | 0.85 |
| 1:F:126:ASN:HD21 | 1:F:129:ASP:HB2 | 1.39 | 0.85 |
| 2:G:12:ILE:HG22 | 2:G:13:LYS:N | 1.92 | 0.85 |
| 2:L:18:ILE:HG22 | 2:L:19:ASP:H | 1.41 | 0.85 |
| 1:B:261:MET:HG2 | 1:B:262:LYS:N | 1.91 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:39:LEU:HD13 | 1:A:304:LEU:HD12 | 1.58 | 0.85 |
| 1:C:140:LEU:CD2 | 1:C:292:GLY:HA2 | 2.07 | 0.84 |
| 1:F:268:PRO:HD3 | 6:F:3075:HOH:O | 1.76 | 0.84 |
| 1:B:161:GLY:HA3 | 1:B:228:THR:OG1 | 1.76 | 0.84 |
| 1:E:45:ALA:HB2 | 1:E:99:VAL:HG11 | 1.58 | 0.84 |
| 1:A:88:LEU:HD23 | 1:A:114:LEU:HD23 | 1.59 | 0.84 |
| 2:L:14:ARG:HH21 | 2:L:88:ASN:HD22 | 1.25 | 0.84 |
| 2:I:15:GLY:HA2 | 2:I:63:ASN:H | 1.42 | 0.84 |
| 2:G:12:ILE:N | 2:G:60:LYS:HZ3 | 1.76 | 0.84 |
| 2:H:19:ASP:HA | 2:H:58:LEU:HD23 | 1.60 | 0.84 |
| 1:D:105:ARG:HD2 | 1:D:128:GLY:HA3 | 1.60 | 0.84 |
| 2:I:109:CYS:SG | 2:I:114:CYS:HB3 | 2.11 | 0.84 |
| 1:C:161:GLY:HA3 | 1:C:228:THR:OG1 | 1.76 | 0.84 |
| 1:E:108:GLN:HB2 | 2:K:113:ASN:O | 1.76 | 0.83 |
| 1:B:132:ASN:O | 1:B:167:ARG:HB2 | 1.77 | 0.83 |
| 2:K:12:ILE:CG2 | 2:K:13:LYS:H | 1.86 | 0.83 |
| 1:F:81:LEU:HD12 | 1:F:86:GLU:O | 1.79 | 0.83 |
| 1:B:200:ASP:HB3 | 2:H:128:ARG:HH22 | 1.44 | 0.83 |
| 2:L:83:VAL:HG11 | 2:L:94:LYS:CB | 2.08 | 0.83 |
| 2:I:46:LEU:HB2 | 2:L:42:ILE:HG13 | 1.60 | 0.83 |
| 2:J:12:ILE:HG22 | 2:J:13:LYS:H | 1.43 | 0.83 |
| 1:A:54:ARG:HH21 | 1:A:268:PRO:HG3 | 1.44 | 0.83 |
| 1:E:266:PRO:HB3 | 3:E:2005:FLC:HG1 | 1.59 | 0.83 |
| 1:B:140:LEU:HD22 | 1:B:292:GLY:HA2 | 1.61 | 0.82 |
| 1:D:132:ASN:O | 1:D:167:ARG:HB2 | 1.79 | 0.82 |
| 2:L:14:ARG:CG | 2:L:88:ASN:HA | 2.09 | 0.82 |
| 2:K:14:ARG:HB3 | 2:K:14:ARG:NH1 | 1.93 | 0.82 |
| 2:J:48:LEU:HD12 | 2:J:58:LEU:HG | 1.62 | 0.82 |
| 2:I:107:LEU:HA | 2:I:152:ALA:HB2 | 1.61 | 0.82 |
| 1:D:120:GLY:O | 1:D:122:VAL:HG23 | 1.79 | 0.81 |
| 2:I:55:ARG:HH11 | 2:L:39:ASP:HB3 | 1.45 | 0.81 |
| 1:B:59:PHE:CD1 | 1:B:296:ARG:HD3 | 2.15 | 0.81 |
| 2:G:141:CYS:O | 2:G:141:CYS:SG | 2.38 | 0.81 |
| 2:H:35:LEU:HD13 | 2:H:61:ILE:HD11 | 1.61 | 0.81 |
| 2:G:83:VAL:HG22 | 2:G:84:ASN:H | 1.45 | 0.81 |
| 1:F:59:PHE:HE1 | 1:F:136:THR:HG21 | 1.46 | 0.81 |
| 2:G:32:LEU:HD13 | 2:G:152:ALA:HB1 | 1.61 | 0.81 |
| 1:F:45:ALA:HB2 | 1:F:99:VAL:HG11 | 1.61 | 0.81 |
| 2:L:22:PRO:HD2 | 2:L:57:ASP:CB | 2.09 | 0.80 |
| 1:C:17:ARG:HH11 | 1:C:17:ARG:HG2 | 1.45 | 0.80 |
| 1:A:109:GLU:HB3 | 2:G:141:CYS:HB2 | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:170:HIS:O | 1:D:174:GLN:HG3 | 1.81 | 0.80 |
| 2:G:17:VAL:HG13 | 2:G:60:LYS:HG2 | 1.63 | 0.80 |
| 1:C:257:ALA:CB | 1:C:261:MET:CE | 2.59 | 0.80 |
| 1:E:237:PRO:HA | 1:E:240:TYR:CE2 | 2.17 | 0.80 |
| 1:F:114:LEU:CD2 | 2:L:115:ILE:HD13 | 2.05 | 0.80 |
| 2:L:15:GLY:O | 2:L:86:ILE:HB | 1.82 | 0.80 |
| 2:I:13:LYS:HG3 | 2:I:88:ASN:HA | 1.63 | 0.79 |
| 1:F:59:PHE:CD1 | 1:F:296:ARG:HD3 | 2.17 | 0.79 |
| 2:K:12:ILE:HD11 | 2:K:60:LYS:HB2 | 1.63 | 0.79 |
| 2:I:44:ILE:HB | 2:L:44:ILE:CG2 | 2.13 | 0.79 |
| 1:F:63:MET:HG3 | 1:F:300:LEU:HD11 | 1.65 | 0.79 |
| 1:B:174:GLN:HA | 1:B:201:MET:CE | 2.13 | 0.79 |
| 1:D:267:LEU:HD12 | 1:F:94:VAL:HG12 | 1.64 | 0.79 |
| 2:L:17:VAL:HG23 | 2:L:86:ILE:HD12 | 1.64 | 0.79 |
| 1:F:265:HIS:H | 1:F:288:GLN:NE2 | 1.81 | 0.78 |
| 2:L:114:CYS:SG | 2:L:116:SER:OG | 2.40 | 0.78 |
| 2:H:109:CYS:SG | 2:H:111:ASN:HB3 | 2.22 | 0.78 |
| 1:E:229:ARG:HH11 | 1:E:232:LYS:HE2 | 1.45 | 0.78 |
| 1:C:160:VAL:HB | 1:C:227:MET:HG2 | 1.65 | 0.78 |
| 1:A:114:LEU:HD22 | 2:G:115:ILE:HG21 | 1.64 | 0.78 |
| 1:E:59:PHE:HE1 | 1:E:136:THR:HG21 | 1.48 | 0.78 |
| 2:I:12:ILE:HD12 | 2:I:61:ILE:O | 1.84 | 0.78 |
| 2:J:104:ASP:CB | 2:J:124:SER:HA | 2.13 | 0.78 |
| 2:L:71:VAL:HG21 | 2:L:85:ARG:HE | 1.49 | 0.78 |
| 1:B:45:ALA:HB2 | 1:B:99:VAL:HG11 | 1.63 | 0.78 |
| 1:B:239:GLU:C | 1:B:241:ALA:H | 1.86 | 0.78 |
| 1:F:131:SER:HB2 | 1:F:234:ARG:HD3 | 1.64 | 0.78 |
| 2:J:43:THR:HB | 2:J:60:LYS:HB2 | 1.64 | 0.78 |
| 2:H:85:ARG:C | 2:H:86:ILE:HG12 | 2.03 | 0.78 |
| 1:F:55:THR:O | 1:F:59:PHE:HB2 | 1.83 | 0.77 |
| 2:J:67:SER:H | 2:J:70:GLN:HE21 | 1.30 | 0.77 |
| 2:I:87:ASP:OD2 | 2:I:92:VAL:HG21 | 1.85 | 0.77 |
| 1:C:109:GLU:HG3 | 1:C:130:GLY:O | 1.85 | 0.77 |
| 1:E:35:GLN:NE2 | 1:E:309:VAL:HG23 | 2.00 | 0.77 |
| 1:A:81:LEU:HD12 | 1:A:86:GLU:O | 1.84 | 0.77 |
| 1:A:237:PRO:HA | 1:A:240:TYR:CE2 | 2.18 | 0.77 |
| 2:I:86:ILE:HG23 | 2:I:91:VAL:HA | 1.66 | 0.77 |
| 1:D:214:SER:OG | 1:D:217:GLU:HG3 | 1.84 | 0.77 |
| 2:H:27:PHE:HZ | 2:K:31:SER:HB2 | 1.49 | 0.76 |
| 1:D:59:PHE:HE1 | 1:D:136:THR:HG21 | 1.48 | 0.76 |
| 1:C:120:GLY:O | 1:C:122:VAL:HG23 | 1.84 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:106:HIS:ND1 | 1:C:107:PRO:HD2 | 1.99 | 0.76 |
| 1:F:265:HIS:ND1 | 1:F:266:PRO:O | 2.17 | 0.76 |
| 1:E:44:ILE:HD12 | 1:E:63:MET:HG2 | 1.66 | 0.76 |
| 2:L:86:ILE:HD13 | 2:L:92:VAL:HA | 1.68 | 0.76 |
| 1:B:106:HIS:CE1 | 2:H:115:ILE:HD11 | 2.21 | 0.76 |
| 2:J:21:ILE:O | 2:J:56:LYS:HA | 1.86 | 0.76 |
| 2:G:70:GLN:O | 2:G:73:GLN:HG2 | 1.85 | 0.76 |
| 2:L:86:ILE:HG23 | 2:L:93:GLY:N | 2.01 | 0.76 |
| 1:B:131:SER:HB3 | 1:B:234:ARG:HD3 | 1.65 | 0.76 |
| 1:B:267:LEU:HD13 | 1:B:289:ALA:HB2 | 1.68 | 0.76 |
| 2:L:83:VAL:CG1 | 2:L:95:SER:H | 1.98 | 0.76 |
| 1:C:257:ALA:HB1 | 1:C:261:MET:HE2 | 1.67 | 0.76 |
| 1:C:43:VAL:HG22 | 1:C:69:SER:HB2 | 1.66 | 0.76 |
| 2:K:84:ASN:HB3 | 2:K:91:VAL:HG13 | 1.68 | 0.76 |
| 2:I:138:CYS:HB2 | 2:I:141:CYS:SG | 2.25 | 0.76 |
| 2:I:19:ASP:HB2 | 2:I:56:LYS:HZ1 | 1.49 | 0.76 |
| 1:C:59:PHE:CD1 | 1:C:296:ARG:HD3 | 2.21 | 0.75 |
| 1:F:225:LEU:HD21 | 1:F:227:MET:CE | 2.17 | 0.75 |
| 2:L:14:ARG:HD3 | 2:L:65:PHE:CZ | 2.20 | 0.75 |
| 1:D:94:VAL:CG1 | 1:E:267:LEU:HD22 | 2.16 | 0.75 |
| 1:B:59:PHE:HE1 | 1:B:136:THR:HG21 | 1.50 | 0.75 |
| 2:J:34:LYS:HB3 | 2:J:37:GLU:HG2 | 1.69 | 0.75 |
| 1:E:137:GLN:HG2 | 1:E:168:THR:HG22 | 1.68 | 0.75 |
| 2:L:18:ILE:HG22 | 2:L:19:ASP:N | 2.01 | 0.75 |
| 2:J:41:ARG:HB3 | 2:J:62:GLU:OE1 | 1.85 | 0.75 |
| 1:C:137:GLN:HG2 | 1:C:168:THR:HG22 | 1.69 | 0.75 |
| 2:G:85:ARG:HB3 | 2:G:93:GLY:H | 1.50 | 0.75 |
| 1:E:44:ILE:HB | 1:E:63:MET:CE | 2.16 | 0.75 |
| 1:D:237:PRO:HA | 1:D:240:TYR:CE1 | 2.22 | 0.75 |
| 2:L:62:GLU:HA | 6:L:1049:HOH:O | 1.85 | 0.74 |
| 1:B:111:ALA:HB2 | 2:H:115:ILE:HD12 | 1.68 | 0.74 |
| 1:C:109:GLU:HA | 1:C:129:ASP:OD1 | 1.86 | 0.74 |
| 1:D:109:GLU:OE2 | 1:D:131:SER:HB3 | 1.88 | 0.74 |
| 1:B:48:PHE:CE2 | 1:B:56:ARG:HB2 | 2.23 | 0.74 |
| 2:G:16:THR:HB | 2:G:65:PHE:HD2 | 1.53 | 0.74 |
| 1:D:189:PRO:HB3 | 1:D:246:GLN:HE22 | 1.53 | 0.74 |
| 1:D:63:MET:HE2 | 1:D:70:VAL:HG22 | 1.68 | 0.74 |
| 1:A:29:LYS:O | 1:A:32:ALA:N | 2.21 | 0.74 |
| 2:I:18:ILE:HG12 | 2:I:83:VAL:HG23 | 1.70 | 0.74 |
| 2:I:19:ASP:HB2 | 2:I:56:LYS:NZ | 2.02 | 0.74 |
| 2:L:46:LEU:HD23 | 2:L:57:ASP:OD1 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L:86:ILE:HG23 | 2:L:93:GLY:H | 1.53 | 0.73 |
| 2:H:14:ARG:HB3 | 2:H:63:ASN:HD22 | 1.52 | 0.73 |
| 1:A:109:GLU:OE1 | 2:G:113:ASN:HB3 | 1.88 | 0.73 |
| 2:I:40:GLN:HG3 | 2:I:62:GLU:HB2 | 1.68 | 0.73 |
| 2:L:14:ARG:CD | 2:L:65:PHE:HZ | 2.00 | 0.73 |
| 2:L:83:VAL:HG12 | 2:L:84:ASN:N | 2.03 | 0.73 |
| 1:F:126:ASN:ND2 | 1:F:129:ASP:HB2 | 2.03 | 0.73 |
| 2:J:34:LYS:HB3 | 2:J:37:GLU:CG | 2.18 | 0.73 |
| 1:E:170:HIS:O | 1:E:174:GLN:HG3 | 1.88 | 0.73 |
| 1:A:140:LEU:HD22 | 1:A:292:GLY:HA2 | 1.70 | 0.73 |
| 2:I:132:ASN:O | 2:I:133:ASP:HB2 | 1.87 | 0.73 |
| 2:J:141:CYS:O | 2:J:141:CYS:SG | 2.46 | 0.73 |
| 1:B:214:SER:OG | 1:B:217:GLU:HG3 | 1.88 | 0.73 |
| 1:B:293:ILE:O | 1:B:297:GLN:HB2 | 1.89 | 0.73 |
| 2:K:102:ARG:NH1 | 2:K:102:ARG:HB3 | 2.04 | 0.73 |
| 2:K:12:ILE:CG2 | 2:K:62:GLU:HG2 | 2.17 | 0.73 |
| 1:D:35:GLN:NE2 | 1:D:309:VAL:HG23 | 2.04 | 0.73 |
| 2:J:17:VAL:HG11 | 2:J:86:ILE:HD12 | 1.71 | 0.73 |
| 1:B:131:SER:HB3 | 1:B:234:ARG:CD | 2.18 | 0.73 |
| 1:A:53:THR:N | 5:A:3001:PO4:O1 | 2.22 | 0.73 |
| 2:J:110:PRO:HD2 | 2:J:145:PHE:CE2 | 2.24 | 0.73 |
| 1:F:10:ILE:HD12 | 1:F:112:ALA:HB1 | 1.71 | 0.73 |
| 1:F:54:ARG:HD3 | 1:F:267:LEU:HB2 | 1.71 | 0.72 |
| 1:B:267:LEU:CD1 | 1:B:289:ALA:HB2 | 2.19 | 0.72 |
| 2:G:76:LEU:HD11 | 2:G:103:ILE:HD13 | 1.70 | 0.72 |
| 2:G:111:ASN:HD22 | 2:G:113:ASN:H | 1.37 | 0.72 |
| 2:J:14:ARG:O | 2:J:14:ARG:HG3 | 1.89 | 0.72 |
| 1:F:237:PRO:HA | 1:F:240:TYR:CE2 | 2.24 | 0.72 |
| 2:L:61:ILE:CG2 | 2:L:64:THR:HB | 2.19 | 0.72 |
| 2:L:86:ILE:HG21 | 2:L:91:VAL:O | 1.89 | 0.72 |
| 2:L:86:ILE:HG22 | 2:L:87:ASP:N | 2.05 | 0.72 |
| 2:L:12:ILE:HD11 | 2:L:15:GLY:HA2 | 1.70 | 0.72 |
| 1:D:120:GLY:O | 1:D:122:VAL:N | 2.23 | 0.72 |
| 2:G:19:ASP:HA | 2:G:58:LEU:CD1 | 2.20 | 0.72 |
| 1:C:65:ARG:HH11 | 1:C:293:ILE:HG21 | 1.54 | 0.72 |
| 2:L:16:THR:HA | 2:L:86:ILE:HG13 | 1.72 | 0.72 |
| 2:I:110:PRO:HD2 | 2:I:145:PHE:CE2 | 2.25 | 0.72 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CE2 | 2.25 | 0.72 |
| 1:B:35:GLN:NE2 | 1:B:309:VAL:HG23 | 2.04 | 0.72 |
| 1:E:59:PHE:CE1 | 1:E:136:THR:HG21 | 2.25 | 0.72 |
| 1:C:65:ARG:NH1 | 1:C:293:ILE:HG21 | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:120:GLY:O | 1:E:122:VAL:HG23 | 1.89 | 0.72 |
| 2:L:23:ALA:N | 2:L:25:ILE:HG12 | 2.04 | 0.71 |
| 1:C:54:ARG:CZ | 1:C:267:LEU:HB3 | 2.19 | 0.71 |
| 2:K:18:ILE:O | 2:K:58:LEU:HD12 | 1.89 | 0.71 |
| 1:C:104:MET:CE | 1:C:112:ALA:HA | 2.19 | 0.71 |
| 1:C:114:LEU:HD13 | 2:I:121:VAL:HG11 | 1.72 | 0.71 |
| 1:C:17:ARG:HG2 | 1:C:17:ARG:NH1 | 2.00 | 0.71 |
| 2:I:56:LYS:HE3 | 2:I:58:LEU:HG | 1.72 | 0.71 |
| 2:G:12:ILE:H | 2:G:60:LYS:NZ | 1.89 | 0.71 |
| 2:G:76:LEU:CD1 | 2:G:103:ILE:HD13 | 2.19 | 0.71 |
| 1:C:106:HIS:HD2 | 6:C:3063:HOH:O | 1.72 | 0.71 |
| 1:C:188:ALA:HA | 1:C:247:PHE:HE2 | 1.55 | 0.71 |
| 1:C:189:PRO:HB3 | 1:C:246:GLN:OE1 | 1.90 | 0.71 |
| 1:D:45:ALA:HB2 | 1:D:99:VAL:HG11 | 1.72 | 0.71 |
| 1:A:138:THR:O | 1:A:142:LEU:HG | 1.90 | 0.71 |
| 2:K:26:GLY:O | 2:K:30:LEU:HB2 | 1.91 | 0.71 |
| 1:E:109:GLU:HG3 | 1:E:130:GLY:O | 1.91 | 0.71 |
| 2:I:30:LEU:HD23 | 2:I:35:LEU:HD12 | 1.70 | 0.71 |
| 2:L:71:VAL:HG12 | 2:L:97:PRO:HG2 | 1.73 | 0.71 |
| 1:D:40:LYS:HG2 | 1:D:41:HIS:CD2 | 2.26 | 0.71 |
| 2:I:107:LEU:HD23 | 2:I:152:ALA:HB2 | 1.72 | 0.71 |
| 2:I:82:THR:HG22 | 2:I:96:ARG:HB3 | 1.73 | 0.71 |
| 2:J:30:LEU:HD11 | 2:J:44:ILE:HD13 | 1.73 | 0.71 |
| 1:C:59:PHE:HE1 | 1:C:136:THR:HG21 | 1.56 | 0.70 |
| 2:K:114:CYS:SG | 2:K:141:CYS:HB3 | 2.31 | 0.70 |
| 1:F:225:LEU:HD21 | 1:F:227:MET:HE1 | 1.73 | 0.70 |
| 2:L:16:THR:HG21 | 2:L:84:ASN:HA | 1.74 | 0.70 |
| 2:I:107:LEU:HA | 2:I:152:ALA:CB | 2.21 | 0.70 |
| 2:K:129:LYS:HA | 2:K:134:ILE:HG22 | 1.74 | 0.70 |
| 1:E:214:SER:OG | 1:E:217:GLU:HG3 | 1.91 | 0.70 |
| 1:C:293:ILE:O | 1:C:297:GLN:HB2 | 1.91 | 0.70 |
| 1:F:293:ILE:O | 1:F:297:GLN:HB2 | 1.92 | 0.70 |
| 2:L:17:VAL:C | 2:L:18:ILE:HG12 | 2.12 | 0.70 |
| 1:D:189:PRO:HB3 | 1:D:246:GLN:NE2 | 2.07 | 0.70 |
| 1:C:284:TRP:HA | 1:C:287:GLN:OE1 | 1.92 | 0.70 |
| 2:L:18:ILE:HG13 | 2:L:83:VAL:HB | 1.72 | 0.70 |
| 2:H:19:ASP:HA | 2:H:58:LEU:CD2 | 2.21 | 0.70 |
| 1:B:239:GLU:O | 1:B:241:ALA:N | 2.25 | 0.70 |
| 2:K:130:ARG:HB2 | 2:K:133:ASP:O | 1.91 | 0.70 |
| 1:E:114:LEU:HD21 | 2:K:119:GLU:HG3 | 1.74 | 0.69 |
| 2:L:115:ILE:HD11 | 2:L:119:GLU:HG3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:110:PRO:HD2 | 2:H:145:PHE:CE2 | 2.27 | 0.69 |
| 1:F:262:LYS:HE2 | 6:F:3069:HOH:O | 1.91 | 0.69 |
| 2:J:104:ASP:HB2 | 2:J:123:SER:O | 1.92 | 0.69 |
| 2:G:103:ILE:CD1 | 2:G:107:LEU:HD11 | 2.21 | 0.69 |
| 2:J:46:LEU:HD22 | 2:J:57:ASP:OD2 | 1.92 | 0.69 |
| 1:B:90:ASP:O | 1:B:94:VAL:HG22 | 1.92 | 0.69 |
| 2:L:75:ALA:HB1 | 2:L:98:SER:O | 1.93 | 0.69 |
| 2:G:12:ILE:CG2 | 2:G:13:LYS:H | 1.98 | 0.69 |
| 2:I:75:ALA:O | 2:I:79:PRO:HG3 | 1.93 | 0.69 |
| 2:G:27:PHE:HZ | 2:J:31:SER:HB3 | 1.58 | 0.69 |
| 2:K:53:MET:HG2 | 2:K:54:GLY:H | 1.58 | 0.69 |
| 1:C:257:ALA:CB | 1:C:261:MET:HE1 | 2.23 | 0.69 |
| 1:B:174:GLN:HA | 1:B:201:MET:HE1 | 1.75 | 0.69 |
| 2:G:46:LEU:HA | 2:G:57:ASP:OD1 | 1.92 | 0.69 |
| 1:D:44:ILE:HD12 | 1:D:63:MET:HG2 | 1.74 | 0.69 |
| 1:B:156:HIS:HD2 | 1:B:185:TYR:OH | 1.76 | 0.69 |
| 1:D:199:LEU:HD13 | 1:D:209:TRP:CH2 | 2.27 | 0.69 |
| 1:A:32:ALA:O | 1:A:34:PRO:HD3 | 1.92 | 0.68 |
| 2:K:43:THR:HB | 2:K:60:LYS:CG | 2.23 | 0.68 |
| 2:I:111:ASN:ND2 | 2:I:113:ASN:H | 1.91 | 0.68 |
| 1:B:267:LEU:HD21 | 1:B:285:TYR:O | 1.93 | 0.68 |
| 1:A:54:ARG:HB2 | 5:A:3001:PO4:O3 | 1.93 | 0.68 |
| 1:D:59:PHE:CD1 | 1:D:296:ARG:HD3 | 2.28 | 0.68 |
| 2:J:146:SER:O | 2:J:149:VAL:HG22 | 1.93 | 0.68 |
| 2:K:52:GLU:HG3 | 6:K:1034:HOH:O | 1.92 | 0.68 |
| 2:L:109:CYS:SG | 2:L:138:CYS:HB2 | 2.33 | 0.68 |
| 1:A:214:SER:OG | 1:A:217:GLU:HG3 | 1.94 | 0.68 |
| 1:E:66:LEU:HD21 | 1:E:297:GLN:HE21 | 1.57 | 0.68 |
| 1:B:75:ASP:OD2 | 1:B:77:ALA:HB3 | 1.94 | 0.68 |
| 1:F:189:PRO:HG3 | 1:F:246:GLN:OE1 | 1.94 | 0.68 |
| 1:C:264:LEU:O | 1:C:265:HIS:HB2 | 1.94 | 0.68 |
| 2:I:76:LEU:HD13 | 2:I:103:ILE:HD11 | 1.74 | 0.68 |
| 1:B:159:MET:CE | 1:B:173:THR:OG1 | 2.42 | 0.68 |
| 2:I:109:CYS:SG | 2:I:114:CYS:HB2 | 2.23 | 0.68 |
| 2:J:12:ILE:HG22 | 2:J:13:LYS:N | 2.08 | 0.68 |
| 1:D:94:VAL:HG11 | 1:E:267:LEU:HD22 | 1.74 | 0.68 |
| 2:J:53:MET:HG3 | 2:J:54:GLY:H | 1.58 | 0.68 |
| 1:B:232:LYS:HA | 1:B:235:LEU:HD12 | 1.76 | 0.68 |
| 2:I:30:LEU:HD21 | 2:I:59:ILE:HD13 | 1.76 | 0.67 |
| 1:D:267:LEU:CD1 | 1:F:94:VAL:HG12 | 2.23 | 0.67 |
| 1:F:284:TRP:HA | 1:F:287:GLN:OE1 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:44:ILE:O | 2:L:44:ILE:HB | 1.95 | 0.67 |
| 1:A:111:ALA:HA | 2:G:115:ILE:HD12 | 1.76 | 0.67 |
| 2:I:92:VAL:HG12 | 2:I:93:GLY:N | 2.10 | 0.67 |
| 2:I:107:LEU:HD23 | 2:I:152:ALA:CB | 2.25 | 0.67 |
| 2:G:41:ARG:HD3 | 2:G:62:GLU:OE1 | 1.94 | 0.67 |
| 2:G:78:ALA:HB1 | 2:G:81:ALA:HB2 | 1.75 | 0.67 |
| 2:L:57:ASP:OD2 | 2:L:58:LEU:N | 2.27 | 0.67 |
| 2:J:14:ARG:O | 2:J:63:ASN:HA | 1.94 | 0.67 |
| 1:B:12:ILE:HG13 | 1:B:171:SER:HB3 | 1.76 | 0.67 |
| 1:F:35:GLN:HE22 | 1:F:309:VAL:HG23 | 1.60 | 0.67 |
| 1:D:69:SER:HA | 6:D:3063:HOH:O | 1.93 | 0.67 |
| 1:E:270:VAL:O | 1:E:270:VAL:HG12 | 1.94 | 0.67 |
| 2:G:138:CYS:HB3 | 2:G:141:CYS:O | 1.94 | 0.67 |
| 2:I:106:VAL:O | 2:I:152:ALA:HB1 | 1.95 | 0.67 |
| 2:J:18:ILE:HG22 | 2:J:21:ILE:HD11 | 1.76 | 0.67 |
| 1:E:83:LYS:HG3 | 1:F:51:ALA:HB2 | 1.76 | 0.67 |
| 2:J:114:CYS:SG | 2:J:116:SER:HB2 | 2.32 | 0.67 |
| 1:A:55:THR:O | 1:A:59:PHE:HB2 | 1.94 | 0.67 |
| 2:I:107:LEU:HD22 | 2:I:150:VAL:HG12 | 1.75 | 0.67 |
| 1:B:209:TRP:HZ3 | 1:B:211:LEU:HD21 | 1.60 | 0.67 |
| 1:D:188:ALA:HB1 | 1:D:189:PRO:HD2 | 1.75 | 0.67 |
| 2:J:51:GLY:C | 2:J:53:MET:H | 1.98 | 0.67 |
| 1:B:54:ARG:NH2 | 1:C:80:SER:OG | 2.28 | 0.67 |
| 2:I:38:THR:O | 2:L:47:ASN:ND2 | 2.27 | 0.67 |
| 2:I:88:ASN:C | 2:I:90:GLU:H | 1.97 | 0.66 |
| 1:E:49:PHE:HE2 | 1:E:81:LEU:HD22 | 1.60 | 0.66 |
| 1:A:240:TYR:O | 1:A:243:VAL:HG23 | 1.95 | 0.66 |
| 1:B:168:THR:HG21 | 1:B:266:PRO:HB3 | 1.77 | 0.66 |
| 1:D:51:ALA:HB2 | 1:F:83:LYS:HG3 | 1.75 | 0.66 |
| 1:A:104:MET:HE1 | 1:A:112:ALA:HA | 1.77 | 0.66 |
| 2:I:105:ASN:OD1 | 2:I:122:SER:HB3 | 1.96 | 0.66 |
| 1:B:106:HIS:HE1 | 1:B:108:GLN:HG2 | 1.60 | 0.66 |
| 2:L:14:ARG:HH21 | 2:L:88:ASN:ND2 | 1.92 | 0.66 |
| 1:B:265:HIS:ND1 | 1:B:266:PRO:O | 2.19 | 0.66 |
| 1:F:63:MET:HG3 | 1:F:300:LEU:CD1 | 2.26 | 0.66 |
| 2:J:103:ILE:HD11 | 2:J:107:LEU:HG | 1.78 | 0.66 |
| 1:F:170:HIS:O | 1:F:174:GLN:HG3 | 1.96 | 0.66 |
| 2:K:99:LEU:HD12 | 2:K:129:LYS:HE2 | 1.78 | 0.66 |
| 1:C:55:THR:O | 1:C:59:PHE:HB2 | 1.96 | 0.66 |
| 1:B:170:HIS:O | 1:B:174:GLN:HG3 | 1.96 | 0.66 |
| 1:E:265:HIS:C | 1:E:266:PRO:O | 2.30 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:219:MET:CE | 1:A:254:LEU:HD23 | 2.25 | 0.66 |
| 1:A:75:ASP:OD2 | 1:A:77:ALA:HB3 | 1.96 | 0.66 |
| 2:I:109:CYS:CB | 2:I:138:CYS:SG | 2.84 | 0.66 |
| 2:G:134:ILE:HB | 2:G:147:HIS:HD2 | 1.60 | 0.66 |
| 1:F:59:PHE:CE1 | 1:F:136:THR:HG21 | 2.31 | 0.66 |
| 1:C:81:LEU:HD13 | 1:C:86:GLU:O | 1.96 | 0.66 |
| 2:H:86:ILE:HG23 | 2:H:91:VAL:HA | 1.77 | 0.65 |
| 2:L:22:PRO:HD3 | 2:L:57:ASP:O | 1.95 | 0.65 |
| 1:E:132:ASN:O | 1:E:167:ARG:HB2 | 1.96 | 0.65 |
| 1:E:299:LEU:O | 1:E:303:VAL:HG23 | 1.96 | 0.65 |
| 2:J:105:ASN:OD1 | 2:J:122:SER:HB3 | 1.97 | 0.65 |
| 1:F:159:MET:HE3 | 1:F:172:LEU:HD23 | 1.79 | 0.65 |
| 1:B:237:PRO:HA | 1:B:240:TYR:CD1 | 2.31 | 0.65 |
| 1:A:60:GLU:HG2 | 1:A:70:VAL:HG11 | 1.78 | 0.65 |
| 2:H:14:ARG:HB3 | 2:H:63:ASN:ND2 | 2.11 | 0.65 |
| 1:B:111:ALA:CB | 2:H:115:ILE:HD12 | 2.27 | 0.65 |
| 1:E:55:THR:O | 1:E:59:PHE:HB2 | 1.97 | 0.65 |
| 1:B:166:GLY:O | 1:B:169:VAL:HG22 | 1.97 | 0.65 |
| 2:H:46:LEU:HA | 2:H:57:ASP:OD1 | 1.96 | 0.65 |
| 2:L:23:ALA:H | 2:L:25:ILE:HG12 | 1.61 | 0.65 |
| 2:G:71:VAL:HG22 | 2:G:97:PRO:HG3 | 1.78 | 0.65 |
| 2:I:28:LYS:HE3 | 2:I:77:TYR:HE2 | 1.62 | 0.65 |
| 1:B:203:ASP:HB3 | 6:B:3061:HOH:O | 1.95 | 0.65 |
| 1:C:75:ASP:OD2 | 1:C:77:ALA:HB3 | 1.97 | 0.65 |
| 2:J:136:LEU:O | 2:J:144:GLU:HA | 1.97 | 0.65 |
| 1:A:44:ILE:HB | 1:A:63:MET:CE | 2.27 | 0.65 |
| 2:J:30:LEU:CD1 | 2:J:44:ILE:HD13 | 2.27 | 0.64 |
| 2:J:53:MET:CG | 2:J:54:GLY:H | 2.09 | 0.64 |
| 1:F:154:ASN:HA | 1:F:181:GLY:O | 1.97 | 0.64 |
| 1:D:105:ARG:NH2 | 3:D:2004:FLC:OB2 | 2.30 | 0.64 |
| 1:B:126:ASN:HD21 | 1:B:129:ASP:HB2 | 1.61 | 0.64 |
| 1:B:106:HIS:CE1 | 1:B:108:GLN:HG2 | 2.32 | 0.64 |
| 1:B:54:ARG:NH2 | 1:C:86:GLU:OE1 | 2.29 | 0.64 |
| 1:F:75:ASP:OD2 | 1:F:77:ALA:HB3 | 1.97 | 0.64 |
| 1:A:84:LYS:NZ | 3:C:2003:FLC:OHB | 2.30 | 0.64 |
| 2:L:115:ILE:C | 2:L:117:HIS:H | 2.01 | 0.64 |
| 2:L:17:VAL:O | 2:L:18:ILE:HG12 | 1.98 | 0.64 |
| 1:C:35:GLN:NE2 | 1:C:309:VAL:HG23 | 2.13 | 0.64 |
| 1:B:58:SER:HB3 | 1:C:98:TYR:CZ | 2.32 | 0.64 |
| 2:I:88:ASN:O | 2:I:90:GLU:N | 2.30 | 0.64 |
| 1:A:109:GLU:CB | 2:G:141:CYS:HB2 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:276:ASP:HB3 | 6:E:3077:HOH:O | 1.97 | 0.64 |
| 1:A:104:MET:CE | 1:A:112:ALA:HA | 2.28 | 0.64 |
| 1:B:54:ARG:HD3 | 1:B:267:LEU:CB | 2.27 | 0.64 |
| 1:C:49:PHE:HE2 | 1:C:81:LEU:HD23 | 1.61 | 0.64 |
| 2:G:94:LYS:HE2 | 2:G:96:ARG:HH21 | 1.62 | 0.64 |
| 1:F:94:VAL:HG23 | 1:F:95:ILE:N | 2.13 | 0.64 |
| 1:E:44:ILE:HB | 1:E:63:MET:HE3 | 1.79 | 0.64 |
| 2:H:39:ASP:HB3 | 2:K:55:ARG:NH1 | 2.13 | 0.64 |
| 2:J:6:LYS:O | 2:J:6:LYS:HG3 | 1.98 | 0.63 |
| 2:I:30:LEU:CD2 | 2:I:35:LEU:HD12 | 2.27 | 0.63 |
| 2:L:22:PRO:HB3 | 2:L:25:ILE:HB | 1.80 | 0.63 |
| 1:A:63:MET:HE1 | 1:A:70:VAL:HG22 | 1.80 | 0.63 |
| 2:I:55:ARG:HH11 | 2:L:39:ASP:CB | 2.12 | 0.63 |
| 1:E:26:THR:HG22 | 1:E:30:LEU:HD12 | 1.80 | 0.63 |
| 1:E:63:MET:HE1 | 1:E:70:VAL:HG22 | 1.79 | 0.63 |
| 1:E:132:ASN:ND2 | 1:E:133:GLN:H | 1.97 | 0.63 |
| 2:J:137:LYS:HA | 2:J:143:LYS:O | 1.97 | 0.63 |
| 2:K:12:ILE:HG13 | 2:K:60:LYS:HE2 | 1.79 | 0.63 |
| 2:I:42:ILE:HD12 | 2:I:44:ILE:HD11 | 1.80 | 0.63 |
| 1:B:109:GLU:HB3 | 2:H:141:CYS:HA | 1.78 | 0.63 |
| 2:K:137:LYS:HD3 | 2:K:144:GLU:HG3 | 1.81 | 0.63 |
| 1:F:134:HIS:CE1 | 1:F:137:GLN:HB2 | 2.33 | 0.63 |
| 2:G:30:LEU:HD21 | 2:G:59:ILE:HD13 | 1.81 | 0.63 |
| 1:F:91:THR:O | 1:F:94:VAL:HG22 | 1.98 | 0.63 |
| 1:A:69:SER:HA | 6:A:3041:HOH:O | 1.97 | 0.63 |
| 1:D:63:MET:HG3 | 1:D:300:LEU:CD1 | 2.27 | 0.63 |
| 2:K:75:ALA:O | 2:K:79:PRO:HG3 | 1.98 | 0.63 |
| 1:E:166:GLY:O | 1:E:169:VAL:HG22 | 1.97 | 0.63 |
| 1:F:140:LEU:HD23 | 1:F:295:ALA:HB3 | 1.81 | 0.63 |
| 2:L:12:ILE:CD1 | 2:L:15:GLY:HA2 | 2.29 | 0.63 |
| 2:I:76:LEU:HD13 | 2:I:103:ILE:CD1 | 2.28 | 0.63 |
| 2:G:25:ILE:HG22 | 2:G:29:LEU:HG | 1.81 | 0.63 |
| 1:B:174:GLN:HA | 1:B:201:MET:HE2 | 1.80 | 0.63 |
| 1:E:44:ILE:HB | 1:E:63:MET:HE2 | 1.79 | 0.63 |
| 1:F:114:LEU:HD23 | 2:L:115:ILE:HD11 | 1.77 | 0.63 |
| 2:K:30:LEU:CD2 | 2:K:44:ILE:HG12 | 2.25 | 0.63 |
| 1:A:43:VAL:HG11 | 1:C:61:THR:HG23 | 1.81 | 0.63 |
| 1:B:23:VAL:HG11 | 1:B:139:LEU:HD13 | 1.80 | 0.63 |
| 1:A:50:GLU:HB3 | 1:A:105:ARG:HG2 | 1.80 | 0.63 |
| 2:I:30:LEU:HD21 | 2:I:59:ILE:HG21 | 1.82 | 0.62 |
| 2:I:46:LEU:HB2 | 2:L:42:ILE:CG1 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:59:PHE:CE2 | 1:D:103:VAL:HG21 | 2.34 | 0.62 |
| 1:D:66:LEU:HD21 | 1:D:297:GLN:HG2 | 1.81 | 0.62 |
| 2:I:110:PRO:HD2 | 2:I:145:PHE:CD2 | 2.34 | 0.62 |
| 1:E:126:ASN:HD21 | 1:E:129:ASP:HB2 | 1.63 | 0.62 |
| 1:A:54:ARG:NH2 | 1:A:268:PRO:HG3 | 2.13 | 0.62 |
| 1:D:129:ASP:O | 1:D:129:ASP:OD1 | 2.17 | 0.62 |
| 2:K:2:THR:O | 2:K:4:ASP:N | 2.32 | 0.62 |
| 1:F:218:VAL:O | 1:F:222:VAL:HG13 | 1.99 | 0.62 |
| 1:A:132:ASN:O | 1:A:167:ARG:HB2 | 1.99 | 0.62 |
| 2:G:71:VAL:HG13 | 2:G:72:ASP:N | 2.13 | 0.62 |
| 1:F:219:MET:HE3 | 1:F:254:LEU:HD23 | 1.81 | 0.62 |
| 2:H:134:ILE:HD12 | 2:H:134:ILE:N | 2.14 | 0.62 |
| 2:I:51:GLY:HA2 | 6:I:1014:HOH:O | 1.99 | 0.62 |
| 1:E:114:LEU:CD2 | 2:K:119:GLU:HG3 | 2.28 | 0.62 |
| 1:B:189:PRO:HB3 | 1:B:246:GLN:OE1 | 2.00 | 0.62 |
| 2:L:18:ILE:CG2 | 2:L:19:ASP:H | 2.12 | 0.62 |
| 2:L:83:VAL:CG1 | 2:L:94:LYS:HB2 | 2.20 | 0.62 |
| 2:G:12:ILE:HD13 | 2:G:62:GLU:OE1 | 2.00 | 0.62 |
| 1:A:29:LYS:O | 1:A:31:LYS:N | 2.33 | 0.62 |
| 2:J:30:LEU:HA | 2:J:35:LEU:HD12 | 1.80 | 0.62 |
| 2:K:29:LEU:HD21 | 2:K:77:TYR:HB2 | 1.82 | 0.62 |
| 1:B:308:LEU:O | 1:B:310:LEU:N | 2.32 | 0.62 |
| 2:H:116:SER:HA | 2:H:121:VAL:HG21 | 1.82 | 0.62 |
| 2:H:14:ARG:HG3 | 2:H:65:PHE:CZ | 2.34 | 0.62 |
| 2:K:16:THR:HG22 | 2:K:17:VAL:N | 2.15 | 0.62 |
| 2:H:111:ASN:C | 2:H:113:ASN:H | 2.04 | 0.62 |
| 1:C:257:ALA:CB | 1:C:261:MET:HE2 | 2.25 | 0.62 |
| 1:B:108:GLN:CB | 2:H:115:ILE:HG13 | 2.29 | 0.62 |
| 2:L:86:ILE:HG21 | 2:L:92:VAL:HA | 1.82 | 0.61 |
| 1:D:227:MET:HE1 | 1:D:272:GLU:O | 2.00 | 0.61 |
| 2:I:100:PRO:O | 2:I:127:VAL:HB | 1.99 | 0.61 |
| 2:J:104:ASP:O | 2:J:105:ASN:HB2 | 1.99 | 0.61 |
| 1:C:229:ARG:HB3 | 3:C:2003:FLC:OA2 | 2.00 | 0.61 |
| 2:H:86:ILE:HG22 | 2:H:90:GLU:C | 2.21 | 0.61 |
| 1:F:44:ILE:HB | 1:F:63:MET:CE | 2.29 | 0.61 |
| 1:F:47:CYS:O | 1:F:104:MET:HA | 2.00 | 0.61 |
| 2:I:70:GLN:HB2 | 6:I:1007:HOH:O | 2.00 | 0.61 |
| 1:D:261:MET:HG2 | 1:D:262:LYS:N | 2.15 | 0.61 |
| 2:H:12:ILE:HG22 | 2:H:13:LYS:N | 2.15 | 0.61 |
| 2:H:109:CYS:N | 2:H:125:PHE:HZ | 1.98 | 0.61 |
| 1:B:162:ASP:HB2 | 1:B:192:LEU:HD13 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:214:SER:OG | 1:F:217:GLU:HG3 | 2.00 | 0.61 |
| 1:E:23:VAL:HG11 | 1:E:139:LEU:HD13 | 1.81 | 0.61 |
| 2:L:58:LEU:O | 2:L:59:ILE:HG13 | 2.00 | 0.61 |
| 1:C:265:HIS:ND1 | 1:C:267:LEU:HD12 | 2.16 | 0.61 |
| 1:E:105:ARG:HG3 | 1:E:128:GLY:HA3 | 1.82 | 0.61 |
| 1:C:12:ILE:HG13 | 1:C:171:SER:HB3 | 1.83 | 0.61 |
| 2:L:21:ILE:O | 2:L:21:ILE:CG1 | 2.46 | 0.61 |
| 1:D:132:ASN:O | 1:D:167:ARG:CB | 2.48 | 0.61 |
| 1:C:49:PHE:CE2 | 1:C:81:LEU:HD23 | 2.36 | 0.61 |
| 2:L:28:LYS:HE2 | 2:L:32:LEU:HD11 | 1.82 | 0.61 |
| 1:F:31:LYS:HE2 | 1:F:294:PHE:CE2 | 2.35 | 0.61 |
| 2:G:68:GLU:O | 2:G:70:GLN:N | 2.34 | 0.61 |
| 1:A:109:GLU:OE2 | 1:A:131:SER:HB3 | 2.00 | 0.61 |
| 1:B:54:ARG:HD3 | 1:B:267:LEU:HB3 | 1.83 | 0.61 |
| 1:A:279:LYS:HG2 | 1:A:279:LYS:O | 2.00 | 0.61 |
| 1:D:167:ARG:HE | 3:D:2004:FLC:HA1 | 1.65 | 0.61 |
| 2:G:30:LEU:HA | 2:G:35:LEU:HD12 | 1.83 | 0.61 |
| 2:K:9:VAL:HG11 | 2:K:58:LEU:HD23 | 1.83 | 0.61 |
| 1:E:77:ALA:O | 1:E:83:LYS:HE2 | 2.01 | 0.61 |
| 1:F:196:GLN:HG3 | 1:F:200:ASP:OD2 | 2.01 | 0.61 |
| 1:B:231:GLN:HE22 | 3:B:2002:FLC:HA1 | 1.66 | 0.61 |
| 1:C:26:THR:HG23 | 1:C:309:VAL:CG1 | 2.31 | 0.60 |
| 1:F:110:GLY:HA3 | 2:L:140:TYR:HB3 | 1.82 | 0.60 |
| 1:F:12:ILE:HG13 | 1:F:171:SER:HB3 | 1.82 | 0.60 |
| 2:G:111:ASN:HD22 | 2:G:111:ASN:C | 2.02 | 0.60 |
| 1:A:39:LEU:CD1 | 1:A:304:LEU:HD12 | 2.29 | 0.60 |
| 3:A:2001:FLC:OG1 | 5:A:3001:PO4:P | 2.60 | 0.60 |
| 1:C:267:LEU:HD13 | 1:C:285:TYR:HB2 | 1.84 | 0.60 |
| 2:G:101:GLU:O | 2:G:127:VAL:HG23 | 2.01 | 0.60 |
| 2:J:102:ARG:HB2 | 2:J:125:PHE:O | 2.01 | 0.60 |
| 2:H:111:ASN:HB2 | 2:H:145:PHE:HZ | 1.66 | 0.60 |
| 1:A:107:PRO:O | 1:A:130:GLY:HA3 | 2.01 | 0.60 |
| 2:H:15:GLY:HA3 | 2:H:61:ILE:O | 2.02 | 0.60 |
| 2:I:92:VAL:HG12 | 2:I:93:GLY:H | 1.66 | 0.60 |
| 1:E:11:SER:CB | 1:E:133:GLN:HG3 | 2.32 | 0.60 |
| 2:J:111:ASN:C | 2:J:113:ASN:H | 2.05 | 0.60 |
| 1:B:160:VAL:HG12 | 1:B:160:VAL:O | 2.00 | 0.60 |
| 1:E:63:MET:CE | 1:E:70:VAL:HG22 | 2.32 | 0.60 |
| 1:B:54:ARG:HD2 | 5:B:3002:PO4:O3 | 2.02 | 0.60 |
| 1:B:44:ILE:HG21 | 1:B:63:MET:CE | 2.32 | 0.60 |
| 1:B:159:MET:HE1 | 1:B:173:THR:OG1 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:13:LYS:HE3 | 2:I:88:ASN:CG | 2.22 | 0.60 |
| 1:B:200:ASP:HB3 | 2:H:128:ARG:NH2 | 2.17 | 0.60 |
| 1:D:196:GLN:HG3 | 1:D:200:ASP:OD2 | 2.01 | 0.60 |
| 1:F:43:VAL:HG22 | 1:F:69:SER:HB2 | 1.83 | 0.60 |
| 1:F:52:SER:HB2 | 1:F:105:ARG:NH1 | 2.17 | 0.60 |
| 1:A:101:ALA:HB2 | 1:A:304:LEU:HD21 | 1.83 | 0.59 |
| 1:A:111:ALA:HA | 2:G:115:ILE:CD1 | 2.32 | 0.59 |
| 2:L:14:ARG:HH11 | 2:L:65:PHE:HZ | 1.48 | 0.59 |
| 1:C:264:LEU:HB3 | 1:C:288:GLN:NE2 | 2.17 | 0.59 |
| 1:D:160:VAL:O | 1:D:161:GLY:O | 2.20 | 0.59 |
| 1:E:105:ARG:CZ | 1:E:167:ARG:NH2 | 2.65 | 0.59 |
| 2:K:125:PHE:HB3 | 2:K:136:LEU:HB3 | 1.83 | 0.59 |
| 2:L:12:ILE:HD13 | 2:L:62:GLU:HA | 1.84 | 0.59 |
| 1:B:45:ALA:HA | 1:B:71:VAL:O | 2.02 | 0.59 |
| 1:D:43:VAL:HG22 | 1:D:69:SER:HB2 | 1.82 | 0.59 |
| 1:F:114:LEU:HD23 | 2:L:115:ILE:CD1 | 2.30 | 0.59 |
| 1:D:52:SER:OG | 1:D:105:ARG:NH1 | 2.34 | 0.59 |
| 2:G:76:LEU:CD1 | 2:G:103:ILE:HG21 | 2.24 | 0.59 |
| 2:G:21:ILE:HB | 2:G:57:ASP:HB2 | 1.84 | 0.59 |
| 2:L:86:ILE:HG22 | 2:L:87:ASP:H | 1.68 | 0.59 |
| 2:H:13:LYS:HD3 | 2:H:13:LYS:C | 2.23 | 0.59 |
| 2:H:27:PHE:CZ | 2:K:31:SER:HB2 | 2.34 | 0.59 |
| 2:J:141:CYS:O | 2:J:143:LYS:N | 2.36 | 0.59 |
| 1:B:308:LEU:O | 1:B:310:LEU:HG | 2.02 | 0.59 |
| 2:I:71:VAL:O | 2:I:74:LEU:HG | 2.02 | 0.59 |
| 2:L:34:LYS:HB3 | 2:L:37:GLU:OE1 | 2.03 | 0.59 |
| 2:H:30:LEU:CD1 | 2:H:44:ILE:HD13 | 2.32 | 0.59 |
| 2:H:136:LEU:O | 2:H:144:GLU:HA | 2.03 | 0.59 |
| 1:A:131:SER:HB2 | 1:A:234:ARG:HD3 | 1.84 | 0.59 |
| 2:K:102:ARG:CZ | 2:K:102:ARG:HB3 | 2.32 | 0.59 |
| 2:J:17:VAL:CG1 | 2:J:86:ILE:HD12 | 2.32 | 0.59 |
| 1:D:31:LYS:HG3 | 1:D:294:PHE:CE1 | 2.38 | 0.59 |
| 2:J:94:LYS:CE | 2:J:96:ARG:HG3 | 2.32 | 0.59 |
| 2:G:69:ASP:HB3 | 6:G:1041:HOH:O | 2.01 | 0.59 |
| 1:D:81:LEU:HD12 | 1:D:86:GLU:O | 2.02 | 0.59 |
| 2:L:115:ILE:O | 2:L:117:HIS:N | 2.36 | 0.59 |
| 1:F:53:THR:N | 5:F:3006:PO4:O3 | 2.33 | 0.59 |
| 2:G:16:THR:HG22 | 2:G:64:THR:O | 2.03 | 0.59 |
| 1:E:12:ILE:HG13 | 1:E:171:SER:HB3 | 1.85 | 0.59 |
| 1:C:226:TYR:OH | 1:C:266:PRO:HG3 | 2.02 | 0.59 |
| 2:K:14:ARG:HA | 2:K:87:ASP:OD2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:267:LEU:HD12 | 1:F:94:VAL:CG1 | 2.33 | 0.59 |
| 1:A:267:LEU:O | 1:A:267:LEU:HG | 2.03 | 0.59 |
| 2:G:49:PRO:HA | 2:G:55:ARG:HG2 | 1.83 | 0.59 |
| 2:J:41:ARG:O | 2:J:62:GLU:HB3 | 2.02 | 0.59 |
| 1:E:229:ARG:NH1 | 1:E:232:LYS:HE2 | 2.17 | 0.59 |
| 2:L:83:VAL:HG22 | 2:L:95:SER:O | 2.03 | 0.58 |
| 1:E:232:LYS:HA | 1:E:235:LEU:HD12 | 1.85 | 0.58 |
| 1:A:79:THR:OG1 | 1:A:81:LEU:HB3 | 2.03 | 0.58 |
| 2:J:94:LYS:HE2 | 2:J:96:ARG:HG3 | 1.85 | 0.58 |
| 1:C:265:HIS:O | 1:C:266:PRO:C | 2.39 | 0.58 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CD2 | 2.38 | 0.58 |
| 1:E:140:LEU:HD13 | 1:E:292:GLY:HA2 | 1.86 | 0.58 |
| 1:F:217:GLU:HG2 | 6:F:3047:HOH:O | 2.03 | 0.58 |
| 1:B:120:GLY:O | 1:B:122:VAL:HG23 | 2.03 | 0.58 |
| 1:D:10:ILE:HD12 | 1:D:112:ALA:HB1 | 1.84 | 0.58 |
| 1:A:44:ILE:HG23 | 1:A:101:ALA:HB3 | 1.84 | 0.58 |
| 1:D:84:LYS:NZ | 3:E:2005:FLC:OHB | 2.36 | 0.58 |
| 1:B:81:LEU:HD13 | 1:B:86:GLU:O | 2.04 | 0.58 |
| 1:C:216:GLU:H | 1:C:216:GLU:CD | 2.06 | 0.58 |
| 2:L:17:VAL:HA | 2:L:60:LYS:HE2 | 1.85 | 0.58 |
| 1:B:110:GLY:HA3 | 2:H:140:TYR:HB3 | 1.86 | 0.58 |
| 1:B:111:ALA:HB2 | 2:H:115:ILE:CD1 | 2.34 | 0.58 |
| 2:J:16:THR:HG23 | 2:J:64:THR:O | 2.03 | 0.58 |
| 1:E:265:HIS:O | 1:E:266:PRO:O | 2.22 | 0.58 |
| 1:E:110:GLY:N | 1:E:129:ASP:OD1 | 2.37 | 0.58 |
| 1:F:120:GLY:O | 1:F:122:VAL:HG23 | 2.03 | 0.58 |
| 2:H:49:PRO:HG3 | 2:H:55:ARG:NH1 | 2.19 | 0.58 |
| 2:G:26:GLY:O | 2:G:30:LEU:HG | 2.04 | 0.58 |
| 1:F:267:LEU:N | 6:F:3075:HOH:O | 2.36 | 0.58 |
| 1:D:2:ASN:HB3 | 1:D:5:TYR:HB2 | 1.85 | 0.58 |
| 2:I:146:SER:O | 2:I:149:VAL:HG22 | 2.04 | 0.58 |
| 2:L:137:LYS:O | 2:L:137:LYS:HG3 | 2.03 | 0.58 |
| 2:I:19:ASP:O | 2:I:21:ILE:HD12 | 2.04 | 0.58 |
| 1:E:38:LEU:HD11 | 1:E:305:ASN:ND2 | 2.19 | 0.58 |
| 1:A:35:GLN:NE2 | 1:A:309:VAL:HG23 | 2.19 | 0.58 |
| 1:D:12:ILE:HG21 | 1:D:175:ALA:HB2 | 1.86 | 0.58 |
| 2:J:25:ILE:O | 2:J:29:LEU:HG | 2.04 | 0.58 |
| 1:D:227:MET:CE | 1:D:272:GLU:O | 2.51 | 0.57 |
| 2:G:115:ILE:O | 2:G:117:HIS:N | 2.37 | 0.57 |
| 1:B:132:ASN:O | 1:B:167:ARG:CB | 2.52 | 0.57 |
| 2:I:86:ILE:HG23 | 2:I:91:VAL:CA | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:26:THR:HG23 | 1:A:309:VAL:CG1 | 2.34 | 0.57 |
| 1:A:293:ILE:HG22 | 1:A:297:GLN:OE1 | 2.04 | 0.57 |
| 1:A:231:GLN:O | 1:A:235:LEU:HG | 2.05 | 0.57 |
| 1:A:290:GLY:C | 1:A:292:GLY:H | 2.07 | 0.57 |
| 1:B:81:LEU:CD1 | 1:B:86:GLU:O | 2.52 | 0.57 |
| 1:F:278:ASP:OD1 | 1:F:278:ASP:N | 2.37 | 0.57 |
| 1:A:44:ILE:HB | 1:A:63:MET:HE3 | 1.86 | 0.57 |
| 2:L:113:ASN:O | 2:L:113:ASN:OD1 | 2.21 | 0.57 |
| 1:D:189:PRO:HG2 | 1:D:192:LEU:HB2 | 1.86 | 0.57 |
| 1:F:140:LEU:CD2 | 1:F:292:GLY:HA2 | 2.19 | 0.57 |
| 1:F:110:GLY:N | 1:F:129:ASP:OD1 | 2.37 | 0.57 |
| 2:K:24:GLN:HA | 6:K:1008:HOH:O | 2.03 | 0.57 |
| 2:H:138:CYS:HB3 | 2:H:142:GLU:H | 1.69 | 0.57 |
| 1:E:88:LEU:H | 2:K:119:GLU:CD | 2.08 | 0.57 |
| 1:F:166:GLY:O | 1:F:169:VAL:HG22 | 2.04 | 0.57 |
| 2:H:106:VAL:HG12 | 2:H:107:LEU:HD23 | 1.84 | 0.57 |
| 1:D:229:ARG:NH2 | 1:F:84:LYS:HD3 | 2.20 | 0.57 |
| 1:D:159:MET:HA | 1:D:226:TYR:O | 2.05 | 0.57 |
| 2:L:114:CYS:CB | 2:L:141:CYS:SG | 2.85 | 0.57 |
| 2:L:18:ILE:CG1 | 2:L:83:VAL:HB | 2.34 | 0.57 |
| 1:A:63:MET:HE1 | 1:A:70:VAL:HG13 | 1.86 | 0.57 |
| 2:I:19:ASP:HB3 | 2:I:58:LEU:HD21 | 1.86 | 0.57 |
| 2:L:14:ARG:HE | 2:L:88:ASN:ND2 | 2.02 | 0.57 |
| 1:B:200:ASP:CB | 2:H:128:ARG:HH22 | 2.16 | 0.57 |
| 1:A:29:LYS:O | 1:A:30:LEU:C | 2.43 | 0.57 |
| 1:D:132:ASN:CG | 1:D:133:GLN:H | 2.08 | 0.57 |
| 1:C:35:GLN:NE2 | 1:C:309:VAL:CG2 | 2.67 | 0.57 |
| 2:I:55:ARG:NH1 | 2:L:39:ASP:HB3 | 2.18 | 0.57 |
| 2:G:18:ILE:HA | 2:G:83:VAL:HA | 1.86 | 0.57 |
| 2:K:138:CYS:HB2 | 2:K:142:GLU:H | 1.69 | 0.57 |
| 1:D:75:ASP:OD2 | 1:D:77:ALA:HB3 | 2.04 | 0.57 |
| 1:E:306:ARG:HB2 | 1:E:306:ARG:NH1 | 2.20 | 0.57 |
| 2:G:91:VAL:HG22 | 6:G:1046:HOH:O | 2.03 | 0.57 |
| 2:L:83:VAL:HG13 | 2:L:95:SER:O | 2.05 | 0.57 |
| 2:G:106:VAL:HG23 | 2:G:107:LEU:CD2 | 2.35 | 0.57 |
| 1:D:109:GLU:HA | 1:D:129:ASP:OD1 | 2.05 | 0.57 |
| 1:C:267:LEU:O | 1:C:267:LEU:HG | 2.04 | 0.57 |
| 1:E:266:PRO:HB2 | 3:E:2005:FLC:HA2 | 1.86 | 0.57 |
| 1:E:80:SER:HB3 | 1:E:84:LYS:HD2 | 1.86 | 0.57 |
| 1:D:134:HIS:NE2 | 3:D:2004:FLC:OB1 | 2.38 | 0.56 |
| 1:F:63:MET:HE1 | 1:F:70:VAL:HG13 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L:13:LYS:O | 2:L:14:ARG:HB2 | 2.04 | 0.56 |
| 2:G:109:CYS:SG | 2:G:111:ASN:HB3 | 2.45 | 0.56 |
| 2:J:103:ILE:HD11 | 2:J:107:LEU:CG | 2.35 | 0.56 |
| 1:B:9:ILE:HG21 | 1:B:299:LEU:HD21 | 1.88 | 0.56 |
| 1:C:54:ARG:NH1 | 1:C:267:LEU:HB3 | 2.20 | 0.56 |
| 2:H:86:ILE:HG22 | 2:H:90:GLU:O | 2.04 | 0.56 |
| 1:B:261:MET:HG2 | 1:B:262:LYS:H | 1.70 | 0.56 |
| 1:D:88:LEU:HD23 | 1:D:114:LEU:HD23 | 1.87 | 0.56 |
| 2:H:131:ALA:O | 2:H:132:ASN:HB3 | 2.04 | 0.56 |
| 1:B:117:GLU:OE1 | 2:H:139:LYS:NZ | 2.36 | 0.56 |
| 1:D:94:VAL:HG21 | 1:E:54:ARG:HH11 | 1.71 | 0.56 |
| 1:B:198:ILE:O | 1:B:202:LEU:HG | 2.05 | 0.56 |
| 1:B:19:ASP:O | 1:B:22:LEU:HB3 | 2.05 | 0.56 |
| 1:A:126:ASN:HD21 | 1:A:129:ASP:HB2 | 1.69 | 0.56 |
| 1:D:230:VAL:O | 1:D:232:LYS:N | 2.38 | 0.56 |
| 2:K:8:GLN:O | 2:K:9:VAL:HG13 | 2.05 | 0.56 |
| 1:C:106:HIS:ND1 | 1:C:107:PRO:CD | 2.69 | 0.56 |
| 1:A:110:GLY:N | 1:A:129:ASP:OD1 | 2.33 | 0.56 |
| 1:C:131:SER:HB3 | 1:C:234:ARG:HD3 | 1.87 | 0.56 |
| 2:L:130:ARG:HH11 | 2:L:130:ARG:HG2 | 1.71 | 0.56 |
| 1:E:106:HIS:ND1 | 1:E:107:PRO:HD2 | 2.20 | 0.56 |
| 1:C:188:ALA:HA | 1:C:247:PHE:CE2 | 2.39 | 0.56 |
| 2:G:110:PRO:HD2 | 2:G:145:PHE:CD2 | 2.41 | 0.56 |
| 1:D:105:ARG:NE | 1:D:167:ARG:HH22 | 2.04 | 0.56 |
| 2:G:103:ILE:HD11 | 2:G:136:LEU:HD13 | 1.87 | 0.56 |
| 1:B:239:GLU:C | 1:B:241:ALA:N | 2.54 | 0.56 |
| 1:D:109:GLU:HG3 | 1:D:130:GLY:O | 2.06 | 0.56 |
| 2:H:139:LYS:O | 2:H:139:LYS:HG2 | 2.05 | 0.56 |
| 1:E:29:LYS:HD3 | 1:E:310:LEU:O | 2.06 | 0.56 |
| 1:D:167:ARG:HH21 | 3:D:2004:FLC:CBC | 2.18 | 0.55 |
| 2:I:111:ASN:O | 2:I:117:HIS:CD2 | 2.59 | 0.55 |
| 1:C:59:PHE:CE1 | 1:C:136:THR:HG21 | 2.39 | 0.55 |
| 1:E:26:THR:HG23 | 1:E:309:VAL:HG11 | 1.89 | 0.55 |
| 2:I:50:SER:HB3 | 2:I:56:LYS:HE2 | 1.86 | 0.55 |
| 2:K:138:CYS:HB2 | 2:K:142:GLU:N | 2.20 | 0.55 |
| 1:A:219:MET:HE1 | 1:A:254:LEU:HD23 | 1.87 | 0.55 |
| 2:K:78:ALA:C | 2:K:80:GLN:H | 2.09 | 0.55 |
| 1:C:174:GLN:HA | 1:C:201:MET:HE1 | 1.87 | 0.55 |
| 2:H:30:LEU:HD21 | 2:H:59:ILE:HG23 | 1.86 | 0.55 |
| 1:E:35:GLN:HE22 | 1:E:309:VAL:HG23 | 1.70 | 0.55 |
| 1:F:174:GLN:HA | 1:F:201:MET:HE3 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:46:LEU:HB2 | 2:K:42:ILE:HB | 1.87 | 0.55 |
| 1:E:17:ARG:HD2 | 1:E:179:PHE:CE1 | 2.40 | 0.55 |
| 2:L:75:ALA:CB | 2:L:98:SER:O | 2.54 | 0.55 |
| 3:A:2001:FLC:OG1 | 5:A:3001:PO4:O4 | 2.24 | 0.55 |
| 1:A:219:MET:HE3 | 1:A:254:LEU:HD23 | 1.87 | 0.55 |
| 1:C:131:SER:CB | 1:C:234:ARG:HD3 | 2.36 | 0.55 |
| 1:C:264:LEU:HB3 | 1:C:288:GLN:HE22 | 1.72 | 0.55 |
| 2:I:20:HIS:HA | 2:I:56:LYS:HD2 | 1.88 | 0.55 |
| 1:D:63:MET:HG3 | 1:D:300:LEU:HD11 | 1.87 | 0.55 |
| 1:C:188:ALA:HB1 | 1:C:189:PRO:HD2 | 1.88 | 0.55 |
| 1:A:11:SER:HB3 | 1:A:14:ASP:OD2 | 2.06 | 0.55 |
| 1:B:101:ALA:HB2 | 1:B:304:LEU:HD21 | 1.89 | 0.55 |
| 2:L:14:ARG:CD | 2:L:65:PHE:CZ | 2.86 | 0.55 |
| 1:D:120:GLY:C | 1:D:122:VAL:H | 2.09 | 0.55 |
| 1:B:116:THR:HG22 | 1:B:124:VAL:HB | 1.88 | 0.55 |
| 2:I:42:ILE:O | 2:I:42:ILE:HG13 | 2.05 | 0.55 |
| 2:I:44:ILE:HB | 2:L:44:ILE:CB | 2.37 | 0.55 |
| 1:C:129:ASP:O | 1:C:130:GLY:C | 2.42 | 0.55 |
| 2:H:115:ILE:O | 2:H:115:ILE:HG22 | 2.06 | 0.55 |
| 1:D:55:THR:O | 1:D:59:PHE:HB2 | 2.07 | 0.55 |
| 1:D:63:MET:HE2 | 1:D:70:VAL:CG2 | 2.37 | 0.55 |
| 2:K:107:LEU:HD13 | 2:K:150:VAL:HG11 | 1.87 | 0.55 |
| 2:L:43:THR:O | 2:L:59:ILE:HG12 | 2.06 | 0.55 |
| 2:G:48:LEU:CD2 | 2:J:41:ARG:HD2 | 2.33 | 0.55 |
| 2:J:47:ASN:HB3 | 2:J:55:ARG:CD | 2.37 | 0.55 |
| 1:C:267:LEU:O | 1:C:269:ARG:N | 2.40 | 0.55 |
| 1:E:237:PRO:HA | 1:E:240:TYR:CD2 | 2.42 | 0.55 |
| 1:C:234:ARG:HH11 | 1:C:234:ARG:HG2 | 1.72 | 0.55 |
| 1:A:166:GLY:O | 1:A:169:VAL:HG22 | 2.06 | 0.55 |
| 2:J:104:ASP:HB2 | 2:J:123:SER:C | 2.27 | 0.55 |
| 1:F:77:ALA:O | 1:F:83:LYS:HE2 | 2.06 | 0.55 |
| 1:F:137:GLN:HG2 | 1:F:168:THR:HG22 | 1.88 | 0.55 |
| 1:F:11:SER:HB3 | 1:F:14:ASP:OD2 | 2.07 | 0.55 |
| 1:B:264:LEU:HB3 | 1:B:288:GLN:NE2 | 2.22 | 0.55 |
| 2:G:71:VAL:CG1 | 2:G:72:ASP:N | 2.70 | 0.55 |
| 2:K:111:ASN:ND2 | 2:K:143:LYS:HE2 | 2.22 | 0.55 |
| 2:G:102:ARG:HD3 | 6:G:1003:HOH:O | 2.06 | 0.55 |
| 1:C:170:HIS:O | 1:C:174:GLN:HG3 | 2.06 | 0.54 |
| 1:B:50:GLU:HB3 | 1:B:105:ARG:HG2 | 1.89 | 0.54 |
| 2:J:115:ILE:HD11 | 2:J:119:GLU:HG3 | 1.88 | 0.54 |
| 1:C:140:LEU:HD22 | 1:C:292:GLY:CA | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:265:HIS:C | 1:B:266:PRO:O | 2.38 | 0.54 |
| 2:K:25:ILE:HG22 | 2:K:29:LEU:HG | 1.89 | 0.54 |
| 2:G:100:PRO:O | 2:G:127:VAL:HB | 2.07 | 0.54 |
| 2:H:102:ARG:HB3 | 2:H:126:ALA:HA | 1.89 | 0.54 |
| 1:D:134:HIS:CE1 | 1:D:137:GLN:HB2 | 2.42 | 0.54 |
| 2:L:12:ILE:HD13 | 2:L:62:GLU:HB2 | 1.87 | 0.54 |
| 2:L:16:THR:O | 2:L:60:LYS:HD3 | 2.07 | 0.54 |
| 1:E:267:LEU:O | 1:E:268:PRO:C | 2.42 | 0.54 |
| 2:I:38:THR:HG22 | 2:I:40:GLN:CB | 2.36 | 0.54 |
| 1:D:45:ALA:HA | 1:D:71:VAL:O | 2.07 | 0.54 |
| 2:L:99:LEU:HG | 2:L:127:VAL:HG11 | 1.87 | 0.54 |
| 1:D:17:ARG:HG2 | 1:D:17:ARG:HH11 | 1.72 | 0.54 |
| 1:C:299:LEU:O | 1:C:303:VAL:HG23 | 2.08 | 0.54 |
| 2:I:44:ILE:HB | 2:L:44:ILE:HB | 1.89 | 0.54 |
| 2:G:68:GLU:C | 2:G:70:GLN:N | 2.61 | 0.54 |
| 1:F:285:TYR:O | 1:F:288:GLN:HG2 | 2.07 | 0.54 |
| 1:B:114:LEU:HD13 | 2:H:121:VAL:HG12 | 1.89 | 0.54 |
| 1:D:168:THR:HG21 | 1:D:266:PRO:HG2 | 1.89 | 0.54 |
| 2:J:67:SER:H | 2:J:70:GLN:NE2 | 2.03 | 0.54 |
| 1:E:105:ARG:NH2 | 1:E:167:ARG:HH21 | 2.04 | 0.54 |
| 1:C:109:GLU:O | 2:I:115:ILE:HB | 2.07 | 0.54 |
| 2:L:20:HIS:HE1 | 2:L:84:ASN:HD21 | 1.55 | 0.54 |
| 1:D:267:LEU:HD21 | 1:D:285:TYR:CB | 2.37 | 0.54 |
| 1:B:161:GLY:CA | 1:B:228:THR:OG1 | 2.52 | 0.54 |
| 2:I:18:ILE:HG22 | 2:I:21:ILE:HD11 | 1.89 | 0.54 |
| 1:D:26:THR:HG23 | 1:D:309:VAL:CG1 | 2.37 | 0.54 |
| 1:C:114:LEU:CD1 | 2:I:121:VAL:HG11 | 2.37 | 0.54 |
| 1:D:29:LYS:HD3 | 1:D:310:LEU:O | 2.08 | 0.54 |
| 1:F:44:ILE:HB | 1:F:63:MET:HE3 | 1.90 | 0.54 |
| 1:D:199:LEU:HD22 | 1:D:209:TRP:CZ3 | 2.43 | 0.54 |
| 1:F:225:LEU:CD2 | 1:F:227:MET:CE | 2.86 | 0.54 |
| 1:B:137:GLN:HG2 | 1:B:168:THR:HG22 | 1.89 | 0.54 |
| 1:F:138:THR:O | 1:F:142:LEU:HG | 2.07 | 0.54 |
| 2:L:146:SER:OG | 2:L:149:VAL:HG23 | 2.08 | 0.54 |
| 2:H:76:LEU:HD12 | 2:H:103:ILE:HD11 | 1.89 | 0.54 |
| 2:L:41:ARG:C | 2:L:42:ILE:HG12 | 2.28 | 0.54 |
| 2:G:68:GLU:C | 2:G:70:GLN:H | 2.11 | 0.54 |
| 1:C:265:HIS:ND1 | 1:C:266:PRO:O | 2.41 | 0.54 |
| 2:H:111:ASN:O | 2:H:113:ASN:N | 2.38 | 0.54 |
| 2:G:106:VAL:HG23 | 2:G:107:LEU:HD23 | 1.89 | 0.54 |
| 2:G:46:LEU:HD13 | 2:J:36:THR:HG23 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:27:PHE:CB | 2:L:36:THR:HG21 | 2.38 | 0.54 |
| 2:I:44:ILE:HB | 2:L:44:ILE:HG22 | 1.90 | 0.54 |
| 2:L:83:VAL:HG12 | 2:L:84:ASN:H | 1.71 | 0.54 |
| 2:L:91:VAL:HG12 | 2:L:92:VAL:N | 2.22 | 0.54 |
| 2:K:9:VAL:HG11 | 2:K:58:LEU:CD2 | 2.38 | 0.54 |
| 1:B:108:GLN:HB2 | 2:H:115:ILE:CG1 | 2.33 | 0.54 |
| 1:E:140:LEU:HD13 | 1:E:292:GLY:CA | 2.38 | 0.54 |
| 1:D:83:LYS:HG3 | 1:E:51:ALA:HB2 | 1.89 | 0.54 |
| 1:C:204:GLU:HG2 | 1:C:205:LYS:N | 2.22 | 0.54 |
| 2:G:14:ARG:HA | 2:G:86:ILE:O | 2.08 | 0.54 |
| 1:A:12:ILE:HG13 | 1:A:171:SER:HB3 | 1.90 | 0.54 |
| 1:D:110:GLY:O | 2:J:115:ILE:HG21 | 2.08 | 0.53 |
| 2:L:86:ILE:CG2 | 2:L:87:ASP:N | 2.71 | 0.53 |
| 1:C:49:PHE:CZ | 1:C:73:PHE:HZ | 2.25 | 0.53 |
| 1:E:140:LEU:HD11 | 1:E:288:GLN:O | 2.08 | 0.53 |
| 2:L:150:VAL:HG12 | 2:L:150:VAL:O | 2.08 | 0.53 |
| 1:B:10:ILE:HD12 | 1:B:112:ALA:HB1 | 1.89 | 0.53 |
| 2:K:41:ARG:HD3 | 2:K:62:GLU:OE2 | 2.08 | 0.53 |
| 2:K:17:VAL:HG21 | 2:K:86:ILE:CD1 | 2.37 | 0.53 |
| 1:B:58:SER:HB3 | 1:C:98:TYR:CE1 | 2.44 | 0.53 |
| 1:D:77:ALA:O | 1:D:83:LYS:HE2 | 2.08 | 0.53 |
| 1:F:301:ALA:O | 1:F:305:ASN:HB2 | 2.09 | 0.53 |
| 1:B:198:ILE:O | 1:B:201:MET:HG2 | 2.09 | 0.53 |
| 1:E:59:PHE:CD1 | 1:E:296:ARG:HD3 | 2.43 | 0.53 |
| 2:K:104:ASP:O | 2:K:106:VAL:HG23 | 2.08 | 0.53 |
| 1:F:267:LEU:O | 1:F:269:ARG:N | 2.40 | 0.53 |
| 1:D:161:GLY:HA3 | 1:D:228:THR:O | 2.08 | 0.53 |
| 1:D:63:MET:CE | 1:D:70:VAL:HG22 | 2.38 | 0.53 |
| 1:A:162:ASP:OD1 | 1:A:162:ASP:C | 2.46 | 0.53 |
| 1:E:216:GLU:HG3 | 1:E:219:MET:CB | 2.38 | 0.53 |
| 1:F:198:ILE:O | 1:F:202:LEU:HG | 2.07 | 0.53 |
| 2:I:12:ILE:HD13 | 2:I:61:ILE:N | 2.24 | 0.53 |
| 2:H:30:LEU:HD11 | 2:H:44:ILE:HD13 | 1.90 | 0.53 |
| 1:A:229:ARG:HD3 | 3:A:2001:FLC:OA1 | 2.09 | 0.53 |
| 1:D:35:GLN:HE22 | 1:D:309:VAL:HG23 | 1.72 | 0.53 |
| 2:G:119:GLU:HB3 | 2:G:120:PRO:CD | 2.38 | 0.53 |
| 1:D:267:LEU:O | 1:D:269:ARG:N | 2.41 | 0.53 |
| 1:C:137:GLN:HG2 | 1:C:168:THR:CG2 | 2.39 | 0.53 |
| 2:J:111:ASN:HD22 | 2:J:114:CYS:N | 2.07 | 0.53 |
| 2:L:86:ILE:CG2 | 2:L:93:GLY:H | 2.21 | 0.53 |
| 2:H:12:ILE:CG2 | 2:H:13:LYS:N | 2.71 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:40:GLN:HG2 | 2:J:63:ASN:HB3 | 1.91 | 0.53 |
| 1:B:44:ILE:CG2 | 1:B:63:MET:HE1 | 2.38 | 0.53 |
| 2:J:114:CYS:O | 2:J:116:SER:N | 2.42 | 0.53 |
| 2:L:83:VAL:CG1 | 2:L:84:ASN:N | 2.71 | 0.53 |
| 1:F:160:VAL:HG22 | 1:F:187:ILE:HB | 1.91 | 0.53 |
| 2:I:22:PRO:HB2 | 2:I:25:ILE:HG13 | 1.89 | 0.53 |
| 1:A:117:GLU:OE1 | 2:G:139:LYS:HE2 | 2.08 | 0.53 |
| 1:A:250:ARG:HG2 | 1:A:250:ARG:HH11 | 1.73 | 0.53 |
| 2:I:43:THR:HB | 2:I:60:LYS:HB2 | 1.90 | 0.53 |
| 1:B:126:ASN:ND2 | 1:B:129:ASP:HB2 | 2.24 | 0.53 |
| 1:E:63:MET:HE1 | 1:E:70:VAL:HG13 | 1.90 | 0.53 |
| 1:F:174:GLN:HG2 | 1:F:201:MET:HE1 | 1.91 | 0.53 |
| 1:F:23:VAL:HA | 1:F:302:LEU:HD11 | 1.91 | 0.53 |
| 2:K:43:THR:HB | 2:K:60:LYS:HG2 | 1.91 | 0.53 |
| 2:L:18:ILE:HD12 | 2:L:94:LYS:HE3 | 1.91 | 0.53 |
| 2:I:38:THR:HG22 | 2:I:40:GLN:HB3 | 1.90 | 0.53 |
| 2:I:28:LYS:HE3 | 2:I:77:TYR:CE2 | 2.44 | 0.53 |
| 1:B:44:ILE:HG21 | 1:B:63:MET:HE1 | 1.91 | 0.53 |
| 1:C:290:GLY:C | 1:C:292:GLY:N | 2.62 | 0.52 |
| 2:I:111:ASN:HB3 | 2:I:114:CYS:HB2 | 1.91 | 0.52 |
| 1:C:267:LEU:O | 1:C:268:PRO:C | 2.44 | 0.52 |
| 2:G:103:ILE:HG13 | 2:G:103:ILE:O | 2.10 | 0.52 |
| 2:H:17:VAL:HG23 | 2:H:86:ILE:HD11 | 1.89 | 0.52 |
| 2:K:86:ILE:C | 2:K:87:ASP:OD1 | 2.48 | 0.52 |
| 1:C:247:PHE:HB2 | 6:C:3043:HOH:O | 2.08 | 0.52 |
| 2:K:78:ALA:O | 2:K:80:GLN:N | 2.38 | 0.52 |
| 1:E:160:VAL:HG13 | 1:E:187:ILE:HB | 1.91 | 0.52 |
| 1:B:104:MET:HE1 | 1:B:115:ALA:HB3 | 1.91 | 0.52 |
| 2:I:12:ILE:CD1 | 2:I:61:ILE:H | 2.22 | 0.52 |
| 1:A:44:ILE:HB | 1:A:63:MET:HE2 | 1.90 | 0.52 |
| 1:A:187:ILE:O | 1:A:188:ALA:HB2 | 2.10 | 0.52 |
| 1:D:52:SER:HA | 5:D:3004:PO4:O1 | 2.08 | 0.52 |
| 2:K:38:THR:HG22 | 2:K:39:ASP:N | 2.24 | 0.52 |
| 2:I:88:ASN:C | 2:I:90:GLU:N | 2.61 | 0.52 |
| 2:L:104:ASP:O | 2:L:106:VAL:HG23 | 2.09 | 0.52 |
| 2:J:105:ASN:N | 2:J:123:SER:HB3 | 2.16 | 0.52 |
| 1:A:131:SER:O | 1:A:131:SER:OG | 2.28 | 0.52 |
| 1:B:55:THR:O | 1:B:59:PHE:HB2 | 2.10 | 0.52 |
| 1:B:265:HIS:O | 1:B:266:PRO:C | 2.42 | 0.52 |
| 1:B:188:ALA:HB1 | 1:B:189:PRO:HD2 | 1.92 | 0.52 |
| 1:D:49:PHE:HB2 | 1:D:107:PRO:HD3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:141:ASP:O | 1:B:145:ILE:HG13 | 2.09 | 0.52 |
| 1:C:230:VAL:O | 1:C:232:LYS:N | 2.38 | 0.52 |
| 1:B:295:ALA:O | 1:B:298:ALA:HB3 | 2.09 | 0.52 |
| 2:G:9:VAL:HG12 | 2:G:10:GLU:H | 1.75 | 0.52 |
| 1:A:53:THR:CG2 | 1:A:54:ARG:N | 2.72 | 0.52 |
| 1:A:189:PRO:HB3 | 1:A:246:GLN:NE2 | 2.24 | 0.52 |
| 2:G:28:LYS:HZ3 | 2:G:77:TYR:HE2 | 1.57 | 0.52 |
| 2:L:16:THR:CG2 | 2:L:84:ASN:HA | 2.38 | 0.52 |
| 1:C:50:GLU:HB2 | 1:C:107:PRO:HG3 | 1.91 | 0.52 |
| 1:F:104:MET:HE1 | 1:F:112:ALA:HA | 1.91 | 0.52 |
| 2:J:51:GLY:O | 2:J:53:MET:N | 2.41 | 0.52 |
| 2:H:25:ILE:O | 2:H:28:LYS:HB3 | 2.10 | 0.52 |
| 1:C:87:THR:HB | 2:I:119:GLU:OE2 | 2.10 | 0.52 |
| 2:L:67:SER:C | 2:L:69:ASP:H | 2.12 | 0.52 |
| 1:C:290:GLY:C | 1:C:292:GLY:H | 2.12 | 0.52 |
| 2:L:77:TYR:O | 2:L:78:ALA:HB2 | 2.10 | 0.52 |
| 1:F:234:ARG:HH11 | 1:F:234:ARG:HG2 | 1.74 | 0.52 |
| 2:I:37:GLU:HG2 | 2:I:37:GLU:O | 2.09 | 0.52 |
| 1:D:54:ARG:HH11 | 1:F:94:VAL:HG11 | 1.75 | 0.52 |
| 1:B:8:HIS:O | 1:B:9:ILE:HD13 | 2.09 | 0.52 |
| 1:A:65:ARG:NH1 | 1:B:43:VAL:HG23 | 2.25 | 0.52 |
| 1:A:106:HIS:ND1 | 1:A:107:PRO:HD2 | 2.25 | 0.52 |
| 1:E:63:MET:HG3 | 1:E:300:LEU:CD1 | 2.40 | 0.52 |
| 1:D:94:VAL:HG13 | 1:E:267:LEU:HD22 | 1.88 | 0.52 |
| 1:A:218:VAL:O | 1:A:222:VAL:HG13 | 2.10 | 0.52 |
| 1:E:202:LEU:HB3 | 1:E:207:ILE:HB | 1.92 | 0.52 |
| 2:L:90:GLU:O | 2:L:90:GLU:HG3 | 2.10 | 0.52 |
| 1:B:54:ARG:HD3 | 1:B:267:LEU:HB2 | 1.91 | 0.52 |
| 1:E:130:GLY:O | 1:E:131:SER:HB3 | 2.10 | 0.52 |
| 1:C:136:THR:HB | 1:C:296:ARG:HE | 1.74 | 0.51 |
| 2:G:1:MET:HG2 | 2:G:89:TYR:HB3 | 1.91 | 0.51 |
| 2:G:152:ALA:O | 2:G:153:ASN:OXT | 2.28 | 0.51 |
| 1:C:160:VAL:HB | 1:C:227:MET:CG | 2.38 | 0.51 |
| 2:G:101:GLU:O | 2:G:127:VAL:N | 2.37 | 0.51 |
| 1:D:31:LYS:HE2 | 1:D:294:PHE:CE2 | 2.45 | 0.51 |
| 2:H:146:SER:C | 2:H:148:ASN:H | 2.12 | 0.51 |
| 2:H:33:PHE:O | 2:H:34:LYS:C | 2.49 | 0.51 |
| 2:L:111:ASN:HB3 | 2:L:114:CYS:CB | 2.40 | 0.51 |
| 1:C:126:ASN:HD21 | 1:C:129:ASP:HB2 | 1.76 | 0.51 |
| 2:L:16:THR:HA | 2:L:86:ILE:CG1 | 2.37 | 0.51 |
| 2:H:19:ASP:OD1 | 2:H:20:HIS:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:45:GLY:O | 2:H:46:LEU:HD23 | 2.10 | 0.51 |
| 2:H:107:LEU:O | 2:H:108:VAL:HG13 | 2.10 | 0.51 |
| 2:H:108:VAL:CG2 | 2:H:153:ASN:HB3 | 2.41 | 0.51 |
| 2:I:92:VAL:O | 2:I:93:GLY:O | 2.28 | 0.51 |
| 1:E:132:ASN:O | 1:E:167:ARG:CB | 2.57 | 0.51 |
| 1:D:117:GLU:OE1 | 2:J:139:LYS:HE2 | 2.10 | 0.51 |
| 2:H:9:VAL:O | 2:H:10:GLU:HG3 | 2.11 | 0.51 |
| 1:F:183:ARG:NH1 | 1:F:185:TYR:HE1 | 2.08 | 0.51 |
| 2:I:111:ASN:O | 2:I:117:HIS:HD2 | 1.94 | 0.51 |
| 2:L:20:HIS:HA | 2:L:82:THR:OG1 | 2.11 | 0.51 |
| 1:B:140:LEU:CD2 | 1:B:292:GLY:HA2 | 2.38 | 0.51 |
| 1:E:63:MET:HG3 | 1:E:300:LEU:HD11 | 1.92 | 0.51 |
| 1:C:44:ILE:HG21 | 1:C:63:MET:HE2 | 1.92 | 0.51 |
| 1:C:199:LEU:HD13 | 1:C:209:TRP:CH2 | 2.44 | 0.51 |
| 2:G:17:VAL:CG2 | 2:G:60:LYS:HE3 | 2.36 | 0.51 |
| 1:B:309:VAL:HG22 | 1:B:309:VAL:O | 2.09 | 0.51 |
| 2:I:130:ARG:HD3 | 2:I:133:ASP:HB3 | 1.92 | 0.51 |
| 1:B:214:SER:HG | 1:B:217:GLU:HG3 | 1.76 | 0.51 |
| 2:G:147:HIS:O | 2:G:150:VAL:HG22 | 2.10 | 0.51 |
| 1:D:114:LEU:HD12 | 2:J:121:VAL:HG11 | 1.93 | 0.51 |
| 1:A:120:GLY:O | 1:A:121:ASN:HB2 | 2.10 | 0.51 |
| 1:B:286:PHE:CE1 | 1:C:93:SER:HB2 | 2.45 | 0.51 |
| 2:G:66:LEU:HB3 | 2:G:70:GLN:NE2 | 2.25 | 0.51 |
| 2:L:16:THR:HG23 | 2:L:84:ASN:C | 2.31 | 0.51 |
| 2:I:7:LEU:HD13 | 2:I:50:SER:HA | 1.92 | 0.51 |
| 2:H:108:VAL:HG21 | 2:H:153:ASN:HB3 | 1.91 | 0.51 |
| 1:F:195:PRO:O | 1:F:199:LEU:HG | 2.10 | 0.51 |
| 2:G:131:ALA:O | 2:G:132:ASN:CB | 2.59 | 0.51 |
| 2:L:91:VAL:CG1 | 2:L:92:VAL:N | 2.73 | 0.51 |
| 1:B:129:ASP:O | 1:B:130:GLY:C | 2.48 | 0.51 |
| 1:F:129:ASP:O | 1:F:130:GLY:C | 2.49 | 0.51 |
| 2:I:130:ARG:HG3 | 2:I:131:ALA:N | 2.26 | 0.51 |
| 2:K:146:SER:O | 2:K:150:VAL:HG23 | 2.11 | 0.51 |
| 1:E:222:VAL:HG23 | 1:E:261:MET:SD | 2.51 | 0.51 |
| 1:A:241:ALA:HB2 | 1:E:241:ALA:CB | 2.40 | 0.51 |
| 1:C:105:ARG:HB2 | 1:C:127:ALA:HB3 | 1.92 | 0.51 |
| 2:L:111:ASN:HB3 | 2:L:114:CYS:HB2 | 1.92 | 0.51 |
| 1:C:47:CYS:O | 1:C:104:MET:HA | 2.09 | 0.51 |
| 1:C:134:HIS:CE1 | 1:C:137:GLN:HB2 | 2.46 | 0.51 |
| 2:J:47:ASN:HB3 | 2:J:55:ARG:HD2 | 1.93 | 0.51 |
| 1:F:35:GLN:NE2 | 1:F:309:VAL:HG23 | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:132:ASN:O | 1:A:133:GLN:O | 2.28 | 0.51 |
| 1:F:183:ARG:HH22 | 1:F:210:SER:HB3 | 1.76 | 0.51 |
| 1:C:162:ASP:OD1 | 1:C:162:ASP:C | 2.49 | 0.51 |
| 2:L:55:ARG:HG2 | 2:L:56:LYS:N | 2.25 | 0.51 |
| 2:J:135:ALA:O | 2:J:136:LEU:HD23 | 2.11 | 0.51 |
| 1:A:237:PRO:HA | 1:A:240:TYR:CD2 | 2.46 | 0.51 |
| 1:A:51:ALA:HB2 | 1:B:83:LYS:HG3 | 1.92 | 0.51 |
| 2:G:125:PHE:HA | 2:G:137:LYS:O | 2.10 | 0.51 |
| 2:J:109:CYS:CA | 2:J:125:PHE:HZ | 2.24 | 0.51 |
| 2:L:20:HIS:HE1 | 2:L:84:ASN:ND2 | 2.09 | 0.51 |
| 2:J:17:VAL:CG2 | 2:J:84:ASN:HB2 | 2.41 | 0.51 |
| 1:E:17:ARG:HH11 | 1:E:17:ARG:HG2 | 1.75 | 0.51 |
| 2:J:75:ALA:HB2 | 2:J:97:PRO:HB3 | 1.92 | 0.51 |
| 2:K:16:THR:HG22 | 2:K:17:VAL:H | 1.74 | 0.50 |
| 1:E:243:VAL:CG1 | 1:E:244:LYS:HD2 | 2.33 | 0.50 |
| 2:J:14:ARG:O | 2:J:14:ARG:CG | 2.57 | 0.50 |
| 2:G:83:VAL:HG12 | 2:G:95:SER:O | 2.11 | 0.50 |
| 1:F:160:VAL:HG12 | 1:F:161:GLY:N | 2.26 | 0.50 |
| 2:K:1:MET:HB2 | 2:K:11:ALA:CB | 2.42 | 0.50 |
| 2:L:12:ILE:HD13 | 2:L:62:GLU:CB | 2.41 | 0.50 |
| 2:L:18:ILE:HD11 | 2:L:94:LYS:HB3 | 1.93 | 0.50 |
| 1:D:54:ARG:CD | 1:D:267:LEU:HB2 | 2.34 | 0.50 |
| 1:E:137:GLN:NE2 | 1:E:140:LEU:HD23 | 2.26 | 0.50 |
| 1:D:17:ARG:HG2 | 1:D:17:ARG:NH1 | 2.26 | 0.50 |
| 1:C:157:VAL:HG13 | 1:C:224:ILE:HB | 1.94 | 0.50 |
| 2:H:6:LYS:HE3 | 2:K:10:GLU:OE2 | 2.09 | 0.50 |
| 2:G:66:LEU:HD13 | 2:G:70:GLN:OE1 | 2.11 | 0.50 |
| 1:A:267:LEU:HD21 | 1:A:286:PHE:CE1 | 2.46 | 0.50 |
| 1:A:49:PHE:HE2 | 1:A:81:LEU:HD22 | 1.77 | 0.50 |
| 1:C:81:LEU:HD12 | 1:C:81:LEU:O | 2.11 | 0.50 |
| 1:E:129:ASP:HB3 | 1:E:132:ASN:HB3 | 1.94 | 0.50 |
| 2:G:147:HIS:ND1 | 2:G:148:ASN:N | 2.60 | 0.50 |
| 2:H:21:ILE:CG2 | 2:H:25:ILE:HG22 | 2.41 | 0.50 |
| 2:J:7:LEU:O | 2:J:8:GLN:HB2 | 2.11 | 0.50 |
| 2:H:72:ASP:HB3 | 2:H:100:PRO:HG3 | 1.93 | 0.50 |
| 2:H:14:ARG:HA | 2:H:86:ILE:O | 2.11 | 0.50 |
| 1:C:17:ARG:HG3 | 1:C:17:ARG:O | 2.11 | 0.50 |
| 1:A:241:ALA:HB2 | 1:E:241:ALA:HB2 | 1.92 | 0.50 |
| 1:C:257:ALA:HB1 | 1:C:261:MET:SD | 2.51 | 0.50 |
| 2:L:78:ALA:CB | 2:L:81:ALA:HB2 | 2.35 | 0.50 |
| 1:A:268:PRO:HD3 | 3:A:2001:FLC:HG2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:165:TYR:O | 1:C:231:GLN:HG3 | 2.11 | 0.50 |
| 1:B:32:ALA:C | 1:B:34:PRO:HD3 | 2.31 | 0.50 |
| 1:E:26:THR:HG23 | 1:E:309:VAL:CG1 | 2.41 | 0.50 |
| 2:H:105:ASN:OD1 | 2:H:122:SER:HB3 | 2.12 | 0.50 |
| 2:L:21:ILE:HG21 | 2:L:56:LYS:CE | 2.42 | 0.50 |
| 2:G:50:SER:O | 2:G:54:GLY:O | 2.30 | 0.50 |
| 2:G:46:LEU:HD13 | 2:J:36:THR:CG2 | 2.42 | 0.50 |
| 1:F:225:LEU:CD2 | 1:F:227:MET:HE2 | 2.41 | 0.50 |
| 1:B:77:ALA:O | 1:B:83:LYS:HE2 | 2.11 | 0.50 |
| 2:K:77:TYR:C | 2:K:79:PRO:HD3 | 2.32 | 0.50 |
| 2:G:8:GLN:HE21 | 2:J:10:GLU:HA | 1.76 | 0.50 |
| 1:D:132:ASN:CG | 1:D:133:GLN:N | 2.64 | 0.50 |
| 2:G:76:LEU:HD13 | 2:G:103:ILE:HD13 | 1.93 | 0.50 |
| 2:L:70:GLN:HA | 2:L:73:GLN:HE21 | 1.71 | 0.50 |
| 1:A:265:HIS:HD2 | 1:A:267:LEU:HD12 | 1.77 | 0.50 |
| 1:C:187:ILE:O | 1:C:188:ALA:HB2 | 2.12 | 0.50 |
| 2:L:5:ASN:C | 2:L:6:LYS:HG3 | 2.33 | 0.50 |
| 1:B:196:GLN:O | 1:B:199:LEU:N | 2.45 | 0.50 |
| 2:H:135:ALA:O | 2:H:136:LEU:HD23 | 2.12 | 0.50 |
| 2:G:48:LEU:HB2 | 2:G:56:LYS:O | 2.10 | 0.50 |
| 1:F:233:GLU:HG3 | 1:F:234:ARG:HG3 | 1.92 | 0.50 |
| 1:A:265:HIS:O | 1:A:266:PRO:C | 2.49 | 0.50 |
| 2:J:45:GLY:O | 2:J:46:LEU:HD23 | 2.11 | 0.50 |
| 1:E:87:THR:HB | 2:K:119:GLU:OE1 | 2.11 | 0.50 |
| 2:G:110:PRO:HD2 | 2:G:145:PHE:CE2 | 2.46 | 0.50 |
| 1:F:22:LEU:O | 1:F:25:ALA:HB3 | 2.10 | 0.50 |
| 2:H:50:SER:HB2 | 2:H:56:LYS:CG | 2.42 | 0.50 |
| 2:H:77:TYR:C | 2:H:79:PRO:HD3 | 2.32 | 0.50 |
| 2:G:49:PRO:CD | 2:J:41:ARG:HD3 | 2.42 | 0.49 |
| 1:E:132:ASN:CG | 1:E:133:GLN:H | 2.15 | 0.49 |
| 2:L:115:ILE:C | 2:L:117:HIS:N | 2.65 | 0.49 |
| 2:L:21:ILE:CG2 | 2:L:56:LYS:CD | 2.79 | 0.49 |
| 2:I:30:LEU:HD21 | 2:I:59:ILE:CG2 | 2.41 | 0.49 |
| 1:A:268:PRO:CD | 3:A:2001:FLC:HG2 | 2.42 | 0.49 |
| 1:D:120:GLY:C | 1:D:122:VAL:N | 2.65 | 0.49 |
| 1:D:44:ILE:HB | 1:D:63:MET:CE | 2.42 | 0.49 |
| 2:H:50:SER:HB2 | 2:H:56:LYS:HG2 | 1.93 | 0.49 |
| 2:L:72:ASP:CB | 2:L:100:PRO:HG2 | 2.23 | 0.49 |
| 2:J:51:GLY:C | 2:J:53:MET:N | 2.66 | 0.49 |
| 1:B:229:ARG:HG2 | 1:B:230:VAL:O | 2.12 | 0.49 |
| 1:A:159:MET:HE2 | 1:A:169:VAL:HG12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L:21:ILE:HG22 | 2:L:56:LYS:HB3 | 1.94 | 0.49 |
| 2:J:111:ASN:C | 2:J:113:ASN:N | 2.66 | 0.49 |
| 2:J:66:LEU:HA | 2:J:70:GLN:NE2 | 2.27 | 0.49 |
| 1:E:59:PHE:O | 1:E:62:SER:HB2 | 2.12 | 0.49 |
| 2:I:91:VAL:HB | 6:I:1041:HOH:O | 2.12 | 0.49 |
| 2:I:67:SER:O | 2:I:71:VAL:HG13 | 2.13 | 0.49 |
| 1:D:104:MET:HE1 | 1:D:112:ALA:HA | 1.93 | 0.49 |
| 1:A:23:VAL:HG11 | 1:A:139:LEU:HD13 | 1.94 | 0.49 |
| 1:E:116:THR:HG22 | 1:E:124:VAL:HB | 1.93 | 0.49 |
| 2:K:76:LEU:CD2 | 2:K:134:ILE:HD11 | 2.42 | 0.49 |
| 2:K:69:ASP:HA | 2:K:72:ASP:HB2 | 1.95 | 0.49 |
| 2:J:16:THR:CG2 | 2:J:65:PHE:HA | 2.43 | 0.49 |
| 2:K:12:ILE:CD1 | 2:K:60:LYS:HB2 | 2.39 | 0.49 |
| 2:L:18:ILE:HG13 | 2:L:83:VAL:CB | 2.42 | 0.49 |
| 1:D:245:ALA:HB3 | 1:D:271:ASP:OD1 | 2.12 | 0.49 |
| 1:F:49:PHE:CE2 | 1:F:81:LEU:HD22 | 2.47 | 0.49 |
| 1:E:35:GLN:N | 1:E:36:PRO:HD3 | 2.27 | 0.49 |
| 1:B:237:PRO:HA | 1:B:240:TYR:CE1 | 2.46 | 0.49 |
| 2:H:21:ILE:HB | 2:H:57:ASP:HB2 | 1.95 | 0.49 |
| 1:D:114:LEU:CD1 | 2:J:121:VAL:HG11 | 2.42 | 0.49 |
| 2:J:121:VAL:O | 2:J:121:VAL:HG23 | 2.11 | 0.49 |
| 1:D:266:PRO:O | 1:D:268:PRO:HD2 | 2.13 | 0.49 |
| 1:B:201:MET:CG | 1:B:202:LEU:N | 2.76 | 0.49 |
| 2:H:71:VAL:HG13 | 2:H:97:PRO:HG3 | 1.95 | 0.49 |
| 2:I:124:SER:C | 2:I:125:PHE:CD1 | 2.86 | 0.49 |
| 1:E:159:MET:HB3 | 1:E:226:TYR:HB3 | 1.94 | 0.49 |
| 2:L:86:ILE:CG2 | 2:L:87:ASP:H | 2.25 | 0.49 |
| 1:A:39:LEU:HD13 | 1:A:304:LEU:CD1 | 2.39 | 0.49 |
| 1:F:94:VAL:CG2 | 1:F:95:ILE:N | 2.75 | 0.49 |
| 1:D:35:GLN:N | 1:D:36:PRO:HD3 | 2.28 | 0.49 |
| 1:E:38:LEU:CD1 | 1:E:305:ASN:ND2 | 2.76 | 0.49 |
| 2:H:6:LYS:O | 2:H:6:LYS:HG2 | 2.11 | 0.49 |
| 1:A:161:GLY:HA3 | 1:A:228:THR:OG1 | 2.13 | 0.49 |
| 1:A:148:THR:HG21 | 1:A:262:LYS:HG3 | 1.94 | 0.49 |
| 2:K:43:THR:O | 2:K:60:LYS:HG2 | 2.12 | 0.49 |
| 2:L:20:HIS:N | 2:L:82:THR:HG21 | 2.28 | 0.49 |
| 2:H:114:CYS:C | 2:H:116:SER:N | 2.66 | 0.49 |
| 1:E:236:ASP:OD1 | 1:E:237:PRO:HD2 | 2.13 | 0.49 |
| 1:B:52:SER:HB2 | 1:B:105:ARG:NH1 | 2.28 | 0.49 |
| 1:F:183:ARG:HG2 | 1:F:208:ALA:HB3 | 1.95 | 0.49 |
| 1:F:258:LYS:HE2 | 1:F:260:ASN:OD1 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:38:LEU:HD11 | 1:A:305:ASN:ND2 | 2.27 | 0.49 |
| 2:H:149:VAL:CG1 | 6:H:1039:HOH:O | 2.61 | 0.49 |
| 2:I:55:ARG:NH1 | 2:L:39:ASP:CB | 2.75 | 0.49 |
| 1:D:240:TYR:HB3 | 6:D:3030:HOH:O | 2.13 | 0.49 |
| 2:J:53:MET:CG | 2:J:54:GLY:N | 2.74 | 0.49 |
| 1:D:159:MET:HE2 | 1:D:169:VAL:HG12 | 1.94 | 0.49 |
| 2:G:47:ASN:O | 2:G:49:PRO:HD3 | 2.13 | 0.48 |
| 2:H:35:LEU:C | 2:H:37:GLU:H | 2.16 | 0.48 |
| 1:E:49:PHE:CE2 | 1:E:81:LEU:HD22 | 2.46 | 0.48 |
| 1:E:12:ILE:CG1 | 1:E:171:SER:HB3 | 2.42 | 0.48 |
| 1:B:49:PHE:HE2 | 1:B:81:LEU:HD23 | 1.76 | 0.48 |
| 1:E:17:ARG:NH1 | 1:E:17:ARG:HG2 | 2.27 | 0.48 |
| 2:I:24:GLN:OE1 | 2:L:36:THR:HG22 | 2.13 | 0.48 |
| 1:D:58:SER:HB3 | 1:F:98:TYR:CZ | 2.48 | 0.48 |
| 1:B:146:GLN:O | 1:B:146:GLN:HG2 | 2.13 | 0.48 |
| 2:H:40:GLN:OE1 | 2:H:63:ASN:HB2 | 2.12 | 0.48 |
| 2:G:83:VAL:HG22 | 2:G:84:ASN:N | 2.21 | 0.48 |
| 1:F:35:GLN:N | 1:F:36:PRO:HD3 | 2.27 | 0.48 |
| 1:E:81:LEU:HG | 1:E:81:LEU:O | 2.11 | 0.48 |
| 1:D:2:ASN:HD21 | 1:D:302:LEU:HB3 | 1.78 | 0.48 |
| 2:G:130:ARG:HD2 | 2:G:133:ASP:OD2 | 2.13 | 0.48 |
| 1:F:140:LEU:HD11 | 1:F:296:ARG:NH1 | 2.27 | 0.48 |
| 2:G:68:GLU:O | 2:G:71:VAL:N | 2.47 | 0.48 |
| 1:D:269:ARG:HH11 | 1:D:273:ILE:HG22 | 1.78 | 0.48 |
| 2:G:45:GLY:O | 2:G:57:ASP:HA | 2.13 | 0.48 |
| 1:D:192:LEU:HD21 | 1:D:235:LEU:HD21 | 1.95 | 0.48 |
| 1:D:117:GLU:OE1 | 2:J:139:LYS:CE | 2.60 | 0.48 |
| 2:L:14:ARG:HE | 2:L:88:ASN:CG | 2.16 | 0.48 |
| 2:J:123:SER:O | 2:J:124:SER:HB2 | 2.14 | 0.48 |
| 2:G:111:ASN:HD21 | 2:G:113:ASN:CB | 2.26 | 0.48 |
| 1:A:59:PHE:CE2 | 1:A:103:VAL:HG21 | 2.48 | 0.48 |
| 2:J:25:ILE:HD13 | 2:J:77:TYR:HB3 | 1.95 | 0.48 |
| 2:G:132:ASN:O | 2:G:133:ASP:HB3 | 2.12 | 0.48 |
| 1:F:279:LYS:O | 1:F:279:LYS:HG2 | 2.13 | 0.48 |
| 1:E:15:LEU:O | 1:E:178:LYS:HE3 | 2.12 | 0.48 |
| 2:L:14:ARG:HA | 2:L:88:ASN:O | 2.14 | 0.48 |
| 2:K:48:LEU:O | 2:K:55:ARG:HA | 2.13 | 0.48 |
| 2:H:149:VAL:O | 2:H:149:VAL:HG12 | 2.14 | 0.48 |
| 1:A:8:HIS:HE1 | 1:A:122:VAL:O | 1.96 | 0.48 |
| 1:E:249:LEU:HD23 | 1:E:273:ILE:HG23 | 1.95 | 0.48 |
| 2:G:126:ALA:O | 2:G:136:LEU:HA | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:136:LEU:N | 2:H:145:PHE:O | 2.39 | 0.48 |
| 2:L:70:GLN:O | 2:L:73:GLN:HB2 | 2.12 | 0.48 |
| 1:A:266:PRO:HB3 | 3:A:2001:FLC:HG1 | 1.96 | 0.48 |
| 2:I:92:VAL:CG1 | 2:I:93:GLY:N | 2.77 | 0.48 |
| 1:D:167:ARG:NE | 3:D:2004:FLC:HA1 | 2.29 | 0.48 |
| 2:G:61:ILE:HG22 | 2:G:64:THR:HB | 1.95 | 0.48 |
| 1:D:166:GLY:O | 1:D:169:VAL:HG22 | 2.13 | 0.48 |
| 2:H:12:ILE:HG12 | 2:H:60:LYS:HD3 | 1.96 | 0.48 |
| 1:F:249:LEU:HD11 | 1:F:254:LEU:HD21 | 1.94 | 0.48 |
| 1:F:237:PRO:HA | 1:F:240:TYR:CD2 | 2.48 | 0.48 |
| 1:F:134:HIS:N | 1:F:135:PRO:HD3 | 2.28 | 0.48 |
| 1:D:129:ASP:O | 1:D:132:ASN:HB3 | 2.13 | 0.48 |
| 2:J:114:CYS:O | 2:J:114:CYS:SG | 2.72 | 0.48 |
| 2:L:14:ARG:N | 2:L:88:ASN:O | 2.46 | 0.48 |
| 2:H:111:ASN:HB2 | 2:H:145:PHE:CZ | 2.48 | 0.48 |
| 1:D:271:ASP:C | 1:D:273:ILE:N | 2.67 | 0.48 |
| 1:A:59:PHE:CE1 | 1:A:136:THR:HG21 | 2.30 | 0.48 |
| 2:G:48:LEU:HD23 | 2:J:41:ARG:CD | 2.38 | 0.48 |
| 1:B:12:ILE:N | 1:B:133:GLN:OE1 | 2.45 | 0.48 |
| 1:A:227:MET:O | 1:A:265:HIS:ND1 | 2.41 | 0.48 |
| 2:J:145:PHE:HB3 | 2:J:149:VAL:CG2 | 2.44 | 0.48 |
| 1:F:112:ALA:O | 1:F:116:THR:HG23 | 2.14 | 0.48 |
| 2:H:73:GLN:OE1 | 2:H:103:ILE:HG23 | 2.13 | 0.48 |
| 1:A:251:ALA:N | 1:A:276:ASP:OD1 | 2.43 | 0.48 |
| 2:H:123:SER:OG | 2:H:125:PHE:HE1 | 1.96 | 0.48 |
| 1:A:49:PHE:CZ | 1:A:73:PHE:HZ | 2.31 | 0.48 |
| 2:K:81:ALA:O | 2:K:97:PRO:HD3 | 2.14 | 0.48 |
| 1:F:38:LEU:HD11 | 1:F:305:ASN:ND2 | 2.29 | 0.48 |
| 1:A:15:LEU:O | 1:A:178:LYS:HE3 | 2.14 | 0.48 |
| 2:H:14:ARG:HG3 | 2:H:65:PHE:HZ | 1.75 | 0.47 |
| 1:D:59:PHE:CE2 | 1:D:103:VAL:CG2 | 2.97 | 0.47 |
| 1:E:187:ILE:O | 1:E:188:ALA:HB2 | 2.14 | 0.47 |
| 2:J:114:CYS:O | 2:J:115:ILE:C | 2.52 | 0.47 |
| 2:I:42:ILE:CD1 | 2:I:44:ILE:HD11 | 2.44 | 0.47 |
| 2:G:39:ASP:O | 2:J:55:ARG:NH1 | 2.47 | 0.47 |
| 2:K:138:CYS:CB | 2:K:142:GLU:H | 2.27 | 0.47 |
| 2:H:146:SER:OG | 2:H:148:ASN:ND2 | 2.47 | 0.47 |
| 2:I:72:ASP:HB3 | 2:I:98:SER:O | 2.14 | 0.47 |
| 1:B:110:GLY:N | 1:B:129:ASP:OD1 | 2.43 | 0.47 |
| 2:J:67:SER:O | 2:J:68:GLU:C | 2.52 | 0.47 |
| 1:B:63:MET:HG2 | 1:B:300:LEU:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:194:MET:SD | 1:F:195:PRO:HD2 | 2.54 | 0.47 |
| 1:B:287:GLN:HA | 6:C:3061:HOH:O | 2.14 | 0.47 |
| 2:J:109:CYS:N | 2:J:125:PHE:HZ | 2.11 | 0.47 |
| 2:I:46:LEU:HD12 | 2:L:42:ILE:HG21 | 1.97 | 0.47 |
| 2:I:19:ASP:O | 2:I:81:ALA:HB1 | 2.14 | 0.47 |
| 2:I:103:ILE:HG13 | 2:I:127:VAL:CG2 | 2.44 | 0.47 |
| 1:C:94:VAL:HG23 | 1:C:95:ILE:N | 2.30 | 0.47 |
| 2:L:13:LYS:O | 2:L:14:ARG:CB | 2.62 | 0.47 |
| 1:F:49:PHE:HE2 | 1:F:81:LEU:HD22 | 1.79 | 0.47 |
| 2:K:78:ALA:HB1 | 2:K:81:ALA:HB2 | 1.96 | 0.47 |
| 2:K:107:LEU:HD22 | 2:K:151:LEU:O | 2.15 | 0.47 |
| 2:H:32:LEU:HD21 | 2:H:77:TYR:CE1 | 2.50 | 0.47 |
| 1:B:11:SER:O | 1:B:14:ASP:N | 2.33 | 0.47 |
| 1:D:38:LEU:HD11 | 1:D:305:ASN:ND2 | 2.30 | 0.47 |
| 2:I:30:LEU:CD2 | 2:I:59:ILE:HD13 | 2.44 | 0.47 |
| 1:C:130:GLY:O | 1:C:132:ASN:N | 2.47 | 0.47 |
| 1:F:267:LEU:HD21 | 1:F:285:TYR:HB2 | 1.96 | 0.47 |
| 1:E:237:PRO:HA | 1:E:240:TYR:CZ | 2.49 | 0.47 |
| 2:G:111:ASN:HD22 | 2:G:112:SER:N | 2.13 | 0.47 |
| 1:B:131:SER:HB3 | 1:B:234:ARG:HD2 | 1.97 | 0.47 |
| 2:G:16:THR:HB | 2:G:65:PHE:CD2 | 2.41 | 0.47 |
| 1:E:75:ASP:OD2 | 1:E:77:ALA:HB3 | 2.14 | 0.47 |
| 1:F:19:ASP:O | 1:F:22:LEU:HB3 | 2.14 | 0.47 |
| 2:I:102:ARG:HG2 | 2:I:126:ALA:HA | 1.95 | 0.47 |
| 2:H:44:ILE:HB | 2:K:44:ILE:HB | 1.96 | 0.47 |
| 2:K:8:GLN:HG3 | 2:K:48:LEU:HD22 | 1.96 | 0.47 |
| 2:I:15:GLY:HA2 | 2:I:63:ASN:N | 2.21 | 0.47 |
| 1:A:265:HIS:C | 1:A:266:PRO:O | 2.49 | 0.47 |
| 2:I:130:ARG:HG2 | 2:I:133:ASP:O | 2.14 | 0.47 |
| 1:E:66:LEU:HD21 | 1:E:297:GLN:NE2 | 2.26 | 0.47 |
| 2:H:102:ARG:CB | 2:H:126:ALA:HA | 2.45 | 0.47 |
| 1:A:161:GLY:O | 1:A:163:LEU:HG | 2.15 | 0.47 |
| 1:C:213:SER:HB2 | 6:C:3092:HOH:O | 2.14 | 0.47 |
| 1:E:164:LYS:HD3 | 1:E:165:TYR:CE2 | 2.50 | 0.47 |
| 1:D:201:MET:O | 1:D:201:MET:HG2 | 2.14 | 0.47 |
| 2:G:68:GLU:OE1 | 2:G:68:GLU:N | 2.36 | 0.47 |
| 2:L:12:ILE:HD13 | 2:L:62:GLU:CA | 2.45 | 0.47 |
| 2:H:12:ILE:HD11 | 2:H:60:LYS:HB3 | 1.97 | 0.47 |
| 1:C:161:GLY:CA | 1:C:228:THR:OG1 | 2.58 | 0.47 |
| 1:C:40:LYS:HG2 | 1:C:41:HIS:CD2 | 2.50 | 0.47 |
| 1:A:172:LEU:HG | 1:A:176:LEU:HD12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:135:PRO:O | 1:D:138:THR:HB | 2.14 | 0.47 |
| 1:A:63:MET:HG3 | 1:A:300:LEU:CD1 | 2.45 | 0.47 |
| 2:K:9:VAL:O | 2:K:9:VAL:HG23 | 2.15 | 0.47 |
| 2:I:20:HIS:O | 2:I:81:ALA:HB2 | 2.15 | 0.47 |
| 2:L:137:LYS:HB3 | 2:L:144:GLU:HG2 | 1.97 | 0.47 |
| 2:K:14:ARG:HH11 | 2:K:14:ARG:CB | 2.21 | 0.47 |
| 1:C:17:ARG:HD2 | 1:C:179:PHE:CE1 | 2.50 | 0.47 |
| 1:D:81:LEU:HA | 1:D:86:GLU:HB3 | 1.96 | 0.47 |
| 2:L:135:ALA:HA | 2:L:146:SER:HA | 1.96 | 0.47 |
| 2:H:146:SER:C | 2:H:148:ASN:N | 2.67 | 0.47 |
| 1:C:146:GLN:O | 1:C:150:GLY:N | 2.48 | 0.47 |
| 1:C:45:ALA:HB2 | 1:C:99:VAL:HG11 | 1.97 | 0.47 |
| 2:G:31:SER:HB3 | 2:J:27:PHE:HZ | 1.80 | 0.47 |
| 2:H:48:LEU:O | 2:H:55:ARG:HA | 2.15 | 0.46 |
| 1:F:140:LEU:HD11 | 1:F:296:ARG:HH12 | 1.80 | 0.46 |
| 2:G:43:THR:HB | 2:G:60:LYS:HB2 | 1.96 | 0.46 |
| 2:H:123:SER:O | 2:H:124:SER:HB2 | 2.15 | 0.46 |
| 2:J:42:ILE:CG2 | 2:J:43:THR:N | 2.78 | 0.46 |
| 1:C:232:LYS:HA | 1:C:235:LEU:HD12 | 1.96 | 0.46 |
| 1:F:292:GLY:O | 1:F:296:ARG:HG3 | 2.15 | 0.46 |
| 2:G:1:MET:HG3 | 2:G:1:MET:O | 2.15 | 0.46 |
| 1:B:54:ARG:CD | 1:B:267:LEU:HB2 | 2.45 | 0.46 |
| 1:D:63:MET:CE | 1:D:70:VAL:HG13 | 2.46 | 0.46 |
| 1:A:30:LEU:C | 1:A:32:ALA:H | 2.18 | 0.46 |
| 2:J:103:ILE:HD11 | 2:J:107:LEU:CD1 | 2.45 | 0.46 |
| 2:L:82:THR:CG2 | 2:L:83:VAL:N | 2.47 | 0.46 |
| 2:K:8:GLN:OE1 | 2:K:8:GLN:HA | 2.14 | 0.46 |
| 1:C:227:MET:CE | 1:C:249:LEU:HD22 | 2.44 | 0.46 |
| 1:E:170:HIS:NE2 | 1:E:195:PRO:HG2 | 2.31 | 0.46 |
| 2:G:131:ALA:O | 2:G:132:ASN:HB3 | 2.15 | 0.46 |
| 1:D:138:THR:O | 1:D:142:LEU:HG | 2.16 | 0.46 |
| 2:I:31:SER:CB | 2:L:27:PHE:HZ | 2.28 | 0.46 |
| 1:C:196:GLN:HG3 | 1:C:200:ASP:OD2 | 2.16 | 0.46 |
| 1:D:234:ARG:HG2 | 1:D:234:ARG:HH11 | 1.81 | 0.46 |
| 1:D:267:LEU:HD21 | 1:D:285:TYR:HB3 | 1.96 | 0.46 |
| 2:J:53:MET:HG3 | 2:J:54:GLY:N | 2.29 | 0.46 |
| 1:D:49:PHE:CE2 | 1:D:81:LEU:HD22 | 2.50 | 0.46 |
| 1:E:216:GLU:HA | 1:E:219:MET:HB2 | 1.96 | 0.46 |
| 2:I:102:ARG:HA | 2:I:125:PHE:O | 2.16 | 0.46 |
| 2:G:33:PHE:CE2 | 2:G:73:GLN:HG3 | 2.50 | 0.46 |
| 2:K:17:VAL:HG21 | 2:K:86:ILE:HD12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:108:GLN:HA | 2:L:113:ASN:OD1 | 2.16 | 0.46 |
| 2:K:109:CYS:HB2 | 2:K:138:CYS:SG | 2.54 | 0.46 |
| 1:D:49:PHE:HE2 | 1:D:81:LEU:HD22 | 1.79 | 0.46 |
| 2:H:78:ALA:HB1 | 2:H:81:ALA:HB2 | 1.98 | 0.46 |
| 1:F:277:VAL:O | 1:F:283:ALA:HB2 | 2.16 | 0.46 |
| 1:E:161:GLY:O | 1:E:163:LEU:HG | 2.15 | 0.46 |
| 2:J:111:ASN:ND2 | 2:J:114:CYS:N | 2.63 | 0.46 |
| 2:I:13:LYS:HB2 | 2:I:89:TYR:CZ | 2.49 | 0.46 |
| 2:K:125:PHE:HA | 2:K:137:LYS:O | 2.16 | 0.46 |
| 1:D:105:ARG:CZ | 3:D:2004:FLC:OB2 | 2.64 | 0.46 |
| 1:D:167:ARG:HE | 3:D:2004:FLC:CA | 2.28 | 0.46 |
| 2:L:14:ARG:NH2 | 2:L:88:ASN:HD22 | 2.04 | 0.46 |
| 1:A:63:MET:CE | 1:A:70:VAL:HG22 | 2.43 | 0.46 |
| 1:A:132:ASN:CG | 1:A:133:GLN:H | 2.19 | 0.46 |
| 1:B:162:ASP:C | 1:B:162:ASP:OD1 | 2.54 | 0.46 |
| 1:B:49:PHE:HE2 | 1:B:81:LEU:CD2 | 2.29 | 0.46 |
| 2:K:19:ASP:OD1 | 2:K:20:HIS:N | 2.49 | 0.46 |
| 2:L:115:ILE:CD1 | 2:L:119:GLU:HG3 | 2.45 | 0.46 |
| 2:J:111:ASN:HD21 | 2:J:113:ASN:HB3 | 1.80 | 0.46 |
| 2:L:8:GLN:CD | 2:L:58:LEU:HD11 | 2.36 | 0.46 |
| 1:C:109:GLU:OE1 | 2:I:113:ASN:HB3 | 2.15 | 0.46 |
| 2:I:109:CYS:O | 2:I:117:HIS:NE2 | 2.49 | 0.46 |
| 2:L:98:SER:C | 2:L:100:PRO:HD3 | 2.37 | 0.46 |
| 2:H:114:CYS:HB3 | 2:H:116:SER:OG | 2.15 | 0.46 |
| 1:D:264:LEU:O | 1:D:265:HIS:HB2 | 2.15 | 0.46 |
| 2:H:19:ASP:HB3 | 2:H:82:THR:CG2 | 2.46 | 0.46 |
| 1:D:59:PHE:CE1 | 1:D:136:THR:HG21 | 2.38 | 0.46 |
| 1:D:236:ASP:OD1 | 1:D:237:PRO:HD2 | 2.15 | 0.46 |
| 1:E:129:ASP:O | 1:E:130:GLY:C | 2.53 | 0.46 |
| 2:G:94:LYS:O | 2:G:94:LYS:HG2 | 2.16 | 0.46 |
| 1:A:26:THR:HG23 | 1:A:309:VAL:HG11 | 1.97 | 0.46 |
| 1:F:183:ARG:NH1 | 1:F:185:TYR:CE1 | 2.83 | 0.46 |
| 2:H:87:ASP:O | 2:H:88:ASN:C | 2.54 | 0.46 |
| 2:H:1:MET:O | 2:H:3:HIS:N | 2.47 | 0.46 |
| 1:A:98:TYR:CZ | 1:C:58:SER:HB3 | 2.51 | 0.46 |
| 2:K:50:SER:HB3 | 2:K:53:MET:C | 2.36 | 0.46 |
| 1:C:309:VAL:O | 1:C:310:LEU:HB3 | 2.16 | 0.46 |
| 1:B:53:THR:HB | 1:B:54:ARG:HH21 | 1.81 | 0.46 |
| 2:I:132:ASN:O | 2:I:133:ASP:CB | 2.59 | 0.46 |
| 1:E:49:PHE:CZ | 1:E:73:PHE:HZ | 2.33 | 0.46 |
| 1:D:104:MET:CE | 1:D:112:ALA:HA | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:23:ALA:O | 2:K:24:GLN:HB2 | 2.15 | 0.46 |
| 2:H:146:SER:O | 2:H:148:ASN:N | 2.49 | 0.46 |
| 1:E:104:MET:CE | 1:E:112:ALA:HA | 2.45 | 0.46 |
| 1:C:250:ARG:O | 1:C:253:ASP:HB2 | 2.16 | 0.46 |
| 1:C:132:ASN:CG | 1:C:133:GLN:N | 2.69 | 0.46 |
| 1:F:156:HIS:HD2 | 1:F:185:TYR:OH | 1.99 | 0.46 |
| 2:H:48:LEU:CD2 | 2:K:41:ARG:HE | 2.28 | 0.45 |
| 1:A:290:GLY:C | 1:A:292:GLY:N | 2.70 | 0.45 |
| 2:K:109:CYS:SG | 2:K:109:CYS:O | 2.73 | 0.45 |
| 2:J:94:LYS:HE3 | 2:J:96:ARG:HG3 | 1.98 | 0.45 |
| 1:F:25:ALA:O | 1:F:28:ALA:HB3 | 2.16 | 0.45 |
| 1:E:106:HIS:CE1 | 1:E:107:PRO:HD2 | 2.51 | 0.45 |
| 2:H:35:LEU:O | 2:H:37:GLU:N | 2.49 | 0.45 |
| 1:A:11:SER:CB | 1:A:133:GLN:HG3 | 2.45 | 0.45 |
| 2:I:42:ILE:HG22 | 2:I:61:ILE:HG23 | 1.98 | 0.45 |
| 1:B:132:ASN:CG | 1:B:133:GLN:H | 2.19 | 0.45 |
| 2:I:107:LEU:HD22 | 2:I:150:VAL:CG1 | 2.44 | 0.45 |
| 1:B:53:THR:HB | 1:C:80:SER:OG | 2.17 | 0.45 |
| 2:K:96:ARG:HH11 | 2:K:96:ARG:HG3 | 1.80 | 0.45 |
| 2:G:119:GLU:HB3 | 2:G:120:PRO:HD2 | 1.98 | 0.45 |
| 1:D:100:ASP:O | 1:D:101:ALA:HB2 | 2.16 | 0.45 |
| 1:C:5:TYR:O | 1:C:6:GLN:HB2 | 2.17 | 0.45 |
| 2:I:109:CYS:C | 2:I:111:ASN:H | 2.19 | 0.45 |
| 2:H:65:PHE:CD2 | 2:H:85:ARG:HD3 | 2.52 | 0.45 |
| 2:G:111:ASN:ND2 | 2:G:113:ASN:N | 2.53 | 0.45 |
| 1:D:270:VAL:O | 1:D:271:ASP:CG | 2.54 | 0.45 |
| 1:D:63:MET:HG3 | 1:D:300:LEU:HD13 | 1.97 | 0.45 |
| 2:G:134:ILE:HB | 2:G:147:HIS:CD2 | 2.47 | 0.45 |
| 2:G:71:VAL:CG1 | 2:G:72:ASP:H | 2.29 | 0.45 |
| 2:K:48:LEU:O | 2:K:56:LYS:N | 2.49 | 0.45 |
| 1:A:234:ARG:HG2 | 1:A:234:ARG:HH11 | 1.80 | 0.45 |
| 2:I:92:VAL:CG1 | 2:I:93:GLY:H | 2.29 | 0.45 |
| 2:J:18:ILE:CG2 | 2:J:21:ILE:HD11 | 2.44 | 0.45 |
| 2:I:28:LYS:O | 2:I:32:LEU:HB2 | 2.16 | 0.45 |
| 1:C:215:ILE:O | 1:C:217:GLU:N | 2.50 | 0.45 |
| 2:K:16:THR:OG1 | 2:K:65:PHE:HA | 2.17 | 0.45 |
| 1:E:43:VAL:O | 1:E:99:VAL:HB | 2.17 | 0.45 |
| 1:B:146:GLN:HB2 | 1:B:152:LEU:HG | 1.99 | 0.45 |
| 1:C:110:GLY:HA3 | 2:I:140:TYR:O | 2.16 | 0.45 |
| 2:K:21:ILE:HB | 2:K:57:ASP:O | 2.16 | 0.45 |
| 1:C:148:THR:HG21 | 1:C:262:LYS:HG3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:280:THR:HA | 1:C:281:PRO:HD3 | 1.80 | 0.45 |
| 1:F:154:ASN:HB3 | 6:F:3088:HOH:O | 2.16 | 0.45 |
| 1:F:120:GLY:O | 1:F:121:ASN:HB2 | 2.17 | 0.45 |
| 2:H:131:ALA:O | 2:H:132:ASN:CB | 2.65 | 0.45 |
| 1:B:33:ASN:N | 1:B:34:PRO:HD3 | 2.32 | 0.45 |
| 1:E:47:CYS:O | 1:E:104:MET:HA | 2.16 | 0.45 |
| 1:F:141:ASP:O | 1:F:145:ILE:HG13 | 2.16 | 0.45 |
| 2:K:92:VAL:HB | 2:K:93:GLY:H | 1.49 | 0.45 |
| 2:L:109:CYS:HB2 | 2:L:138:CYS:SG | 2.56 | 0.45 |
| 2:I:17:VAL:HG22 | 2:I:60:LYS:HD3 | 1.98 | 0.45 |
| 2:K:86:ILE:O | 2:K:87:ASP:OD1 | 2.35 | 0.45 |
| 1:D:160:VAL:HB | 1:D:227:MET:HG2 | 1.99 | 0.45 |
| 2:J:12:ILE:CG2 | 2:J:13:LYS:N | 2.79 | 0.45 |
| 1:A:54:ARG:NE | 5:A:3001:PO4:O3 | 2.50 | 0.45 |
| 2:L:71:VAL:HG11 | 2:L:85:ARG:HH21 | 1.81 | 0.45 |
| 2:J:21:ILE:HA | 2:J:22:PRO:HD3 | 1.83 | 0.45 |
| 1:C:81:LEU:CG | 1:C:81:LEU:O | 2.65 | 0.45 |
| 2:I:48:LEU:O | 2:I:56:LYS:HG2 | 2.17 | 0.45 |
| 1:C:246:GLN:HG2 | 1:C:246:GLN:O | 2.16 | 0.45 |
| 1:A:132:ASN:O | 1:A:133:GLN:C | 2.53 | 0.45 |
| 2:K:107:LEU:HD13 | 2:K:150:VAL:CG1 | 2.46 | 0.45 |
| 1:E:254:LEU:HD13 | 1:E:282:HIS:CD2 | 2.50 | 0.45 |
| 1:A:284:TRP:HA | 1:A:287:GLN:OE1 | 2.17 | 0.45 |
| 1:B:278:ASP:HB3 | 6:B:3077:HOH:O | 2.16 | 0.45 |
| 1:D:105:ARG:CD | 1:D:128:GLY:HA3 | 2.41 | 0.45 |
| 2:H:110:PRO:HD2 | 2:H:145:PHE:CD2 | 2.51 | 0.45 |
| 2:J:12:ILE:HD12 | 2:J:41:ARG:NH2 | 2.32 | 0.45 |
| 2:G:32:LEU:O | 2:G:32:LEU:HD12 | 2.16 | 0.45 |
| 1:A:137:GLN:HA | 1:A:140:LEU:HG | 1.98 | 0.45 |
| 1:F:30:LEU:HD22 | 1:F:297:GLN:HE21 | 1.81 | 0.45 |
| 2:K:78:ALA:N | 2:K:79:PRO:HD3 | 2.32 | 0.45 |
| 2:L:26:GLY:O | 2:L:30:LEU:HG | 2.17 | 0.45 |
| 2:I:30:LEU:HD13 | 2:I:44:ILE:HG12 | 1.99 | 0.45 |
| 1:B:114:LEU:CD1 | 2:H:121:VAL:HG12 | 2.47 | 0.45 |
| 1:D:286:PHE:O | 1:D:287:GLN:C | 2.54 | 0.45 |
| 2:I:107:LEU:HB3 | 2:I:150:VAL:CG1 | 2.47 | 0.45 |
| 1:F:227:MET:HE3 | 1:F:249:LEU:HB2 | 1.97 | 0.45 |
| 1:A:31:LYS:CG | 1:A:31:LYS:O | 2.64 | 0.45 |
| 1:D:51:ALA:CB | 1:F:83:LYS:HG3 | 2.46 | 0.45 |
| 1:F:215:ILE:C | 1:F:217:GLU:H | 2.19 | 0.45 |
| 1:D:75:ASP:OD1 | 1:D:77:ALA:CB | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:250:ARG:NH1 | 1:A:250:ARG:HG2 | 2.32 | 0.45 |
| 1:E:196:GLN:O | 1:E:199:LEU:N | 2.50 | 0.45 |
| 1:D:11:SER:HB2 | 2:J:142:GLU:OE2 | 2.17 | 0.45 |
| 2:L:103:ILE:O | 2:L:124:SER:HA | 2.17 | 0.45 |
| 1:E:28:ALA:HB2 | 6:E:3024:HOH:O | 2.16 | 0.45 |
| 1:D:129:ASP:O | 1:D:130:GLY:C | 2.56 | 0.44 |
| 2:J:137:LYS:HG2 | 2:J:144:GLU:HB3 | 2.00 | 0.44 |
| 2:I:42:ILE:HD11 | 2:L:46:LEU:CD1 | 2.36 | 0.44 |
| 2:H:114:CYS:C | 2:H:116:SER:H | 2.18 | 0.44 |
| 2:J:40:GLN:HG2 | 2:J:62:GLU:O | 2.16 | 0.44 |
| 2:J:16:THR:HG21 | 2:J:65:PHE:HA | 1.99 | 0.44 |
| 2:J:47:ASN:O | 2:J:55:ARG:HD3 | 2.17 | 0.44 |
| 1:A:11:SER:HA | 1:A:133:GLN:HG3 | 1.99 | 0.44 |
| 2:L:130:ARG:HG2 | 2:L:131:ALA:H | 1.82 | 0.44 |
| 1:B:264:LEU:HB3 | 1:B:288:GLN:HE22 | 1.81 | 0.44 |
| 2:J:128:ARG:HH11 | 2:J:128:ARG:HG3 | 1.82 | 0.44 |
| 2:L:42:ILE:HG22 | 2:L:44:ILE:CG1 | 2.33 | 0.44 |
| 2:K:30:LEU:HD13 | 2:K:59:ILE:HD13 | 1.99 | 0.44 |
| 1:A:54:ARG:HG2 | 1:B:98:TYR:OH | 2.16 | 0.44 |
| 2:I:19:ASP:C | 2:I:21:ILE:HD12 | 2.37 | 0.44 |
| 1:E:109:GLU:OE1 | 2:K:111:ASN:ND2 | 2.40 | 0.44 |
| 1:B:211:LEU:O | 1:B:212:HIS:CG | 2.70 | 0.44 |
| 1:C:229:ARG:NE | 3:C:2003:FLC:OA1 | 2.49 | 0.44 |
| 1:A:132:ASN:O | 1:A:167:ARG:CB | 2.65 | 0.44 |
| 1:D:223:ASP:O | 1:D:261:MET:HA | 2.18 | 0.44 |
| 1:C:277:VAL:O | 1:C:277:VAL:HG12 | 2.17 | 0.44 |
| 1:D:194:MET:SD | 1:D:198:ILE:HG21 | 2.57 | 0.44 |
| 2:I:111:ASN:O | 2:I:114:CYS:HB3 | 2.17 | 0.44 |
| 2:L:86:ILE:HD13 | 2:L:92:VAL:CA | 2.43 | 0.44 |
| 2:H:41:ARG:NE | 2:K:8:GLN:HE21 | 2.11 | 0.44 |
| 1:B:133:GLN:NE2 | 1:B:174:GLN:OE1 | 2.50 | 0.44 |
| 2:I:83:VAL:O | 2:I:83:VAL:HG13 | 2.18 | 0.44 |
| 1:A:290:GLY:O | 1:A:292:GLY:N | 2.51 | 0.44 |
| 2:G:94:LYS:CE | 2:G:96:ARG:HH21 | 2.28 | 0.44 |
| 2:K:34:LYS:HA | 6:K:1011:HOH:O | 2.16 | 0.44 |
| 1:B:88:LEU:O | 1:B:92:ILE:HG12 | 2.17 | 0.44 |
| 2:G:34:LYS:HB3 | 2:G:37:GLU:HG2 | 1.96 | 0.44 |
| 1:C:58:SER:OG | 1:C:296:ARG:NH1 | 2.51 | 0.44 |
| 2:G:56:LYS:HD2 | 2:G:56:LYS:C | 2.37 | 0.44 |
| 2:L:61:ILE:HD13 | 6:L:1047:HOH:O | 2.18 | 0.44 |
| 2:H:134:ILE:HB | 2:H:147:HIS:CD2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:138:THR:OG1 | 1:F:171:SER:HB2 | 2.17 | 0.44 |
| 2:H:104:ASP:O | 2:H:106:VAL:N | 2.51 | 0.44 |
| 1:D:138:THR:OG1 | 1:D:171:SER:HB2 | 2.17 | 0.44 |
| 2:I:6:LYS:O | 2:I:6:LYS:HG2 | 2.16 | 0.44 |
| 1:F:44:ILE:HB | 1:F:63:MET:HE2 | 1.99 | 0.44 |
| 1:A:54:ARG:CZ | 1:A:267:LEU:HB3 | 2.48 | 0.44 |
| 1:D:76:SER:HB2 | 1:D:81:LEU:HD23 | 1.99 | 0.44 |
| 1:E:277:VAL:O | 1:E:283:ALA:HB2 | 2.18 | 0.44 |
| 1:B:17:ARG:HH11 | 1:B:17:ARG:HG2 | 1.83 | 0.44 |
| 1:C:153:ASP:OD1 | 1:C:153:ASP:N | 2.50 | 0.44 |
| 2:H:42:ILE:HA | 2:H:60:LYS:O | 2.18 | 0.44 |
| 1:F:268:PRO:CD | 6:F:3075:HOH:O | 2.50 | 0.44 |
| 2:H:125:PHE:N | 2:H:125:PHE:CD1 | 2.86 | 0.44 |
| 1:D:265:HIS:O | 1:D:267:LEU:N | 2.51 | 0.44 |
| 2:G:49:PRO:HD2 | 2:J:41:ARG:HD3 | 1.98 | 0.44 |
| 2:J:86:ILE:CG2 | 2:J:87:ASP:N | 2.80 | 0.44 |
| 2:J:145:PHE:HB3 | 2:J:149:VAL:HG21 | 1.99 | 0.44 |
| 1:A:132:ASN:CG | 1:A:133:GLN:N | 2.71 | 0.44 |
| 1:B:187:ILE:O | 1:B:188:ALA:HB2 | 2.18 | 0.44 |
| 1:B:229:ARG:HB3 | 3:B:2002:FLC:OA2 | 2.16 | 0.44 |
| 1:E:151:ARG:HD2 | 1:E:153:ASP:O | 2.17 | 0.44 |
| 1:C:291:ASN:HA | 1:C:294:PHE:HD2 | 1.83 | 0.44 |
| 2:I:16:THR:N | 2:I:61:ILE:O | 2.44 | 0.44 |
| 1:C:284:TRP:O | 1:C:288:GLN:HB3 | 2.18 | 0.44 |
| 2:G:11:ALA:HA | 2:G:60:LYS:NZ | 2.33 | 0.44 |
| 1:D:284:TRP:HA | 1:D:287:GLN:OE1 | 2.18 | 0.44 |
| 2:I:32:LEU:C | 2:I:34:LYS:H | 2.21 | 0.44 |
| 2:G:70:GLN:O | 2:G:73:GLN:CG | 2.60 | 0.44 |
| 2:L:18:ILE:CB | 2:L:83:VAL:HB | 2.47 | 0.44 |
| 1:F:63:MET:HE1 | 1:F:70:VAL:HG22 | 1.99 | 0.44 |
| 2:G:115:ILE:C | 2:G:117:HIS:N | 2.71 | 0.44 |
| 2:J:57:ASP:C | 2:J:58:LEU:HD23 | 2.38 | 0.44 |
| 1:E:32:ALA:O | 1:E:34:PRO:HD3 | 2.16 | 0.44 |
| 2:I:41:ARG:HB3 | 2:I:62:GLU:CD | 2.37 | 0.44 |
| 2:K:109:CYS:SG | 2:K:114:CYS:CB | 3.05 | 0.44 |
| 1:E:66:LEU:HG | 1:E:297:GLN:HG3 | 1.99 | 0.44 |
| 2:K:32:LEU:HD11 | 2:K:106:VAL:CG1 | 2.47 | 0.44 |
| 1:B:160:VAL:HG13 | 1:B:187:ILE:HB | 2.00 | 0.44 |
| 2:J:25:ILE:O | 2:J:25:ILE:CG2 | 2.66 | 0.44 |
| 1:F:160:VAL:HG22 | 1:F:187:ILE:HD12 | 1.99 | 0.44 |
| 1:D:25:ALA:O | 1:D:28:ALA:HB3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:61:THR:O | 1:F:62:SER:C | 2.56 | 0.44 |
| 2:I:111:ASN:HD22 | 2:I:111:ASN:C | 2.20 | 0.44 |
| 2:K:134:ILE:O | 2:K:134:ILE:HG13 | 2.17 | 0.44 |
| 1:F:265:HIS:N | 1:F:288:GLN:HE22 | 1.93 | 0.44 |
| 1:F:54:ARG:N | 5:F:3006:PO4:O3 | 2.51 | 0.44 |
| 2:I:13:LYS:O | 2:I:14:ARG:HB3 | 2.18 | 0.44 |
| 1:C:120:GLY:O | 1:C:121:ASN:CG | 2.57 | 0.44 |
| 2:I:21:ILE:HB | 2:I:57:ASP:O | 2.17 | 0.44 |
| 2:K:137:LYS:HE2 | 2:K:142:GLU:C | 2.38 | 0.44 |
| 1:B:166:GLY:O | 1:B:168:THR:N | 2.51 | 0.44 |
| 1:C:229:ARG:NH2 | 3:C:2003:FLC:OA1 | 2.48 | 0.44 |
| 1:B:49:PHE:CE2 | 1:B:81:LEU:HD23 | 2.53 | 0.44 |
| 2:L:38:THR:HG22 | 2:L:40:GLN:HG3 | 2.00 | 0.44 |
| 2:H:36:THR:HG22 | 2:K:46:LEU:CD1 | 2.47 | 0.44 |
| 2:L:125:PHE:HB3 | 2:L:136:LEU:HB3 | 2.00 | 0.44 |
| 2:I:12:ILE:HD11 | 2:I:17:VAL:CG2 | 2.48 | 0.43 |
| 2:L:14:ARG:HA | 2:L:88:ASN:C | 2.39 | 0.43 |
| 2:G:83:VAL:O | 2:G:84:ASN:HB2 | 2.18 | 0.43 |
| 2:I:40:GLN:HG3 | 2:I:62:GLU:CB | 2.43 | 0.43 |
| 1:E:49:PHE:CD1 | 1:E:49:PHE:N | 2.85 | 0.43 |
| 1:A:189:PRO:HB3 | 1:A:246:GLN:HE22 | 1.82 | 0.43 |
| 2:L:21:ILE:CG2 | 2:L:56:LYS:CE | 2.95 | 0.43 |
| 2:L:20:HIS:CE1 | 2:L:84:ASN:HD21 | 2.36 | 0.43 |
| 2:G:138:CYS:CB | 2:G:141:CYS:O | 2.64 | 0.43 |
| 1:C:30:LEU:CD2 | 1:C:309:VAL:HG21 | 2.39 | 0.43 |
| 1:D:273:ILE:HD13 | 1:D:285:TYR:CE2 | 2.53 | 0.43 |
| 2:L:71:VAL:HG21 | 2:L:85:ARG:NE | 2.25 | 0.43 |
| 1:A:31:LYS:HG2 | 1:A:31:LYS:O | 2.18 | 0.43 |
| 2:G:130:ARG:O | 2:G:133:ASP:O | 2.36 | 0.43 |
| 2:L:52:GLU:O | 2:L:53:MET:HG3 | 2.18 | 0.43 |
| 2:L:115:ILE:HG23 | 2:L:116:SER:N | 2.32 | 0.43 |
| 2:L:55:ARG:O | 2:L:56:LYS:HG2 | 2.18 | 0.43 |
| 1:F:59:PHE:O | 1:F:62:SER:HB2 | 2.18 | 0.43 |
| 1:A:267:LEU:O | 1:A:267:LEU:CG | 2.66 | 0.43 |
| 2:G:20:HIS:C | 2:G:21:ILE:HG13 | 2.37 | 0.43 |
| 2:G:46:LEU:HB2 | 2:J:42:ILE:HB | 1.99 | 0.43 |
| 1:E:134:HIS:CE1 | 1:E:137:GLN:HB2 | 2.53 | 0.43 |
| 1:C:114:LEU:CD1 | 2:I:121:VAL:CG1 | 2.97 | 0.43 |
| 1:A:308:LEU:O | 1:A:309:VAL:C | 2.57 | 0.43 |
| 2:H:79:PRO:HG2 | 6:H:1035:HOH:O | 2.16 | 0.43 |
| 1:E:37:GLU:OE2 | 1:E:37:GLU:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:98:SER:O | 2:G:99:LEU:C | 2.56 | 0.43 |
| 1:D:109:GLU:OE1 | 2:J:113:ASN:HB3 | 2.19 | 0.43 |
| 2:J:114:CYS:HB2 | 2:J:141:CYS:HB3 | 2.00 | 0.43 |
| 2:I:47:ASN:O | 2:I:48:LEU:HD23 | 2.18 | 0.43 |
| 2:I:81:ALA:O | 2:I:97:PRO:HD2 | 2.18 | 0.43 |
| 2:J:33:PHE:O | 2:J:34:LYS:C | 2.55 | 0.43 |
| 2:J:47:ASN:HB3 | 2:J:55:ARG:HD3 | 2.00 | 0.43 |
| 2:I:66:LEU:HB3 | 2:I:70:GLN:HB3 | 2.00 | 0.43 |
| 2:I:27:PHE:HB3 | 2:L:36:THR:HG21 | 2.00 | 0.43 |
| 2:L:125:PHE:CD1 | 2:L:125:PHE:N | 2.86 | 0.43 |
| 2:I:135:ALA:HB1 | 2:I:144:GLU:CD | 2.38 | 0.43 |
| 1:A:277:VAL:HG12 | 1:A:277:VAL:O | 2.17 | 0.43 |
| 2:L:12:ILE:CG1 | 2:L:62:GLU:HB2 | 2.47 | 0.43 |
| 1:F:266:PRO:C | 6:F:3075:HOH:O | 2.56 | 0.43 |
| 2:G:83:VAL:HG13 | 2:G:84:ASN:N | 2.33 | 0.43 |
| 1:D:191:ALA:O | 1:D:192:LEU:HD23 | 2.18 | 0.43 |
| 1:F:261:MET:HG2 | 1:F:262:LYS:N | 2.34 | 0.43 |
| 1:A:230:VAL:O | 1:A:232:LYS:N | 2.52 | 0.43 |
| 2:L:38:THR:C | 2:L:40:GLN:H | 2.21 | 0.43 |
| 1:A:151:ARG:HD2 | 1:A:153:ASP:O | 2.19 | 0.43 |
| 2:K:108:VAL:O | 2:K:110:PRO:HD3 | 2.19 | 0.43 |
| 1:A:83:LYS:HG3 | 1:C:51:ALA:HB2 | 2.00 | 0.43 |
| 1:C:267:LEU:CG | 1:C:267:LEU:O | 2.66 | 0.43 |
| 2:L:16:THR:O | 2:L:17:VAL:HG22 | 2.19 | 0.43 |
| 2:L:83:VAL:CG1 | 2:L:84:ASN:H | 2.30 | 0.43 |
| 2:K:38:THR:HG22 | 2:K:40:GLN:N | 2.09 | 0.43 |
| 2:I:63:ASN:CB | 6:I:1042:HOH:O | 2.67 | 0.43 |
| 2:H:134:ILE:CD1 | 2:H:134:ILE:N | 2.82 | 0.43 |
| 2:J:25:ILE:HG12 | 2:J:28:LYS:HD2 | 2.01 | 0.43 |
| 2:L:149:VAL:O | 2:L:149:VAL:HG12 | 2.19 | 0.43 |
| 1:E:216:GLU:OE2 | 1:E:255:HIS:NE2 | 2.51 | 0.43 |
| 1:A:176:LEU:O | 1:A:182:ASN:ND2 | 2.50 | 0.43 |
| 1:D:9:ILE:HB | 1:D:125:LEU:HD22 | 2.00 | 0.43 |
| 2:G:3:HIS:CD2 | 2:G:6:LYS:HA | 2.54 | 0.43 |
| 1:F:188:ALA:HA | 1:F:247:PHE:HE2 | 1.83 | 0.43 |
| 2:G:70:GLN:O | 2:G:73:GLN:NE2 | 2.51 | 0.43 |
| 2:G:7:LEU:HG | 2:G:9:VAL:HG23 | 1.99 | 0.43 |
| 1:C:26:THR:HG23 | 1:C:309:VAL:HG11 | 2.01 | 0.43 |
| 2:K:138:CYS:CB | 2:K:141:CYS:SG | 3.01 | 0.43 |
| 1:F:174:GLN:HA | 1:F:201:MET:CE | 2.48 | 0.43 |
| 2:K:110:PRO:HD2 | 2:K:145:PHE:HD1 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:28:LYS:HD2 | 2:K:28:LYS:HA | 1.92 | 0.43 |
| 2:L:109:CYS:O | 2:L:117:HIS:NE2 | 2.52 | 0.43 |
| 1:D:129:ASP:CG | 1:D:132:ASN:HD22 | 2.22 | 0.43 |
| 2:I:12:ILE:CD1 | 2:I:61:ILE:N | 2.82 | 0.43 |
| 2:L:83:VAL:HA | 2:L:95:SER:O | 2.19 | 0.43 |
| 1:D:267:LEU:CD1 | 1:F:94:VAL:CG1 | 2.95 | 0.43 |
| 1:D:270:VAL:H | 1:D:272:GLU:CD | 2.21 | 0.43 |
| 1:B:223:ASP:O | 1:B:261:MET:HA | 2.19 | 0.43 |
| 1:E:229:ARG:HB3 | 3:E:2005:FLC:OA2 | 2.19 | 0.43 |
| 1:E:267:LEU:O | 1:E:269:ARG:N | 2.51 | 0.43 |
| 1:F:105:ARG:HG3 | 1:F:128:GLY:HA3 | 2.01 | 0.43 |
| 2:H:106:VAL:C | 2:H:107:LEU:HD23 | 2.39 | 0.43 |
| 1:C:151:ARG:HD2 | 1:C:153:ASP:O | 2.19 | 0.43 |
| 1:C:291:ASN:HA | 1:C:294:PHE:CD2 | 2.54 | 0.43 |
| 1:A:144:THR:HG21 | 1:A:288:GLN:HB2 | 2.01 | 0.43 |
| 1:C:156:HIS:HD2 | 1:C:185:TYR:OH | 2.02 | 0.43 |
| 2:G:33:PHE:O | 2:G:34:LYS:C | 2.57 | 0.43 |
| 2:K:85:ARG:O | 2:K:87:ASP:OD1 | 2.36 | 0.43 |
| 2:L:61:ILE:HG22 | 2:L:64:THR:HB | 1.98 | 0.43 |
| 2:H:25:ILE:O | 2:H:25:ILE:HG23 | 2.18 | 0.43 |
| 2:J:114:CYS:C | 2:J:116:SER:N | 2.71 | 0.43 |
| 2:J:35:LEU:HD22 | 2:J:61:ILE:CD1 | 2.49 | 0.43 |
| 2:J:106:VAL:HG23 | 2:J:107:LEU:HG | 2.00 | 0.43 |
| 1:F:215:ILE:O | 1:F:217:GLU:N | 2.52 | 0.43 |
| 1:D:61:THR:HG23 | 1:F:43:VAL:HG11 | 2.01 | 0.43 |
| 2:H:99:LEU:HA | 2:H:100:PRO:HD3 | 1.87 | 0.43 |
| 2:K:28:LYS:HG2 | 6:K:1007:HOH:O | 2.19 | 0.43 |
| 1:F:250:ARG:HB3 | 6:F:3008:HOH:O | 2.18 | 0.43 |
| 2:K:67:SER:O | 2:K:70:GLN:N | 2.48 | 0.43 |
| 1:C:306:ARG:NH1 | 1:C:306:ARG:HB2 | 2.34 | 0.43 |
| 2:G:70:GLN:HA | 2:G:73:GLN:CD | 2.39 | 0.42 |
| 2:L:16:THR:HG22 | 2:L:17:VAL:N | 2.33 | 0.42 |
| 1:A:63:MET:HE1 | 1:A:70:VAL:CG2 | 2.49 | 0.42 |
| 2:K:50:SER:HB3 | 2:K:53:MET:O | 2.19 | 0.42 |
| 2:J:14:ARG:HD2 | 2:J:65:PHE:HZ | 1.83 | 0.42 |
| 1:F:109:GLU:HA | 1:F:129:ASP:OD1 | 2.19 | 0.42 |
| 1:E:34:PRO:C | 1:E:36:PRO:HD3 | 2.39 | 0.42 |
| 2:G:134:ILE:CG2 | 2:G:135:ALA:N | 2.81 | 0.42 |
| 2:J:25:ILE:CG2 | 2:J:77:TYR:HB3 | 2.48 | 0.42 |
| 1:A:246:GLN:CG | 1:A:246:GLN:O | 2.67 | 0.42 |
| 2:H:16:THR:CG2 | 2:H:83:VAL:HG13 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:162:ASP:OD1 | 1:E:162:ASP:C | 2.56 | 0.42 |
| 1:F:140:LEU:HD23 | 1:F:295:ALA:CB | 2.48 | 0.42 |
| 2:L:14:ARG:CA | 2:L:88:ASN:O | 2.68 | 0.42 |
| 1:C:240:TYR:O | 1:C:243:VAL:HG12 | 2.19 | 0.42 |
| 1:A:63:MET:HG3 | 1:A:300:LEU:HD11 | 2.01 | 0.42 |
| 2:K:107:LEU:HA | 2:K:152:ALA:HA | 2.01 | 0.42 |
| 2:H:76:LEU:HD12 | 2:H:103:ILE:CD1 | 2.48 | 0.42 |
| 2:H:149:VAL:HG12 | 6:H:1039:HOH:O | 2.18 | 0.42 |
| 1:B:17:ARG:HD2 | 1:B:179:PHE:CE1 | 2.54 | 0.42 |
| 2:L:38:THR:O | 2:L:40:GLN:N | 2.49 | 0.42 |
| 2:K:16:THR:CG2 | 2:K:17:VAL:N | 2.82 | 0.42 |
| 1:D:63:MET:HE2 | 1:D:70:VAL:HG13 | 2.00 | 0.42 |
| 2:H:122:SER:HB2 | 6:H:1006:HOH:O | 2.19 | 0.42 |
| 2:H:38:THR:O | 2:K:47:ASN:ND2 | 2.51 | 0.42 |
| 1:A:91:THR:O | 1:A:94:VAL:HG22 | 2.19 | 0.42 |
| 2:L:18:ILE:HG13 | 2:L:83:VAL:CG1 | 2.49 | 0.42 |
| 1:A:243:VAL:HG12 | 1:A:244:LYS:N | 2.34 | 0.42 |
| 2:K:22:PRO:HG3 | 2:K:80:GLN:NE2 | 2.35 | 0.42 |
| 1:D:66:LEU:HD21 | 1:D:297:GLN:CG | 2.47 | 0.42 |
| 1:E:19:ASP:O | 1:E:23:VAL:HG23 | 2.19 | 0.42 |
| 2:G:14:ARG:HG2 | 2:G:87:ASP:CB | 2.49 | 0.42 |
| 2:J:80:GLN:O | 2:J:81:ALA:C | 2.58 | 0.42 |
| 1:D:185:TYR:CE2 | 1:D:222:VAL:HG12 | 2.55 | 0.42 |
| 2:K:99:LEU:HA | 2:K:100:PRO:HD3 | 1.91 | 0.42 |
| 2:H:111:ASN:C | 2:H:113:ASN:N | 2.70 | 0.42 |
| 1:D:267:LEU:O | 1:D:268:PRO:C | 2.57 | 0.42 |
| 1:D:267:LEU:HD11 | 1:D:286:PHE:HA | 2.02 | 0.42 |
| 1:E:55:THR:HB | 5:E:3005:PO4:O1 | 2.20 | 0.42 |
| 1:E:267:LEU:HA | 1:E:267:LEU:HD12 | 1.74 | 0.42 |
| 1:B:232:LYS:HA | 1:B:235:LEU:CD1 | 2.48 | 0.42 |
| 1:F:309:VAL:CG2 | 1:F:310:LEU:N | 2.81 | 0.42 |
| 1:F:75:ASP:C | 1:F:77:ALA:H | 2.23 | 0.42 |
| 1:F:159:MET:HE1 | 1:F:172:LEU:HB3 | 2.01 | 0.42 |
| 1:B:231:GLN:HE22 | 3:B:2002:FLC:CA | 2.30 | 0.42 |
| 2:J:80:GLN:O | 2:J:82:THR:N | 2.52 | 0.42 |
| 1:B:51:ALA:HB2 | 1:C:83:LYS:HG3 | 2.01 | 0.42 |
| 1:A:306:ARG:HB2 | 1:A:306:ARG:NH1 | 2.34 | 0.42 |
| 2:I:111:ASN:HD22 | 2:I:112:SER:N | 2.18 | 0.42 |
| 1:E:108:GLN:NE2 | 6:E:3073:HOH:O | 2.53 | 0.42 |
| 1:F:168:THR:HG21 | 3:F:2006:FLC:HG1 | 2.02 | 0.42 |
| 1:B:229:ARG:NE | 3:B:2002:FLC:OA1 | 2.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:81:LEU:HD12 | 1:B:86:GLU:O | 2.19 | 0.42 |
| 2:J:78:ALA:HB1 | 2:J:81:ALA:HB2 | 2.02 | 0.42 |
| 2:I:33:PHE:CE2 | 2:I:73:GLN:HB3 | 2.53 | 0.42 |
| 2:L:14:ARG:HA | 2:L:88:ASN:CA | 2.49 | 0.42 |
| 2:L:20:HIS:HA | 2:L:82:THR:HG21 | 2.01 | 0.42 |
| 2:K:53:MET:CG | 2:K:54:GLY:H | 2.30 | 0.42 |
| 1:D:269:ARG:HH11 | 1:D:273:ILE:CG2 | 2.32 | 0.42 |
| 1:C:120:GLY:O | 1:C:121:ASN:OD1 | 2.37 | 0.42 |
| 1:D:106:HIS:HA | 1:D:107:PRO:HD3 | 1.82 | 0.42 |
| 1:A:162:ASP:HB3 | 1:A:230:VAL:HA | 2.01 | 0.42 |
| 1:B:42:LYS:NZ | 6:B:3014:HOH:O | 2.52 | 0.42 |
| 1:C:285:TYR:CE1 | 1:C:286:PHE:CE2 | 3.07 | 0.42 |
| 2:K:54:GLY:O | 2:K:55:ARG:C | 2.58 | 0.42 |
| 2:G:111:ASN:ND2 | 2:G:111:ASN:C | 2.69 | 0.42 |
| 2:J:34:LYS:HB3 | 2:J:37:GLU:HG3 | 1.97 | 0.42 |
| 1:B:88:LEU:O | 1:B:88:LEU:HG | 2.19 | 0.42 |
| 1:F:162:ASP:HB2 | 1:F:230:VAL:HA | 2.01 | 0.42 |
| 1:E:233:GLU:HG2 | 1:E:234:ARG:HG3 | 2.01 | 0.42 |
| 1:E:64:HIS:O | 1:E:67:GLY:N | 2.38 | 0.42 |
| 2:G:82:THR:HG23 | 2:G:96:ARG:HG2 | 2.01 | 0.42 |
| 2:H:133:ASP:C | 2:H:134:ILE:HD12 | 2.39 | 0.42 |
| 2:K:1:MET:HB2 | 2:K:11:ALA:HB2 | 2.02 | 0.42 |
| 1:A:122:VAL:HA | 1:A:123:PRO:HD3 | 1.77 | 0.42 |
| 2:K:108:VAL:O | 2:K:108:VAL:HG23 | 2.20 | 0.42 |
| 2:G:108:VAL:HB | 2:G:151:LEU:HB3 | 2.02 | 0.42 |
| 1:C:270:VAL:O | 1:C:271:ASP:CG | 2.58 | 0.42 |
| 2:K:12:ILE:CG1 | 2:K:60:LYS:HE2 | 2.48 | 0.42 |
| 1:B:114:LEU:HD13 | 2:H:121:VAL:CG1 | 2.48 | 0.42 |
| 1:E:106:HIS:CE1 | 1:E:108:GLN:HG2 | 2.55 | 0.42 |
| 1:B:233:GLU:HG2 | 1:B:234:ARG:HG3 | 2.02 | 0.42 |
| 2:I:20:HIS:H | 2:I:56:LYS:HD2 | 1.84 | 0.42 |
| 2:K:32:LEU:HD21 | 2:K:77:TYR:OH | 2.20 | 0.42 |
| 2:K:78:ALA:C | 2:K:80:GLN:N | 2.73 | 0.42 |
| 2:J:128:ARG:NH1 | 2:J:128:ARG:HG3 | 2.35 | 0.42 |
| 2:I:30:LEU:CD1 | 2:I:44:ILE:HG12 | 2.49 | 0.41 |
| 1:C:265:HIS:CD2 | 1:C:273:ILE:HD11 | 2.55 | 0.41 |
| 2:H:109:CYS:HA | 2:H:110:PRO:HD3 | 1.59 | 0.41 |
| 2:H:114:CYS:O | 2:H:116:SER:N | 2.47 | 0.41 |
| 1:C:35:GLN:HE22 | 1:C:309:VAL:HG23 | 1.85 | 0.41 |
| 1:D:270:VAL:N | 1:D:272:GLU:OE2 | 2.51 | 0.41 |
| 2:J:65:PHE:C | 2:J:66:LEU:HD23 | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:130:ARG:CG | 2:I:131:ALA:N | 2.81 | 0.41 |
| 1:E:105:ARG:NH2 | 1:E:167:ARG:NH2 | 2.69 | 0.41 |
| 1:D:17:ARG:HD2 | 1:D:179:PHE:CE1 | 2.55 | 0.41 |
| 1:D:249:LEU:HD11 | 1:D:254:LEU:CD2 | 2.50 | 0.41 |
| 1:F:109:GLU:OE2 | 1:F:131:SER:HB3 | 2.20 | 0.41 |
| 1:E:114:LEU:CD1 | 2:K:121:VAL:HG11 | 2.50 | 0.41 |
| 1:E:306:ARG:CB | 1:E:306:ARG:HH11 | 2.33 | 0.41 |
| 2:L:130:ARG:HG2 | 2:L:130:ARG:NH1 | 2.34 | 0.41 |
| 1:E:215:ILE:HD13 | 1:E:249:LEU:HD13 | 2.03 | 0.41 |
| 1:D:132:ASN:O | 1:D:133:GLN:O | 2.39 | 0.41 |
| 1:F:60:GLU:HG2 | 1:F:70:VAL:HG11 | 2.02 | 0.41 |
| 2:G:138:CYS:HB3 | 2:G:141:CYS:C | 2.40 | 0.41 |
| 2:J:12:ILE:CG2 | 2:J:13:LYS:H | 2.22 | 0.41 |
| 2:J:47:ASN:HB3 | 2:J:55:ARG:HH11 | 1.85 | 0.41 |
| 2:G:19:ASP:HA | 2:G:58:LEU:HD13 | 2.01 | 0.41 |
| 1:E:151:ARG:HH11 | 1:E:151:ARG:HG2 | 1.85 | 0.41 |
| 1:C:101:ALA:HB2 | 1:C:304:LEU:HD21 | 2.02 | 0.41 |
| 1:C:219:MET:CE | 1:C:254:LEU:HD23 | 2.50 | 0.41 |
| 2:L:16:THR:HB | 2:L:60:LYS:CB | 2.34 | 0.41 |
| 2:H:111:ASN:HD21 | 2:H:113:ASN:HB3 | 1.85 | 0.41 |
| 1:E:8:HIS:CD2 | 1:E:116:THR:HB | 2.55 | 0.41 |
| 2:G:3:HIS:NE2 | 2:G:6:LYS:HA | 2.36 | 0.41 |
| 6:I:1037:HOH:O | 2:L:7:LEU:HD11 | 2.19 | 0.41 |
| 1:F:91:THR:HG22 | 1:F:95:ILE:HD12 | 2.03 | 0.41 |
| 2:G:49:PRO:HD3 | 2:J:41:ARG:HD3 | 2.02 | 0.41 |
| 1:E:45:ALA:HA | 1:E:71:VAL:O | 2.20 | 0.41 |
| 1:B:131:SER:HA | 1:B:167:ARG:HB3 | 2.01 | 0.41 |
| 1:A:231:GLN:HE22 | 3:A:2001:FLC:CAC | 2.33 | 0.41 |
| 2:L:68:GLU:HG2 | 2:L:85:ARG:NH1 | 2.35 | 0.41 |
| 2:I:40:GLN:HG3 | 2:I:62:GLU:OE1 | 2.20 | 0.41 |
| 1:E:132:ASN:CG | 1:E:133:GLN:N | 2.74 | 0.41 |
| 2:K:29:LEU:HD13 | 2:K:74:LEU:HD22 | 2.03 | 0.41 |
| 1:B:17:ARG:NH1 | 1:B:17:ARG:HG2 | 2.36 | 0.41 |
| 1:A:154:ASN:HA | 1:A:181:GLY:O | 2.21 | 0.41 |
| 2:L:16:THR:HG21 | 2:L:84:ASN:CA | 2.48 | 0.41 |
| 2:L:20:HIS:CA | 2:L:82:THR:HG21 | 2.50 | 0.41 |
| 1:F:227:MET:HB2 | 1:F:273:ILE:HD11 | 2.02 | 0.41 |
| 2:G:40:GLN:O | 2:J:47:ASN:HB2 | 2.20 | 0.41 |
| 1:D:26:THR:HG23 | 1:D:309:VAL:HG11 | 2.01 | 0.41 |
| 1:F:174:GLN:O | 1:F:178:LYS:HG3 | 2.21 | 0.41 |
| 1:B:49:PHE:CD1 | 1:B:49:PHE:N | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:234:ARG:HG2 | 1:E:234:ARG:HH11 | 1.86 | 0.41 |
| 2:L:57:ASP:C | 2:L:57:ASP:OD2 | 2.58 | 0.41 |
| 1:F:94:VAL:HG23 | 1:F:95:ILE:HG13 | 2.02 | 0.41 |
| 2:I:15:GLY:CA | 2:I:63:ASN:H | 2.24 | 0.41 |
| 2:I:63:ASN:O | 2:I:63:ASN:CG | 2.58 | 0.41 |
| 1:A:265:HIS:CD2 | 1:A:266:PRO:O | 2.74 | 0.41 |
| 1:C:81:LEU:HG | 1:C:81:LEU:O | 2.21 | 0.41 |
| 2:I:121:VAL:O | 2:I:121:VAL:HG23 | 2.20 | 0.41 |
| 1:C:246:GLN:CG | 1:C:246:GLN:O | 2.68 | 0.41 |
| 1:A:219:MET:HE3 | 1:A:254:LEU:HA | 2.03 | 0.41 |
| 2:G:94:LYS:HE2 | 2:G:96:ARG:NH2 | 2.33 | 0.41 |
| 2:K:96:ARG:HA | 2:K:97:PRO:HD3 | 1.87 | 0.41 |
| 1:D:106:HIS:HB3 | 1:D:111:ALA:HB3 | 2.02 | 0.41 |
| 1:D:157:VAL:O | 1:D:184:PHE:HA | 2.21 | 0.41 |
| 1:F:119:SER:OG | 1:F:119:SER:O | 2.37 | 0.41 |
| 1:F:140:LEU:CD2 | 1:F:295:ALA:HB3 | 2.49 | 0.41 |
| 2:H:30:LEU:HD13 | 2:H:44:ILE:HD13 | 2.03 | 0.41 |
| 2:K:58:LEU:HG | 2:K:59:ILE:N | 2.36 | 0.41 |
| 1:F:267:LEU:O | 1:F:268:PRO:C | 2.54 | 0.41 |
| 2:H:114:CYS:HB3 | 2:H:116:SER:CB | 2.51 | 0.41 |
| 1:D:199:LEU:HD22 | 1:D:209:TRP:CH2 | 2.55 | 0.41 |
| 2:K:106:VAL:HG12 | 2:K:106:VAL:O | 2.19 | 0.41 |
| 1:C:174:GLN:O | 1:C:178:LYS:HG3 | 2.21 | 0.41 |
| 1:A:160:VAL:HG22 | 1:A:187:ILE:HD12 | 2.02 | 0.41 |
| 1:D:38:LEU:CD1 | 1:D:305:ASN:ND2 | 2.83 | 0.41 |
| 2:I:33:PHE:HE2 | 2:I:73:GLN:HB3 | 1.84 | 0.41 |
| 2:I:65:PHE:CD2 | 2:I:85:ARG:HG3 | 2.55 | 0.41 |
| 2:L:114:CYS:O | 2:L:115:ILE:C | 2.59 | 0.41 |
| 2:I:59:ILE:HG22 | 2:I:61:ILE:HD11 | 2.02 | 0.41 |
| 2:I:115:ILE:C | 2:I:117:HIS:H | 2.24 | 0.41 |
| 2:L:16:THR:C | 2:L:17:VAL:HG22 | 2.41 | 0.41 |
| 2:G:59:ILE:HG22 | 2:G:60:LYS:N | 2.36 | 0.41 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CZ | 2.56 | 0.41 |
| 1:F:109:GLU:OE1 | 2:L:113:ASN:O | 2.39 | 0.41 |
| 1:E:230:VAL:O | 1:E:232:LYS:N | 2.51 | 0.41 |
| 1:A:49:PHE:CE2 | 1:A:81:LEU:HD22 | 2.56 | 0.41 |
| 1:F:227:MET:HG3 | 1:F:273:ILE:HD11 | 2.03 | 0.41 |
| 1:B:48:PHE:CD2 | 1:B:56:ARG:HB2 | 2.55 | 0.41 |
| 1:D:196:GLN:O | 1:D:199:LEU:N | 2.53 | 0.41 |
| 1:B:63:MET:CG | 1:B:300:LEU:HD11 | 2.51 | 0.41 |
| 2:G:91:VAL:O | 2:G:91:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L:130:ARG:HG2 | 2:L:131:ALA:N | 2.36 | 0.41 |
| 1:C:63:MET:SD | 1:C:70:VAL:HG22 | 2.61 | 0.41 |
| 2:H:72:ASP:O | 2:H:75:ALA:CB | 2.69 | 0.41 |
| 1:B:80:SER:HB3 | 1:B:84:LYS:HD2 | 2.03 | 0.41 |
| 1:D:89:ALA:HB1 | 1:D:118:PHE:CZ | 2.55 | 0.41 |
| 2:G:79:PRO:O | 2:G:80:GLN:HB2 | 2.20 | 0.41 |
| 2:H:89:TYR:O | 2:H:89:TYR:CD1 | 2.73 | 0.41 |
| 2:G:10:GLU:HG2 | 2:G:11:ALA:N | 2.36 | 0.41 |
| 2:H:113:ASN:O | 2:H:114:CYS:C | 2.59 | 0.41 |
| 1:B:136:THR:HB | 1:B:296:ARG:HE | 1.86 | 0.41 |
| 1:F:227:MET:CB | 1:F:273:ILE:HD11 | 2.51 | 0.41 |
| 1:F:219:MET:CE | 1:F:254:LEU:HD23 | 2.50 | 0.41 |
| 2:G:40:GLN:HG3 | 2:G:64:THR:OG1 | 2.21 | 0.41 |
| 2:J:110:PRO:HD2 | 2:J:145:PHE:CD2 | 2.56 | 0.41 |
| 1:D:75:ASP:CG | 1:D:77:ALA:HB3 | 2.41 | 0.41 |
| 1:F:236:ASP:O | 1:F:239:GLU:N | 2.49 | 0.41 |
| 1:C:21:ASN:HA | 1:C:21:ASN:HD22 | 1.65 | 0.41 |
| 1:D:110:GLY:C | 2:J:115:ILE:HG21 | 2.40 | 0.40 |
| 2:L:20:HIS:CE1 | 2:L:84:ASN:OD1 | 2.74 | 0.40 |
| 2:H:138:CYS:HB3 | 2:H:142:GLU:N | 2.33 | 0.40 |
| 1:C:106:HIS:CE1 | 1:C:107:PRO:HD2 | 2.53 | 0.40 |
| 2:I:48:LEU:HD23 | 2:I:48:LEU:HA | 1.86 | 0.40 |
| 2:K:102:ARG:NH1 | 2:K:102:ARG:CB | 2.80 | 0.40 |
| 2:K:119:GLU:HA | 2:K:120:PRO:HD3 | 1.87 | 0.40 |
| 2:J:103:ILE:HD11 | 2:J:107:LEU:HD11 | 2.03 | 0.40 |
| 1:A:78:ASN:CG | 1:C:75:ASP:HB2 | 2.41 | 0.40 |
| 2:H:8:GLN:O | 2:H:9:VAL:HG23 | 2.20 | 0.40 |
| 1:C:277:VAL:O | 1:C:280:THR:OG1 | 2.29 | 0.40 |
| 2:I:99:LEU:HA | 2:I:99:LEU:HD23 | 1.88 | 0.40 |
| 2:L:109:CYS:CB | 2:L:138:CYS:SG | 3.01 | 0.40 |
| 2:J:111:ASN:HD22 | 2:J:114:CYS:H | 1.67 | 0.40 |
| 1:A:98:TYR:OH | 1:C:54:ARG:HB3 | 2.21 | 0.40 |
| 2:L:83:VAL:HG13 | 2:L:95:SER:N | 2.09 | 0.40 |
| 2:K:53:MET:HG2 | 2:K:54:GLY:N | 2.30 | 0.40 |
| 1:A:109:GLU:CG | 1:A:130:GLY:O | 2.58 | 0.40 |
| 2:L:85:ARG:HG3 | 2:L:85:ARG:O | 2.22 | 0.40 |
| 1:E:137:GLN:O | 1:E:141:ASP:OD2 | 2.38 | 0.40 |
| 1:B:134:HIS:CE1 | 1:B:137:GLN:HB2 | 2.57 | 0.40 |
| 1:F:215:ILE:C | 1:F:217:GLU:N | 2.74 | 0.40 |
| 1:C:234:ARG:NH1 | 1:C:234:ARG:HG2 | 2.34 | 0.40 |
| 1:D:17:ARG:O | 1:D:20:LEU:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:23:VAL:HG11 | 1:D:139:LEU:HD13 | 2.03 | 0.40 |
| 1:D:129:ASP:OD1 | 1:D:132:ASN:HB3 | 2.21 | 0.40 |
| 1:E:240:TYR:O | 1:E:243:VAL:HG12 | 2.21 | 0.40 |
| 1:E:54:ARG:HD3 | 1:E:267:LEU:HB2 | 2.04 | 0.40 |
| 1:E:120:GLY:O | 1:E:121:ASN:C | 2.60 | 0.40 |
| 2:K:126:ALA:O | 2:K:136:LEU:HA | 2.21 | 0.40 |
| 1:F:38:LEU:HD11 | 1:F:305:ASN:HD21 | 1.87 | 0.40 |
| 1:A:19:ASP:O | 1:A:22:LEU:HB3 | 2.21 | 0.40 |
| 1:E:96:SER:CB | 1:E:119:SER:HA | 2.51 | 0.40 |
| 2:I:39:ASP:HB3 | 2:L:55:ARG:HH12 | 1.87 | 0.40 |
| 2:H:42:ILE:HG22 | 2:H:44:ILE:HG13 | 2.04 | 0.40 |
| 1:A:267:LEU:HD12 | 1:A:267:LEU:HA | 1.87 | 0.40 |
| 1:D:69:SER:HB3 | 1:E:64:HIS:CG | 2.57 | 0.40 |
| 2:H:75:ALA:HB3 | 2:H:100:PRO:HD3 | 2.03 | 0.40 |
| 2:L:66:LEU:HD23 | 2:L:66:LEU:HA | 1.84 | 0.40 |
| 2:L:62:GLU:CG | 2:L:63:ASN:N | 2.85 | 0.40 |
| 2:K:40:GLN:OE1 | 2:K:63:ASN:HB2 | 2.21 | 0.40 |
| 2:I:14:ARG:H | 2:I:88:ASN:H | 1.70 | 0.40 |
| 1:C:49:PHE:CD2 | 1:C:76:SER:HB3 | 2.57 | 0.40 |
| 2:G:65:PHE:CZ | 2:G:85:ARG:NE | 2.87 | 0.40 |
| 2:I:36:THR:O | 2:I:38:THR:N | 2.52 | 0.40 |
| 2:G:102:ARG:HA | 2:G:125:PHE:O | 2.21 | 0.40 |
| 2:J:71:VAL:HG13 | 2:J:83:VAL:HG21 | 2.02 | 0.40 |
| 1:C:4:LEU:HD12 | 1:C:302:LEU:HD13 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 308/310 (99%) | 260 (84%) | 38 (12%) | 10 (3%) | 5 20 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | B | 308/310 (99%) | 257 (83%) | 39 (13%) | 12 (4%) | 4 15 |
| 1 | C | 308/310 (99%) | 260 (84%) | 37 (12%) | 11 (4%) | 4 18 |
| 1 | D | 308/310 (99%) | 265 (86%) | 32 (10%) | 11 (4%) | 4 18 |
| 1 | E | 308/310 (99%) | 262 (85%) | 36 (12%) | 10 (3%) | 5 20 |
| 1 | F | 308/310 (99%) | 263 (85%) | 36 (12%) | 9 (3%) | 6 23 |
| 2 | G | 151/153 (99%) | 105 (70%) | 33 (22%) | 13 (9%) | 1 2 |
| 2 | H | 151/153 (99%) | 104 (69%) | 34 (22%) | 13 (9%) | 1 2 |
| 2 | I | 151/153 (99%) | 112 (74%) | 33 (22%) | 6 (4%) | 4 15 |
| 2 | J | 151/153 (99%) | 104 (69%) | 38 (25%) | 9 (6%) | 2 6 |
| 2 | K | 151/153 (99%) | 125 (83%) | 20 (13%) | 6 (4%) | 4 15 |
| 2 | L | 151/153 (99%) | 94 (62%) | 40 (26%) | 17 (11%) | 0 1 |
| All | All | 2754/2778 (99%) | 2211 (80%) | 416 (15%) | 127 (5%) | 3 11 |

All (127) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 29 | LYS |
| 1 | A | 30 | LEU |
| 1 | A | 133 | GLN |
| 1 | A | 243 | VAL |
| 1 | B | 131 | SER |
| 1 | B | 240 | TYR |
| 1 | B | 271 | ASP |
| 1 | B | 309 | VAL |
| 1 | C | 131 | SER |
| 2 | G | 142 | GLU |
| 2 | H | 36 | THR |
| 2 | H | 105 | ASN |
| 2 | H | 131 | ALA |
| 2 | I | 89 | TYR |
| 2 | I | 93 | GLY |
| 2 | I | 97 | PRO |
| 1 | D | 121 | ASN |
| 1 | D | 130 | GLY |
| 1 | D | 133 | GLN |
| 1 | D | 161 | GLY |
| 1 | E | 231 | GLN |
| 1 | F | 130 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | J | 81 | ALA |
| 2 | J | 142 | GLU |
| 2 | K | 92 | VAL |
| 2 | L | 14 | ARG |
| 2 | L | 41 | ARG |
| 2 | L | 85 | ARG |
| 2 | L | 116 | SER |
| 1 | A | 231 | GLN |
| 1 | A | 291 | ASN |
| 1 | B | 130 | GLY |
| 1 | C | 216 | GLU |
| 1 | C | 231 | GLN |
| 1 | C | 270 | VAL |
| 1 | C | 309 | VAL |
| 2 | G | 34 | LYS |
| 2 | G | 69 | ASP |
| 2 | G | 83 | VAL |
| 2 | G | 116 | SER |
| 2 | H | 6 | LYS |
| 2 | H | 15 | GLY |
| 1 | D | 231 | GLN |
| 1 | D | 238 | SER |
| 1 | E | 130 | GLY |
| 1 | F | 231 | GLN |
| 1 | F | 309 | VAL |
| 2 | J | 52 | GLU |
| 2 | J | 115 | ILE |
| 2 | L | 7 | LEU |
| 2 | L | 17 | VAL |
| 2 | L | 38 | THR |
| 2 | L | 39 | ASP |
| 1 | A | 6 | GLN |
| 1 | A | 34 | PRO |
| 1 | A | 271 | ASP |
| 1 | B | 121 | ASN |
| 1 | B | 167 | ARG |
| 2 | G | 133 | ASP |
| 2 | H | 106 | VAL |
| 2 | H | 111 | ASN |
| 2 | H | 112 | SER |
| 2 | H | 123 | SER |
| 2 | H | 124 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 91 | VAL |
| 1 | D | 36 | PRO |
| 1 | D | 267 | LEU |
| 1 | E | 36 | PRO |
| 1 | E | 266 | PRO |
| 1 | F | 36 | PRO |
| 1 | F | 216 | GLU |
| 2 | J | 6 | LYS |
| 2 | K | 3 | HIS |
| 2 | L | 9 | VAL |
| 2 | L | 19 | ASP |
| 2 | L | 59 | ILE |
| 2 | L | 78 | ALA |
| 1 | A | 128 | GLY |
| 1 | B | 30 | LEU |
| 1 | B | 34 | PRO |
| 1 | B | 128 | GLY |
| 1 | B | 197 | TYR |
| 1 | C | 36 | PRO |
| 2 | G | 84 | ASN |
| 2 | G | 123 | SER |
| 2 | G | 132 | ASN |
| 2 | H | 147 | HIS |
| 1 | D | 271 | ASP |
| 1 | E | 240 | TYR |
| 1 | E | 268 | PRO |
| 1 | E | 293 | ILE |
| 2 | J | 3 | HIS |
| 2 | J | 90 | GLU |
| 2 | L | 123 | SER |
| 2 | L | 142 | GLU |
| 1 | B | 258 | LYS |
| 2 | G | 18 | ILE |
| 2 | H | 11 | ALA |
| 2 | I | 133 | ASP |
| 1 | D | 87 | THR |
| 1 | F | 52 | SER |
| 1 | F | 233 | GLU |
| 2 | J | 124 | SER |
| 2 | L | 54 | GLY |
| 2 | L | 88 | ASN |
| 2 | L | 131 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 161 | GLY |
| 1 | C | 240 | TYR |
| 2 | G | 111 | ASN |
| 2 | I | 120 | PRO |
| 1 | D | 128 | GLY |
| 1 | C | 82 | GLY |
| 1 | C | 265 | HIS |
| 2 | G | 49 | PRO |
| 1 | E | 135 | PRO |
| 2 | J | 22 | PRO |
| 2 | K | 9 | VAL |
| 2 | K | 106 | VAL |
| 2 | H | 79 | PRO |
| 2 | K | 12 | ILE |
| 1 | C | 130 | GLY |
| 2 | G | 12 | ILE |
| 1 | F | 128 | GLY |
| 1 | F | 270 | VAL |
| 2 | K | 79 | PRO |
| 1 | E | 128 | GLY |
| 1 | E | 267 | LEU |

### 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 | 261/261 (100%) | 249 (95%) | 12 (5%) | 33 | 69 |
| 1 | B | 261/261 (100%) | 249 (95%) | 12 (5%) | 33 | 69 |
| 1 | C | 261/261 (100%) | 247 (95%) | 14 (5%) | 27 | 62 |
| 1 | D | 261/261 (100%) | 253 (97%) | 8 (3%) | 47 | 82 |
| 1 | E | 261/261 (100%) | 251 (96%) | 10 (4%) | 40 | 76 |
| 1 | F | 261/261 (100%) | 248 (95%) | 13 (5%) | 30 | 65 |
| 2 | G | 137/137 (100%) | 129 (94%) | 8 (6%) | 25 | 58 |
| 2 | H | 137/137 (100%) | 126 (92%) | 11 (8%) | 15 | 40 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | I | 137/137 (100%) | 127 (93%) | 10 (7%) | 17 45 |
| 2 | J | 137/137 (100%) | 126 (92%) | 11 (8%) | 15 40 |
| 2 | K | 137/137 (100%) | 125 (91%) | 12 (9%) | 12 35 |
| 2 | L | 137/137 (100%) | 128 (93%) | 9 (7%) | 21 51 |
| All | All | 2388/2388 (100%) | 2258 (95%) | 130 (5%) | 27 62 |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 13 | ASN |
| 1 | A | 17 | ARG |
| 1 | A | 18 | ASP |
| 1 | A | 53 | THR |
| 1 | A | 59 | PHE |
| 1 | A | 136 | THR |
| 1 | A | 153 | ASP |
| 1 | A | 162 | ASP |
| 1 | A | 229 | ARG |
| 1 | A | 232 | LYS |
| 1 | A | 253 | ASP |
| 1 | A | 305 | ASN |
| 1 | B | 13 | ASN |
| 1 | B | 17 | ARG |
| 1 | B | 34 | PRO |
| 1 | B | 54 | ARG |
| 1 | B | 74 | SER |
| 1 | B | 80 | SER |
| 1 | B | 94 | VAL |
| 1 | B | 162 | ASP |
| 1 | B | 196 | GLN |
| 1 | B | 201 | MET |
| 1 | B | 253 | ASP |
| 1 | B | 309 | VAL |
| 1 | C | 13 | ASN |
| 1 | C | 17 | ARG |
| 1 | C | 54 | ARG |
| 1 | C | 59 | PHE |
| 1 | C | 86 | GLU |
| 1 | C | 131 | SER |
| 1 | C | 153 | ASP |
| 1 | C | 162 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 169 | VAL |
| 1 | C | 204 | GLU |
| 1 | C | 233 | GLU |
| 1 | C | 237 | PRO |
| 1 | C | 253 | ASP |
| 1 | C | 285 | TYR |
| 2 | G | 16 | THR |
| 2 | G | 36 | THR |
| 2 | G | 69 | ASP |
| 2 | G | 104 | ASP |
| 2 | G | 109 | CYS |
| 2 | G | 111 | ASN |
| 2 | G | 141 | CYS |
| 2 | G | 142 | GLU |
| 2 | H | 25 | ILE |
| 2 | H | 38 | THR |
| 2 | H | 56 | LYS |
| 2 | H | 69 | ASP |
| 2 | H | 84 | ASN |
| 2 | H | 86 | ILE |
| 2 | H | 109 | CYS |
| 2 | H | 111 | ASN |
| 2 | H | 125 | PHE |
| 2 | H | 127 | VAL |
| 2 | H | 133 | ASP |
| 2 | I | 12 | ILE |
| 2 | I | 52 | GLU |
| 2 | I | 57 | ASP |
| 2 | I | 76 | LEU |
| 2 | I | 91 | VAL |
| 2 | I | 97 | PRO |
| 2 | I | 109 | CYS |
| 2 | I | 111 | ASN |
| 2 | I | 114 | CYS |
| 2 | I | 147 | HIS |
| 1 | D | 13 | ASN |
| 1 | D | 17 | ARG |
| 1 | D | 81 | LEU |
| 1 | D | 105 | ARG |
| 1 | D | 147 | GLU |
| 1 | D | 285 | TYR |
| 1 | D | 305 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 309 | VAL |
| 1 | E | 17 | ARG |
| 1 | E | 18 | ASP |
| 1 | E | 59 | PHE |
| 1 | E | 80 | SER |
| 1 | E | 153 | ASP |
| 1 | E | 159 | MET |
| 1 | E | 233 | GLU |
| 1 | E | 253 | ASP |
| 1 | E | 266 | PRO |
| 1 | E | 309 | VAL |
| 1 | F | 13 | ASN |
| 1 | F | 17 | ARG |
| 1 | F | 18 | ASP |
| 1 | F | 59 | PHE |
| 1 | F | 147 | GLU |
| 1 | F | 183 | ARG |
| 1 | F | 237 | PRO |
| 1 | F | 253 | ASP |
| 1 | F | 278 | ASP |
| 1 | F | 285 | TYR |
| 1 | F | 305 | ASN |
| 1 | F | 307 | ASP |
| 1 | F | 309 | VAL |
| 2 | J | 19 | ASP |
| 2 | J | 31 | SER |
| 2 | J | 36 | THR |
| 2 | J | 50 | SER |
| 2 | J | 63 | ASN |
| 2 | J | 103 | ILE |
| 2 | J | 108 | VAL |
| 2 | J | 113 | ASN |
| 2 | J | 114 | CYS |
| 2 | J | 138 | CYS |
| 2 | J | 147 | HIS |
| 2 | K | 4 | ASP |
| 2 | K | 14 | ARG |
| 2 | K | 31 | SER |
| 2 | K | 52 | GLU |
| 2 | K | 57 | ASP |
| 2 | K | 71 | VAL |
| 2 | K | 96 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | K | 109 | CYS |
| 2 | K | 128 | ARG |
| 2 | K | 133 | ASP |
| 2 | K | 143 | LYS |
| 2 | K | 149 | VAL |
| 2 | L | 4 | ASP |
| 2 | L | 17 | VAL |
| 2 | L | 18 | ILE |
| 2 | L | 20 | HIS |
| 2 | L | 85 | ARG |
| 2 | L | 87 | ASP |
| 2 | L | 96 | ARG |
| 2 | L | 109 | CYS |
| 2 | L | 138 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 13 | ASN |
| 1 | A | 21 | ASN |
| 1 | A | 41 | HIS |
| 1 | A | 132 | ASN |
| 1 | A | 156 | HIS |
| 1 | A | 231 | GLN |
| 1 | A | 246 | GLN |
| 1 | A | 291 | ASN |
| 1 | A | 305 | ASN |
| 1 | B | 13 | ASN |
| 1 | B | 21 | ASN |
| 1 | B | 35 | GLN |
| 1 | B | 41 | HIS |
| 1 | B | 108 | GLN |
| 1 | B | 156 | HIS |
| 1 | B | 231 | GLN |
| 1 | B | 291 | ASN |
| 1 | B | 305 | ASN |
| 1 | C | 13 | ASN |
| 1 | C | 21 | ASN |
| 1 | C | 35 | GLN |
| 1 | C | 41 | HIS |
| 1 | C | 132 | ASN |
| 1 | C | 156 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 231 | GLN |
| 1 | C | 291 | ASN |
| 1 | C | 305 | ASN |
| 2 | G | 8 | GLN |
| 2 | G | 111 | ASN |
| 2 | G | 148 | ASN |
| 2 | H | 20 | HIS |
| 2 | H | 63 | ASN |
| 2 | H | 111 | ASN |
| 2 | H | 147 | HIS |
| 2 | H | 148 | ASN |
| 2 | I | 70 | GLN |
| 2 | I | 84 | ASN |
| 2 | I | 111 | ASN |
| 2 | I | 117 | HIS |
| 2 | I | 147 | HIS |
| 1 | D | 13 | ASN |
| 1 | D | 21 | ASN |
| 1 | D | 35 | GLN |
| 1 | D | 41 | HIS |
| 1 | D | 64 | HIS |
| 1 | D | 132 | ASN |
| 1 | D | 246 | GLN |
| 1 | D | 291 | ASN |
| 1 | D | 297 | GLN |
| 1 | D | 305 | ASN |
| 1 | E | 13 | ASN |
| 1 | E | 21 | ASN |
| 1 | E | 35 | GLN |
| 1 | E | 41 | HIS |
| 1 | E | 108 | GLN |
| 1 | E | 126 | ASN |
| 1 | E | 132 | ASN |
| 1 | E | 137 | GLN |
| 1 | E | 246 | GLN |
| 1 | E | 291 | ASN |
| 1 | E | 297 | GLN |
| 1 | E | 305 | ASN |
| 1 | F | 13 | ASN |
| 1 | F | 21 | ASN |
| 1 | F | 35 | GLN |
| 1 | F | 41 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 126 | ASN |
| 1 | F | 156 | HIS |
| 1 | F | 170 | HIS |
| 1 | F | 242 | ASN |
| 1 | F | 288 | GLN |
| 1 | F | 291 | ASN |
| 1 | F | 297 | GLN |
| 1 | F | 305 | ASN |
| 2 | J | 3 | HIS |
| 2 | J | 70 | GLN |
| 2 | J | 84 | ASN |
| 2 | J | 111 | ASN |
| 2 | J | 113 | ASN |
| 2 | J | 153 | ASN |
| 2 | K | 8 | GLN |
| 2 | K | 20 | HIS |
| 2 | K | 80 | GLN |
| 2 | K | 147 | HIS |
| 2 | L | 20 | HIS |
| 2 | L | 84 | ASN |
| 2 | L | 88 | ASN |
| 2 | L | 105 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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 | $\#\|Z\| > 2$ |
| 3 | FLC | A | 2001 | - | 3,12,12 | 4.84 | 2 (66%) | 3,17,17 | 1.98 | 1 (33%) |
| 5 | PO4 | A | 3001 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.44 | 0 |
| 3 | FLC | B | 2002 | - | 3,12,12 | 2.77 | 2 (66%) | 3,17,17 | 1.19 | 0 |
| 5 | PO4 | B | 3002 | - | 4,4,4 | 1.49 | 1 (25%) | 6,6,6 | 0.43 | 0 |
| 3 | FLC | C | 2003 | - | 3,12,12 | 4.28 | 2 (66%) | 3,17,17 | 1.45 | 0 |
| 5 | PO4 | C | 3003 | - | 4,4,4 | 1.14 | 0 | 6,6,6 | 0.39 | 0 |
| 3 | FLC | D | 2004 | - | 3,12,12 | 4.42 | 3 (100%) | 3,17,17 | 1.99 | 1 (33%) |
| 5 | PO4 | D | 3004 | - | 4,4,4 | 0.94 | 0 | 6,6,6 | 0.40 | 0 |
| 3 | FLC | E | 2005 | - | 3,12,12 | 4.71 | 2 (66%) | 3,17,17 | 2.05 | 1 (33%) |
| 5 | PO4 | E | 3005 | - | 4,4,4 | 1.09 | 0 | 6,6,6 | 0.42 | 0 |
| 3 | FLC | F | 2006 | - | 3,12,12 | 4.18 | 2 (66%) | 3,17,17 | 2.69 | 1 (33%) |
| 5 | PO4 | F | 3006 | - | 4,4,4 | 1.03 | 0 | 6,6,6 | 0.41 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | FLC | A | 2001 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | A | 3001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | FLC | B | 2002 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | B | 3002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | FLC | C | 2003 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | C | 3003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | FLC | D | 2004 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | D | 3004 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | FLC | E | 2005 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | E | 3005 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | FLC | F | 2006 | - | - | 0/6/16/16 | 0/0/0/0 |
| 5 | PO4 | F | 3006 | - | - | 0/0/0/0 | 0/0/0/0 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | B | 3002 | PO4 | P-O3 | 2.48 | 1.62 | 1.53 |
| 3 | D | 2004 | FLC | OHB-CB | 2.57 | 1.47 | 1.43 |
| 3 | B | 2002 | FLC | CA-CB | 3.01 | 1.59 | 1.54 |
| 3 | B | 2002 | FLC | CG-CB | 3.72 | 1.60 | 1.54 |
| 3 | C | 2003 | FLC | CA-CB | 3.88 | 1.60 | 1.54 |
| 3 | D | 2004 | FLC | CG-CB | 4.72 | 1.61 | 1.54 |
| 3 | F | 2006 | FLC | CG-CB | 4.81 | 1.62 | 1.54 |
| 3 | F | 2006 | FLC | CA-CB | 5.27 | 1.62 | 1.54 |
| 3 | D | 2004 | FLC | CA-CB | 5.45 | 1.63 | 1.54 |
| 3 | E | 2005 | FLC | CG-CB | 5.50 | 1.63 | 1.54 |
| 3 | A | 2001 | FLC | CG-CB | 5.56 | 1.63 | 1.54 |
| 3 | E | 2005 | FLC | CA-CB | 6.02 | 1.63 | 1.54 |
| 3 | A | 2001 | FLC | CA-CB | 6.07 | 1.63 | 1.54 |
| 3 | C | 2003 | FLC | CG-CB | 6.28 | 1.64 | 1.54 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 2001 | FLC | CB-CA-CAC | 3.11 | 119.93 | 114.96 |
| 3 | E | 2005 | FLC | CB-CA-CAC | 3.22 | 120.10 | 114.96 |
| 3 | D | 2004 | FLC | CB-CA-CAC | 3.24 | 120.14 | 114.96 |
| 3 | F | 2006 | FLC | CB-CA-CAC | 4.55 | 122.23 | 114.96 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 35 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 2001 | FLC | 7 | 0 |
| 5 | A | 3001 | PO4 | 5 | 0 |
| 3 | B | 2002 | FLC | 4 | 0 |
| 5 | B | 3002 | PO4 | 1 | 0 |
| 3 | C | 2003 | FLC | 4 | 0 |
| 3 | D | 2004 | FLC | 7 | 0 |
| 5 | D | 3004 | PO4 | 1 | 0 |
| 3 | E | 2005 | FLC | 4 | 0 |
| 5 | E | 3005 | PO4 | 1 | 0 |
| 3 | F | 2006 | FLC | 1 | 0 |
| 5 | F | 3006 | PO4 | 2 | 0 |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 310/310 (100%) | -0.36 | 1 (0%) 94 94 | 15, 42, 66, 78 | 0 |
| 1 | B | 310/310 (100%) | -0.12 | 4 (1%) 79 78 | 20, 60, 91, 113 | 0 |
| 1 | C | 310/310 (100%) | -0.30 | 1 (0%) 94 94 | 19, 46, 69, 97 | 0 |
| 1 | D | 310/310 (100%) | -0.18 | 3 (0%) 84 82 | 31, 59, 83, 109 | 0 |
| 1 | E | 310/310 (100%) | -0.18 | 3 (0%) 84 82 | 34, 54, 85, 103 | 0 |
| 1 | F | 310/310 (100%) | -0.11 | 5 (1%) 74 72 | 36, 66, 91, 118 | 0 |
| 2 | G | 153/153 (100%) | 0.60 | 21 (13%) 4 2 | 45, 92, 161, 182 | 0 |
| 2 | H | 153/153 (100%) | 0.07 | 9 (5%) 26 19 | 40, 63, 133, 171 | 0 |
| 2 | I | 153/153 (100%) | 0.64 | 23 (15%) 3 2 | 57, 99, 144, 161 | 0 |
| 2 | J | 153/153 (100%) | 0.64 | 15 (9%) 10 6 | 49, 89, 164, 192 | 0 |
| 2 | K | 153/153 (100%) | 0.33 | 13 (8%) 13 8 | 34, 63, 149, 181 | 0 |
| 2 | L | 153/153 (100%) | 1.10 | 34 (22%) 1 0 | 62, 126, 163, 170 | 0 |
| All | All | 2778/2778 (100%) | 0.05 | 132 (4%) 34 28 | 15, 61, 130, 192 | 0 |

All (132) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | K | 3 | HIS | 11.7 |
| 2 | J | 1 | MET | 11.2 |
| 2 | G | 1 | MET | 10.4 |
| 2 | J | 7 | LEU | 10.1 |
| 2 | K | 4 | ASP | 9.5 |
| 2 | L | 17 | VAL | 8.3 |
| 2 | J | 2 | THR | 7.9 |
| 2 | I | 153 | ASN | 7.6 |
| 2 | J | 9 | VAL | 7.6 |
| 2 | G | 2 | THR | 7.4 |
| 2 | K | 2 | THR | 7.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | H | 4 | ASP | 7.1 |
| 2 | J | 6 | LYS | 6.9 |
| 2 | I | 2 | THR | 6.9 |
| 2 | J | 10 | GLU | 6.6 |
| 2 | L | 8 | GLN | 6.6 |
| 2 | K | 9 | VAL | 6.4 |
| 2 | G | 5 | ASN | 6.4 |
| 2 | I | 152 | ALA | 6.0 |
| 2 | G | 9 | VAL | 6.0 |
| 2 | G | 3 | HIS | 6.0 |
| 2 | K | 6 | LYS | 5.8 |
| 2 | G | 153 | ASN | 5.8 |
| 2 | K | 5 | ASN | 5.7 |
| 2 | L | 79 | PRO | 5.7 |
| 2 | J | 95 | SER | 5.6 |
| 2 | H | 1 | MET | 5.6 |
| 1 | F | 310 | LEU | 5.5 |
| 2 | G | 11 | ALA | 5.3 |
| 2 | L | 10 | GLU | 5.3 |
| 2 | H | 10 | GLU | 5.1 |
| 2 | K | 153 | ASN | 5.0 |
| 2 | K | 8 | GLN | 4.9 |
| 2 | K | 10 | GLU | 4.8 |
| 2 | G | 10 | GLU | 4.7 |
| 2 | L | 16 | THR | 4.7 |
| 2 | I | 49 | PRO | 4.6 |
| 2 | H | 6 | LYS | 4.6 |
| 2 | L | 80 | GLN | 4.6 |
| 1 | C | 309 | VAL | 4.6 |
| 2 | J | 11 | ALA | 4.5 |
| 2 | L | 75 | ALA | 4.4 |
| 2 | I | 1 | MET | 4.4 |
| 2 | J | 8 | GLN | 4.3 |
| 2 | H | 5 | ASN | 4.2 |
| 2 | L | 76 | LEU | 4.1 |
| 2 | G | 8 | GLN | 4.1 |
| 2 | K | 1 | MET | 4.1 |
| 2 | G | 53 | MET | 4.0 |
| 2 | H | 153 | ASN | 3.9 |
| 2 | I | 63 | ASN | 3.9 |
| 2 | I | 50 | SER | 3.9 |
| 2 | L | 9 | VAL | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | G | 152 | ALA | 3.8 |
| 2 | G | 4 | ASP | 3.7 |
| 2 | L | 87 | ASP | 3.7 |
| 2 | I | 8 | GLN | 3.7 |
| 2 | L | 151 | LEU | 3.7 |
| 1 | A | 310 | LEU | 3.7 |
| 2 | J | 5 | ASN | 3.6 |
| 2 | I | 30 | LEU | 3.6 |
| 2 | G | 51 | GLY | 3.6 |
| 1 | B | 255 | HIS | 3.5 |
| 2 | L | 5 | ASN | 3.4 |
| 2 | L | 152 | ALA | 3.4 |
| 2 | G | 151 | LEU | 3.4 |
| 2 | H | 2 | THR | 3.4 |
| 2 | L | 131 | ALA | 3.3 |
| 2 | I | 66 | LEU | 3.3 |
| 2 | K | 7 | LEU | 3.3 |
| 2 | I | 9 | VAL | 3.2 |
| 2 | L | 3 | HIS | 3.2 |
| 1 | E | 271 | ASP | 3.2 |
| 2 | L | 18 | ILE | 3.2 |
| 2 | L | 4 | ASP | 3.1 |
| 2 | L | 1 | MET | 3.1 |
| 1 | F | 208 | ALA | 3.1 |
| 1 | D | 255 | HIS | 3.1 |
| 2 | I | 54 | GLY | 3.0 |
| 2 | L | 153 | ASN | 3.0 |
| 2 | H | 3 | HIS | 3.0 |
| 2 | L | 77 | TYR | 3.0 |
| 2 | L | 85 | ARG | 3.0 |
| 2 | I | 64 | THR | 2.9 |
| 1 | D | 254 | LEU | 2.9 |
| 2 | G | 7 | LEU | 2.8 |
| 2 | G | 92 | VAL | 2.8 |
| 2 | L | 74 | LEU | 2.8 |
| 2 | I | 99 | LEU | 2.8 |
| 2 | L | 61 | ILE | 2.8 |
| 2 | J | 132 | ASN | 2.8 |
| 2 | I | 35 | LEU | 2.7 |
| 1 | E | 309 | VAL | 2.7 |
| 2 | L | 82 | THR | 2.7 |
| 2 | L | 92 | VAL | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | J | 153 | ASN | 2.6 |
| 2 | J | 3 | HIS | 2.6 |
| 2 | L | 66 | LEU | 2.5 |
| 2 | L | 62 | GLU | 2.5 |
| 2 | J | 92 | VAL | 2.5 |
| 2 | J | 106 | VAL | 2.5 |
| 1 | B | 240 | TYR | 2.4 |
| 2 | G | 97 | PRO | 2.4 |
| 2 | I | 5 | ASN | 2.4 |
| 2 | G | 52 | GLU | 2.4 |
| 2 | K | 11 | ALA | 2.4 |
| 2 | L | 128 | ARG | 2.4 |
| 2 | K | 77 | TYR | 2.4 |
| 2 | G | 6 | LYS | 2.4 |
| 1 | F | 254 | LEU | 2.3 |
| 2 | H | 76 | LEU | 2.3 |
| 2 | G | 76 | LEU | 2.3 |
| 2 | I | 37 | GLU | 2.2 |
| 2 | I | 103 | ILE | 2.2 |
| 2 | I | 53 | MET | 2.2 |
| 2 | L | 127 | VAL | 2.2 |
| 2 | G | 131 | ALA | 2.2 |
| 1 | D | 219 | MET | 2.2 |
| 2 | L | 2 | THR | 2.2 |
| 2 | I | 10 | GLU | 2.1 |
| 1 | F | 309 | VAL | 2.1 |
| 2 | L | 100 | PRO | 2.1 |
| 1 | F | 220 | ALA | 2.1 |
| 2 | I | 65 | PHE | 2.1 |
| 2 | L | 67 | SER | 2.1 |
| 2 | L | 99 | LEU | 2.1 |
| 2 | I | 52 | GLU | 2.0 |
| 1 | B | 243 | VAL | 2.0 |
| 1 | E | 310 | LEU | 2.0 |
| 2 | L | 149 | VAL | 2.0 |
| 2 | I | 87 | ASP | 2.0 |
| 1 | B | 254 | LEU | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 4 | ZN | I | 1003 | 1/1 | 0.87 | 0.17 | 1.40 | 67,67,67,67 | 0 |
| 3 | FLC | D | 2004 | 13/13 | 0.88 | 0.23 | 1.16 | 63,65,68,70 | 0 |
| 3 | FLC | C | 2003 | 13/13 | 0.91 | 0.22 | 1.16 | 46,50,55,55 | 0 |
| 5 | PO4 | C | 3003 | 5/5 | 0.98 | 0.23 | 1.14 | 38,39,41,41 | 0 |
| 5 | PO4 | B | 3002 | 5/5 | 0.98 | 0.28 | 0.98 | 37,37,40,41 | 0 |
| 3 | FLC | F | 2006 | 13/13 | 0.93 | 0.24 | 0.82 | 61,64,67,68 | 0 |
| 3 | FLC | E | 2005 | 13/13 | 0.93 | 0.23 | 0.81 | 68,70,72,72 | 0 |
| 3 | FLC | B | 2002 | 13/13 | 0.91 | 0.27 | 0.81 | 65,68,69,71 | 0 |
| 3 | FLC | A | 2001 | 13/13 | 0.91 | 0.23 | 0.77 | 34,48,52,55 | 0 |
| 5 | PO4 | F | 3006 | 5/5 | 0.96 | 0.23 | 0.40 | 49,49,51,51 | 0 |
| 4 | ZN | K | 1005 | 1/1 | 0.93 | 0.16 | 0.30 | 64,64,64,64 | 0 |
| 5 | PO4 | E | 3005 | 5/5 | 0.97 | 0.23 | 0.26 | 41,41,42,43 | 0 |
| 4 | ZN | H | 1002 | 1/1 | 0.99 | 0.14 | -0.01 | 56,56,56,56 | 0 |
| 4 | ZN | L | 1006 | 1/1 | 0.97 | 0.14 | -0.02 | 63,63,63,63 | 0 |
| 5 | PO4 | A | 3001 | 5/5 | 0.98 | 0.20 | -0.11 | 26,26,30,32 | 0 |
| 4 | ZN | G | 1001 | 1/1 | 0.99 | 0.11 | -0.25 | 57,57,57,57 | 0 |
| 5 | PO4 | D | 3004 | 5/5 | 0.99 | 0.19 | -0.49 | 29,30,33,34 | 0 |
| 4 | ZN | J | 1004 | 1/1 | 0.81 | 0.09 | -2.61 | 52,52,52,52 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.