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

Jan 31, 2016 – 09:32 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1PD5 |
| Title | : | Crystal structure of E.coli chloramphenicol acetyltransferase type I at 2.5 Angstrom resolution |
| Authors | : | Roidis, A.; Kokkinidis, M. |
| Deposited on | : | 2003-05-19 |
| Resolution | : | 2.50 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:

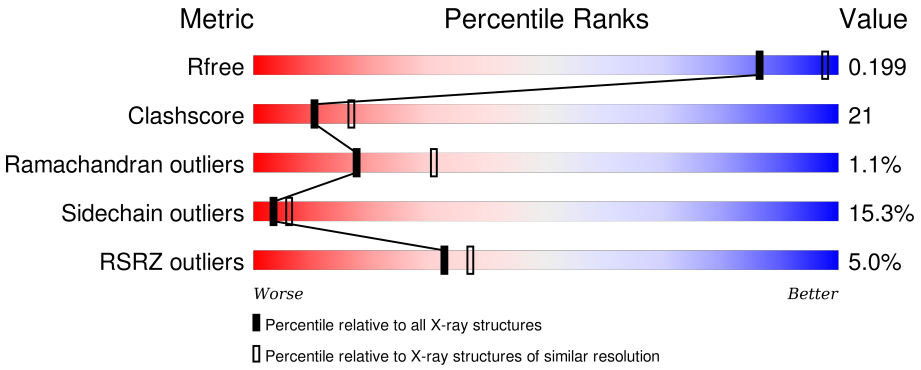
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 2.50 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 3553 (2.50-2.50) |
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |
| RSRZ outliers | 91569 | 3562 (2.50-2.50) |

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 | 219 | 45% 37% 12% |
| 1 | B | 219 | 57% 29% 9% |
| 1 | C | 219 | 47% 38% 9% |
| 1 | D | 219 | 46% 40% 8% |
| 1 | E | 219 | 54% 35% 8% |

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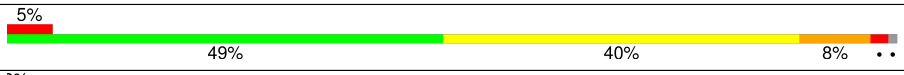
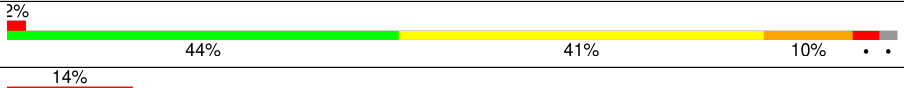
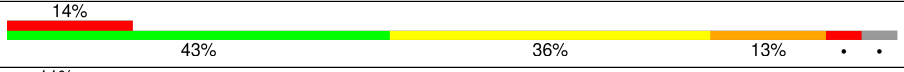
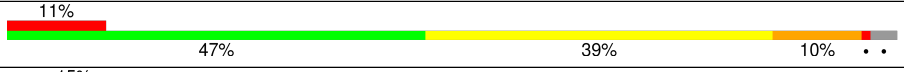
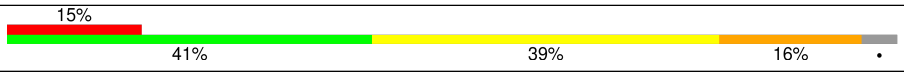
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 219 |   |
| 1 | G | 219 |   |
| 1 | H | 219 |   |
| 1 | I | 219 |   |
| 1 | J | 219 |   |
| 1 | K | 219 |   |
| 1 | L | 219 |   |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21418 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 Chloramphenicol acetyltransferase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1144 | 290 | 316 | 13 | | | |
| 1 | B | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1789 | 1162 | 295 | 319 | 13 | | | |
| 1 | C | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1144 | 290 | 316 | 13 | | | |
| 1 | D | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1144 | 290 | 316 | 13 | | | |
| 1 | E | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1785 | 1160 | 294 | 318 | 13 | | | |
| 1 | F | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1759 | 1142 | 289 | 315 | 13 | | | |
| 1 | G | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1144 | 290 | 316 | 13 | | | |
| 1 | H | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1785 | 1159 | 294 | 319 | 13 | | | |
| 1 | I | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1776 | 1154 | 292 | 317 | 13 | | | |
| 1 | J | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1755 | 1140 | 288 | 314 | 13 | | | |
| 1 | K | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1147 | 289 | 314 | 13 | | | |
| 1 | L | 210 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1746 | 1135 | 286 | 312 | 13 | | | |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 19 | Total | O | 0 | 0 |
| | | | 19 | 19 | | |
| 2 | B | 22 | Total | O | 0 | 0 |
| | | | 22 | 22 | | |

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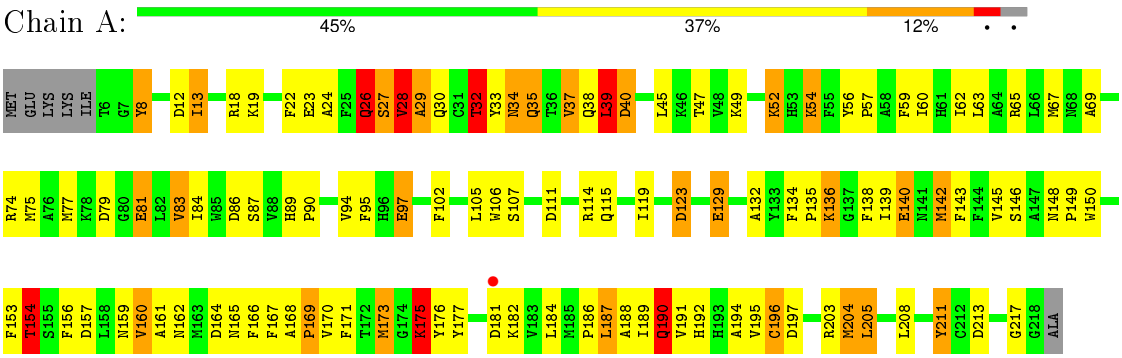
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | C | 19 | Total O<br>19 19 | 0 | 0 |
| 2 | D | 21 | Total O<br>21 21 | 0 | 0 |
| 2 | E | 15 | Total O<br>15 15 | 0 | 0 |
| 2 | F | 16 | Total O<br>16 16 | 0 | 0 |
| 2 | G | 20 | Total O<br>20 20 | 0 | 0 |
| 2 | H | 36 | Total O<br>36 36 | 0 | 0 |
| 2 | I | 17 | Total O<br>17 17 | 0 | 0 |
| 2 | J | 11 | Total O<br>11 11 | 0 | 0 |
| 2 | K | 4 | Total O<br>4 4 | 0 | 0 |
| 2 | L | 8 | Total O<br>8 8 | 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.

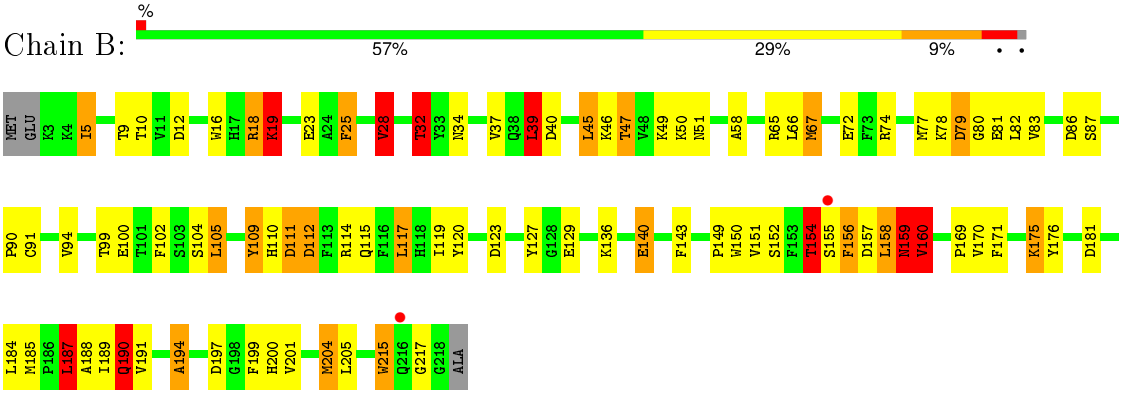
- Molecule 1: Chloramphenicol acetyltransferase

Chain A:



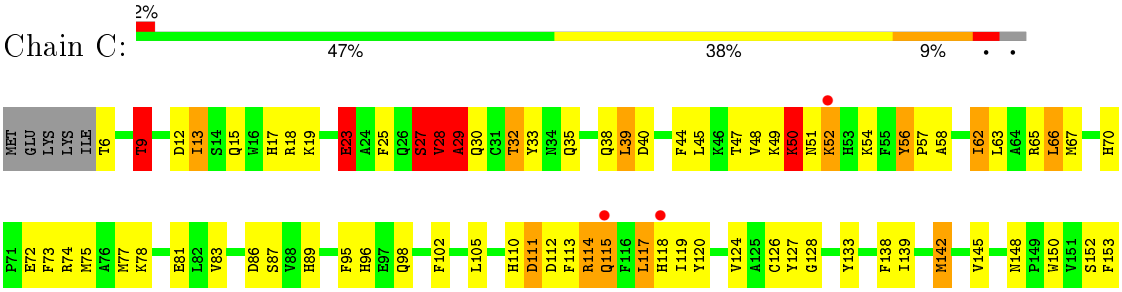

- Molecule 1: Chloramphenicol acetyltransferase

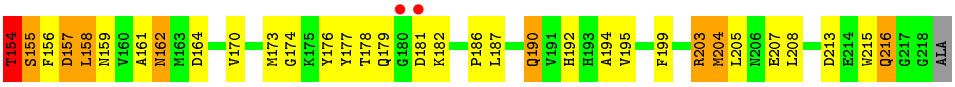
Chain B:




- Molecule 1: Chloramphenicol acetyltransferase

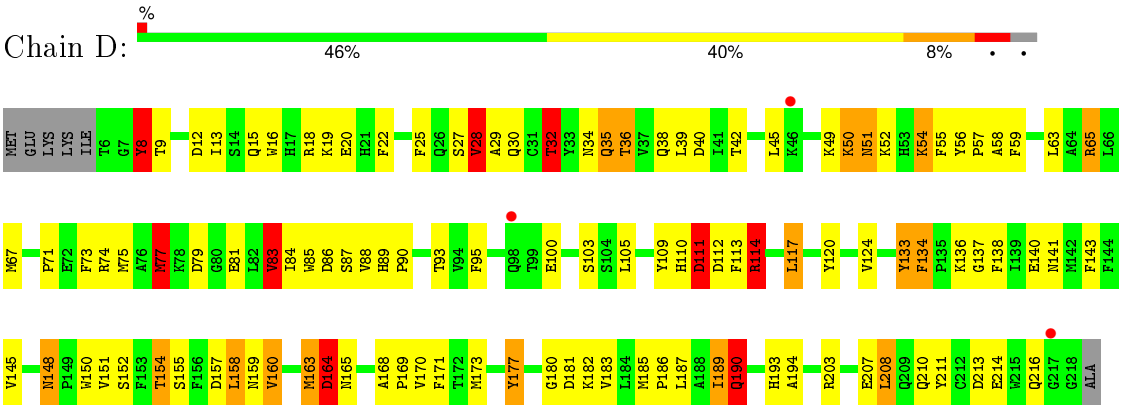
Chain C:





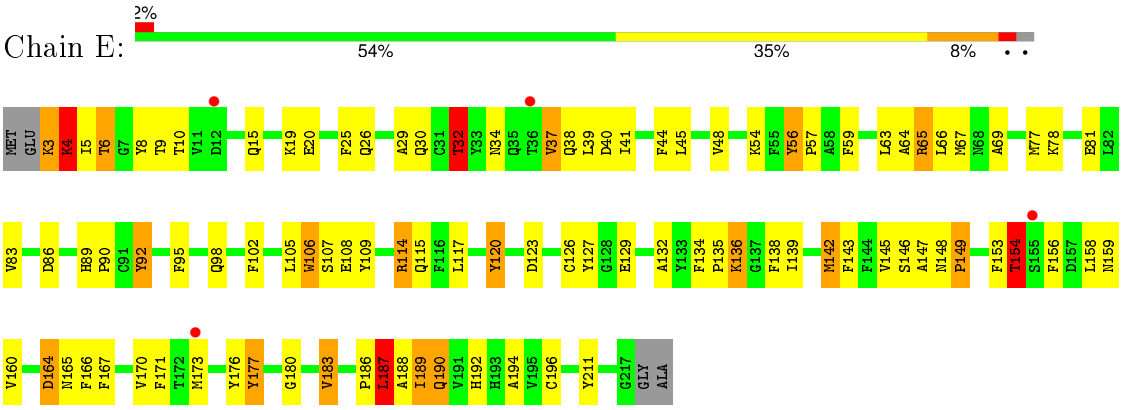
• Molecule 1: Chloramphenicol acetyltransferase

Chain D:



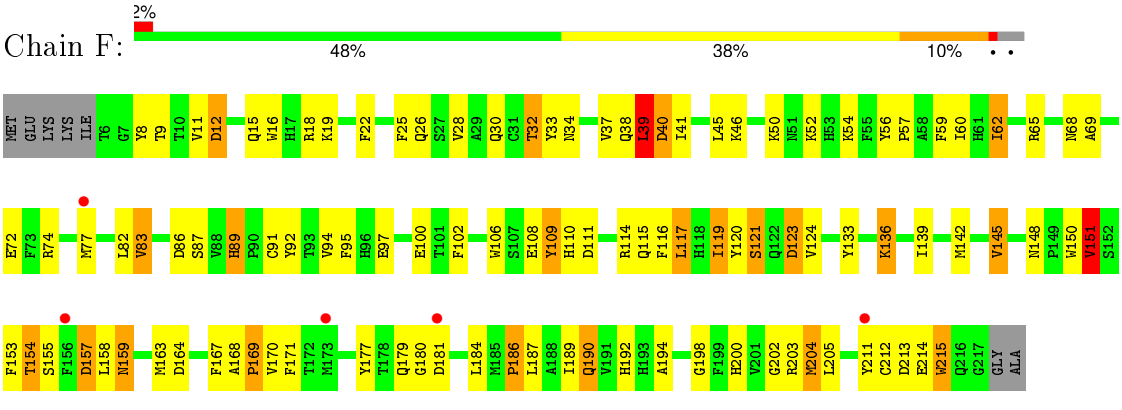

• Molecule 1: Chloramphenicol acetyltransferase

Chain E:



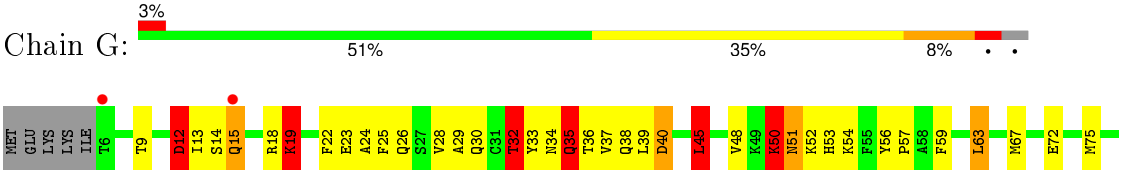

• Molecule 1: Chloramphenicol acetyltransferase

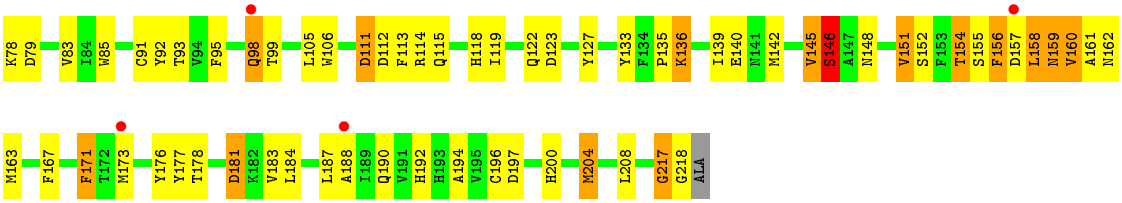
Chain F:




• Molecule 1: Chloramphenicol acetyltransferase

Chain G:

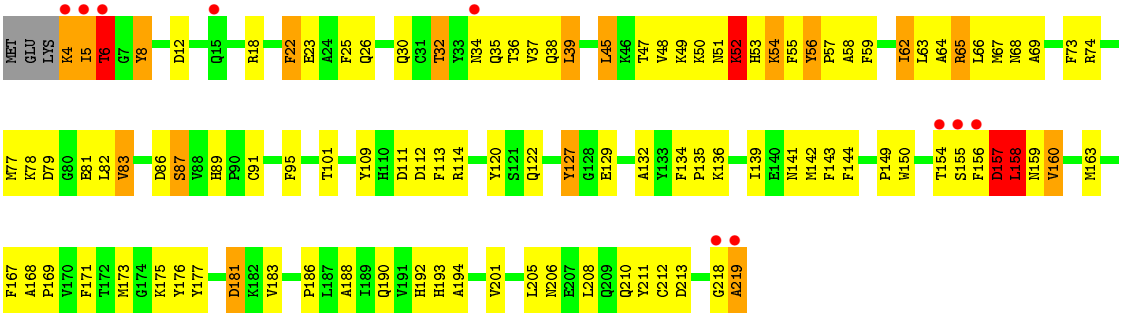






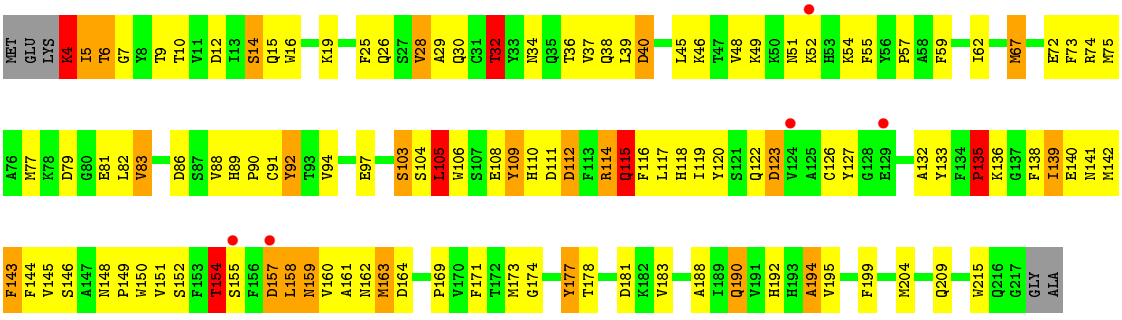
• Molecule 1: Chloramphenicol acetyltransferase

Chain H:

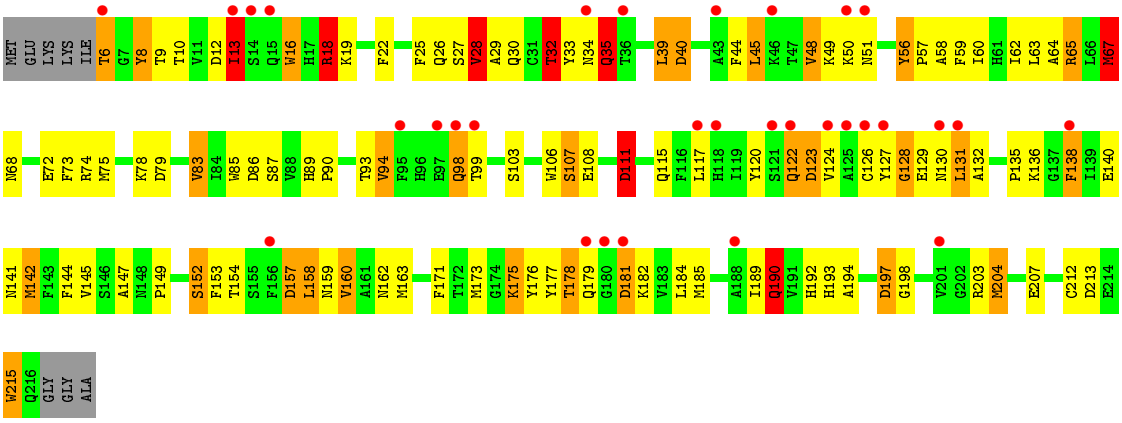
• Molecule 1: Chloramphenicol acetyltransferase

Chain I:

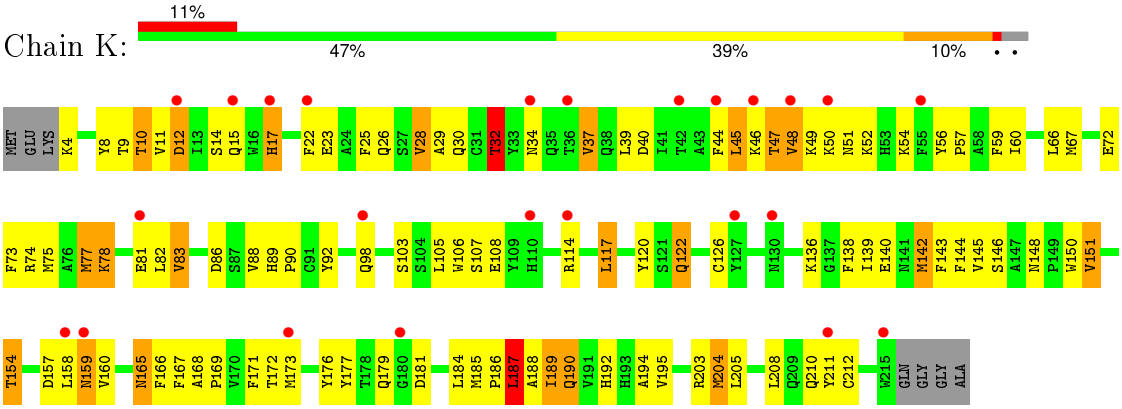
• Molecule 1: Chloramphenicol acetyltransferase

Chain J:

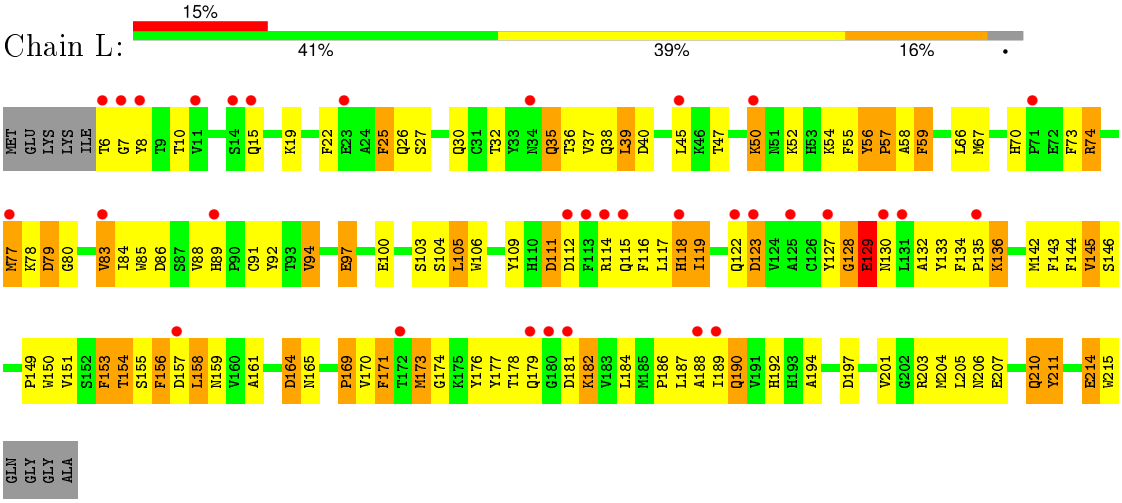
• Molecule 1: Chloramphenicol acetyltransferase

Chain K:




• Molecule 1: Chloramphenicol acetyltransferase

Chain L:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 115.74Å 129.70Å 117.98Å<br>90.00° 108.38° 90.00° | Depositor |
| Resolution (Å) | 10.00 – 2.50<br>39.33 – 2.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.6 (10.00-2.50)<br>98.7 (39.33-2.50) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | 0.06 | Depositor |
| $< I/\sigma(I) >$ [1] | 3.61 (at 2.51Å) | Xtriage |
| Refinement program | REFMAC 5.1.24 | Depositor |
| R, $R_{free}$ | 0.195 , 0.281<br>0.207 , 0.199 | Depositor<br>DCC |
| $R_{free}$ test set | 5598 reflections (5.32%) | DCC |
| Wilson B-factor (Å$^2$) | 37.9 | Xtriage |
| Anisotropy | 0.643 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 51.5 | EDS |
| Estimated twinning fraction | 0.012 for l,-k,h | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.34$ | Xtriage |
| Outliers | 0 of 112711 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 21418 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 46.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.31 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.2096e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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 | 2.04 | 58/1822 (3.2%) | 1.62 | 38/2473 (1.5%) |
| 1 | B | 1.76 | 22/1848 (1.2%) | 1.59 | 34/2506 (1.4%) |
| 1 | C | 1.84 | 35/1822 (1.9%) | 1.58 | 36/2473 (1.5%) |
| 1 | D | 1.83 | 38/1822 (2.1%) | 1.52 | 25/2473 (1.0%) |
| 1 | E | 1.67 | 20/1844 (1.1%) | 1.39 | 14/2501 (0.6%) |
| 1 | F | 1.76 | 26/1818 (1.4%) | 1.53 | 31/2468 (1.3%) |
| 1 | G | 1.71 | 18/1822 (1.0%) | 1.53 | 30/2473 (1.2%) |
| 1 | H | 1.85 | 33/1844 (1.8%) | 1.55 | 30/2502 (1.2%) |
| 1 | I | 1.85 | 38/1835 (2.1%) | 1.50 | 23/2490 (0.9%) |
| 1 | J | 1.57 | 15/1814 (0.8%) | 1.47 | 26/2463 (1.1%) |
| 1 | K | 1.55 | 14/1822 (0.8%) | 1.35 | 9/2473 (0.4%) |
| 1 | L | 1.67 | 21/1805 (1.2%) | 1.41 | 19/2451 (0.8%) |
| All | All | 1.76 | 338/21918 (1.5%) | 1.51 | 315/29746 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 2 |
| 1 | G | 0 | 1 |
| 1 | I | 0 | 1 |
| 1 | J | 0 | 3 |
| 1 | K | 0 | 1 |
| 1 | L | 0 | 1 |
| All | All | 0 | 10 |

All (338) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 150 | TRP | CE3-CZ3 | 10.79 | 1.56 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 95 | PHE | CE2-CZ | 10.43 | 1.57 | 1.37 |
| 1 | A | 87 | SER | CB-OG | -10.09 | 1.29 | 1.42 |
| 1 | I | 127 | TYR | CD1-CE1 | 10.07 | 1.54 | 1.39 |
| 1 | I | 140 | GLU | CD-OE1 | 9.99 | 1.36 | 1.25 |
| 1 | E | 146 | SER | CB-OG | 9.66 | 1.54 | 1.42 |
| 1 | G | 151 | VAL | CB-CG2 | 9.36 | 1.72 | 1.52 |
| 1 | I | 28 | VAL | CB-CG2 | 9.03 | 1.71 | 1.52 |
| 1 | I | 183 | VAL | CB-CG1 | 9.00 | 1.71 | 1.52 |
| 1 | F | 171 | PHE | CE2-CZ | 8.93 | 1.54 | 1.37 |
| 1 | A | 28 | VAL | CB-CG1 | 8.76 | 1.71 | 1.52 |
| 1 | F | 145 | VAL | CB-CG1 | 8.62 | 1.71 | 1.52 |
| 1 | K | 151 | VAL | CB-CG2 | 8.49 | 1.70 | 1.52 |
| 1 | C | 95 | PHE | CE1-CZ | 8.35 | 1.53 | 1.37 |
| 1 | C | 28 | VAL | CB-CG2 | 8.33 | 1.70 | 1.52 |
| 1 | F | 116 | PHE | CE2-CZ | 8.24 | 1.53 | 1.37 |
| 1 | I | 144 | PHE | CD1-CE1 | 8.23 | 1.55 | 1.39 |
| 1 | A | 35 | GLN | CB-CG | -8.21 | 1.30 | 1.52 |
| 1 | J | 94 | VAL | CB-CG2 | 8.21 | 1.70 | 1.52 |
| 1 | A | 177 | TYR | CE1-CZ | 8.19 | 1.49 | 1.38 |
| 1 | J | 177 | TYR | CD2-CE2 | -8.13 | 1.27 | 1.39 |
| 1 | H | 69 | ALA | CA-CB | 8.12 | 1.69 | 1.52 |
| 1 | B | 159 | ASN | CB-CG | 8.07 | 1.69 | 1.51 |
| 1 | F | 211 | TYR | CD2-CE2 | 8.05 | 1.51 | 1.39 |
| 1 | D | 58 | ALA | CA-CB | 8.04 | 1.69 | 1.52 |
| 1 | A | 33 | TYR | CD1-CE1 | 8.03 | 1.51 | 1.39 |
| 1 | D | 35 | GLN | CB-CG | -7.99 | 1.30 | 1.52 |
| 1 | A | 162 | ASN | CB-CG | 7.94 | 1.69 | 1.51 |
| 1 | A | 129 | GLU | CD-OE1 | 7.81 | 1.34 | 1.25 |
| 1 | J | 198 | GLY | C-O | 7.71 | 1.35 | 1.23 |
| 1 | E | 160 | VAL | CB-CG1 | -7.67 | 1.36 | 1.52 |
| 1 | L | 143 | PHE | CE1-CZ | 7.66 | 1.51 | 1.37 |
| 1 | A | 24 | ALA | C-O | 7.63 | 1.37 | 1.23 |
| 1 | A | 86 | ASP | CB-CG | 7.62 | 1.67 | 1.51 |
| 1 | A | 156 | PHE | CE2-CZ | 7.62 | 1.51 | 1.37 |
| 1 | F | 211 | TYR | CD1-CE1 | 7.61 | 1.50 | 1.39 |
| 1 | I | 109 | TYR | CB-CG | -7.59 | 1.40 | 1.51 |
| 1 | C | 162 | ASN | CB-CG | -7.49 | 1.33 | 1.51 |
| 1 | F | 170 | VAL | CB-CG2 | 7.47 | 1.68 | 1.52 |
| 1 | C | 98 | GLN | CG-CD | 7.45 | 1.68 | 1.51 |
| 1 | C | 195 | VAL | CB-CG1 | 7.44 | 1.68 | 1.52 |
| 1 | J | 160 | VAL | CB-CG2 | 7.42 | 1.68 | 1.52 |
| 1 | B | 160 | VAL | CB-CG1 | -7.39 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 157 | ASP | CB-CG | -7.38 | 1.36 | 1.51 |
| 1 | B | 28 | VAL | CB-CG2 | 7.38 | 1.68 | 1.52 |
| 1 | I | 111 | ASP | CB-CG | 7.38 | 1.67 | 1.51 |
| 1 | F | 150 | TRP | CB-CG | -7.26 | 1.37 | 1.50 |
| 1 | C | 87 | SER | CB-OG | -7.22 | 1.32 | 1.42 |
| 1 | B | 102 | PHE | CE2-CZ | 7.17 | 1.50 | 1.37 |
| 1 | E | 166 | PHE | CD1-CE1 | 7.16 | 1.53 | 1.39 |
| 1 | A | 69 | ALA | CA-CB | 7.14 | 1.67 | 1.52 |
| 1 | A | 81 | GLU | CG-CD | 7.14 | 1.62 | 1.51 |
| 1 | K | 211 | TYR | CD1-CE1 | 7.13 | 1.50 | 1.39 |
| 1 | I | 162 | ASN | C-O | -7.12 | 1.09 | 1.23 |
| 1 | H | 81 | GLU | CD-OE2 | 7.11 | 1.33 | 1.25 |
| 1 | A | 195 | VAL | CB-CG1 | 7.11 | 1.67 | 1.52 |
| 1 | I | 152 | SER | CB-OG | 7.10 | 1.51 | 1.42 |
| 1 | B | 199 | PHE | CE1-CZ | 7.08 | 1.50 | 1.37 |
| 1 | F | 102 | PHE | CD1-CE1 | 7.08 | 1.53 | 1.39 |
| 1 | G | 176 | TYR | CD1-CE1 | 7.08 | 1.50 | 1.39 |
| 1 | I | 55 | PHE | CE2-CZ | 7.07 | 1.50 | 1.37 |
| 1 | F | 167 | PHE | CG-CD2 | 7.06 | 1.49 | 1.38 |
| 1 | A | 8 | TYR | CD1-CE1 | -7.04 | 1.28 | 1.39 |
| 1 | A | 95 | PHE | CE2-CZ | 7.02 | 1.50 | 1.37 |
| 1 | A | 161 | ALA | CA-CB | -6.97 | 1.37 | 1.52 |
| 1 | C | 156 | PHE | CE2-CZ | 6.96 | 1.50 | 1.37 |
| 1 | I | 116 | PHE | CE1-CZ | 6.92 | 1.50 | 1.37 |
| 1 | H | 134 | PHE | CD1-CE1 | 6.91 | 1.53 | 1.39 |
| 1 | L | 174 | GLY | C-O | 6.90 | 1.34 | 1.23 |
| 1 | K | 98 | GLN | CG-CD | 6.89 | 1.66 | 1.51 |
| 1 | I | 103 | SER | C-O | 6.88 | 1.36 | 1.23 |
| 1 | L | 176 | TYR | CG-CD1 | 6.86 | 1.48 | 1.39 |
| 1 | K | 144 | PHE | CD1-CE1 | 6.85 | 1.52 | 1.39 |
| 1 | I | 106 | TRP | CB-CG | 6.84 | 1.62 | 1.50 |
| 1 | I | 199 | PHE | CE1-CZ | 6.80 | 1.50 | 1.37 |
| 1 | H | 22 | PHE | CE1-CZ | 6.79 | 1.50 | 1.37 |
| 1 | I | 6 | THR | CB-CG2 | 6.79 | 1.74 | 1.52 |
| 1 | H | 143 | PHE | CE2-CZ | 6.78 | 1.50 | 1.37 |
| 1 | D | 190 | GLN | CB-CG | -6.75 | 1.34 | 1.52 |
| 1 | G | 159 | ASN | CB-CG | 6.74 | 1.66 | 1.51 |
| 1 | B | 215 | TRP | CG-CD1 | 6.71 | 1.46 | 1.36 |
| 1 | L | 171 | PHE | CE2-CZ | 6.71 | 1.50 | 1.37 |
| 1 | C | 176 | TYR | CG-CD1 | 6.71 | 1.47 | 1.39 |
| 1 | E | 143 | PHE | CD2-CE2 | 6.70 | 1.52 | 1.39 |
| 1 | E | 37 | VAL | CB-CG1 | -6.65 | 1.38 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 54 | LYS | CE-NZ | 6.64 | 1.65 | 1.49 |
| 1 | B | 28 | VAL | CB-CG1 | 6.64 | 1.66 | 1.52 |
| 1 | L | 177 | TYR | CE1-CZ | 6.62 | 1.47 | 1.38 |
| 1 | I | 215 | TRP | CB-CG | -6.60 | 1.38 | 1.50 |
| 1 | H | 176 | TYR | CG-CD1 | 6.60 | 1.47 | 1.39 |
| 1 | E | 102 | PHE | CE2-CZ | 6.53 | 1.49 | 1.37 |
| 1 | B | 170 | VAL | CB-CG2 | 6.52 | 1.66 | 1.52 |
| 1 | C | 15 | GLN | CG-CD | 6.51 | 1.66 | 1.51 |
| 1 | H | 78 | LYS | CE-NZ | 6.51 | 1.65 | 1.49 |
| 1 | G | 181 | ASP | CB-CG | 6.51 | 1.65 | 1.51 |
| 1 | D | 95 | PHE | CG-CD1 | 6.47 | 1.48 | 1.38 |
| 1 | L | 116 | PHE | CE1-CZ | 6.47 | 1.49 | 1.37 |
| 1 | E | 143 | PHE | CD1-CE1 | 6.47 | 1.52 | 1.39 |
| 1 | I | 72 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 1 | A | 54 | LYS | CD-CE | 6.45 | 1.67 | 1.51 |
| 1 | D | 177 | TYR | CD1-CE1 | 6.40 | 1.49 | 1.39 |
| 1 | F | 95 | PHE | CE1-CZ | 6.37 | 1.49 | 1.37 |
| 1 | C | 33 | TYR | CB-CG | -6.36 | 1.42 | 1.51 |
| 1 | C | 81 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | G | 176 | TYR | CE1-CZ | 6.34 | 1.46 | 1.38 |
| 1 | E | 196 | CYS | CB-SG | -6.31 | 1.71 | 1.82 |
| 1 | A | 150 | TRP | CE3-CZ3 | 6.28 | 1.49 | 1.38 |
| 1 | F | 69 | ALA | CA-CB | 6.27 | 1.65 | 1.52 |
| 1 | E | 56 | TYR | CG-CD1 | -6.27 | 1.31 | 1.39 |
| 1 | A | 74 | ARG | CB-CG | 6.26 | 1.69 | 1.52 |
| 1 | H | 183 | VAL | CB-CG2 | 6.26 | 1.66 | 1.52 |
| 1 | H | 55 | PHE | CE1-CZ | 6.26 | 1.49 | 1.37 |
| 1 | I | 37 | VAL | CB-CG2 | -6.25 | 1.39 | 1.52 |
| 1 | D | 54 | LYS | CD-CE | 6.24 | 1.66 | 1.51 |
| 1 | L | 153 | PHE | CE1-CZ | 6.23 | 1.49 | 1.37 |
| 1 | H | 167 | PHE | CB-CG | 6.23 | 1.61 | 1.51 |
| 1 | B | 176 | TYR | CG-CD1 | 6.22 | 1.47 | 1.39 |
| 1 | I | 55 | PHE | CD1-CE1 | 6.22 | 1.51 | 1.39 |
| 1 | C | 176 | TYR | CD1-CE1 | 6.22 | 1.48 | 1.39 |
| 1 | G | 146 | SER | CB-OG | -6.19 | 1.34 | 1.42 |
| 1 | B | 16 | TRP | CG-CD1 | 6.19 | 1.45 | 1.36 |
| 1 | J | 190 | GLN | CB-CG | 6.17 | 1.69 | 1.52 |
| 1 | H | 206 | ASN | C-O | 6.16 | 1.35 | 1.23 |
| 1 | H | 160 | VAL | CA-CB | 6.15 | 1.67 | 1.54 |
| 1 | F | 151 | VAL | CB-CG2 | -6.14 | 1.40 | 1.52 |
| 1 | A | 166 | PHE | CE1-CZ | 6.13 | 1.49 | 1.37 |
| 1 | A | 153 | PHE | CD1-CE1 | 6.13 | 1.51 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 126 | CYS | CB-SG | -6.12 | 1.71 | 1.82 |
| 1 | B | 67 | MET | CB-CG | 6.11 | 1.70 | 1.51 |
| 1 | A | 22 | PHE | CE2-CZ | 6.10 | 1.49 | 1.37 |
| 1 | D | 211 | TYR | CB-CG | -6.10 | 1.42 | 1.51 |
| 1 | H | 157 | ASP | CA-CB | -6.10 | 1.40 | 1.53 |
| 1 | C | 23 | GLU | CG-CD | 6.09 | 1.61 | 1.51 |
| 1 | C | 27 | SER | C-O | 6.09 | 1.34 | 1.23 |
| 1 | D | 22 | PHE | CE1-CZ | 6.09 | 1.49 | 1.37 |
| 1 | I | 92 | TYR | CE2-CZ | 6.08 | 1.46 | 1.38 |
| 1 | D | 138 | PHE | CE2-CZ | 6.07 | 1.48 | 1.37 |
| 1 | K | 177 | TYR | CE2-CZ | 6.07 | 1.46 | 1.38 |
| 1 | L | 97 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 |
| 1 | D | 8 | TYR | CG-CD1 | 6.07 | 1.47 | 1.39 |
| 1 | J | 140 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | L | 153 | PHE | CD1-CE1 | 6.02 | 1.51 | 1.39 |
| 1 | G | 24 | ALA | CA-CB | -6.02 | 1.39 | 1.52 |
| 1 | K | 159 | ASN | CB-CG | 6.01 | 1.64 | 1.51 |
| 1 | C | 153 | PHE | CE1-CZ | 5.99 | 1.48 | 1.37 |
| 1 | A | 95 | PHE | CE1-CZ | 5.99 | 1.48 | 1.37 |
| 1 | C | 127 | TYR | CD1-CE1 | 5.98 | 1.48 | 1.39 |
| 1 | I | 177 | TYR | CD1-CE1 | 5.97 | 1.48 | 1.39 |
| 1 | A | 26 | GLN | CB-CG | -5.96 | 1.36 | 1.52 |
| 1 | I | 159 | ASN | CB-CG | 5.93 | 1.64 | 1.51 |
| 1 | I | 183 | VAL | CB-CG2 | 5.93 | 1.65 | 1.52 |
| 1 | H | 64 | ALA | CA-CB | -5.92 | 1.40 | 1.52 |
| 1 | B | 194 | ALA | CA-CB | 5.92 | 1.64 | 1.52 |
| 1 | D | 134 | PHE | CE1-CZ | 5.92 | 1.48 | 1.37 |
| 1 | I | 4 | LYS | CB-CG | 5.92 | 1.68 | 1.52 |
| 1 | H | 56 | TYR | CD2-CE2 | 5.92 | 1.48 | 1.39 |
| 1 | A | 140 | GLU | CD-OE1 | 5.92 | 1.32 | 1.25 |
| 1 | A | 169 | PRO | CA-C | 5.92 | 1.64 | 1.52 |
| 1 | I | 4 | LYS | N-CA | 5.90 | 1.58 | 1.46 |
| 1 | G | 171 | PHE | CD1-CE1 | 5.89 | 1.51 | 1.39 |
| 1 | A | 134 | PHE | CB-CG | 5.88 | 1.61 | 1.51 |
| 1 | A | 176 | TYR | CE2-CZ | 5.88 | 1.46 | 1.38 |
| 1 | A | 191 | VAL | CA-CB | -5.88 | 1.42 | 1.54 |
| 1 | I | 114 | ARG | CG-CD | 5.87 | 1.66 | 1.51 |
| 1 | D | 210 | GLN | CG-CD | 5.86 | 1.64 | 1.51 |
| 1 | D | 216 | GLN | CG-CD | 5.85 | 1.64 | 1.51 |
| 1 | H | 176 | TYR | CD1-CE1 | 5.85 | 1.48 | 1.39 |
| 1 | D | 111 | ASP | CB-CG | -5.85 | 1.39 | 1.51 |
| 1 | B | 109 | TYR | CD1-CE1 | 5.85 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 28 | VAL | CB-CG1 | 5.85 | 1.65 | 1.52 |
| 1 | D | 105 | LEU | CG-CD1 | 5.84 | 1.73 | 1.51 |
| 1 | H | 144 | PHE | C-O | 5.82 | 1.34 | 1.23 |
| 1 | B | 190 | GLN | CB-CG | -5.82 | 1.36 | 1.52 |
| 1 | F | 109 | TYR | CD2-CE2 | -5.81 | 1.30 | 1.39 |
| 1 | E | 170 | VAL | CB-CG2 | 5.80 | 1.65 | 1.52 |
| 1 | A | 95 | PHE | CG-CD2 | 5.80 | 1.47 | 1.38 |
| 1 | F | 22 | PHE | CE2-CZ | 5.79 | 1.48 | 1.37 |
| 1 | D | 177 | TYR | CG-CD2 | 5.78 | 1.46 | 1.39 |
| 1 | B | 200 | HIS | C-O | -5.78 | 1.12 | 1.23 |
| 1 | G | 167 | PHE | CG-CD2 | 5.78 | 1.47 | 1.38 |
| 1 | D | 133 | TYR | CG-CD1 | 5.75 | 1.46 | 1.39 |
| 1 | K | 189 | ILE | CA-CB | 5.75 | 1.68 | 1.54 |
| 1 | H | 167 | PHE | CD1-CE1 | 5.75 | 1.50 | 1.39 |
| 1 | D | 211 | TYR | C-O | -5.74 | 1.12 | 1.23 |
| 1 | A | 167 | PHE | CB-CG | 5.73 | 1.61 | 1.51 |
| 1 | H | 79 | ASP | CB-CG | 5.72 | 1.63 | 1.51 |
| 1 | J | 16 | TRP | CG-CD1 | 5.72 | 1.44 | 1.36 |
| 1 | C | 102 | PHE | CD1-CE1 | 5.71 | 1.50 | 1.39 |
| 1 | C | 83 | VAL | CB-CG1 | -5.71 | 1.40 | 1.52 |
| 1 | D | 145 | VAL | CB-CG2 | -5.70 | 1.40 | 1.52 |
| 1 | I | 140 | GLU | CG-CD | 5.70 | 1.60 | 1.51 |
| 1 | A | 59 | PHE | CD1-CE1 | 5.70 | 1.50 | 1.39 |
| 1 | D | 114 | ARG | CG-CD | 5.69 | 1.66 | 1.51 |
| 1 | I | 194 | ALA | C-O | 5.68 | 1.34 | 1.23 |
| 1 | A | 95 | PHE | CG-CD1 | 5.66 | 1.47 | 1.38 |
| 1 | I | 15 | GLN | CB-CG | 5.66 | 1.67 | 1.52 |
| 1 | C | 127 | TYR | CE2-CZ | 5.66 | 1.46 | 1.38 |
| 1 | D | 170 | VAL | CA-CB | -5.62 | 1.43 | 1.54 |
| 1 | H | 150 | TRP | CE3-CZ3 | 5.62 | 1.48 | 1.38 |
| 1 | A | 196 | CYS | CB-SG | -5.62 | 1.72 | 1.81 |
| 1 | I | 195 | VAL | CB-CG1 | 5.61 | 1.64 | 1.52 |
| 1 | D | 171 | PHE | C-O | 5.60 | 1.33 | 1.23 |
| 1 | D | 109 | TYR | CD2-CE2 | 5.60 | 1.47 | 1.39 |
| 1 | H | 219 | ALA | N-CA | 5.59 | 1.57 | 1.46 |
| 1 | K | 12 | ASP | CB-CG | 5.59 | 1.63 | 1.51 |
| 1 | C | 65 | ARG | CG-CD | -5.59 | 1.38 | 1.51 |
| 1 | L | 176 | TYR | CD1-CE1 | 5.58 | 1.47 | 1.39 |
| 1 | K | 98 | GLN | CB-CG | 5.58 | 1.67 | 1.52 |
| 1 | H | 55 | PHE | CD2-CE2 | 5.57 | 1.50 | 1.39 |
| 1 | A | 65 | ARG | NE-CZ | 5.56 | 1.40 | 1.33 |
| 1 | B | 127 | TYR | CZ-OH | 5.56 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | J | 48 | VAL | CB-CG2 | -5.56 | 1.41 | 1.52 |
| 1 | B | 58 | ALA | CA-CB | 5.55 | 1.64 | 1.52 |
| 1 | L | 94 | VAL | CA-CB | 5.55 | 1.66 | 1.54 |
| 1 | G | 171 | PHE | CE2-CZ | 5.55 | 1.47 | 1.37 |
| 1 | I | 4 | LYS | CG-CD | 5.55 | 1.71 | 1.52 |
| 1 | D | 183 | VAL | CB-CG2 | 5.54 | 1.64 | 1.52 |
| 1 | F | 8 | TYR | CD1-CE1 | -5.53 | 1.31 | 1.39 |
| 1 | H | 74 | ARG | CZ-NH1 | 5.53 | 1.40 | 1.33 |
| 1 | F | 170 | VAL | C-O | 5.53 | 1.33 | 1.23 |
| 1 | G | 162 | ASN | CB-CG | 5.52 | 1.63 | 1.51 |
| 1 | B | 140 | GLU | CG-CD | 5.52 | 1.60 | 1.51 |
| 1 | E | 102 | PHE | CD1-CE1 | 5.52 | 1.50 | 1.39 |
| 1 | G | 156 | PHE | CE1-CZ | -5.51 | 1.26 | 1.37 |
| 1 | I | 104 | SER | CB-OG | -5.49 | 1.35 | 1.42 |
| 1 | L | 55 | PHE | CB-CG | -5.49 | 1.42 | 1.51 |
| 1 | K | 81 | GLU | CG-CD | 5.48 | 1.60 | 1.51 |
| 1 | F | 95 | PHE | CE2-CZ | 5.48 | 1.47 | 1.37 |
| 1 | I | 133 | TYR | CB-CG | -5.47 | 1.43 | 1.51 |
| 1 | A | 156 | PHE | CD1-CE1 | 5.46 | 1.50 | 1.39 |
| 1 | G | 95 | PHE | C-O | -5.46 | 1.12 | 1.23 |
| 1 | I | 88 | VAL | CB-CG2 | -5.46 | 1.41 | 1.52 |
| 1 | A | 143 | PHE | CD2-CE2 | -5.45 | 1.28 | 1.39 |
| 1 | H | 186 | PRO | C-O | 5.45 | 1.34 | 1.23 |
| 1 | A | 23 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | C | 58 | ALA | CA-CB | 5.44 | 1.63 | 1.52 |
| 1 | G | 28 | VAL | CB-CG1 | 5.44 | 1.64 | 1.52 |
| 1 | E | 92 | TYR | CD2-CE2 | 5.44 | 1.47 | 1.39 |
| 1 | J | 28 | VAL | CB-CG2 | 5.43 | 1.64 | 1.52 |
| 1 | E | 106 | TRP | CE3-CZ3 | 5.42 | 1.47 | 1.38 |
| 1 | A | 211 | TYR | CG-CD1 | 5.42 | 1.46 | 1.39 |
| 1 | J | 74 | ARG | CB-CG | 5.39 | 1.67 | 1.52 |
| 1 | B | 25 | PHE | CE2-CZ | -5.39 | 1.27 | 1.37 |
| 1 | D | 88 | VAL | CA-CB | -5.39 | 1.43 | 1.54 |
| 1 | D | 133 | TYR | CE1-CZ | 5.39 | 1.45 | 1.38 |
| 1 | K | 28 | VAL | CB-CG2 | 5.39 | 1.64 | 1.52 |
| 1 | A | 134 | PHE | CD1-CE1 | 5.37 | 1.50 | 1.39 |
| 1 | C | 138 | PHE | CD1-CE1 | 5.35 | 1.50 | 1.39 |
| 1 | L | 156 | PHE | CD2-CE2 | -5.35 | 1.28 | 1.39 |
| 1 | H | 109 | TYR | CD1-CE1 | -5.35 | 1.31 | 1.39 |
| 1 | A | 59 | PHE | CE2-CZ | 5.35 | 1.47 | 1.37 |
| 1 | H | 68 | ASN | CB-CG | 5.35 | 1.63 | 1.51 |
| 1 | H | 95 | PHE | CE2-CZ | 5.35 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 84 | ILE | CB-CG2 | 5.34 | 1.69 | 1.52 |
| 1 | I | 48 | VAL | CB-CG1 | 5.34 | 1.64 | 1.52 |
| 1 | L | 176 | TYR | CE1-CZ | 5.34 | 1.45 | 1.38 |
| 1 | E | 176 | TYR | CD1-CE1 | 5.33 | 1.47 | 1.39 |
| 1 | C | 102 | PHE | CE2-CZ | 5.33 | 1.47 | 1.37 |
| 1 | A | 160 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 1 | C | 95 | PHE | CG-CD1 | 5.31 | 1.46 | 1.38 |
| 1 | L | 145 | VAL | CB-CG2 | -5.29 | 1.41 | 1.52 |
| 1 | C | 95 | PHE | CG-CD2 | 5.29 | 1.46 | 1.38 |
| 1 | I | 55 | PHE | CG-CD2 | 5.29 | 1.46 | 1.38 |
| 1 | C | 75 | MET | C-O | 5.27 | 1.33 | 1.23 |
| 1 | D | 100 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | I | 115 | GLN | CG-CD | 5.26 | 1.63 | 1.51 |
| 1 | A | 33 | TYR | CE2-CZ | 5.25 | 1.45 | 1.38 |
| 1 | F | 28 | VAL | CB-CG2 | 5.25 | 1.63 | 1.52 |
| 1 | A | 54 | LYS | CG-CD | 5.24 | 1.70 | 1.52 |
| 1 | C | 177 | TYR | CG-CD2 | 5.24 | 1.46 | 1.39 |
| 1 | B | 156 | PHE | CD2-CE2 | 5.24 | 1.49 | 1.39 |
| 1 | J | 144 | PHE | CE2-CZ | 5.24 | 1.47 | 1.37 |
| 1 | A | 138 | PHE | CD1-CE1 | 5.24 | 1.49 | 1.39 |
| 1 | G | 152 | SER | CA-CB | 5.23 | 1.60 | 1.52 |
| 1 | H | 127 | TYR | CD1-CE1 | 5.23 | 1.47 | 1.39 |
| 1 | I | 90 | PRO | CG-CD | 5.22 | 1.67 | 1.50 |
| 1 | F | 154 | THR | N-CA | -5.22 | 1.35 | 1.46 |
| 1 | C | 44 | PHE | CE2-CZ | -5.22 | 1.27 | 1.37 |
| 1 | K | 144 | PHE | CD2-CE2 | 5.21 | 1.49 | 1.39 |
| 1 | C | 133 | TYR | CE2-CZ | 5.20 | 1.45 | 1.38 |
| 1 | H | 56 | TYR | CD1-CE1 | 5.20 | 1.47 | 1.39 |
| 1 | D | 143 | PHE | CE2-CZ | 5.20 | 1.47 | 1.37 |
| 1 | A | 34 | ASN | CG-ND2 | 5.19 | 1.45 | 1.32 |
| 1 | G | 33 | TYR | CG-CD1 | 5.19 | 1.45 | 1.39 |
| 1 | A | 29 | ALA | N-CA | -5.19 | 1.35 | 1.46 |
| 1 | L | 133 | TYR | CE2-CZ | 5.19 | 1.45 | 1.38 |
| 1 | A | 175 | LYS | CB-CG | 5.18 | 1.66 | 1.52 |
| 1 | E | 69 | ALA | CA-CB | 5.18 | 1.63 | 1.52 |
| 1 | A | 81 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | D | 55 | PHE | CE1-CZ | 5.17 | 1.47 | 1.37 |
| 1 | F | 33 | TYR | C-O | 5.16 | 1.33 | 1.23 |
| 1 | A | 132 | ALA | CA-CB | 5.16 | 1.63 | 1.52 |
| 1 | G | 176 | TYR | CG-CD1 | 5.16 | 1.45 | 1.39 |
| 1 | J | 8 | TYR | CE2-CZ | 5.15 | 1.45 | 1.38 |
| 1 | D | 95 | PHE | CE2-CZ | 5.15 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 108 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |
| 1 | L | 143 | PHE | CG-CD1 | 5.15 | 1.46 | 1.38 |
| 1 | D | 124 | VAL | CB-CG1 | 5.14 | 1.63 | 1.52 |
| 1 | L | 25 | PHE | CE1-CZ | 5.14 | 1.47 | 1.37 |
| 1 | L | 59 | PHE | CD1-CE1 | 5.14 | 1.49 | 1.39 |
| 1 | C | 161 | ALA | CA-CB | -5.14 | 1.41 | 1.52 |
| 1 | K | 23 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | E | 149 | PRO | CA-C | -5.12 | 1.42 | 1.52 |
| 1 | D | 83 | VAL | CA-CB | -5.12 | 1.44 | 1.54 |
| 1 | E | 180 | GLY | C-O | 5.12 | 1.31 | 1.23 |
| 1 | C | 170 | VAL | C-O | 5.11 | 1.33 | 1.23 |
| 1 | D | 211 | TYR | CZ-OH | -5.11 | 1.29 | 1.37 |
| 1 | C | 56 | TYR | CB-CG | 5.10 | 1.59 | 1.51 |
| 1 | F | 109 | TYR | CD1-CE1 | -5.10 | 1.31 | 1.39 |
| 1 | B | 46 | LYS | CB-CG | 5.10 | 1.66 | 1.52 |
| 1 | A | 47 | THR | C-O | 5.09 | 1.33 | 1.23 |
| 1 | J | 35 | GLN | C-O | 5.08 | 1.33 | 1.23 |
| 1 | F | 167 | PHE | CE1-CZ | 5.08 | 1.47 | 1.37 |
| 1 | D | 49 | LYS | CE-NZ | 5.08 | 1.61 | 1.49 |
| 1 | E | 177 | TYR | CE1-CZ | 5.08 | 1.45 | 1.38 |
| 1 | A | 102 | PHE | CD2-CE2 | -5.08 | 1.29 | 1.39 |
| 1 | L | 35 | GLN | CB-CG | -5.07 | 1.38 | 1.52 |
| 1 | A | 134 | PHE | CE1-CZ | 5.07 | 1.47 | 1.37 |
| 1 | E | 95 | PHE | CG-CD2 | 5.07 | 1.46 | 1.38 |
| 1 | D | 88 | VAL | CB-CG1 | 5.06 | 1.63 | 1.52 |
| 1 | G | 196 | CYS | CB-SG | -5.06 | 1.73 | 1.81 |
| 1 | D | 28 | VAL | CB-CG2 | 5.06 | 1.63 | 1.52 |
| 1 | H | 167 | PHE | CE2-CZ | 5.06 | 1.47 | 1.37 |
| 1 | J | 33 | TYR | CE2-CZ | 5.05 | 1.45 | 1.38 |
| 1 | H | 171 | PHE | CE2-CZ | 5.05 | 1.47 | 1.37 |
| 1 | A | 28 | VAL | CB-CG2 | 5.04 | 1.63 | 1.52 |
| 1 | F | 74 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.33 |
| 1 | F | 159 | ASN | CB-CG | 5.04 | 1.62 | 1.51 |
| 1 | A | 52 | LYS | CD-CE | 5.04 | 1.63 | 1.51 |
| 1 | F | 16 | TRP | CB-CG | 5.04 | 1.59 | 1.50 |
| 1 | D | 151 | VAL | CA-CB | 5.03 | 1.65 | 1.54 |
| 1 | A | 23 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 |
| 1 | L | 143 | PHE | CG-CD2 | 5.01 | 1.46 | 1.38 |
| 1 | H | 62 | ILE | CA-C | 5.01 | 1.66 | 1.52 |
| 1 | A | 167 | PHE | CD2-CE2 | 5.00 | 1.49 | 1.39 |
| 1 | B | 72 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |
| 1 | J | 13 | ILE | CA-CB | 5.00 | 1.66 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 98 | GLN | CB-CG | 5.00 | 1.66 | 1.52 |

All (315) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 111 | ASP | CB-CG-OD2 | 13.02 | 130.02 | 118.30 |
| 1 | A | 65 | ARG | NE-CZ-NH1 | 11.59 | 126.09 | 120.30 |
| 1 | C | 157 | ASP | CB-CG-OD2 | 11.45 | 128.60 | 118.30 |
| 1 | C | 18 | ARG | NE-CZ-NH1 | 11.39 | 126.00 | 120.30 |
| 1 | I | 181 | ASP | CB-CG-OD2 | 11.01 | 128.21 | 118.30 |
| 1 | A | 197 | ASP | CB-CG-OD1 | 10.86 | 128.07 | 118.30 |
| 1 | B | 112 | ASP | CB-CG-OD1 | 10.58 | 127.82 | 118.30 |
| 1 | J | 111 | ASP | CB-CG-OD1 | 10.52 | 127.77 | 118.30 |
| 1 | J | 40 | ASP | CB-CG-OD2 | 10.32 | 127.59 | 118.30 |
| 1 | B | 111 | ASP | CB-CG-OD2 | 10.26 | 127.53 | 118.30 |
| 1 | J | 86 | ASP | CB-CG-OD2 | 10.22 | 127.50 | 118.30 |
| 1 | F | 40 | ASP | CB-CG-OD2 | 10.10 | 127.39 | 118.30 |
| 1 | B | 18 | ARG | NE-CZ-NH2 | -9.95 | 115.33 | 120.30 |
| 1 | D | 157 | ASP | CB-CG-OD2 | 9.80 | 127.12 | 118.30 |
| 1 | C | 86 | ASP | CB-CG-OD2 | 9.77 | 127.09 | 118.30 |
| 1 | C | 18 | ARG | NE-CZ-NH2 | -9.76 | 115.42 | 120.30 |
| 1 | H | 86 | ASP | CB-CG-OD2 | 9.56 | 126.90 | 118.30 |
| 1 | J | 197 | ASP | CB-CG-OD2 | 9.41 | 126.77 | 118.30 |
| 1 | J | 157 | ASP | CB-CG-OD1 | -9.39 | 109.85 | 118.30 |
| 1 | D | 40 | ASP | CB-CG-OD2 | 9.39 | 126.75 | 118.30 |
| 1 | I | 67 | MET | CG-SD-CE | -9.27 | 85.37 | 100.20 |
| 1 | H | 213 | ASP | CB-CG-OD2 | 9.22 | 126.60 | 118.30 |
| 1 | I | 163 | MET | CG-SD-CE | 9.21 | 114.93 | 100.20 |
| 1 | B | 111 | ASP | CB-CG-OD1 | -9.19 | 110.03 | 118.30 |
| 1 | B | 123 | ASP | CB-CG-OD2 | 9.17 | 126.55 | 118.30 |
| 1 | F | 213 | ASP | CB-CG-OD2 | 9.08 | 126.47 | 118.30 |
| 1 | L | 111 | ASP | CB-CG-OD2 | 9.05 | 126.44 | 118.30 |
| 1 | H | 5 | ILE | C-N-CA | 8.99 | 144.17 | 121.70 |
| 1 | G | 45 | LEU | CB-CG-CD2 | 8.98 | 126.27 | 111.00 |
| 1 | K | 40 | ASP | CB-CG-OD2 | 8.98 | 126.38 | 118.30 |
| 1 | E | 86 | ASP | CB-CG-OD2 | 8.96 | 126.36 | 118.30 |
| 1 | A | 217 | GLY | C-N-CA | -8.92 | 103.56 | 122.30 |
| 1 | K | 86 | ASP | CB-CG-OD2 | 8.70 | 126.13 | 118.30 |
| 1 | H | 111 | ASP | CB-CG-OD1 | 8.68 | 126.11 | 118.30 |
| 1 | H | 39 | LEU | CB-CG-CD2 | 8.68 | 125.75 | 111.00 |
| 1 | L | 181 | ASP | CB-CG-OD2 | 8.62 | 126.06 | 118.30 |
| 1 | J | 157 | ASP | CB-CG-OD2 | 8.59 | 126.03 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | L | 79 | ASP | CB-CG-OD2 | 8.52 | 125.97 | 118.30 |
| 1 | G | 111 | ASP | CB-CG-OD1 | -8.52 | 110.64 | 118.30 |
| 1 | G | 157 | ASP | CB-CG-OD2 | 8.43 | 125.89 | 118.30 |
| 1 | A | 32 | THR | N-CA-CB | -8.42 | 94.30 | 110.30 |
| 1 | B | 187 | LEU | CB-CG-CD2 | 8.36 | 125.22 | 111.00 |
| 1 | D | 65 | ARG | NE-CZ-NH2 | -8.36 | 116.12 | 120.30 |
| 1 | F | 86 | ASP | CB-CG-OD2 | 8.33 | 125.80 | 118.30 |
| 1 | G | 181 | ASP | CB-CG-OD2 | 8.27 | 125.74 | 118.30 |
| 1 | F | 12 | ASP | CB-CG-OD2 | 8.19 | 125.67 | 118.30 |
| 1 | C | 203 | ARG | NE-CZ-NH1 | -8.11 | 116.24 | 120.30 |
| 1 | G | 40 | ASP | CB-CG-OD2 | 8.06 | 125.56 | 118.30 |
| 1 | H | 112 | ASP | CB-CG-OD1 | 8.01 | 125.51 | 118.30 |
| 1 | F | 181 | ASP | CB-CG-OD2 | 7.97 | 125.47 | 118.30 |
| 1 | H | 66 | LEU | CB-CG-CD2 | -7.95 | 97.49 | 111.00 |
| 1 | H | 52 | LYS | CA-C-N | -7.94 | 99.73 | 117.20 |
| 1 | F | 12 | ASP | CB-CG-OD1 | -7.88 | 111.21 | 118.30 |
| 1 | H | 39 | LEU | CA-CB-CG | 7.87 | 133.40 | 115.30 |
| 1 | I | 164 | ASP | CB-CG-OD2 | 7.85 | 125.37 | 118.30 |
| 1 | G | 12 | ASP | CB-CG-OD1 | 7.78 | 125.30 | 118.30 |
| 1 | J | 74 | ARG | NE-CZ-NH1 | -7.71 | 116.45 | 120.30 |
| 1 | H | 157 | ASP | CB-CG-OD1 | -7.67 | 111.40 | 118.30 |
| 1 | H | 6 | THR | N-CA-C | 7.66 | 131.67 | 111.00 |
| 1 | B | 28 | VAL | N-CA-CB | 7.65 | 128.33 | 111.50 |
| 1 | J | 157 | ASP | CB-CA-C | -7.63 | 95.14 | 110.40 |
| 1 | C | 181 | ASP | CB-CG-OD2 | 7.56 | 125.10 | 118.30 |
| 1 | A | 18 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 1 | I | 79 | ASP | CB-CG-OD2 | 7.55 | 125.10 | 118.30 |
| 1 | D | 158 | LEU | CB-CG-CD2 | -7.51 | 98.22 | 111.00 |
| 1 | J | 32 | THR | OG1-CB-CG2 | -7.50 | 92.74 | 110.00 |
| 1 | F | 151 | VAL | CG1-CB-CG2 | -7.49 | 98.91 | 110.90 |
| 1 | A | 12 | ASP | CB-CG-OD2 | 7.46 | 125.02 | 118.30 |
| 1 | I | 28 | VAL | CG1-CB-CG2 | 7.46 | 122.84 | 110.90 |
| 1 | J | 12 | ASP | CB-CG-OD2 | 7.33 | 124.90 | 118.30 |
| 1 | G | 111 | ASP | CB-CG-OD2 | 7.33 | 124.89 | 118.30 |
| 1 | J | 128 | GLY | N-CA-C | -7.31 | 94.82 | 113.10 |
| 1 | G | 32 | THR | N-CA-CB | -7.30 | 96.43 | 110.30 |
| 1 | I | 28 | VAL | CB-CA-C | 7.25 | 125.17 | 111.40 |
| 1 | C | 157 | ASP | CB-CG-OD1 | -7.24 | 111.79 | 118.30 |
| 1 | E | 154 | THR | N-CA-CB | -7.18 | 96.66 | 110.30 |
| 1 | D | 181 | ASP | CB-CG-OD2 | 7.17 | 124.76 | 118.30 |
| 1 | H | 87 | SER | CB-CA-C | -7.17 | 96.49 | 110.10 |
| 1 | J | 6 | THR | C-N-CA | -7.14 | 107.30 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 97 | GLU | CB-CA-C | -7.08 | 96.25 | 110.40 |
| 1 | H | 12 | ASP | CB-CG-OD2 | 7.08 | 124.67 | 118.30 |
| 1 | A | 111 | ASP | CB-CG-OD2 | 7.05 | 124.64 | 118.30 |
| 1 | D | 12 | ASP | CB-CG-OD2 | 7.05 | 124.64 | 118.30 |
| 1 | F | 123 | ASP | CB-CG-OD2 | 7.04 | 124.64 | 118.30 |
| 1 | L | 164 | ASP | CB-CG-OD2 | 7.03 | 124.62 | 118.30 |
| 1 | C | 86 | ASP | CB-CG-OD1 | -6.95 | 112.05 | 118.30 |
| 1 | A | 39 | LEU | CB-CG-CD2 | 6.90 | 122.73 | 111.00 |
| 1 | H | 8 | TYR | CB-CG-CD2 | 6.84 | 125.11 | 121.00 |
| 1 | C | 87 | SER | CB-CA-C | -6.81 | 97.17 | 110.10 |
| 1 | H | 6 | THR | N-CA-CB | -6.78 | 97.41 | 110.30 |
| 1 | J | 67 | MET | CG-SD-CE | 6.77 | 111.03 | 100.20 |
| 1 | H | 83 | VAL | N-CA-CB | -6.77 | 96.61 | 111.50 |
| 1 | L | 187 | LEU | CA-CB-CG | -6.76 | 99.76 | 115.30 |
| 1 | J | 65 | ARG | NE-CZ-NH1 | -6.75 | 116.93 | 120.30 |
| 1 | B | 40 | ASP | CB-CG-OD2 | 6.75 | 124.37 | 118.30 |
| 1 | A | 197 | ASP | OD1-CG-OD2 | -6.74 | 110.49 | 123.30 |
| 1 | A | 49 | LYS | CD-CE-NZ | -6.74 | 96.20 | 111.70 |
| 1 | C | 213 | ASP | CB-CG-OD2 | 6.73 | 124.36 | 118.30 |
| 1 | A | 97 | GLU | CA-CB-CG | 6.73 | 128.20 | 113.40 |
| 1 | G | 112 | ASP | CB-CG-OD2 | 6.70 | 124.33 | 118.30 |
| 1 | E | 187 | LEU | CB-CG-CD2 | 6.70 | 122.39 | 111.00 |
| 1 | E | 40 | ASP | CB-CG-OD2 | 6.69 | 124.33 | 118.30 |
| 1 | I | 12 | ASP | CB-CG-OD2 | 6.67 | 124.30 | 118.30 |
| 1 | H | 219 | ALA | N-CA-CB | 6.64 | 119.39 | 110.10 |
| 1 | E | 187 | LEU | CA-CB-CG | -6.62 | 100.08 | 115.30 |
| 1 | A | 181 | ASP | CB-CG-OD2 | 6.61 | 124.25 | 118.30 |
| 1 | J | 18 | ARG | CG-CD-NE | 6.60 | 125.65 | 111.80 |
| 1 | H | 5 | ILE | CA-C-N | -6.59 | 102.71 | 117.20 |
| 1 | I | 40 | ASP | CB-CG-OD2 | 6.57 | 124.22 | 118.30 |
| 1 | A | 203 | ARG | NE-CZ-NH2 | -6.56 | 117.02 | 120.30 |
| 1 | C | 39 | LEU | CB-CG-CD2 | 6.56 | 122.15 | 111.00 |
| 1 | F | 121 | SER | N-CA-CB | 6.55 | 120.33 | 110.50 |
| 1 | B | 51 | ASN | C-N-CA | -6.53 | 105.38 | 121.70 |
| 1 | D | 213 | ASP | CB-CG-OD2 | 6.51 | 124.16 | 118.30 |
| 1 | C | 176 | TYR | CB-CG-CD2 | -6.51 | 117.10 | 121.00 |
| 1 | B | 74 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 1 | E | 32 | THR | N-CA-CB | -6.49 | 97.97 | 110.30 |
| 1 | G | 51 | ASN | N-CA-C | -6.46 | 93.56 | 111.00 |
| 1 | L | 39 | LEU | CA-CB-CG | 6.45 | 130.12 | 115.30 |
| 1 | B | 181 | ASP | CB-CG-OD2 | 6.44 | 124.10 | 118.30 |
| 1 | D | 54 | LYS | CD-CE-NZ | 6.43 | 126.48 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 123 | ASP | CB-CG-OD2 | 6.42 | 124.08 | 118.30 |
| 1 | C | 32 | THR | N-CA-CB | -6.38 | 98.17 | 110.30 |
| 1 | B | 105 | LEU | CB-CG-CD2 | -6.38 | 100.15 | 111.00 |
| 1 | A | 213 | ASP | CB-CG-OD2 | 6.37 | 124.03 | 118.30 |
| 1 | G | 197 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 |
| 1 | D | 32 | THR | N-CA-CB | -6.36 | 98.21 | 110.30 |
| 1 | H | 52 | LYS | C-N-CA | 6.36 | 137.60 | 121.70 |
| 1 | D | 51 | ASN | C-N-CA | -6.36 | 105.81 | 121.70 |
| 1 | A | 217 | GLY | O-C-N | -6.34 | 112.42 | 123.20 |
| 1 | F | 18 | ARG | NE-CZ-NH2 | -6.29 | 117.15 | 120.30 |
| 1 | A | 86 | ASP | CB-CG-OD2 | 6.29 | 123.96 | 118.30 |
| 1 | A | 87 | SER | CB-CA-C | -6.29 | 98.15 | 110.10 |
| 1 | B | 77 | MET | CG-SD-CE | -6.29 | 90.14 | 100.20 |
| 1 | G | 63 | LEU | CB-CG-CD1 | 6.28 | 121.68 | 111.00 |
| 1 | I | 123 | ASP | CB-CG-OD2 | 6.27 | 123.94 | 118.30 |
| 1 | C | 12 | ASP | CB-CG-OD2 | 6.26 | 123.94 | 118.30 |
| 1 | K | 187 | LEU | CA-CB-CG | -6.25 | 100.92 | 115.30 |
| 1 | D | 52 | LYS | CB-CA-C | 6.24 | 122.89 | 110.40 |
| 1 | B | 86 | ASP | CB-CG-OD2 | 6.24 | 123.92 | 118.30 |
| 1 | B | 12 | ASP | CB-CG-OD2 | 6.24 | 123.91 | 118.30 |
| 1 | G | 45 | LEU | CA-CB-CG | 6.23 | 129.63 | 115.30 |
| 1 | D | 111 | ASP | N-CA-CB | -6.23 | 99.39 | 110.60 |
| 1 | A | 205 | LEU | CB-CG-CD1 | -6.23 | 100.41 | 111.00 |
| 1 | A | 79 | ASP | CB-CG-OD2 | 6.22 | 123.90 | 118.30 |
| 1 | B | 39 | LEU | CB-CA-C | -6.22 | 98.38 | 110.20 |
| 1 | G | 145 | VAL | CB-CA-C | -6.21 | 99.61 | 111.40 |
| 1 | G | 146 | SER | CB-CA-C | -6.19 | 98.34 | 110.10 |
| 1 | L | 187 | LEU | CB-CG-CD1 | 6.19 | 121.52 | 111.00 |
| 1 | I | 105 | LEU | CB-CG-CD1 | -6.17 | 100.52 | 111.00 |
| 1 | F | 94 | VAL | N-CA-C | -6.16 | 94.36 | 111.00 |
| 1 | F | 117 | LEU | CB-CG-CD2 | 6.16 | 121.47 | 111.00 |
| 1 | F | 163 | MET | CG-SD-CE | -6.16 | 90.34 | 100.20 |
| 1 | D | 74 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |
| 1 | A | 75 | MET | CG-SD-CE | 6.16 | 110.06 | 100.20 |
| 1 | C | 154 | THR | N-CA-CB | -6.16 | 98.60 | 110.30 |
| 1 | H | 114 | ARG | NE-CZ-NH2 | 6.16 | 123.38 | 120.30 |
| 1 | G | 19 | LYS | CB-CA-C | -6.14 | 98.11 | 110.40 |
| 1 | A | 27 | SER | CB-CA-C | -6.09 | 98.52 | 110.10 |
| 1 | B | 154 | THR | CA-CB-CG2 | 6.09 | 120.92 | 112.40 |
| 1 | C | 162 | ASN | CB-CA-C | -6.09 | 98.23 | 110.40 |
| 1 | B | 19 | LYS | CD-CE-NZ | -6.08 | 97.72 | 111.70 |
| 1 | G | 196 | CYS | CA-CB-SG | -6.07 | 103.07 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 136 | LYS | CB-CA-C | -6.06 | 98.28 | 110.40 |
| 1 | L | 169 | PRO | N-CD-CG | -6.06 | 94.11 | 103.20 |
| 1 | J | 213 | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | B | 18 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 1 | F | 39 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | C | 40 | ASP | CB-CG-OD2 | 6.04 | 123.73 | 118.30 |
| 1 | D | 77 | MET | CG-SD-CE | -6.04 | 90.54 | 100.20 |
| 1 | J | 152 | SER | N-CA-CB | -6.03 | 101.45 | 110.50 |
| 1 | G | 50 | LYS | CD-CE-NZ | -6.03 | 97.83 | 111.70 |
| 1 | A | 62 | ILE | CG1-CB-CG2 | -6.03 | 98.14 | 111.40 |
| 1 | A | 105 | LEU | CB-CG-CD2 | -6.03 | 100.75 | 111.00 |
| 1 | I | 135 | PRO | N-CD-CG | -6.02 | 94.16 | 103.20 |
| 1 | J | 131 | LEU | CA-CB-CG | 6.02 | 129.15 | 115.30 |
| 1 | D | 86 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 1 | A | 40 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 1 | F | 74 | ARG | NE-CZ-NH2 | -6.01 | 117.30 | 120.30 |
| 1 | J | 79 | ASP | CB-CG-OD2 | 6.01 | 123.71 | 118.30 |
| 1 | J | 123 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 1 | E | 114 | ARG | NE-CZ-NH1 | 5.99 | 123.29 | 120.30 |
| 1 | K | 37 | VAL | N-CA-C | -5.99 | 94.84 | 111.00 |
| 1 | A | 154 | THR | N-CA-CB | -5.96 | 98.98 | 110.30 |
| 1 | C | 78 | LYS | CD-CE-NZ | -5.95 | 98.01 | 111.70 |
| 1 | F | 65 | ARG | NE-CZ-NH2 | -5.93 | 117.33 | 120.30 |
| 1 | G | 217 | GLY | N-CA-C | -5.92 | 98.30 | 113.10 |
| 1 | B | 123 | ASP | CB-CG-OD1 | -5.90 | 112.99 | 118.30 |
| 1 | B | 28 | VAL | CA-CB-CG2 | 5.89 | 119.74 | 110.90 |
| 1 | F | 158 | LEU | CB-CG-CD1 | -5.89 | 100.99 | 111.00 |
| 1 | L | 123 | ASP | CB-CG-OD2 | 5.88 | 123.59 | 118.30 |
| 1 | J | 181 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | A | 187 | LEU | CB-CG-CD2 | 5.85 | 120.94 | 111.00 |
| 1 | F | 186 | PRO | N-CD-CG | -5.84 | 94.43 | 103.20 |
| 1 | C | 83 | VAL | CG1-CB-CG2 | 5.82 | 120.22 | 110.90 |
| 1 | C | 158 | LEU | CB-CG-CD2 | 5.82 | 120.89 | 111.00 |
| 1 | K | 187 | LEU | CB-CG-CD2 | 5.81 | 120.88 | 111.00 |
| 1 | A | 175 | LYS | CD-CE-NZ | -5.80 | 98.35 | 111.70 |
| 1 | L | 203 | ARG | NE-CZ-NH1 | -5.79 | 117.40 | 120.30 |
| 1 | L | 74 | ARG | NE-CZ-NH1 | 5.77 | 123.18 | 120.30 |
| 1 | B | 32 | THR | N-CA-CB | -5.75 | 99.37 | 110.30 |
| 1 | K | 12 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | C | 117 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | C | 74 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | C | 152 | SER | N-CA-C | -5.72 | 95.55 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 158 | LEU | CB-CG-CD2 | 5.72 | 120.73 | 111.00 |
| 1 | K | 208 | LEU | CB-CG-CD2 | -5.72 | 101.27 | 111.00 |
| 1 | C | 178 | THR | CA-CB-CG2 | -5.72 | 104.39 | 112.40 |
| 1 | D | 111 | ASP | CB-CA-C | -5.72 | 98.97 | 110.40 |
| 1 | E | 123 | ASP | CB-CG-OD2 | 5.69 | 123.42 | 118.30 |
| 1 | B | 47 | THR | OG1-CB-CG2 | -5.68 | 96.93 | 110.00 |
| 1 | A | 187 | LEU | CB-CG-CD1 | -5.63 | 101.44 | 111.00 |
| 1 | A | 54 | LYS | CD-CE-NZ | 5.62 | 124.63 | 111.70 |
| 1 | D | 51 | ASN | O-C-N | -5.62 | 113.70 | 122.70 |
| 1 | G | 51 | ASN | C-N-CA | -5.61 | 107.68 | 121.70 |
| 1 | B | 90 | PRO | N-CD-CG | -5.60 | 94.81 | 103.20 |
| 1 | I | 143 | PHE | N-CA-C | -5.58 | 95.92 | 111.00 |
| 1 | L | 176 | TYR | CB-CG-CD1 | 5.58 | 124.35 | 121.00 |
| 1 | C | 77 | MET | CG-SD-CE | -5.58 | 91.28 | 100.20 |
| 1 | A | 37 | VAL | CG1-CB-CG2 | 5.58 | 119.82 | 110.90 |
| 1 | J | 178 | THR | OG1-CB-CG2 | -5.56 | 97.21 | 110.00 |
| 1 | A | 65 | ARG | NH1-CZ-NH2 | -5.56 | 113.29 | 119.40 |
| 1 | C | 203 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | L | 173 | MET | CB-CG-SD | -5.54 | 95.78 | 112.40 |
| 1 | F | 94 | VAL | CG1-CB-CG2 | -5.54 | 102.04 | 110.90 |
| 1 | I | 5 | ILE | N-CA-C | 5.53 | 125.92 | 111.00 |
| 1 | B | 136 | LYS | CD-CE-NZ | -5.51 | 99.02 | 111.70 |
| 1 | D | 49 | LYS | CD-CE-NZ | 5.50 | 124.36 | 111.70 |
| 1 | G | 79 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | I | 9 | THR | OG1-CB-CG2 | -5.49 | 97.37 | 110.00 |
| 1 | E | 189 | ILE | CG1-CB-CG2 | -5.49 | 99.32 | 111.40 |
| 1 | B | 117 | LEU | CA-CB-CG | 5.48 | 127.90 | 115.30 |
| 1 | C | 127 | TYR | CD1-CE1-CZ | -5.48 | 114.87 | 119.80 |
| 1 | A | 13 | ILE | CG1-CB-CG2 | -5.47 | 99.36 | 111.40 |
| 1 | K | 32 | THR | N-CA-CB | -5.44 | 99.96 | 110.30 |
| 1 | B | 28 | VAL | CG1-CB-CG2 | 5.44 | 119.60 | 110.90 |
| 1 | D | 79 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | H | 52 | LYS | O-C-N | 5.43 | 131.38 | 122.70 |
| 1 | E | 211 | TYR | CB-CG-CD1 | -5.41 | 117.75 | 121.00 |
| 1 | E | 183 | VAL | CB-CA-C | -5.41 | 101.12 | 111.40 |
| 1 | D | 208 | LEU | CB-CG-CD2 | 5.40 | 120.18 | 111.00 |
| 1 | H | 65 | ARG | NE-CZ-NH2 | 5.36 | 122.98 | 120.30 |
| 1 | H | 143 | PHE | N-CA-C | -5.36 | 96.52 | 111.00 |
| 1 | B | 117 | LEU | CB-CG-CD2 | 5.35 | 120.10 | 111.00 |
| 1 | I | 178 | THR | OG1-CB-CG2 | -5.35 | 97.70 | 110.00 |
| 1 | G | 98 | GLN | CA-CB-CG | 5.34 | 125.15 | 113.40 |
| 1 | D | 160 | VAL | CB-CA-C | 5.33 | 121.54 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 89 | HIS | CB-CA-C | 5.33 | 121.06 | 110.40 |
| 1 | C | 27 | SER | CB-CA-C | -5.32 | 99.99 | 110.10 |
| 1 | I | 74 | ARG | NE-CZ-NH2 | 5.32 | 122.96 | 120.30 |
| 1 | G | 178 | THR | OG1-CB-CG2 | -5.31 | 97.78 | 110.00 |
| 1 | L | 211 | TYR | CB-CG-CD1 | 5.31 | 124.19 | 121.00 |
| 1 | D | 89 | HIS | CB-CA-C | 5.31 | 121.01 | 110.40 |
| 1 | F | 117 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | G | 158 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 1 | A | 87 | SER | CA-CB-OG | -5.29 | 96.90 | 111.20 |
| 1 | J | 39 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 1 | C | 111 | ASP | N-CA-CB | -5.28 | 101.10 | 110.60 |
| 1 | F | 187 | LEU | CA-CB-CG | -5.28 | 103.16 | 115.30 |
| 1 | C | 118 | HIS | N-CA-CB | 5.27 | 120.09 | 110.60 |
| 1 | H | 77 | MET | N-CA-C | -5.27 | 96.76 | 111.00 |
| 1 | I | 111 | ASP | CB-CG-OD2 | 5.27 | 123.05 | 118.30 |
| 1 | A | 111 | ASP | OD1-CG-OD2 | -5.26 | 113.30 | 123.30 |
| 1 | G | 160 | VAL | CG1-CB-CG2 | 5.25 | 119.30 | 110.90 |
| 1 | H | 5 | ILE | O-C-N | 5.25 | 131.10 | 122.70 |
| 1 | B | 150 | TRP | C-N-CA | -5.25 | 108.58 | 121.70 |
| 1 | D | 36 | THR | OG1-CB-CG2 | -5.25 | 97.93 | 110.00 |
| 1 | I | 32 | THR | N-CA-CB | -5.23 | 100.36 | 110.30 |
| 1 | G | 37 | VAL | CG1-CB-CG2 | -5.23 | 102.53 | 110.90 |
| 1 | L | 57 | PRO | N-CD-CG | -5.23 | 95.35 | 103.20 |
| 1 | B | 154 | THR | N-CA-CB | -5.22 | 100.38 | 110.30 |
| 1 | H | 218 | GLY | C-N-CA | -5.21 | 108.66 | 121.70 |
| 1 | I | 16 | TRP | CA-CB-CG | 5.20 | 123.58 | 113.70 |
| 1 | B | 77 | MET | CA-CB-CG | -5.20 | 104.46 | 113.30 |
| 1 | G | 35 | GLN | CA-CB-CG | 5.20 | 124.84 | 113.40 |
| 1 | K | 208 | LEU | CB-CG-CD1 | 5.20 | 119.83 | 111.00 |
| 1 | D | 90 | PRO | N-CD-CG | -5.20 | 95.41 | 103.20 |
| 1 | H | 181 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 1 | C | 142 | MET | CG-SD-CE | 5.19 | 108.50 | 100.20 |
| 1 | J | 204 | MET | CG-SD-CE | -5.19 | 91.90 | 100.20 |
| 1 | F | 46 | LYS | CD-CE-NZ | -5.18 | 99.78 | 111.70 |
| 1 | A | 18 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 1 | E | 164 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | I | 4 | LYS | N-CA-C | 5.17 | 124.97 | 111.00 |
| 1 | I | 154 | THR | N-CA-CB | -5.17 | 100.48 | 110.30 |
| 1 | L | 211 | TYR | CB-CG-CD2 | -5.16 | 117.90 | 121.00 |
| 1 | E | 63 | LEU | CB-CG-CD1 | -5.16 | 102.23 | 111.00 |
| 1 | F | 91 | CYS | CB-CA-C | 5.16 | 120.72 | 110.40 |
| 1 | J | 86 | ASP | CB-CG-OD1 | -5.15 | 113.67 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 157 | ASP | CB-CG-OD1 | 5.14 | 122.93 | 118.30 |
| 1 | L | 40 | ASP | CB-CG-OD2 | 5.14 | 122.93 | 118.30 |
| 1 | A | 170 | VAL | CA-CB-CG2 | -5.14 | 103.19 | 110.90 |
| 1 | C | 29 | ALA | N-CA-C | 5.13 | 124.86 | 111.00 |
| 1 | E | 65 | ARG | N-CA-CB | 5.11 | 119.79 | 110.60 |
| 1 | H | 86 | ASP | CB-CG-OD1 | -5.10 | 113.71 | 118.30 |
| 1 | A | 190 | GLN | C-N-CA | -5.10 | 108.95 | 121.70 |
| 1 | F | 83 | VAL | N-CA-CB | -5.08 | 100.31 | 111.50 |
| 1 | L | 112 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | L | 118 | HIS | N-CA-C | -5.07 | 97.31 | 111.00 |
| 1 | B | 45 | LEU | CB-CG-CD1 | 5.07 | 119.61 | 111.00 |
| 1 | C | 9 | THR | CA-CB-CG2 | 5.06 | 119.48 | 112.40 |
| 1 | F | 123 | ASP | CB-CG-OD1 | -5.05 | 113.75 | 118.30 |
| 1 | F | 18 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | C | 66 | LEU | CB-CG-CD2 | -5.05 | 102.42 | 111.00 |
| 1 | A | 123 | ASP | CB-CG-OD1 | 5.04 | 122.83 | 118.30 |
| 1 | J | 142 | MET | CB-CA-C | -5.03 | 100.34 | 110.40 |
| 1 | D | 114 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | C | 187 | LEU | CB-CG-CD2 | 5.02 | 119.53 | 111.00 |
| 1 | C | 95 | PHE | CB-CA-C | 5.02 | 120.43 | 110.40 |
| 1 | B | 184 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 1 | G | 105 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 1 | F | 169 | PRO | N-CD-CG | -5.01 | 95.68 | 103.20 |
| 1 | H | 18 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 1 | B | 65 | ARG | NE-CZ-NH1 | -5.01 | 117.80 | 120.30 |
| 1 | F | 62 | ILE | CG1-CB-CG2 | 5.01 | 122.41 | 111.40 |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 168 | ALA | Mainchain |
| 1 | C | 28 | VAL | Peptide |
| 1 | C | 52 | LYS | Peptide |
| 1 | G | 217 | GLY | Peptide |
| 1 | I | 4 | LYS | Peptide |
| 1 | J | 127 | TYR | Peptide |
| 1 | J | 13 | ILE | Peptide |
| 1 | J | 153 | PHE | Peptide |
| 1 | K | 50 | LYS | Peptide |
| 1 | L | 128 | GLY | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1763 | 0 | 1647 | 72 | 0 |
| 1 | B | 1789 | 0 | 1684 | 58 | 0 |
| 1 | C | 1763 | 0 | 1647 | 83 | 0 |
| 1 | D | 1763 | 0 | 1647 | 79 | 0 |
| 1 | E | 1785 | 0 | 1681 | 61 | 0 |
| 1 | F | 1759 | 0 | 1644 | 56 | 0 |
| 1 | G | 1763 | 0 | 1647 | 83 | 0 |
| 1 | H | 1785 | 0 | 1675 | 72 | 0 |
| 1 | I | 1776 | 0 | 1668 | 104 | 0 |
| 1 | J | 1755 | 0 | 1641 | 115 | 0 |
| 1 | K | 1763 | 0 | 1657 | 92 | 0 |
| 1 | L | 1746 | 0 | 1633 | 94 | 0 |
| 2 | A | 19 | 0 | 0 | 1 | 0 |
| 2 | B | 22 | 0 | 0 | 1 | 0 |
| 2 | C | 19 | 0 | 0 | 1 | 0 |
| 2 | D | 21 | 0 | 0 | 2 | 0 |
| 2 | E | 15 | 0 | 0 | 1 | 0 |
| 2 | F | 16 | 0 | 0 | 1 | 0 |
| 2 | G | 20 | 0 | 0 | 3 | 0 |
| 2 | H | 36 | 0 | 0 | 3 | 0 |
| 2 | I | 17 | 0 | 0 | 0 | 0 |
| 2 | J | 11 | 0 | 0 | 5 | 0 |
| 2 | K | 4 | 0 | 0 | 1 | 0 |
| 2 | L | 8 | 0 | 0 | 0 | 0 |
| All | All | 21418 | 0 | 19871 | 881 | 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 21.

All (881) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:13:ILE:CG1 | 1:C:13:ILE:CD1 | 1.83 | 1.56 |
| 1:I:6:THR:CG2 | 1:I:6:THR:CB | 1.74 | 1.55 |
| 1:I:139:ILE:N | 1:I:142:MET:HE3 | 1.19 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:139:ILE:H | 1:I:142:MET:CE | 1.36 | 1.37 |
| 1:I:171:PHE:CZ | 1:I:204:MET:HE3 | 1.61 | 1.35 |
| 1:I:171:PHE:HZ | 1:I:204:MET:CE | 1.41 | 1.34 |
| 1:I:171:PHE:CZ | 1:I:204:MET:CE | 2.12 | 1.31 |
| 1:A:67:MET:CE | 1:A:171:PHE:HE1 | 1.46 | 1.26 |
| 1:C:145:VAL:CG1 | 1:C:173:MET:CE | 2.18 | 1.21 |
| 1:E:59:PHE:HD2 | 1:E:173:MET:CE | 1.57 | 1.17 |
| 1:G:32:THR:HG22 | 1:I:159:ASN:HB3 | 1.26 | 1.17 |
| 1:I:6:THR:HG21 | 1:I:141:ASN:HD21 | 1.11 | 1.15 |
| 1:H:67:MET:HE3 | 1:H:73:PHE:HB3 | 1.18 | 1.15 |
| 1:B:158:LEU:CD1 | 1:B:160:VAL:HG23 | 1.77 | 1.13 |
| 1:C:145:VAL:HG12 | 1:C:173:MET:HE3 | 1.32 | 1.12 |
| 1:C:145:VAL:CG1 | 1:C:173:MET:HE2 | 1.80 | 1.11 |
| 1:A:67:MET:CE | 1:A:171:PHE:CE1 | 2.34 | 1.11 |
| 1:J:154:THR:HG22 | 1:K:154:THR:O | 1.47 | 1.11 |
| 1:K:154:THR:HG23 | 1:L:154:THR:O | 1.50 | 1.11 |
| 1:A:67:MET:HE2 | 1:A:171:PHE:CE1 | 1.87 | 1.08 |
| 1:J:159:ASN:HB3 | 1:K:32:THR:HG22 | 1.34 | 1.06 |
| 1:C:67:MET:CE | 1:C:73:PHE:CG | 2.39 | 1.06 |
| 1:A:67:MET:HE2 | 1:A:171:PHE:HE1 | 0.96 | 1.05 |
| 1:K:8:TYR:CZ | 1:K:78:LYS:HD3 | 1.91 | 1.05 |
| 1:L:129:GLU:OE2 | 1:L:129:GLU:HA | 1.36 | 1.05 |
| 1:E:59:PHE:HD2 | 1:E:173:MET:HE1 | 1.20 | 1.04 |
| 1:I:138:PHE:HA | 1:I:142:MET:HE1 | 1.41 | 1.03 |
| 1:I:67:MET:HE1 | 1:I:169:PRO:HG2 | 1.07 | 1.03 |
| 1:I:171:PHE:HZ | 1:I:204:MET:HE3 | 0.92 | 1.02 |
| 1:C:67:MET:HE1 | 1:C:73:PHE:CG | 1.95 | 1.02 |
| 1:C:67:MET:HE3 | 1:C:73:PHE:CB | 1.90 | 1.02 |
| 1:E:59:PHE:CD2 | 1:E:173:MET:CE | 2.44 | 1.01 |
| 1:H:67:MET:CE | 1:H:73:PHE:HB3 | 1.90 | 1.01 |
| 1:I:67:MET:CE | 1:I:169:PRO:HG2 | 1.89 | 1.01 |
| 1:J:159:ASN:HD22 | 1:L:159:ASN:HD21 | 1.02 | 1.00 |
| 1:A:159:ASN:HB3 | 1:B:32:THR:HG22 | 1.39 | 0.98 |
| 1:A:154:THR:HG23 | 1:B:154:THR:O | 1.61 | 0.98 |
| 1:J:67:MET:HA | 1:J:67:MET:HE2 | 1.41 | 0.97 |
| 1:A:154:THR:O | 1:C:154:THR:HG23 | 1.65 | 0.96 |
| 1:D:67:MET:CE | 1:D:169:PRO:HG2 | 1.95 | 0.96 |
| 1:L:67:MET:HE3 | 1:L:73:PHE:HB3 | 1.43 | 0.96 |
| 1:H:32:THR:HG21 | 2:H:224:HOH:O | 1.65 | 0.95 |
| 1:C:67:MET:CE | 1:C:73:PHE:HB3 | 1.95 | 0.95 |
| 1:B:158:LEU:HD11 | 1:B:160:VAL:HG23 | 1.45 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:159:ASN:ND2 | 1:L:159:ASN:HD21 | 1.65 | 0.95 |
| 1:L:106:TRP:CD1 | 1:L:142:MET:HE3 | 2.02 | 0.94 |
| 1:I:171:PHE:CZ | 1:I:204:MET:HE1 | 2.02 | 0.94 |
| 1:A:123:ASP:OD1 | 1:A:136:LYS:NZ | 2.01 | 0.93 |
| 1:C:67:MET:CE | 1:C:73:PHE:CB | 2.45 | 0.93 |
| 1:I:112:ASP:OD2 | 1:I:115:GLN:HG2 | 1.68 | 0.93 |
| 1:B:149:PRO:O | 1:B:175:LYS:HG3 | 1.67 | 0.93 |
| 1:C:145:VAL:HG11 | 1:C:173:MET:CE | 1.98 | 0.93 |
| 1:H:67:MET:HE3 | 1:H:73:PHE:CB | 1.99 | 0.92 |
| 1:A:56:TYR:HE1 | 1:A:173:MET:HE3 | 1.31 | 0.92 |
| 1:B:67:MET:CE | 1:B:169:PRO:HG2 | 1.99 | 0.92 |
| 1:J:67:MET:HA | 1:J:67:MET:CE | 1.98 | 0.92 |
| 1:K:148:ASN:HD22 | 1:K:150:TRP:HE3 | 1.17 | 0.92 |
| 1:C:56:TYR:HB3 | 1:C:57:PRO:HD3 | 1.51 | 0.92 |
| 1:A:56:TYR:CD1 | 1:A:173:MET:HE1 | 2.03 | 0.92 |
| 1:G:59:PHE:HD2 | 1:G:173:MET:CE | 1.82 | 0.92 |
| 1:F:110:HIS:HD2 | 1:F:119:ILE:HD11 | 1.34 | 0.91 |
| 1:G:32:THR:CG2 | 1:I:159:ASN:HB3 | 1.99 | 0.91 |
| 1:D:154:THR:O | 1:F:154:THR:HG23 | 1.71 | 0.91 |
| 1:I:6:THR:HG21 | 1:I:141:ASN:ND2 | 1.84 | 0.90 |
| 1:E:59:PHE:CD2 | 1:E:173:MET:SD | 2.65 | 0.90 |
| 1:J:154:THR:CG2 | 1:K:154:THR:O | 2.19 | 0.90 |
| 1:D:163:MET:O | 1:D:164:ASP:HB2 | 1.71 | 0.90 |
| 1:A:67:MET:HE1 | 1:A:171:PHE:CE1 | 2.04 | 0.90 |
| 1:H:192:HIS:HD1 | 1:H:194:ALA:H | 1.14 | 0.89 |
| 1:E:139:ILE:H | 1:E:142:MET:HE3 | 1.35 | 0.89 |
| 1:I:67:MET:HE1 | 1:I:169:PRO:CG | 1.99 | 0.89 |
| 1:L:7:GLY:HA3 | 1:L:86:ASP:OD1 | 1.70 | 0.88 |
| 1:H:54:LYS:HD3 | 2:H:249:HOH:O | 1.73 | 0.88 |
| 1:L:67:MET:CE | 1:L:169:PRO:HG2 | 2.04 | 0.88 |
| 1:A:56:TYR:CE1 | 1:A:173:MET:HE3 | 2.09 | 0.88 |
| 1:H:91:CYS:HB2 | 1:H:142:MET:HE2 | 1.55 | 0.88 |
| 1:C:114:ARG:HH11 | 1:C:114:ARG:CG | 1.86 | 0.88 |
| 1:C:114:ARG:HH11 | 1:C:114:ARG:HG2 | 1.40 | 0.86 |
| 1:C:216:GLN:HA | 1:C:216:GLN:HE21 | 1.40 | 0.86 |
| 1:G:59:PHE:CD2 | 1:G:173:MET:CE | 2.59 | 0.85 |
| 1:D:67:MET:HE3 | 1:D:73:PHE:HB3 | 1.59 | 0.85 |
| 1:J:106:TRP:CD1 | 1:J:142:MET:HE3 | 2.12 | 0.84 |
| 1:J:154:THR:O | 1:L:154:THR:HG23 | 1.78 | 0.84 |
| 1:K:47:THR:O | 1:K:49:LYS:N | 2.11 | 0.84 |
| 1:I:171:PHE:CE2 | 1:I:204:MET:CE | 2.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:59:PHE:HD2 | 1:G:173:MET:HE1 | 1.43 | 0.83 |
| 1:J:30:GLN:NE2 | 1:J:163:MET:O | 2.11 | 0.83 |
| 1:K:171:PHE:CZ | 1:K:204:MET:CE | 2.63 | 0.82 |
| 1:E:59:PHE:CD2 | 1:E:173:MET:HE1 | 2.07 | 0.82 |
| 2:A:220:HOH:O | 1:C:159:ASN:HB2 | 1.79 | 0.82 |
| 1:D:67:MET:HE1 | 1:D:169:PRO:HG2 | 1.60 | 0.82 |
| 1:A:56:TYR:HD1 | 1:A:173:MET:HE1 | 1.43 | 0.82 |
| 1:D:8:TYR:N | 1:D:8:TYR:CD2 | 2.44 | 0.82 |
| 1:F:106:TRP:CD1 | 1:F:142:MET:CE | 2.62 | 0.81 |
| 1:A:56:TYR:CE1 | 1:A:173:MET:CE | 2.64 | 0.81 |
| 1:C:49:LYS:O | 1:C:51:ASN:N | 2.13 | 0.81 |
| 1:C:145:VAL:CG1 | 1:C:173:MET:HE3 | 1.95 | 0.81 |
| 1:J:159:ASN:HD21 | 1:K:159:ASN:ND2 | 1.80 | 0.80 |
| 1:G:154:THR:HG23 | 1:H:154:THR:O | 1.82 | 0.80 |
| 1:D:67:MET:CE | 1:D:73:PHE:HB3 | 2.11 | 0.80 |
| 1:F:110:HIS:CD2 | 1:F:119:ILE:HD11 | 2.17 | 0.80 |
| 1:L:91:CYS:HB2 | 1:L:142:MET:HE2 | 1.63 | 0.79 |
| 1:K:154:THR:CG2 | 1:L:154:THR:O | 2.28 | 0.79 |
| 1:L:192:HIS:HD1 | 1:L:194:ALA:H | 1.30 | 0.79 |
| 1:C:145:VAL:HG11 | 1:C:173:MET:HE2 | 1.56 | 0.79 |
| 1:I:139:ILE:N | 1:I:142:MET:CE | 2.13 | 0.79 |
| 1:G:171:PHE:HZ | 1:G:204:MET:HE3 | 1.47 | 0.79 |
| 1:A:192:HIS:HD1 | 1:A:194:ALA:H | 1.29 | 0.79 |
| 1:J:138:PHE:CD2 | 1:J:138:PHE:O | 2.36 | 0.79 |
| 1:J:89:HIS:CE1 | 1:J:108:GLU:HG3 | 2.18 | 0.79 |
| 1:K:171:PHE:CZ | 1:K:204:MET:HE3 | 2.19 | 0.78 |
| 1:G:171:PHE:CZ | 1:G:204:MET:HE3 | 2.18 | 0.78 |
| 1:K:25:PHE:O | 1:K:30:GLN:HG3 | 1.84 | 0.78 |
| 1:G:50:LYS:C | 1:G:51:ASN:O | 2.12 | 0.78 |
| 1:E:106:TRP:CE2 | 1:E:136:LYS:HD2 | 2.18 | 0.78 |
| 1:D:154:THR:HG23 | 1:E:154:THR:O | 1.84 | 0.77 |
| 1:J:192:HIS:HD1 | 1:J:194:ALA:H | 1.33 | 0.77 |
| 1:F:100:GLU:OE1 | 1:J:6:THR:HG22 | 1.85 | 0.77 |
| 1:B:67:MET:HE1 | 1:B:169:PRO:HG2 | 1.63 | 0.77 |
| 1:F:192:HIS:HD1 | 1:F:194:ALA:H | 1.29 | 0.77 |
| 1:C:145:VAL:HG13 | 1:C:173:MET:HE2 | 1.65 | 0.77 |
| 1:L:106:TRP:CD1 | 1:L:142:MET:CE | 2.68 | 0.77 |
| 1:K:8:TYR:CE2 | 1:K:78:LYS:HD3 | 2.19 | 0.77 |
| 1:E:67:MET:HE3 | 1:E:171:PHE:CE1 | 2.20 | 0.77 |
| 1:E:34:ASN:ND2 | 1:E:190:GLN:HB3 | 2.00 | 0.77 |
| 1:G:91:CYS:SG | 1:G:142:MET:HE2 | 2.25 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:192:HIS:HD1 | 1:G:194:ALA:H | 1.33 | 0.76 |
| 1:I:171:PHE:CE2 | 1:I:204:MET:HE3 | 2.17 | 0.76 |
| 1:C:112:ASP:HB3 | 1:C:115:GLN:HG3 | 1.68 | 0.75 |
| 1:A:154:THR:CG2 | 1:B:154:THR:O | 2.35 | 0.75 |
| 1:E:67:MET:CE | 1:E:171:PHE:CE1 | 2.70 | 0.75 |
| 1:L:67:MET:HE1 | 1:L:169:PRO:HG2 | 1.67 | 0.75 |
| 1:D:159:ASN:HB3 | 1:E:32:THR:HG22 | 1.68 | 0.75 |
| 1:J:10:THR:HG23 | 1:J:10:THR:O | 1.86 | 0.75 |
| 1:G:171:PHE:CZ | 1:G:204:MET:CE | 2.70 | 0.74 |
| 1:G:15:GLN:HA | 1:G:15:GLN:HE21 | 1.51 | 0.74 |
| 1:J:6:THR:O | 1:J:6:THR:HG23 | 1.84 | 0.74 |
| 1:K:59:PHE:CD2 | 1:K:173:MET:SD | 2.80 | 0.74 |
| 1:J:40:ASP:HA | 1:J:184:LEU:HD23 | 1.67 | 0.74 |
| 1:G:13:ILE:O | 1:G:19:LYS:HG3 | 1.86 | 0.74 |
| 1:K:10:THR:OG1 | 1:K:83:VAL:HG23 | 1.87 | 0.74 |
| 1:B:154:THR:HG23 | 1:C:154:THR:O | 1.88 | 0.74 |
| 1:L:106:TRP:HB3 | 1:L:142:MET:HE2 | 1.70 | 0.74 |
| 1:A:56:TYR:CD1 | 1:A:173:MET:CE | 2.71 | 0.73 |
| 1:E:139:ILE:O | 1:E:142:MET:SD | 2.46 | 0.73 |
| 1:F:106:TRP:O | 1:F:136:LYS:NZ | 2.22 | 0.73 |
| 1:J:190:GLN:C | 1:J:190:GLN:HE21 | 1.91 | 0.73 |
| 1:C:67:MET:HE3 | 1:C:73:PHE:CG | 2.19 | 0.73 |
| 1:E:59:PHE:HD2 | 1:E:173:MET:SD | 2.06 | 0.72 |
| 1:J:106:TRP:CD1 | 1:J:142:MET:CE | 2.72 | 0.72 |
| 1:D:163:MET:O | 1:D:164:ASP:CB | 2.36 | 0.72 |
| 1:J:123:ASP:OD1 | 1:J:136:LYS:HE2 | 1.88 | 0.72 |
| 1:J:159:ASN:CB | 1:K:32:THR:HG22 | 2.18 | 0.72 |
| 1:D:75:MET:HE3 | 2:D:235:HOH:O | 1.88 | 0.72 |
| 1:J:35:GLN:HG3 | 1:L:156:PHE:HD1 | 1.54 | 0.72 |
| 1:C:67:MET:HE2 | 1:C:73:PHE:HB3 | 1.70 | 0.72 |
| 1:L:129:GLU:OE2 | 1:L:129:GLU:CA | 2.26 | 0.72 |
| 1:J:35:GLN:HG3 | 1:L:156:PHE:CD1 | 2.24 | 0.71 |
| 1:B:155:SER:HB2 | 1:C:155:SER:HB2 | 1.71 | 0.71 |
| 1:K:45:LEU:HD22 | 1:K:49:LYS:HD2 | 1.71 | 0.71 |
| 1:K:106:TRP:CD1 | 1:K:142:MET:CE | 2.74 | 0.71 |
| 1:L:59:PHE:CD2 | 1:L:173:MET:HE1 | 2.26 | 0.71 |
| 1:I:171:PHE:CE2 | 1:I:204:MET:HE1 | 2.22 | 0.71 |
| 1:H:47:THR:O | 1:H:51:ASN:ND2 | 2.24 | 0.71 |
| 1:G:159:ASN:ND2 | 1:I:159:ASN:ND2 | 2.39 | 0.70 |
| 1:D:65:ARG:CD | 1:J:111:ASP:OD2 | 2.39 | 0.70 |
| 1:E:3:LYS:O | 1:E:4:LYS:HG2 | 1.90 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:154:THR:O | 1:C:154:THR:CG2 | 2.39 | 0.70 |
| 1:K:72:GLU:HA | 1:K:75:MET:HE2 | 1.72 | 0.70 |
| 1:C:145:VAL:HG12 | 1:C:173:MET:CE | 1.94 | 0.70 |
| 1:G:171:PHE:HZ | 1:G:204:MET:CE | 2.03 | 0.70 |
| 1:L:59:PHE:HD2 | 1:L:173:MET:HE1 | 1.57 | 0.70 |
| 1:I:59:PHE:CD2 | 1:I:173:MET:SD | 2.84 | 0.70 |
| 1:B:34:ASN:CG | 1:B:157:ASP:HB2 | 2.12 | 0.70 |
| 1:H:149:PRO:O | 1:H:175:LYS:HD3 | 1.91 | 0.69 |
| 1:B:204:MET:HE1 | 1:B:205:LEU:HD23 | 1.73 | 0.69 |
| 1:A:34:ASN:HB2 | 1:A:157:ASP:OD2 | 1.93 | 0.69 |
| 1:H:159:ASN:HB3 | 1:I:32:THR:HG22 | 1.74 | 0.69 |
| 1:D:65:ARG:HD3 | 1:J:111:ASP:OD2 | 1.92 | 0.69 |
| 1:F:190:GLN:C | 1:F:190:GLN:HE21 | 1.96 | 0.69 |
| 1:G:59:PHE:CD2 | 1:G:173:MET:HE1 | 2.24 | 0.69 |
| 1:G:154:THR:O | 1:I:154:THR:HG23 | 1.93 | 0.69 |
| 1:C:67:MET:HE1 | 1:C:73:PHE:CD2 | 2.28 | 0.69 |
| 1:A:204:MET:HE2 | 1:A:205:LEU:HG | 1.73 | 0.69 |
| 1:J:159:ASN:ND2 | 1:K:159:ASN:ND2 | 2.40 | 0.68 |
| 1:E:67:MET:CE | 1:E:171:PHE:HE1 | 2.06 | 0.68 |
| 1:I:59:PHE:HD2 | 1:I:173:MET:HE1 | 1.58 | 0.68 |
| 1:E:132:ALA:O | 1:E:135:PRO:HD3 | 1.92 | 0.68 |
| 1:I:138:PHE:CA | 1:I:142:MET:HE1 | 2.21 | 0.68 |
| 1:L:8:TYR:HB2 | 1:L:83:VAL:HG13 | 1.74 | 0.68 |
| 1:C:13:ILE:H | 1:C:13:ILE:HD12 | 1.58 | 0.68 |
| 1:E:159:ASN:HB3 | 1:F:32:THR:HG22 | 1.76 | 0.68 |
| 1:D:34:ASN:ND2 | 1:D:158:LEU:H | 1.92 | 0.68 |
| 1:C:57:PRO:HG3 | 1:C:120:TYR:CE2 | 2.29 | 0.68 |
| 1:J:35:GLN:HA | 1:L:155:SER:O | 1.94 | 0.68 |
| 1:H:67:MET:CE | 1:H:169:PRO:HG2 | 2.24 | 0.68 |
| 1:I:145:VAL:HG11 | 1:I:173:MET:CE | 2.24 | 0.67 |
| 1:J:44:PHE:HB2 | 1:J:212:CYS:O | 1.95 | 0.67 |
| 1:C:67:MET:HE3 | 1:C:73:PHE:HB3 | 1.59 | 0.67 |
| 1:H:91:CYS:HB2 | 1:H:142:MET:CE | 2.24 | 0.67 |
| 1:F:34:ASN:ND2 | 1:F:190:GLN:HB2 | 2.08 | 0.67 |
| 1:C:192:HIS:HD1 | 1:C:194:ALA:H | 1.40 | 0.67 |
| 1:J:171:PHE:CZ | 1:J:204:MET:HE3 | 2.29 | 0.67 |
| 1:F:110:HIS:HD2 | 1:F:119:ILE:CD1 | 2.06 | 0.67 |
| 1:A:32:THR:HG22 | 1:C:159:ASN:HB3 | 1.77 | 0.67 |
| 1:F:92:TYR:HA | 1:F:145:VAL:O | 1.94 | 0.67 |
| 1:L:214:GLU:O | 1:L:215:TRP:C | 2.33 | 0.67 |
| 1:F:214:GLU:O | 1:F:215:TRP:C | 2.32 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:171:PHE:HZ | 1:J:204:MET:HE3 | 1.60 | 0.66 |
| 1:H:67:MET:HE1 | 1:H:73:PHE:CD2 | 2.30 | 0.66 |
| 1:B:34:ASN:ND2 | 1:B:190:GLN:HB3 | 2.11 | 0.66 |
| 1:H:113:PHE:H | 1:H:219:ALA:HB3 | 1.59 | 0.66 |
| 1:E:3:LYS:O | 1:E:4:LYS:CG | 2.42 | 0.66 |
| 1:B:156:PHE:O | 1:B:157:ASP:HB3 | 1.95 | 0.66 |
| 1:J:65:ARG:HD3 | 2:J:229:HOH:O | 1.95 | 0.66 |
| 1:F:30:GLN:HE22 | 1:F:164:ASP:HA | 1.60 | 0.66 |
| 1:I:6:THR:CG2 | 1:I:6:THR:CA | 2.69 | 0.66 |
| 1:F:120:TYR:O | 1:F:124:VAL:HG23 | 1.95 | 0.66 |
| 1:I:145:VAL:HG11 | 1:I:173:MET:HE3 | 1.77 | 0.66 |
| 1:J:16:TRP:CE2 | 1:J:18:ARG:HB2 | 2.30 | 0.66 |
| 1:J:10:THR:CG2 | 1:J:10:THR:O | 2.44 | 0.65 |
| 1:G:30:GLN:HB3 | 1:I:161:ALA:HB3 | 1.78 | 0.65 |
| 1:H:56:TYR:HD1 | 1:H:173:MET:HE1 | 1.61 | 0.65 |
| 1:J:176:TYR:HB3 | 1:J:185:MET:HB2 | 1.77 | 0.65 |
| 1:I:7:GLY:CA | 1:I:86:ASP:OD1 | 2.44 | 0.65 |
| 1:H:67:MET:HE1 | 1:H:169:PRO:HG2 | 1.78 | 0.65 |
| 1:F:106:TRP:CD1 | 1:F:142:MET:HE3 | 2.31 | 0.65 |
| 1:I:7:GLY:C | 1:I:86:ASP:OD1 | 2.36 | 0.65 |
| 1:D:32:THR:HG21 | 2:D:220:HOH:O | 1.96 | 0.64 |
| 1:K:67:MET:HE2 | 1:K:67:MET:HA | 1.79 | 0.64 |
| 1:C:110:HIS:CD2 | 1:C:119:ILE:HD13 | 2.32 | 0.64 |
| 1:H:56:TYR:CD1 | 1:H:173:MET:HE1 | 2.32 | 0.64 |
| 1:J:13:ILE:HG22 | 1:J:19:LYS:HD2 | 1.80 | 0.64 |
| 1:A:56:TYR:O | 1:A:60:ILE:HG13 | 1.99 | 0.63 |
| 1:L:123:ASP:OD1 | 1:L:136:LYS:HE3 | 1.97 | 0.63 |
| 1:L:59:PHE:HD2 | 1:L:173:MET:CE | 2.10 | 0.63 |
| 1:I:139:ILE:HG13 | 1:I:142:MET:CE | 2.28 | 0.63 |
| 1:G:159:ASN:HD22 | 1:I:159:ASN:CG | 2.01 | 0.63 |
| 1:A:56:TYR:N | 1:A:57:PRO:HD2 | 2.13 | 0.63 |
| 1:G:154:THR:O | 1:I:154:THR:CG2 | 2.47 | 0.63 |
| 1:A:204:MET:HE1 | 1:A:205:LEU:CD2 | 2.29 | 0.63 |
| 1:J:106:TRP:HB3 | 1:J:142:MET:HE2 | 1.81 | 0.63 |
| 1:E:106:TRP:CZ2 | 1:E:136:LYS:HD2 | 2.33 | 0.63 |
| 1:F:40:ASP:HA | 1:F:184:LEU:HD23 | 1.81 | 0.63 |
| 1:H:22:PHE:CE2 | 1:H:82:LEU:HD22 | 2.34 | 0.63 |
| 1:H:91:CYS:SG | 1:H:142:MET:HE1 | 2.38 | 0.63 |
| 1:K:57:PRO:HG3 | 1:K:120:TYR:CE2 | 2.34 | 0.63 |
| 1:K:159:ASN:HB3 | 1:L:32:THR:HG23 | 1.80 | 0.62 |
| 1:K:56:TYR:HB3 | 1:K:57:PRO:HD3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:148:ASN:ND2 | 1:K:150:TRP:HE3 | 1.92 | 0.62 |
| 1:E:139:ILE:H | 1:E:142:MET:CE | 2.10 | 0.62 |
| 1:D:34:ASN:HD21 | 1:D:158:LEU:H | 1.46 | 0.62 |
| 1:I:190:GLN:HE21 | 1:I:190:GLN:C | 2.01 | 0.62 |
| 1:C:114:ARG:CG | 1:C:114:ARG:NH1 | 2.51 | 0.62 |
| 1:J:10:THR:HB | 2:J:225:HOH:O | 2.00 | 0.62 |
| 1:L:115:GLN:O | 1:L:118:HIS:O | 2.17 | 0.62 |
| 1:H:57:PRO:HG3 | 1:H:120:TYR:CE2 | 2.35 | 0.62 |
| 1:F:179:GLN:O | 1:F:180:GLY:C | 2.38 | 0.62 |
| 1:I:7:GLY:HA3 | 1:I:86:ASP:OD1 | 1.99 | 0.61 |
| 1:E:67:MET:HE3 | 1:E:171:PHE:HE1 | 1.62 | 0.61 |
| 1:A:34:ASN:OD1 | 1:A:157:ASP:OD2 | 2.18 | 0.61 |
| 1:A:39:LEU:O | 1:A:184:LEU:HA | 2.00 | 0.61 |
| 1:L:66:LEU:CD2 | 1:L:211:TYR:CE2 | 2.83 | 0.61 |
| 1:J:49:LYS:O | 1:J:51:ASN:O | 2.18 | 0.61 |
| 1:L:66:LEU:HD23 | 1:L:211:TYR:CE2 | 2.36 | 0.61 |
| 1:K:117:LEU:HD22 | 1:K:117:LEU:O | 2.00 | 0.61 |
| 1:K:34:ASN:ND2 | 1:K:190:GLN:HB2 | 2.15 | 0.61 |
| 1:A:34:ASN:CB | 1:A:157:ASP:OD2 | 2.49 | 0.61 |
| 1:H:58:ALA:HA | 1:H:113:PHE:CE1 | 2.36 | 0.61 |
| 1:D:59:PHE:CD2 | 1:D:173:MET:SD | 2.94 | 0.61 |
| 1:A:34:ASN:CG | 1:A:157:ASP:OD2 | 2.39 | 0.61 |
| 1:J:158:LEU:HD13 | 1:J:160:VAL:HG23 | 1.81 | 0.61 |
| 1:I:138:PHE:HA | 1:I:142:MET:CE | 2.23 | 0.61 |
| 1:K:171:PHE:HZ | 1:K:204:MET:SD | 2.23 | 0.60 |
| 1:L:26:GLN:HA | 1:L:26:GLN:NE2 | 2.16 | 0.60 |
| 1:A:83:VAL:CG1 | 1:A:84:ILE:N | 2.64 | 0.60 |
| 1:K:171:PHE:CE2 | 1:K:204:MET:HE1 | 2.36 | 0.60 |
| 1:H:65:ARG:HH22 | 1:H:219:ALA:HB1 | 1.66 | 0.60 |
| 1:I:148:ASN:O | 1:I:174:GLY:HA2 | 2.01 | 0.60 |
| 1:I:112:ASP:OD2 | 1:I:115:GLN:CG | 2.48 | 0.60 |
| 1:B:67:MET:HE3 | 1:B:169:PRO:HG2 | 1.84 | 0.60 |
| 1:G:154:THR:CG2 | 1:H:154:THR:O | 2.47 | 0.60 |
| 1:L:59:PHE:CD2 | 1:L:173:MET:CE | 2.84 | 0.60 |
| 1:A:83:VAL:HG13 | 1:A:84:ILE:N | 2.17 | 0.60 |
| 1:I:67:MET:CE | 1:I:169:PRO:CG | 2.71 | 0.59 |
| 1:C:13:ILE:H | 1:C:13:ILE:CD1 | 2.15 | 0.59 |
| 1:L:127:TYR:O | 1:L:129:GLU:N | 2.34 | 0.59 |
| 1:F:139:ILE:HG13 | 1:F:142:MET:HG3 | 1.84 | 0.59 |
| 1:G:59:PHE:CE2 | 1:G:63:LEU:HD11 | 2.37 | 0.59 |
| 1:C:110:HIS:CD2 | 1:C:119:ILE:CD1 | 2.86 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:8:TYR:C | 1:H:8:TYR:CD1 | 2.75 | 0.59 |
| 1:E:154:THR:CG2 | 1:F:154:THR:O | 2.51 | 0.58 |
| 1:D:57:PRO:HG3 | 1:D:120:TYR:CE2 | 2.38 | 0.58 |
| 1:A:67:MET:HE3 | 1:A:169:PRO:HB2 | 1.84 | 0.58 |
| 1:L:106:TRP:HB3 | 1:L:142:MET:CE | 2.33 | 0.58 |
| 1:H:22:PHE:CZ | 1:H:82:LEU:HD22 | 2.38 | 0.58 |
| 1:D:35:GLN:OE1 | 1:F:151:VAL:HG11 | 2.03 | 0.58 |
| 1:E:8:TYR:CE2 | 1:E:78:LYS:HE2 | 2.38 | 0.58 |
| 1:I:138:PHE:C | 1:I:142:MET:HE3 | 2.14 | 0.58 |
| 1:H:139:ILE:HD12 | 1:H:141:ASN:OD1 | 2.03 | 0.58 |
| 1:F:110:HIS:CD2 | 1:F:119:ILE:CD1 | 2.84 | 0.58 |
| 1:H:25:PHE:HB2 | 1:H:194:ALA:HA | 1.85 | 0.58 |
| 1:D:8:TYR:HD1 | 1:D:83:VAL:HG22 | 1.69 | 0.58 |
| 1:L:106:TRP:HD1 | 1:L:142:MET:CE | 2.14 | 0.58 |
| 1:F:57:PRO:HG3 | 1:F:120:TYR:CE2 | 2.39 | 0.58 |
| 1:A:187:LEU:CD2 | 1:A:208:LEU:HD21 | 2.34 | 0.58 |
| 1:C:9:THR:HG22 | 2:C:228:HOH:O | 2.03 | 0.58 |
| 1:B:67:MET:CE | 1:B:169:PRO:CG | 2.79 | 0.58 |
| 1:C:49:LYS:C | 1:C:51:ASN:N | 2.56 | 0.58 |
| 1:H:127:TYR:CE2 | 1:H:136:LYS:HG2 | 2.38 | 0.58 |
| 1:K:47:THR:O | 1:K:48:VAL:C | 2.42 | 0.57 |
| 1:A:204:MET:CE | 1:A:205:LEU:HD23 | 2.33 | 0.57 |
| 1:E:192:HIS:HD1 | 1:E:194:ALA:H | 1.52 | 0.57 |
| 1:G:113:PHE:HD2 | 1:G:218:GLY:HA3 | 1.67 | 0.57 |
| 1:B:158:LEU:HD12 | 1:B:160:VAL:HG23 | 1.82 | 0.57 |
| 1:I:38:GLN:NE2 | 1:I:177:TYR:OH | 2.37 | 0.57 |
| 1:A:204:MET:CE | 1:A:205:LEU:HG | 2.35 | 0.57 |
| 1:G:159:ASN:ND2 | 1:H:159:ASN:ND2 | 2.53 | 0.57 |
| 1:J:149:PRO:O | 1:J:175:LYS:HB2 | 2.04 | 0.57 |
| 1:C:56:TYR:HB3 | 1:C:57:PRO:CD | 2.30 | 0.57 |
| 1:K:106:TRP:CD1 | 1:K:142:MET:HE1 | 2.39 | 0.57 |
| 1:K:171:PHE:HZ | 1:K:204:MET:CE | 2.15 | 0.57 |
| 1:A:204:MET:HE1 | 1:A:205:LEU:HD23 | 1.87 | 0.57 |
| 1:G:72:GLU:N | 1:G:72:GLU:OE2 | 2.30 | 0.57 |
| 1:K:192:HIS:HD1 | 1:K:194:ALA:H | 1.53 | 0.57 |
| 1:J:138:PHE:CG | 1:J:138:PHE:O | 2.57 | 0.57 |
| 1:I:149:PRO:HD2 | 1:I:150:TRP:CZ3 | 2.39 | 0.56 |
| 1:H:4:LYS:HB2 | 1:H:89:HIS:HE2 | 1.70 | 0.56 |
| 1:G:14:SER:HA | 1:G:19:LYS:HE2 | 1.87 | 0.56 |
| 1:G:53:HIS:HE1 | 1:G:114:ARG:NH1 | 2.02 | 0.56 |
| 1:C:49:LYS:O | 1:C:50:LYS:C | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:59:PHE:HD2 | 1:I:173:MET:SD | 2.27 | 0.56 |
| 1:I:59:PHE:HD2 | 1:I:173:MET:CE | 2.18 | 0.56 |
| 1:G:155:SER:O | 1:H:35:GLN:HA | 2.05 | 0.56 |
| 1:E:92:TYR:HA | 1:E:145:VAL:O | 2.05 | 0.56 |
| 1:F:157:ASP:OD2 | 1:F:157:ASP:N | 2.37 | 0.56 |
| 1:D:67:MET:CE | 1:D:169:PRO:CG | 2.79 | 0.56 |
| 1:H:48:VAL:HG13 | 1:H:53:HIS:O | 2.06 | 0.56 |
| 1:C:114:ARG:HG3 | 1:C:114:ARG:NH1 | 2.19 | 0.56 |
| 1:K:171:PHE:CE2 | 1:K:204:MET:CE | 2.89 | 0.56 |
| 1:D:56:TYR:HB3 | 1:D:57:PRO:HD3 | 1.86 | 0.56 |
| 1:L:179:GLN:HE21 | 1:L:184:LEU:HD12 | 1.70 | 0.56 |
| 1:L:30:GLN:HE22 | 1:L:164:ASP:HA | 1.71 | 0.56 |
| 1:B:67:MET:HE1 | 1:B:169:PRO:CG | 2.35 | 0.56 |
| 1:G:59:PHE:HD2 | 1:G:173:MET:HE2 | 1.69 | 0.56 |
| 1:L:45:LEU:HD23 | 1:L:45:LEU:C | 2.25 | 0.56 |
| 1:G:159:ASN:ND2 | 1:I:159:ASN:HD21 | 2.04 | 0.56 |
| 1:L:37:VAL:HG13 | 1:L:38:GLN:N | 2.21 | 0.56 |
| 1:D:8:TYR:CD1 | 1:D:83:VAL:HG22 | 2.40 | 0.56 |
| 1:L:118:HIS:O | 1:L:119:ILE:HB | 2.06 | 0.56 |
| 1:A:89:HIS:O | 1:A:142:MET:HA | 2.06 | 0.56 |
| 1:I:118:HIS:CE1 | 1:I:122:GLN:NE2 | 2.73 | 0.55 |
| 1:J:67:MET:HE1 | 1:J:73:PHE:CG | 2.41 | 0.55 |
| 1:I:77:MET:HE1 | 1:I:82:LEU:HB2 | 1.87 | 0.55 |
| 1:J:106:TRP:HD1 | 1:J:142:MET:CE | 2.19 | 0.55 |
| 1:J:25:PHE:O | 1:J:30:GLN:HG3 | 2.06 | 0.55 |
| 1:D:65:ARG:HD2 | 1:J:111:ASP:OD2 | 2.06 | 0.55 |
| 1:I:118:HIS:ND1 | 1:I:122:GLN:NE2 | 2.53 | 0.55 |
| 1:K:74:ARG:HD2 | 1:K:88:VAL:HG13 | 1.89 | 0.55 |
| 1:L:26:GLN:HA | 1:L:26:GLN:HE21 | 1.70 | 0.55 |
| 1:E:25:PHE:O | 1:E:30:GLN:HG3 | 2.07 | 0.55 |
| 1:L:77:MET:HG3 | 1:L:165:ASN:OD1 | 2.07 | 0.55 |
| 1:H:45:LEU:HD13 | 1:H:49:LYS:NZ | 2.22 | 0.55 |
| 1:K:34:ASN:OD1 | 1:K:157:ASP:HB3 | 2.07 | 0.55 |
| 1:J:57:PRO:HA | 1:J:60:ILE:HB | 1.88 | 0.55 |
| 1:C:49:LYS:C | 1:C:51:ASN:H | 2.10 | 0.55 |
| 1:B:156:PHE:C | 1:B:156:PHE:CD2 | 2.80 | 0.55 |
| 1:I:34:ASN:ND2 | 1:I:158:LEU:H | 2.04 | 0.55 |
| 1:A:115:GLN:O | 1:A:119:ILE:HD12 | 2.07 | 0.55 |
| 1:H:65:ARG:HH22 | 1:H:219:ALA:CB | 2.20 | 0.55 |
| 1:D:203:ARG:O | 1:D:207:GLU:HG3 | 2.07 | 0.55 |
| 1:H:38:GLN:NE2 | 1:H:177:TYR:OH | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:138:PHE:CA | 1:I:142:MET:CE | 2.84 | 0.54 |
| 1:K:90:PRO:HD2 | 1:K:107:SER:O | 2.07 | 0.54 |
| 1:B:204:MET:CE | 1:B:205:LEU:HD23 | 2.37 | 0.54 |
| 1:D:110:HIS:HD2 | 1:D:112:ASP:H | 1.54 | 0.54 |
| 1:J:29:ALA:O | 1:J:30:GLN:C | 2.45 | 0.54 |
| 1:K:106:TRP:CD1 | 1:K:142:MET:HE3 | 2.43 | 0.54 |
| 1:G:72:GLU:HG3 | 1:G:200:HIS:HB3 | 1.89 | 0.54 |
| 1:J:67:MET:HE1 | 1:J:73:PHE:CD1 | 2.42 | 0.54 |
| 1:I:34:ASN:HD21 | 1:I:158:LEU:H | 1.55 | 0.54 |
| 1:I:75:MET:HA | 1:I:83:VAL:O | 2.08 | 0.54 |
| 1:G:159:ASN:HB3 | 1:H:32:THR:HG22 | 1.90 | 0.54 |
| 1:K:159:ASN:HB3 | 1:L:32:THR:CG2 | 2.38 | 0.54 |
| 1:D:25:PHE:O | 1:D:30:GLN:HG3 | 2.08 | 0.54 |
| 1:I:118:HIS:CE1 | 1:I:122:GLN:HE21 | 2.25 | 0.54 |
| 1:C:148:ASN:O | 1:C:174:GLY:HA2 | 2.08 | 0.54 |
| 1:G:159:ASN:HD22 | 1:I:159:ASN:ND2 | 2.06 | 0.54 |
| 1:G:91:CYS:HB2 | 1:G:142:MET:HE2 | 1.90 | 0.54 |
| 1:J:27:SER:OG | 1:J:28:VAL:HG22 | 2.08 | 0.54 |
| 1:G:93:THR:HG23 | 1:G:146:SER:HB3 | 1.90 | 0.54 |
| 1:K:106:TRP:CG | 1:K:142:MET:CE | 2.91 | 0.54 |
| 1:F:11:VAL:HG21 | 1:F:82:LEU:HD23 | 1.89 | 0.54 |
| 1:C:67:MET:HE3 | 1:C:67:MET:HA | 1.90 | 0.54 |
| 1:K:56:TYR:HB3 | 1:K:57:PRO:CD | 2.37 | 0.54 |
| 1:L:66:LEU:HD21 | 1:L:211:TYR:CD2 | 2.43 | 0.54 |
| 1:I:6:THR:CG2 | 1:I:141:ASN:HD21 | 2.01 | 0.53 |
| 1:J:159:ASN:HB3 | 1:K:32:THR:CG2 | 2.24 | 0.53 |
| 1:G:59:PHE:HE2 | 1:G:63:LEU:HD11 | 1.72 | 0.53 |
| 1:H:4:LYS:HB2 | 1:H:89:HIS:NE2 | 2.23 | 0.53 |
| 1:J:62:ILE:HD11 | 1:J:215:TRP:CD1 | 2.43 | 0.53 |
| 1:J:171:PHE:CZ | 1:J:204:MET:CE | 2.91 | 0.53 |
| 1:B:78:LYS:O | 1:B:81:GLU:N | 2.39 | 0.53 |
| 1:G:59:PHE:CD2 | 1:G:173:MET:SD | 3.02 | 0.53 |
| 1:J:40:ASP:HA | 1:J:184:LEU:CD2 | 2.38 | 0.53 |
| 1:E:148:ASN:N | 1:E:149:PRO:HD3 | 2.22 | 0.53 |
| 1:D:190:GLN:O | 1:D:190:GLN:HG3 | 2.06 | 0.53 |
| 1:A:187:LEU:CD2 | 1:A:208:LEU:CD2 | 2.85 | 0.53 |
| 1:F:177:TYR:OH | 2:F:233:HOH:O | 2.19 | 0.53 |
| 1:E:154:THR:HG23 | 1:F:154:THR:O | 2.08 | 0.53 |
| 1:K:171:PHE:CZ | 1:K:204:MET:SD | 3.01 | 0.53 |
| 1:E:44:PHE:O | 1:E:48:VAL:HG23 | 2.09 | 0.53 |
| 1:J:123:ASP:OD1 | 1:J:136:LYS:CE | 2.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:93:THR:CG2 | 1:G:146:SER:HB3 | 2.39 | 0.53 |
| 1:C:190:GLN:C | 1:C:190:GLN:HE21 | 2.12 | 0.53 |
| 1:G:98:GLN:HB2 | 1:G:99:THR:HG23 | 1.90 | 0.53 |
| 1:H:26:GLN:HE21 | 1:H:26:GLN:HA | 1.74 | 0.53 |
| 1:J:30:GLN:NE2 | 2:J:226:HOH:O | 2.41 | 0.53 |
| 1:J:27:SER:OG | 1:J:28:VAL:N | 2.40 | 0.53 |
| 1:H:5:ILE:HA | 1:H:6:THR:HG23 | 1.90 | 0.53 |
| 1:G:139:ILE:HG13 | 1:G:142:MET:CG | 2.38 | 0.53 |
| 1:D:110:HIS:HD2 | 1:D:111:ASP:N | 2.06 | 0.53 |
| 1:K:154:THR:HG22 | 1:L:36:THR:HB | 1.90 | 0.53 |
| 1:J:99:THR:HB | 1:K:17:HIS:HD2 | 1.73 | 0.53 |
| 1:C:216:GLN:HA | 1:C:216:GLN:NE2 | 2.17 | 0.52 |
| 1:A:56:TYR:N | 1:A:57:PRO:CD | 2.71 | 0.52 |
| 1:G:12:ASP:OD2 | 1:G:15:GLN:HG2 | 2.10 | 0.52 |
| 1:H:56:TYR:HB3 | 1:H:57:PRO:HD3 | 1.91 | 0.52 |
| 1:I:143:PHE:HB2 | 1:I:169:PRO:HD2 | 1.92 | 0.52 |
| 1:L:67:MET:HE1 | 1:L:73:PHE:CD2 | 2.44 | 0.52 |
| 1:L:57:PRO:HG2 | 1:L:58:ALA:N | 2.23 | 0.52 |
| 1:E:156:PHE:C | 1:E:156:PHE:CD2 | 2.82 | 0.52 |
| 1:H:30:GLN:NE2 | 1:H:163:MET:HG3 | 2.25 | 0.52 |
| 1:E:187:LEU:HG | 1:E:188:ALA:N | 2.21 | 0.52 |
| 1:K:106:TRP:HB3 | 1:K:142:MET:HE1 | 1.92 | 0.52 |
| 1:J:130:ASN:HB3 | 1:J:135:PRO:HG3 | 1.92 | 0.52 |
| 1:G:187:LEU:CD2 | 1:G:208:LEU:HD21 | 2.40 | 0.52 |
| 1:G:75:MET:HA | 1:G:83:VAL:O | 2.08 | 0.52 |
| 1:L:35:GLN:O | 1:L:188:ALA:HA | 2.09 | 0.52 |
| 1:C:67:MET:HE3 | 1:C:73:PHE:HB2 | 1.88 | 0.52 |
| 1:B:154:THR:HG21 | 1:C:38:GLN:OE1 | 2.10 | 0.52 |
| 1:D:214:GLU:OE2 | 1:J:115:GLN:HG3 | 2.10 | 0.52 |
| 1:K:34:ASN:HD21 | 1:K:190:GLN:HB2 | 1.75 | 0.52 |
| 1:J:59:PHE:HD2 | 1:J:173:MET:HE1 | 1.74 | 0.52 |
| 1:C:47:THR:O | 1:C:48:VAL:C | 2.48 | 0.52 |
| 1:B:187:LEU:HG | 1:B:188:ALA:N | 2.18 | 0.52 |
| 1:C:67:MET:HE1 | 1:C:73:PHE:CD1 | 2.44 | 0.52 |
| 1:D:16:TRP:CE2 | 1:D:18:ARG:HB2 | 2.45 | 0.52 |
| 1:G:133:TYR:O | 1:G:135:PRO:HD3 | 2.10 | 0.52 |
| 1:L:171:PHE:HA | 1:L:188:ALA:O | 2.10 | 0.51 |
| 1:A:56:TYR:HB3 | 1:A:57:PRO:HD3 | 1.92 | 0.51 |
| 1:C:29:ALA:O | 1:C:30:GLN:C | 2.45 | 0.51 |
| 1:A:129:GLU:HA | 1:A:129:GLU:OE1 | 2.10 | 0.51 |
| 1:D:110:HIS:CD2 | 1:D:112:ASP:H | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:189:ILE:O | 1:D:189:ILE:HG23 | 2.10 | 0.51 |
| 1:D:73:PHE:HB3 | 1:D:169:PRO:HG2 | 1.91 | 0.51 |
| 1:L:106:TRP:CG | 1:L:142:MET:HE3 | 2.43 | 0.51 |
| 1:J:145:VAL:CG1 | 1:J:173:MET:HE3 | 2.41 | 0.51 |
| 1:E:90:PRO:HD2 | 1:E:107:SER:O | 2.10 | 0.51 |
| 1:I:30:GLN:NE2 | 1:I:192:HIS:NE2 | 2.47 | 0.51 |
| 1:C:113:PHE:CD2 | 1:C:215:TRP:HZ2 | 2.29 | 0.51 |
| 1:D:27:SER:O | 1:D:28:VAL:C | 2.45 | 0.51 |
| 1:A:204:MET:CE | 1:A:205:LEU:CD2 | 2.88 | 0.51 |
| 1:B:78:LYS:O | 1:B:80:GLY:N | 2.43 | 0.51 |
| 1:G:45:LEU:HD12 | 1:G:183:VAL:HG11 | 1.92 | 0.51 |
| 1:K:59:PHE:HD2 | 1:K:173:MET:CE | 2.24 | 0.51 |
| 1:I:30:GLN:NE2 | 1:I:163:MET:HG3 | 2.26 | 0.51 |
| 1:I:49:LYS:O | 1:I:51:ASN:O | 2.29 | 0.51 |
| 1:F:89:HIS:ND1 | 1:F:109:TYR:HB3 | 2.25 | 0.51 |
| 1:I:25:PHE:O | 1:I:30:GLN:HG3 | 2.10 | 0.51 |
| 1:D:148:ASN:ND2 | 1:D:150:TRP:HE3 | 2.09 | 0.51 |
| 1:K:171:PHE:CZ | 1:K:189:ILE:HD13 | 2.46 | 0.51 |
| 1:D:8:TYR:CD1 | 1:D:83:VAL:CG2 | 2.94 | 0.51 |
| 1:H:59:PHE:CD2 | 1:H:173:MET:SD | 3.04 | 0.51 |
| 1:G:34:ASN:ND2 | 2:G:232:HOH:O | 2.44 | 0.51 |
| 1:B:5:ILE:N | 1:B:5:ILE:CD1 | 2.74 | 0.51 |
| 1:I:110:HIS:HB3 | 1:I:115:GLN:OE1 | 2.11 | 0.50 |
| 1:F:106:TRP:CD1 | 1:F:142:MET:HE2 | 2.45 | 0.50 |
| 1:F:151:VAL:CG1 | 1:F:153:PHE:HB3 | 2.40 | 0.50 |
| 1:G:127:TYR:CE2 | 1:G:136:LYS:HG2 | 2.46 | 0.50 |
| 1:A:77:MET:HG3 | 1:A:165:ASN:OD1 | 2.11 | 0.50 |
| 1:K:172:THR:HB | 1:K:188:ALA:HB3 | 1.93 | 0.50 |
| 1:J:163:MET:SD | 1:L:161:ALA:HB2 | 2.51 | 0.50 |
| 1:E:67:MET:CE | 1:E:171:PHE:CZ | 2.93 | 0.50 |
| 1:K:139:ILE:HG13 | 1:K:142:MET:HG2 | 1.93 | 0.50 |
| 1:E:26:GLN:HA | 1:E:26:GLN:HE21 | 1.76 | 0.50 |
| 1:C:62:ILE:HG21 | 1:C:208:LEU:HD12 | 1.94 | 0.50 |
| 1:I:40:ASP:HB3 | 1:I:209:GLN:OE1 | 2.12 | 0.50 |
| 1:G:159:ASN:ND2 | 1:H:159:ASN:HD21 | 2.10 | 0.50 |
| 1:G:59:PHE:CD2 | 1:G:173:MET:HE2 | 2.42 | 0.50 |
| 1:L:179:GLN:HE21 | 1:L:184:LEU:CD1 | 2.24 | 0.50 |
| 1:D:114:ARG:CG | 1:D:114:ARG:HH11 | 2.25 | 0.50 |
| 1:J:56:TYR:CZ | 1:J:147:ALA:HB2 | 2.46 | 0.50 |
| 1:D:159:ASN:OD1 | 1:E:159:ASN:ND2 | 2.45 | 0.50 |
| 1:D:113:PHE:O | 1:D:117:LEU:HB2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:91:CYS:CB | 1:G:142:MET:HE2 | 2.42 | 0.50 |
| 1:J:159:ASN:ND2 | 1:K:159:ASN:HD22 | 2.10 | 0.50 |
| 1:D:56:TYR:HB3 | 1:D:57:PRO:CD | 2.41 | 0.50 |
| 1:F:68:ASN:OD1 | 1:F:87:SER:HA | 2.10 | 0.50 |
| 1:C:204:MET:CE | 1:C:205:LEU:HD23 | 2.41 | 0.50 |
| 1:I:67:MET:HE1 | 1:I:73:PHE:HB3 | 1.93 | 0.50 |
| 1:J:34:ASN:ND2 | 1:J:190:GLN:HB2 | 2.27 | 0.50 |
| 1:B:34:ASN:CB | 1:B:157:ASP:HB2 | 2.41 | 0.50 |
| 1:L:84:ILE:HG22 | 1:L:85:TRP:O | 2.12 | 0.50 |
| 1:D:30:GLN:HE22 | 1:D:164:ASP:HA | 1.77 | 0.50 |
| 1:G:18:ARG:O | 1:G:19:LYS:C | 2.50 | 0.50 |
| 1:C:110:HIS:HD2 | 1:C:119:ILE:HD13 | 1.76 | 0.50 |
| 1:K:10:THR:O | 1:K:10:THR:CG2 | 2.60 | 0.49 |
| 1:D:148:ASN:ND2 | 1:D:150:TRP:CE3 | 2.81 | 0.49 |
| 1:L:153:PHE:O | 1:L:186:PRO:HB3 | 2.11 | 0.49 |
| 1:J:106:TRP:HB3 | 1:J:142:MET:CE | 2.42 | 0.49 |
| 1:G:91:CYS:SG | 1:G:142:MET:CE | 2.96 | 0.49 |
| 1:L:123:ASP:OD1 | 1:L:136:LYS:CE | 2.60 | 0.49 |
| 1:F:39:LEU:HD13 | 1:F:41:ILE:CG2 | 2.42 | 0.49 |
| 1:K:8:TYR:OH | 1:K:78:LYS:HD3 | 2.12 | 0.49 |
| 1:D:110:HIS:CD2 | 1:D:111:ASP:N | 2.81 | 0.49 |
| 1:D:38:GLN:NE2 | 1:D:177:TYR:OH | 2.44 | 0.49 |
| 1:J:106:TRP:O | 1:J:136:LYS:HE3 | 2.12 | 0.49 |
| 1:J:34:ASN:O | 1:L:157:ASP:N | 2.45 | 0.49 |
| 1:A:13:ILE:HG22 | 1:A:19:LYS:HG3 | 1.95 | 0.49 |
| 1:G:26:GLN:NE2 | 2:G:225:HOH:O | 2.37 | 0.49 |
| 1:H:5:ILE:O | 1:H:5:ILE:HG22 | 2.12 | 0.49 |
| 1:E:56:TYR:HB3 | 1:E:57:PRO:CD | 2.42 | 0.49 |
| 1:K:22:PHE:CE1 | 1:K:26:GLN:HG3 | 2.47 | 0.49 |
| 1:D:67:MET:HE1 | 1:D:169:PRO:CG | 2.40 | 0.49 |
| 1:D:25:PHE:HB2 | 1:D:194:ALA:HA | 1.95 | 0.49 |
| 1:L:8:TYR:HB2 | 1:L:83:VAL:CG1 | 2.41 | 0.49 |
| 1:B:99:THR:O | 1:B:100:GLU:HB2 | 2.12 | 0.49 |
| 1:L:103:SER:HB3 | 1:L:132:ALA:O | 2.12 | 0.49 |
| 1:I:14:SER:HA | 1:I:19:LYS:HD2 | 1.95 | 0.49 |
| 2:B:240:HOH:O | 1:C:17:HIS:HD2 | 1.94 | 0.49 |
| 1:J:179:GLN:O | 1:J:179:GLN:CG | 2.60 | 0.49 |
| 1:J:67:MET:CE | 1:J:73:PHE:CG | 2.96 | 0.49 |
| 1:B:67:MET:HE2 | 1:B:169:PRO:HB2 | 1.94 | 0.49 |
| 1:K:171:PHE:CE2 | 1:K:189:ILE:HD13 | 2.47 | 0.49 |
| 1:E:67:MET:HE2 | 1:E:171:PHE:CE1 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:127:TYR:CE2 | 1:G:136:LYS:CG | 2.95 | 0.49 |
| 1:D:38:GLN:NE2 | 1:D:177:TYR:HE2 | 2.09 | 0.49 |
| 1:B:191:VAL:HG21 | 1:B:201:VAL:HG21 | 1.95 | 0.49 |
| 1:A:90:PRO:HD2 | 1:A:107:SER:O | 2.12 | 0.49 |
| 1:D:38:GLN:NE2 | 1:D:177:TYR:CE2 | 2.81 | 0.49 |
| 1:I:145:VAL:CG1 | 1:I:173:MET:CE | 2.91 | 0.48 |
| 1:K:44:PHE:HB2 | 1:K:212:CYS:HB3 | 1.94 | 0.48 |
| 1:G:92:TYR:HA | 1:G:145:VAL:O | 2.13 | 0.48 |
| 1:D:36:THR:HB | 1:F:155:SER:HB3 | 1.94 | 0.48 |
| 1:L:178:THR:O | 1:L:179:GLN:HB3 | 2.14 | 0.48 |
| 1:J:10:THR:CB | 2:J:225:HOH:O | 2.59 | 0.48 |
| 1:J:44:PHE:O | 1:J:48:VAL:HG23 | 2.13 | 0.48 |
| 1:I:150:TRP:HB2 | 1:I:151:VAL:HG23 | 1.95 | 0.48 |
| 1:I:139:ILE:HG13 | 1:I:142:MET:HE2 | 1.95 | 0.48 |
| 1:I:110:HIS:CD2 | 1:I:119:ILE:HD12 | 2.48 | 0.48 |
| 1:H:25:PHE:O | 1:H:30:GLN:HG3 | 2.13 | 0.48 |
| 1:E:134:PHE:O | 1:E:135:PRO:C | 2.50 | 0.48 |
| 1:D:87:SER:O | 1:D:141:ASN:ND2 | 2.43 | 0.48 |
| 1:B:215:TRP:CZ2 | 1:B:217:GLY:HA2 | 2.49 | 0.48 |
| 1:J:159:ASN:ND2 | 1:L:159:ASN:ND2 | 2.48 | 0.48 |
| 1:I:148:ASN:HD22 | 1:I:150:TRP:HE3 | 1.60 | 0.48 |
| 1:K:138:PHE:CD2 | 1:K:138:PHE:N | 2.81 | 0.48 |
| 1:F:151:VAL:HG12 | 1:F:153:PHE:HD2 | 1.79 | 0.48 |
| 1:K:11:VAL:HG23 | 1:K:82:LEU:O | 2.14 | 0.48 |
| 1:F:123:ASP:OD1 | 1:F:136:LYS:CE | 2.62 | 0.48 |
| 1:E:30:GLN:HE22 | 1:E:164:ASP:HA | 1.79 | 0.48 |
| 1:I:67:MET:CE | 1:I:73:PHE:HB3 | 2.44 | 0.48 |
| 1:G:35:GLN:O | 1:G:188:ALA:HA | 2.14 | 0.48 |
| 1:K:10:THR:HG22 | 1:K:10:THR:O | 2.13 | 0.48 |
| 1:A:157:ASP:HB2 | 1:C:157:ASP:OD2 | 2.14 | 0.48 |
| 1:A:187:LEU:HD22 | 1:A:208:LEU:HD21 | 1.95 | 0.48 |
| 1:J:63:LEU:HD13 | 1:J:171:PHE:CD1 | 2.49 | 0.47 |
| 1:K:67:MET:HG3 | 1:K:143:PHE:CG | 2.48 | 0.47 |
| 1:L:89:HIS:ND1 | 1:L:109:TYR:N | 2.49 | 0.47 |
| 1:K:72:GLU:HA | 1:K:75:MET:CE | 2.41 | 0.47 |
| 1:L:66:LEU:HD23 | 1:L:211:TYR:HE2 | 1.79 | 0.47 |
| 1:G:22:PHE:O | 1:G:23:GLU:C | 2.50 | 0.47 |
| 1:D:136:LYS:O | 1:D:137:GLY:C | 2.51 | 0.47 |
| 1:G:161:ALA:HB2 | 1:H:163:MET:SD | 2.54 | 0.47 |
| 1:G:154:THR:HG22 | 1:H:36:THR:HB | 1.97 | 0.47 |
| 1:J:57:PRO:O | 1:J:58:ALA:C | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:77:MET:HE3 | 1:E:165:ASN:OD1 | 2.15 | 0.47 |
| 1:J:159:ASN:CG | 1:K:159:ASN:HD22 | 2.17 | 0.47 |
| 1:K:92:TYR:HA | 1:K:145:VAL:O | 2.13 | 0.47 |
| 1:A:123:ASP:OD1 | 1:A:136:LYS:CE | 2.62 | 0.47 |
| 1:J:57:PRO:HB3 | 1:J:120:TYR:CE2 | 2.49 | 0.47 |
| 1:B:151:VAL:CG1 | 1:B:152:SER:N | 2.78 | 0.47 |
| 1:F:204:MET:HE2 | 1:F:205:LEU:HA | 1.96 | 0.47 |
| 1:B:109:TYR:O | 1:B:110:HIS:CG | 2.68 | 0.47 |
| 1:I:139:ILE:HG13 | 1:I:142:MET:HE3 | 1.92 | 0.47 |
| 1:C:120:TYR:CZ | 1:C:124:VAL:HG21 | 2.49 | 0.47 |
| 1:J:67:MET:CA | 1:J:67:MET:CE | 2.84 | 0.47 |
| 1:D:67:MET:HE3 | 1:D:169:PRO:HG2 | 1.92 | 0.47 |
| 1:L:67:MET:CE | 1:L:169:PRO:CG | 2.85 | 0.47 |
| 1:I:109:TYR:O | 1:I:110:HIS:CD2 | 2.68 | 0.47 |
| 1:A:192:HIS:HD1 | 1:A:194:ALA:N | 2.05 | 0.47 |
| 1:I:92:TYR:HA | 1:I:145:VAL:O | 2.14 | 0.47 |
| 1:I:59:PHE:CD2 | 1:I:173:MET:HE1 | 2.45 | 0.47 |
| 1:G:30:GLN:HB3 | 1:I:161:ALA:CB | 2.43 | 0.47 |
| 1:A:184:LEU:HD23 | 1:A:184:LEU:HA | 1.63 | 0.47 |
| 1:B:5:ILE:N | 1:B:5:ILE:HD13 | 2.29 | 0.47 |
| 1:A:29:ALA:O | 1:A:30:GLN:C | 2.52 | 0.47 |
| 1:J:85:TRP:CD2 | 1:J:141:ASN:HB3 | 2.50 | 0.47 |
| 1:K:190:GLN:C | 1:K:190:GLN:HE21 | 2.17 | 0.47 |
| 1:K:77:MET:HE2 | 1:K:82:LEU:HD13 | 1.97 | 0.47 |
| 1:D:59:PHE:HD2 | 1:D:173:MET:CE | 2.28 | 0.47 |
| 1:B:67:MET:HG3 | 1:B:143:PHE:CG | 2.50 | 0.46 |
| 1:K:157:ASP:OD2 | 1:L:157:ASP:OD2 | 2.33 | 0.46 |
| 1:D:59:PHE:CE2 | 1:D:63:LEU:HD11 | 2.50 | 0.46 |
| 1:K:8:TYR:CD1 | 1:K:8:TYR:O | 2.68 | 0.46 |
| 1:J:18:ARG:HE | 1:J:197:ASP:CG | 2.19 | 0.46 |
| 1:B:151:VAL:HG12 | 1:B:152:SER:N | 2.29 | 0.46 |
| 1:J:189:ILE:HG23 | 1:J:189:ILE:O | 2.14 | 0.46 |
| 1:A:26:GLN:O | 1:A:26:GLN:HG3 | 2.15 | 0.46 |
| 1:B:171:PHE:HA | 1:B:188:ALA:O | 2.15 | 0.46 |
| 1:K:165:ASN:HA | 1:K:167:PHE:CZ | 2.50 | 0.46 |
| 1:E:153:PHE:O | 1:E:186:PRO:HB3 | 2.16 | 0.46 |
| 1:J:45:LEU:HD23 | 1:J:45:LEU:HA | 1.77 | 0.46 |
| 1:E:56:TYR:HB3 | 1:E:57:PRO:HD3 | 1.97 | 0.46 |
| 1:J:64:ALA:O | 1:J:68:ASN:ND2 | 2.48 | 0.46 |
| 1:F:202:GLY:O | 1:F:203:ARG:C | 2.54 | 0.46 |
| 1:B:39:LEU:O | 1:B:185:MET:N | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:59:PHE:CE2 | 1:E:173:MET:SD | 3.08 | 0.46 |
| 1:L:67:MET:HB3 | 1:L:88:VAL:HG21 | 1.97 | 0.46 |
| 1:B:204:MET:CE | 1:B:205:LEU:HA | 2.45 | 0.46 |
| 1:J:145:VAL:HG11 | 1:J:173:MET:HE3 | 1.97 | 0.46 |
| 1:E:105:LEU:HD21 | 1:E:127:TYR:HB2 | 1.97 | 0.46 |
| 1:J:122:GLN:O | 1:J:126:CYS:HB3 | 2.16 | 0.46 |
| 1:B:155:SER:O | 1:C:35:GLN:HA | 2.16 | 0.46 |
| 1:A:204:MET:HE2 | 1:A:205:LEU:N | 2.31 | 0.46 |
| 1:J:106:TRP:CG | 1:J:142:MET:HE3 | 2.49 | 0.46 |
| 1:E:67:MET:HE2 | 1:E:171:PHE:HE1 | 1.79 | 0.46 |
| 1:D:51:ASN:H | 1:D:51:ASN:ND2 | 2.12 | 0.46 |
| 1:K:154:THR:HG21 | 1:L:38:GLN:OE1 | 2.16 | 0.46 |
| 1:K:34:ASN:HB3 | 1:K:157:ASP:OD1 | 2.16 | 0.46 |
| 1:I:145:VAL:CG1 | 1:I:173:MET:HE2 | 2.46 | 0.46 |
| 1:A:139:ILE:HG12 | 1:A:142:MET:HE3 | 1.98 | 0.46 |
| 1:G:113:PHE:CG | 1:G:113:PHE:O | 2.68 | 0.46 |
| 1:E:26:GLN:HA | 1:E:26:GLN:NE2 | 2.30 | 0.46 |
| 1:E:59:PHE:CD2 | 1:E:173:MET:HE2 | 2.45 | 0.45 |
| 1:I:67:MET:HG3 | 1:I:143:PHE:CG | 2.51 | 0.45 |
| 1:B:105:LEU:HA | 1:B:105:LEU:HD23 | 1.61 | 0.45 |
| 1:J:124:VAL:O | 1:J:128:GLY:CA | 2.65 | 0.45 |
| 1:J:90:PRO:HD2 | 1:J:107:SER:O | 2.16 | 0.45 |
| 1:C:51:ASN:HB3 | 1:C:52:LYS:H | 1.57 | 0.45 |
| 1:H:26:GLN:NE2 | 1:H:26:GLN:HA | 2.30 | 0.45 |
| 1:J:159:ASN:HD22 | 1:L:159:ASN:ND2 | 1.87 | 0.45 |
| 1:F:26:GLN:HA | 1:F:26:GLN:NE2 | 2.31 | 0.45 |
| 1:I:6:THR:CG2 | 1:I:6:THR:OG1 | 2.52 | 0.45 |
| 1:B:158:LEU:HD13 | 1:B:160:VAL:HG23 | 1.87 | 0.45 |
| 1:H:192:HIS:HD1 | 1:H:194:ALA:N | 1.97 | 0.45 |
| 1:K:59:PHE:CE2 | 1:K:173:MET:SD | 3.09 | 0.45 |
| 1:J:63:LEU:HD13 | 1:J:171:PHE:CG | 2.51 | 0.45 |
| 1:A:40:ASP:HA | 1:A:184:LEU:HD23 | 1.98 | 0.45 |
| 1:L:74:ARG:HB2 | 1:L:84:ILE:HG23 | 1.97 | 0.45 |
| 1:B:19:LYS:HE3 | 1:B:23:GLU:OE2 | 2.17 | 0.45 |
| 1:A:35:GLN:O | 1:A:188:ALA:HA | 2.17 | 0.45 |
| 1:A:175:LYS:HZ3 | 1:A:175:LYS:HG3 | 1.40 | 0.45 |
| 1:I:171:PHE:HA | 1:I:188:ALA:O | 2.16 | 0.45 |
| 1:L:182:LYS:HZ2 | 1:L:182:LYS:HG2 | 1.62 | 0.45 |
| 1:L:106:TRP:HD1 | 1:L:142:MET:HE1 | 1.82 | 0.45 |
| 1:A:145:VAL:CG1 | 1:A:173:MET:HE2 | 2.46 | 0.45 |
| 1:J:89:HIS:CE1 | 1:J:108:GLU:CG | 2.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:205:LEU:O | 1:H:208:LEU:HB3 | 2.17 | 0.45 |
| 1:C:56:TYR:CE1 | 1:C:173:MET:HE1 | 2.52 | 0.45 |
| 1:D:36:THR:HG22 | 1:F:154:THR:HG22 | 1.99 | 0.45 |
| 1:G:36:THR:HB | 1:I:155:SER:HB3 | 1.98 | 0.45 |
| 1:L:149:PRO:HD2 | 1:L:150:TRP:CZ3 | 2.52 | 0.45 |
| 1:L:144:PHE:HB2 | 1:L:170:VAL:HG22 | 1.99 | 0.45 |
| 1:C:56:TYR:HE1 | 1:C:173:MET:CE | 2.29 | 0.45 |
| 1:K:49:LYS:C | 1:K:51:ASN:O | 2.55 | 0.45 |
| 1:F:26:GLN:HA | 1:F:26:GLN:HE21 | 1.81 | 0.45 |
| 1:C:96:HIS:CE1 | 1:C:128:GLY:O | 2.70 | 0.45 |
| 1:H:101:THR:HB | 2:H:231:HOH:O | 2.16 | 0.45 |
| 1:C:67:MET:CE | 1:C:73:PHE:CD1 | 2.99 | 0.45 |
| 1:B:204:MET:HE2 | 1:B:205:LEU:HG | 1.99 | 0.45 |
| 1:A:13:ILE:H | 1:A:13:ILE:HD12 | 1.82 | 0.45 |
| 1:F:204:MET:HE2 | 1:F:205:LEU:CA | 2.47 | 0.45 |
| 1:D:77:MET:HB2 | 1:D:165:ASN:HB3 | 1.99 | 0.45 |
| 1:J:93:THR:HA | 1:J:103:SER:O | 2.16 | 0.45 |
| 1:K:205:LEU:HD23 | 1:K:205:LEU:HA | 1.85 | 0.45 |
| 1:J:159:ASN:HD21 | 1:K:159:ASN:HD21 | 1.60 | 0.45 |
| 1:J:6:THR:O | 1:J:6:THR:CG2 | 2.53 | 0.45 |
| 1:J:25:PHE:HB2 | 1:J:194:ALA:HA | 1.99 | 0.44 |
| 1:H:113:PHE:N | 1:H:219:ALA:HB3 | 2.30 | 0.44 |
| 1:G:30:GLN:NE2 | 2:G:225:HOH:O | 2.50 | 0.44 |
| 1:B:78:LYS:O | 1:B:79:ASP:C | 2.55 | 0.44 |
| 1:A:149:PRO:O | 1:A:175:LYS:HB2 | 2.18 | 0.44 |
| 1:J:98:GLN:N | 1:J:98:GLN:HE21 | 2.16 | 0.44 |
| 1:I:57:PRO:HB3 | 1:I:120:TYR:CD2 | 2.52 | 0.44 |
| 1:J:203:ARG:HG2 | 1:J:207:GLU:OE2 | 2.17 | 0.44 |
| 1:J:75:MET:HA | 1:J:83:VAL:O | 2.17 | 0.44 |
| 1:D:67:MET:HE1 | 1:D:73:PHE:HB3 | 1.92 | 0.44 |
| 1:C:30:GLN:HE22 | 1:C:164:ASP:HA | 1.83 | 0.44 |
| 1:H:35:GLN:NE2 | 1:H:201:VAL:HG11 | 2.32 | 0.44 |
| 1:K:187:LEU:HG | 1:K:188:ALA:N | 2.30 | 0.44 |
| 1:E:6:THR:HG21 | 1:E:89:HIS:HE2 | 1.82 | 0.44 |
| 1:H:132:ALA:O | 1:H:135:PRO:HD3 | 2.16 | 0.44 |
| 1:G:171:PHE:HA | 1:G:188:ALA:O | 2.17 | 0.44 |
| 1:D:159:ASN:ND2 | 1:F:159:ASN:CG | 2.70 | 0.44 |
| 1:H:155:SER:HB3 | 1:I:36:THR:HB | 1.98 | 0.44 |
| 1:G:106:TRP:HB3 | 1:G:142:MET:HE3 | 2.00 | 0.44 |
| 1:J:59:PHE:O | 1:J:60:ILE:C | 2.55 | 0.44 |
| 1:J:124:VAL:O | 1:J:128:GLY:HA2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:94:VAL:N | 1:I:103:SER:O | 2.38 | 0.44 |
| 1:H:67:MET:CE | 1:H:73:PHE:CB | 2.73 | 0.44 |
| 1:E:139:ILE:N | 1:E:142:MET:HE3 | 2.18 | 0.44 |
| 1:L:25:PHE:HB2 | 1:L:194:ALA:HA | 2.00 | 0.44 |
| 1:H:57:PRO:HG3 | 1:H:120:TYR:CZ | 2.53 | 0.44 |
| 1:F:59:PHE:O | 1:F:60:ILE:C | 2.55 | 0.44 |
| 1:L:130:ASN:HB2 | 1:L:135:PRO:HB3 | 2.00 | 0.44 |
| 1:A:159:ASN:OD1 | 1:B:159:ASN:ND2 | 2.47 | 0.44 |
| 1:C:63:LEU:HD23 | 1:C:208:LEU:HD13 | 1.99 | 0.44 |
| 1:A:30:GLN:HE22 | 1:A:164:ASP:HA | 1.82 | 0.44 |
| 1:H:34:ASN:ND2 | 1:H:158:LEU:H | 2.15 | 0.44 |
| 1:G:38:GLN:NE2 | 1:G:177:TYR:OH | 2.50 | 0.44 |
| 1:D:163:MET:HG2 | 1:D:163:MET:H | 1.61 | 0.44 |
| 1:K:72:GLU:HG2 | 1:K:73:PHE:H | 1.83 | 0.44 |
| 1:I:149:PRO:HD2 | 1:I:150:TRP:CE3 | 2.52 | 0.44 |
| 1:I:77:MET:CE | 1:I:82:LEU:HB2 | 2.47 | 0.44 |
| 1:D:185:MET:HA | 1:D:186:PRO:HD3 | 1.75 | 0.44 |
| 1:K:66:LEU:HD23 | 1:K:66:LEU:HA | 1.71 | 0.44 |
| 1:D:20:GLU:OE1 | 1:F:133:TYR:N | 2.42 | 0.44 |
| 1:K:59:PHE:O | 1:K:60:ILE:C | 2.56 | 0.44 |
| 1:E:4:LYS:HB3 | 1:E:4:LYS:HE3 | 1.30 | 0.44 |
| 1:G:159:ASN:CG | 1:H:159:ASN:ND2 | 2.72 | 0.43 |
| 1:I:192:HIS:HD1 | 1:I:194:ALA:H | 1.64 | 0.43 |
| 1:G:85:TRP:CH2 | 1:G:140:GLU:HG3 | 2.53 | 0.43 |
| 1:G:29:ALA:O | 1:G:30:GLN:C | 2.56 | 0.43 |
| 1:L:92:TYR:HA | 1:L:145:VAL:O | 2.18 | 0.43 |
| 1:B:66:LEU:O | 1:B:67:MET:C | 2.50 | 0.43 |
| 1:J:32:THR:HG22 | 1:J:163:MET:SD | 2.59 | 0.43 |
| 1:D:85:TRP:CZ2 | 1:D:140:GLU:HB3 | 2.53 | 0.43 |
| 1:D:85:TRP:CG | 1:D:141:ASN:HB3 | 2.53 | 0.43 |
| 1:H:156:PHE:CD2 | 1:H:157:ASP:N | 2.85 | 0.43 |
| 1:G:15:GLN:HA | 1:G:15:GLN:NE2 | 2.25 | 0.43 |
| 1:E:77:MET:HE3 | 1:E:77:MET:HB2 | 1.52 | 0.43 |
| 1:I:91:CYS:HA | 1:I:105:LEU:O | 2.19 | 0.43 |
| 1:H:210:GLN:O | 1:H:211:TYR:C | 2.57 | 0.43 |
| 1:C:203:ARG:O | 1:C:207:GLU:HG3 | 2.18 | 0.43 |
| 1:I:6:THR:CG2 | 1:I:6:THR:N | 2.81 | 0.43 |
| 1:H:168:ALA:HA | 1:H:169:PRO:HD3 | 1.88 | 0.43 |
| 1:D:168:ALA:HA | 1:D:169:PRO:HD3 | 1.79 | 0.43 |
| 1:G:30:GLN:HG2 | 1:G:163:MET:SD | 2.58 | 0.43 |
| 1:J:59:PHE:CD2 | 1:J:173:MET:HE1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:92:TYR:CD1 | 1:L:92:TYR:O | 2.72 | 0.43 |
| 1:I:4:LYS:HB3 | 1:I:5:ILE:HD13 | 2.01 | 0.43 |
| 1:G:50:LYS:HA | 1:G:50:LYS:HD2 | 1.68 | 0.43 |
| 1:H:67:MET:CE | 1:H:73:PHE:CG | 3.02 | 0.43 |
| 1:C:38:GLN:HE22 | 1:C:186:PRO:HG3 | 1.83 | 0.43 |
| 1:J:18:ARG:NH2 | 1:J:193:HIS:O | 2.52 | 0.43 |
| 1:H:45:LEU:HD23 | 1:H:45:LEU:HA | 1.91 | 0.43 |
| 1:L:57:PRO:HG2 | 1:L:58:ALA:H | 1.81 | 0.43 |
| 1:B:47:THR:HG21 | 1:B:215:TRP:O | 2.19 | 0.43 |
| 1:J:22:PHE:O | 1:J:26:GLN:N | 2.47 | 0.43 |
| 1:C:56:TYR:N | 1:C:57:PRO:CD | 2.81 | 0.43 |
| 1:H:25:PHE:CZ | 1:H:193:HIS:CE1 | 3.06 | 0.43 |
| 1:D:159:ASN:ND2 | 1:F:159:ASN:ND2 | 2.67 | 0.43 |
| 1:C:70:HIS:HB3 | 1:C:72:GLU:OE1 | 2.19 | 0.43 |
| 1:C:27:SER:OG | 1:C:28:VAL:N | 2.45 | 0.43 |
| 1:H:63:LEU:O | 1:H:67:MET:HG2 | 2.18 | 0.43 |
| 1:J:171:PHE:CE2 | 1:J:204:MET:CE | 3.01 | 0.43 |
| 1:K:67:MET:HG3 | 1:K:143:PHE:CD2 | 2.54 | 0.43 |
| 1:F:38:GLN:NE2 | 1:F:177:TYR:OH | 2.51 | 0.43 |
| 1:L:56:TYR:HB3 | 1:L:57:PRO:CD | 2.49 | 0.43 |
| 1:D:187:LEU:HD22 | 1:D:208:LEU:CD2 | 2.48 | 0.43 |
| 1:L:66:LEU:HD21 | 1:L:211:TYR:CE2 | 2.51 | 0.43 |
| 1:G:40:ASP:HA | 1:G:184:LEU:HD23 | 2.01 | 0.43 |
| 1:L:206:ASN:O | 1:L:210:GLN:HB2 | 2.19 | 0.43 |
| 1:B:112:ASP:HB3 | 1:B:115:GLN:HB2 | 1.99 | 0.43 |
| 1:L:67:MET:HE1 | 1:L:169:PRO:CG | 2.42 | 0.42 |
| 1:H:25:PHE:HB2 | 1:H:194:ALA:CA | 2.48 | 0.42 |
| 1:J:57:PRO:HB3 | 1:J:120:TYR:CD2 | 2.54 | 0.42 |
| 1:C:105:LEU:HA | 1:C:105:LEU:HD23 | 1.89 | 0.42 |
| 1:C:25:PHE:O | 1:C:30:GLN:HG3 | 2.18 | 0.42 |
| 1:D:93:THR:HA | 1:D:103:SER:O | 2.19 | 0.42 |
| 1:L:47:THR:HA | 1:L:50:LYS:HD3 | 2.01 | 0.42 |
| 1:C:19:LYS:HE2 | 1:C:23:GLU:OE2 | 2.19 | 0.42 |
| 1:C:66:LEU:HD11 | 1:C:208:LEU:HA | 2.01 | 0.42 |
| 1:D:59:PHE:CD2 | 1:D:173:MET:CE | 3.02 | 0.42 |
| 1:J:59:PHE:HD2 | 1:J:173:MET:CE | 2.32 | 0.42 |
| 1:E:147:ALA:C | 1:E:149:PRO:HD3 | 2.39 | 0.42 |
| 1:I:57:PRO:HB3 | 1:I:120:TYR:CE2 | 2.55 | 0.42 |
| 1:C:89:HIS:O | 1:C:142:MET:HA | 2.19 | 0.42 |
| 1:D:42:THR:OG1 | 1:D:182:LYS:HA | 2.20 | 0.42 |
| 1:G:25:PHE:HB2 | 1:G:194:ALA:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:28:VAL:HG23 | 1:A:29:ALA:H | 1.84 | 0.42 |
| 1:D:50:LYS:C | 1:D:51:ASN:O | 2.56 | 0.42 |
| 1:H:34:ASN:HD21 | 1:H:158:LEU:H | 1.67 | 0.42 |
| 1:D:133:TYR:CE2 | 1:D:134:PHE:HE1 | 2.37 | 0.42 |
| 1:I:6:THR:CG2 | 1:I:141:ASN:ND2 | 2.67 | 0.42 |
| 1:C:56:TYR:CE1 | 1:C:173:MET:CE | 3.02 | 0.42 |
| 1:D:29:ALA:O | 1:D:30:GLN:C | 2.57 | 0.42 |
| 1:K:73:PHE:CZ | 1:K:204:MET:HB2 | 2.54 | 0.42 |
| 1:I:132:ALA:O | 1:I:135:PRO:HD3 | 2.20 | 0.42 |
| 1:L:158:LEU:HB3 | 1:L:190:GLN:HG3 | 2.02 | 0.42 |
| 1:A:190:GLN:CG | 1:A:190:GLN:O | 2.66 | 0.42 |
| 1:K:176:TYR:HA | 1:K:184:LEU:O | 2.19 | 0.42 |
| 1:J:154:THR:O | 1:L:154:THR:CG2 | 2.58 | 0.42 |
| 1:A:56:TYR:H | 1:A:57:PRO:HD2 | 1.84 | 0.42 |
| 1:J:34:ASN:HB2 | 1:L:157:ASP:HB2 | 2.01 | 0.42 |
| 1:F:56:TYR:HB3 | 1:F:57:PRO:HD3 | 2.01 | 0.42 |
| 1:G:56:TYR:HB3 | 1:G:57:PRO:CD | 2.49 | 0.42 |
| 1:E:34:ASN:ND2 | 1:E:190:GLN:CB | 2.77 | 0.42 |
| 1:H:35:GLN:O | 1:H:188:ALA:HA | 2.19 | 0.42 |
| 1:B:100:GLU:HG2 | 1:C:199:PHE:CE1 | 2.55 | 0.42 |
| 1:L:197:ASP:O | 1:L:201:VAL:HG23 | 2.19 | 0.42 |
| 1:G:32:THR:HG22 | 1:I:159:ASN:CB | 2.20 | 0.42 |
| 1:A:106:TRP:HB3 | 1:A:142:MET:HE2 | 2.01 | 0.42 |
| 1:F:204:MET:HE2 | 1:F:205:LEU:N | 2.35 | 0.42 |
| 1:G:184:LEU:HD23 | 1:G:184:LEU:HA | 1.71 | 0.42 |
| 1:K:122:GLN:HG3 | 1:K:122:GLN:O | 2.19 | 0.42 |
| 1:E:120:TYR:CD2 | 1:E:120:TYR:C | 2.93 | 0.42 |
| 1:F:25:PHE:O | 1:F:30:GLN:HA | 2.19 | 0.41 |
| 1:L:22:PHE:O | 1:L:26:GLN:HG2 | 2.19 | 0.41 |
| 1:J:132:ALA:O | 1:J:135:PRO:HD3 | 2.19 | 0.41 |
| 1:D:117:LEU:HD23 | 1:D:117:LEU:HA | 1.96 | 0.41 |
| 1:L:105:LEU:HD21 | 1:L:127:TYR:HB2 | 2.02 | 0.41 |
| 1:I:145:VAL:HG11 | 1:I:173:MET:HE2 | 2.01 | 0.41 |
| 1:L:70:HIS:NE2 | 1:L:207:GLU:OE1 | 2.47 | 0.41 |
| 1:G:156:PHE:C | 1:G:156:PHE:CD2 | 2.93 | 0.41 |
| 1:K:57:PRO:HB3 | 1:K:120:TYR:CD2 | 2.56 | 0.41 |
| 1:K:59:PHE:CD2 | 1:K:173:MET:CE | 3.03 | 0.41 |
| 1:D:182:LYS:HZ3 | 1:D:182:LYS:HG3 | 1.46 | 0.41 |
| 1:L:205:LEU:HD23 | 1:L:205:LEU:HA | 1.96 | 0.41 |
| 1:G:139:ILE:HG13 | 1:G:142:MET:HG3 | 2.02 | 0.41 |
| 1:K:89:HIS:O | 1:K:142:MET:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:153:PHE:O | 1:F:186:PRO:HB3 | 2.21 | 0.41 |
| 1:D:114:ARG:CG | 1:D:114:ARG:NH1 | 2.83 | 0.41 |
| 1:D:85:TRP:CD2 | 1:D:141:ASN:HB3 | 2.55 | 0.41 |
| 1:E:165:ASN:HA | 1:E:167:PHE:CE1 | 2.55 | 0.41 |
| 1:A:90:PRO:O | 1:A:106:TRP:HA | 2.21 | 0.41 |
| 1:K:92:TYR:N | 1:K:92:TYR:CD2 | 2.88 | 0.41 |
| 1:B:91:CYS:HA | 1:B:105:LEU:O | 2.21 | 0.41 |
| 1:I:120:TYR:O | 1:I:123:ASP:HB2 | 2.21 | 0.41 |
| 1:G:118:HIS:O | 1:G:122:GLN:HG3 | 2.21 | 0.41 |
| 1:J:162:ASN:HB3 | 2:K:221:HOH:O | 2.20 | 0.41 |
| 1:B:82:LEU:HD12 | 1:B:82:LEU:HA | 1.81 | 0.41 |
| 1:E:66:LEU:HD23 | 1:E:66:LEU:HA | 1.89 | 0.41 |
| 1:E:41:ILE:HG13 | 1:E:183:VAL:O | 2.19 | 0.41 |
| 1:C:25:PHE:HB2 | 1:C:194:ALA:HA | 2.03 | 0.41 |
| 1:F:151:VAL:HG12 | 1:F:151:VAL:O | 2.21 | 0.41 |
| 1:L:171:PHE:CZ | 1:L:189:ILE:HD13 | 2.55 | 0.41 |
| 1:A:38:GLN:HE22 | 1:A:186:PRO:HG3 | 1.86 | 0.41 |
| 1:B:154:THR:CG2 | 1:C:154:THR:O | 2.65 | 0.41 |
| 1:H:154:THR:HG22 | 1:I:154:THR:O | 2.21 | 0.41 |
| 1:L:118:HIS:O | 1:L:119:ILE:CB | 2.69 | 0.41 |
| 1:J:8:TYR:CD1 | 1:J:83:VAL:HG21 | 2.55 | 0.41 |
| 1:F:72:GLU:HG3 | 1:F:200:HIS:HB3 | 2.03 | 0.41 |
| 1:C:67:MET:CE | 1:C:73:PHE:CD2 | 2.94 | 0.41 |
| 1:L:67:MET:HE3 | 1:L:73:PHE:CB | 2.31 | 0.41 |
| 1:K:57:PRO:HA | 1:K:60:ILE:HD12 | 2.02 | 0.41 |
| 1:I:59:PHE:CD2 | 1:I:173:MET:CE | 3.03 | 0.41 |
| 1:I:89:HIS:ND1 | 1:I:108:GLU:HA | 2.36 | 0.41 |
| 1:E:65:ARG:NH2 | 2:E:230:HOH:O | 2.53 | 0.41 |
| 1:B:204:MET:HE3 | 1:B:204:MET:O | 2.21 | 0.41 |
| 1:C:204:MET:HE2 | 1:C:205:LEU:HD23 | 2.02 | 0.41 |
| 1:F:204:MET:CE | 1:F:205:LEU:HA | 2.50 | 0.41 |
| 1:E:64:ALA:HB1 | 1:E:109:TYR:CD1 | 2.56 | 0.41 |
| 1:I:26:GLN:HA | 1:I:26:GLN:HE21 | 1.86 | 0.41 |
| 1:I:138:PHE:C | 1:I:142:MET:CE | 2.82 | 0.40 |
| 1:G:159:ASN:HD21 | 1:I:159:ASN:HD21 | 1.68 | 0.40 |
| 1:H:91:CYS:SG | 1:H:142:MET:CE | 3.07 | 0.40 |
| 1:A:27:SER:OG | 1:A:28:VAL:HG22 | 2.20 | 0.40 |
| 1:G:56:TYR:HB3 | 1:G:57:PRO:HD3 | 2.03 | 0.40 |
| 1:B:18:ARG:NE | 1:B:197:ASP:OD1 | 2.46 | 0.40 |
| 1:B:119:ILE:O | 1:B:120:TYR:C | 2.59 | 0.40 |
| 1:E:38:GLN:NE2 | 1:E:177:TYR:OH | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:136:LYS:NZ | 2:J:223:HOH:O | 2.54 | 0.40 |
| 1:F:106:TRP:HB3 | 1:F:142:MET:HE2 | 2.03 | 0.40 |
| 1:L:134:PHE:O | 1:L:136:LYS:N | 2.55 | 0.40 |
| 1:B:109:TYR:O | 1:B:110:HIS:CD2 | 2.74 | 0.40 |
| 1:K:168:ALA:HA | 1:K:169:PRO:HD3 | 1.96 | 0.40 |
| 1:F:168:ALA:HA | 1:F:169:PRO:HD3 | 1.93 | 0.40 |
| 1:K:154:THR:HG22 | 1:L:36:THR:CB | 2.52 | 0.40 |
| 1:J:67:MET:CE | 1:J:73:PHE:CD1 | 3.04 | 0.40 |
| 1:K:75:MET:HB2 | 1:K:195:VAL:HG11 | 2.03 | 0.40 |
| 1:A:187:LEU:HD23 | 1:A:208:LEU:CD2 | 2.51 | 0.40 |
| 1:B:25:PHE:HB2 | 1:B:194:ALA:HA | 2.02 | 0.40 |
| 1:A:63:LEU:O | 1:A:67:MET:HG2 | 2.21 | 0.40 |
| 1:F:123:ASP:OD1 | 1:F:136:LYS:HE3 | 2.21 | 0.40 |
| 1:B:204:MET:HE3 | 1:B:205:LEU:HA | 2.02 | 0.40 |
| 1:A:8:TYR:HB2 | 1:A:83:VAL:HG13 | 2.04 | 0.40 |
| 1:D:114:ARG:NH1 | 1:D:114:ARG:HG3 | 2.36 | 0.40 |
| 1:K:185:MET:HA | 1:K:186:PRO:HD3 | 1.97 | 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 | 211/219 (96%) | 203 (96%) | 7 (3%) | 1 (0%) | 34 | 55 |
| 1 | B | 214/219 (98%) | 204 (95%) | 8 (4%) | 2 (1%) | 21 | 37 |
| 1 | C | 211/219 (96%) | 200 (95%) | 8 (4%) | 3 (1%) | 14 | 24 |
| 1 | D | 211/219 (96%) | 196 (93%) | 12 (6%) | 3 (1%) | 14 | 24 |
| 1 | E | 213/219 (97%) | 199 (93%) | 12 (6%) | 2 (1%) | 21 | 37 |
| 1 | F | 210/219 (96%) | 195 (93%) | 14 (7%) | 1 (0%) | 34 | 55 |
| 1 | G | 211/219 (96%) | 196 (93%) | 14 (7%) | 1 (0%) | 34 | 55 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | H | 214/219 (98%) | 204 (95%) | 8 (4%) | 2 (1%) | 21 | 37 |
| 1 | I | 212/219 (97%) | 199 (94%) | 11 (5%) | 2 (1%) | 21 | 37 |
| 1 | J | 209/219 (95%) | 191 (91%) | 16 (8%) | 2 (1%) | 19 | 34 |
| 1 | K | 210/219 (96%) | 195 (93%) | 10 (5%) | 5 (2%) | 7 | 11 |
| 1 | L | 208/219 (95%) | 188 (90%) | 16 (8%) | 4 (2%) | 10 | 16 |
| All | All | 2534/2628 (96%) | 2370 (94%) | 136 (5%) | 28 (1%) | 17 | 31 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 28 | VAL |
| 1 | B | 79 | ASP |
| 1 | D | 164 | ASP |
| 1 | K | 48 | VAL |
| 1 | L | 119 | ILE |
| 1 | B | 28 | VAL |
| 1 | C | 29 | ALA |
| 1 | E | 4 | LYS |
| 1 | E | 29 | ALA |
| 1 | K | 166 | PHE |
| 1 | L | 128 | GLY |
| 1 | C | 50 | LYS |
| 1 | D | 50 | LYS |
| 1 | H | 6 | THR |
| 1 | H | 52 | LYS |
| 1 | K | 29 | ALA |
| 1 | I | 29 | ALA |
| 1 | K | 47 | THR |
| 1 | K | 165 | ASN |
| 1 | D | 180 | GLY |
| 1 | G | 19 | LYS |
| 1 | J | 72 | GLU |
| 1 | F | 198 | GLY |
| 1 | L | 129 | GLU |
| 1 | I | 135 | PRO |
| 1 | J | 13 | ILE |
| 1 | L | 80 | GLY |
| 1 | C | 28 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 189/194 (97%) | 160 (85%) | 29 (15%) | 3 | 6 |
| 1 | B | 192/194 (99%) | 163 (85%) | 29 (15%) | 3 | 6 |
| 1 | C | 189/194 (97%) | 163 (86%) | 26 (14%) | 4 | 8 |
| 1 | D | 189/194 (97%) | 162 (86%) | 27 (14%) | 4 | 7 |
| 1 | E | 192/194 (99%) | 161 (84%) | 31 (16%) | 3 | 5 |
| 1 | F | 189/194 (97%) | 161 (85%) | 28 (15%) | 4 | 7 |
| 1 | G | 189/194 (97%) | 164 (87%) | 25 (13%) | 5 | 9 |
| 1 | H | 191/194 (98%) | 171 (90%) | 20 (10%) | 8 | 16 |
| 1 | I | 191/194 (98%) | 163 (85%) | 28 (15%) | 4 | 7 |
| 1 | J | 189/194 (97%) | 158 (84%) | 31 (16%) | 3 | 5 |
| 1 | K | 190/194 (98%) | 150 (79%) | 40 (21%) | 1 | 2 |
| 1 | L | 188/194 (97%) | 154 (82%) | 34 (18%) | 2 | 3 |
| All | All | 2278/2328 (98%) | 1930 (85%) | 348 (15%) | 3 | 6 |

All (348) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 26 | GLN |
| 1 | A | 28 | VAL |
| 1 | A | 32 | THR |
| 1 | A | 37 | VAL |
| 1 | A | 39 | LEU |
| 1 | A | 45 | LEU |
| 1 | A | 52 | LYS |
| 1 | A | 54 | LYS |
| 1 | A | 81 | GLU |
| 1 | A | 83 | VAL |
| 1 | A | 94 | VAL |
| 1 | A | 97 | GLU |
| 1 | A | 114 | ARG |
| 1 | A | 135 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 136 | LYS |
| 1 | A | 140 | GLU |
| 1 | A | 142 | MET |
| 1 | A | 146 | SER |
| 1 | A | 148 | ASN |
| 1 | A | 154 | THR |
| 1 | A | 160 | VAL |
| 1 | A | 173 | MET |
| 1 | A | 175 | LYS |
| 1 | A | 182 | LYS |
| 1 | A | 189 | ILE |
| 1 | A | 190 | GLN |
| 1 | A | 196 | CYS |
| 1 | A | 204 | MET |
| 1 | A | 211 | TYR |
| 1 | B | 5 | ILE |
| 1 | B | 9 | THR |
| 1 | B | 10 | THR |
| 1 | B | 19 | LYS |
| 1 | B | 28 | VAL |
| 1 | B | 32 | THR |
| 1 | B | 37 | VAL |
| 1 | B | 39 | LEU |
| 1 | B | 45 | LEU |
| 1 | B | 49 | LYS |
| 1 | B | 50 | LYS |
| 1 | B | 83 | VAL |
| 1 | B | 87 | SER |
| 1 | B | 94 | VAL |
| 1 | B | 104 | SER |
| 1 | B | 111 | ASP |
| 1 | B | 114 | ARG |
| 1 | B | 117 | LEU |
| 1 | B | 129 | GLU |
| 1 | B | 140 | GLU |
| 1 | B | 154 | THR |
| 1 | B | 158 | LEU |
| 1 | B | 159 | ASN |
| 1 | B | 160 | VAL |
| 1 | B | 175 | LYS |
| 1 | B | 187 | LEU |
| 1 | B | 189 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 190 | GLN |
| 1 | B | 204 | MET |
| 1 | C | 6 | THR |
| 1 | C | 9 | THR |
| 1 | C | 13 | ILE |
| 1 | C | 23 | GLU |
| 1 | C | 27 | SER |
| 1 | C | 32 | THR |
| 1 | C | 39 | LEU |
| 1 | C | 45 | LEU |
| 1 | C | 50 | LYS |
| 1 | C | 54 | LYS |
| 1 | C | 62 | ILE |
| 1 | C | 111 | ASP |
| 1 | C | 114 | ARG |
| 1 | C | 115 | GLN |
| 1 | C | 117 | LEU |
| 1 | C | 126 | CYS |
| 1 | C | 139 | ILE |
| 1 | C | 154 | THR |
| 1 | C | 155 | SER |
| 1 | C | 158 | LEU |
| 1 | C | 162 | ASN |
| 1 | C | 179 | GLN |
| 1 | C | 182 | LYS |
| 1 | C | 190 | GLN |
| 1 | C | 204 | MET |
| 1 | C | 216 | GLN |
| 1 | D | 8 | TYR |
| 1 | D | 9 | THR |
| 1 | D | 13 | ILE |
| 1 | D | 15 | GLN |
| 1 | D | 19 | LYS |
| 1 | D | 28 | VAL |
| 1 | D | 32 | THR |
| 1 | D | 39 | LEU |
| 1 | D | 45 | LEU |
| 1 | D | 54 | LYS |
| 1 | D | 71 | PRO |
| 1 | D | 77 | MET |
| 1 | D | 81 | GLU |
| 1 | D | 83 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 111 | ASP |
| 1 | D | 114 | ARG |
| 1 | D | 117 | LEU |
| 1 | D | 148 | ASN |
| 1 | D | 152 | SER |
| 1 | D | 154 | THR |
| 1 | D | 155 | SER |
| 1 | D | 160 | VAL |
| 1 | D | 163 | MET |
| 1 | D | 164 | ASP |
| 1 | D | 189 | ILE |
| 1 | D | 190 | GLN |
| 1 | D | 193 | HIS |
| 1 | E | 3 | LYS |
| 1 | E | 4 | LYS |
| 1 | E | 5 | ILE |
| 1 | E | 6 | THR |
| 1 | E | 9 | THR |
| 1 | E | 10 | THR |
| 1 | E | 15 | GLN |
| 1 | E | 19 | LYS |
| 1 | E | 20 | GLU |
| 1 | E | 32 | THR |
| 1 | E | 37 | VAL |
| 1 | E | 39 | LEU |
| 1 | E | 45 | LEU |
| 1 | E | 54 | LYS |
| 1 | E | 81 | GLU |
| 1 | E | 83 | VAL |
| 1 | E | 98 | GLN |
| 1 | E | 108 | GLU |
| 1 | E | 114 | ARG |
| 1 | E | 115 | GLN |
| 1 | E | 117 | LEU |
| 1 | E | 120 | TYR |
| 1 | E | 129 | GLU |
| 1 | E | 136 | LYS |
| 1 | E | 138 | PHE |
| 1 | E | 142 | MET |
| 1 | E | 154 | THR |
| 1 | E | 158 | LEU |
| 1 | E | 187 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 189 | ILE |
| 1 | E | 190 | GLN |
| 1 | F | 9 | THR |
| 1 | F | 12 | ASP |
| 1 | F | 15 | GLN |
| 1 | F | 19 | LYS |
| 1 | F | 32 | THR |
| 1 | F | 37 | VAL |
| 1 | F | 39 | LEU |
| 1 | F | 45 | LEU |
| 1 | F | 50 | LYS |
| 1 | F | 52 | LYS |
| 1 | F | 54 | LYS |
| 1 | F | 62 | ILE |
| 1 | F | 77 | MET |
| 1 | F | 83 | VAL |
| 1 | F | 114 | ARG |
| 1 | F | 115 | GLN |
| 1 | F | 117 | LEU |
| 1 | F | 119 | ILE |
| 1 | F | 121 | SER |
| 1 | F | 136 | LYS |
| 1 | F | 148 | ASN |
| 1 | F | 151 | VAL |
| 1 | F | 157 | ASP |
| 1 | F | 189 | ILE |
| 1 | F | 190 | GLN |
| 1 | F | 204 | MET |
| 1 | F | 212 | CYS |
| 1 | F | 215 | TRP |
| 1 | G | 9 | THR |
| 1 | G | 12 | ASP |
| 1 | G | 15 | GLN |
| 1 | G | 32 | THR |
| 1 | G | 35 | GLN |
| 1 | G | 39 | LEU |
| 1 | G | 45 | LEU |
| 1 | G | 48 | VAL |
| 1 | G | 50 | LYS |
| 1 | G | 52 | LYS |
| 1 | G | 54 | LYS |
| 1 | G | 67 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 78 | LYS |
| 1 | G | 111 | ASP |
| 1 | G | 115 | GLN |
| 1 | G | 119 | ILE |
| 1 | G | 146 | SER |
| 1 | G | 148 | ASN |
| 1 | G | 151 | VAL |
| 1 | G | 154 | THR |
| 1 | G | 158 | LEU |
| 1 | G | 160 | VAL |
| 1 | G | 181 | ASP |
| 1 | G | 190 | GLN |
| 1 | G | 204 | MET |
| 1 | H | 4 | LYS |
| 1 | H | 23 | GLU |
| 1 | H | 32 | THR |
| 1 | H | 37 | VAL |
| 1 | H | 39 | LEU |
| 1 | H | 45 | LEU |
| 1 | H | 50 | LYS |
| 1 | H | 52 | LYS |
| 1 | H | 54 | LYS |
| 1 | H | 62 | ILE |
| 1 | H | 83 | VAL |
| 1 | H | 87 | SER |
| 1 | H | 122 | GLN |
| 1 | H | 129 | GLU |
| 1 | H | 157 | ASP |
| 1 | H | 158 | LEU |
| 1 | H | 160 | VAL |
| 1 | H | 181 | ASP |
| 1 | H | 190 | GLN |
| 1 | H | 212 | CYS |
| 1 | I | 4 | LYS |
| 1 | I | 10 | THR |
| 1 | I | 14 | SER |
| 1 | I | 28 | VAL |
| 1 | I | 32 | THR |
| 1 | I | 39 | LEU |
| 1 | I | 45 | LEU |
| 1 | I | 46 | LYS |
| 1 | I | 52 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 54 | LYS |
| 1 | I | 62 | ILE |
| 1 | I | 81 | GLU |
| 1 | I | 83 | VAL |
| 1 | I | 97 | GLU |
| 1 | I | 105 | LEU |
| 1 | I | 112 | ASP |
| 1 | I | 114 | ARG |
| 1 | I | 115 | GLN |
| 1 | I | 117 | LEU |
| 1 | I | 126 | CYS |
| 1 | I | 136 | LYS |
| 1 | I | 139 | ILE |
| 1 | I | 146 | SER |
| 1 | I | 154 | THR |
| 1 | I | 157 | ASP |
| 1 | I | 158 | LEU |
| 1 | I | 160 | VAL |
| 1 | I | 190 | GLN |
| 1 | J | 9 | THR |
| 1 | J | 18 | ARG |
| 1 | J | 28 | VAL |
| 1 | J | 32 | THR |
| 1 | J | 35 | GLN |
| 1 | J | 39 | LEU |
| 1 | J | 45 | LEU |
| 1 | J | 50 | LYS |
| 1 | J | 56 | TYR |
| 1 | J | 67 | MET |
| 1 | J | 78 | LYS |
| 1 | J | 83 | VAL |
| 1 | J | 87 | SER |
| 1 | J | 94 | VAL |
| 1 | J | 98 | GLN |
| 1 | J | 107 | SER |
| 1 | J | 111 | ASP |
| 1 | J | 117 | LEU |
| 1 | J | 122 | GLN |
| 1 | J | 129 | GLU |
| 1 | J | 131 | LEU |
| 1 | J | 138 | PHE |
| 1 | J | 152 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 157 | ASP |
| 1 | J | 158 | LEU |
| 1 | J | 175 | LYS |
| 1 | J | 178 | THR |
| 1 | J | 181 | ASP |
| 1 | J | 182 | LYS |
| 1 | J | 190 | GLN |
| 1 | J | 215 | TRP |
| 1 | K | 4 | LYS |
| 1 | K | 9 | THR |
| 1 | K | 10 | THR |
| 1 | K | 12 | ASP |
| 1 | K | 14 | SER |
| 1 | K | 15 | GLN |
| 1 | K | 17 | HIS |
| 1 | K | 28 | VAL |
| 1 | K | 32 | THR |
| 1 | K | 37 | VAL |
| 1 | K | 39 | LEU |
| 1 | K | 45 | LEU |
| 1 | K | 46 | LYS |
| 1 | K | 52 | LYS |
| 1 | K | 54 | LYS |
| 1 | K | 77 | MET |
| 1 | K | 78 | LYS |
| 1 | K | 83 | VAL |
| 1 | K | 103 | SER |
| 1 | K | 105 | LEU |
| 1 | K | 108 | GLU |
| 1 | K | 114 | ARG |
| 1 | K | 117 | LEU |
| 1 | K | 122 | GLN |
| 1 | K | 126 | CYS |
| 1 | K | 136 | LYS |
| 1 | K | 140 | GLU |
| 1 | K | 142 | MET |
| 1 | K | 146 | SER |
| 1 | K | 151 | VAL |
| 1 | K | 154 | THR |
| 1 | K | 158 | LEU |
| 1 | K | 160 | VAL |
| 1 | K | 179 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 181 | ASP |
| 1 | K | 187 | LEU |
| 1 | K | 190 | GLN |
| 1 | K | 203 | ARG |
| 1 | K | 204 | MET |
| 1 | K | 210 | GLN |
| 1 | L | 6 | THR |
| 1 | L | 10 | THR |
| 1 | L | 15 | GLN |
| 1 | L | 19 | LYS |
| 1 | L | 27 | SER |
| 1 | L | 39 | LEU |
| 1 | L | 50 | LYS |
| 1 | L | 52 | LYS |
| 1 | L | 54 | LYS |
| 1 | L | 56 | TYR |
| 1 | L | 77 | MET |
| 1 | L | 78 | LYS |
| 1 | L | 79 | ASP |
| 1 | L | 83 | VAL |
| 1 | L | 94 | VAL |
| 1 | L | 97 | GLU |
| 1 | L | 100 | GLU |
| 1 | L | 104 | SER |
| 1 | L | 105 | LEU |
| 1 | L | 111 | ASP |
| 1 | L | 114 | ARG |
| 1 | L | 117 | LEU |
| 1 | L | 122 | GLN |
| 1 | L | 129 | GLU |
| 1 | L | 136 | LYS |
| 1 | L | 146 | SER |
| 1 | L | 151 | VAL |
| 1 | L | 154 | THR |
| 1 | L | 158 | LEU |
| 1 | L | 182 | LYS |
| 1 | L | 190 | GLN |
| 1 | L | 204 | MET |
| 1 | L | 210 | GLN |
| 1 | L | 214 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 26 | GLN |
| 1 | A | 30 | GLN |
| 1 | A | 38 | GLN |
| 1 | A | 148 | ASN |
| 1 | A | 159 | ASN |
| 1 | B | 26 | GLN |
| 1 | B | 34 | ASN |
| 1 | B | 38 | GLN |
| 1 | B | 159 | ASN |
| 1 | C | 26 | GLN |
| 1 | C | 30 | GLN |
| 1 | C | 51 | ASN |
| 1 | C | 110 | HIS |
| 1 | C | 159 | ASN |
| 1 | C | 190 | GLN |
| 1 | C | 216 | GLN |
| 1 | D | 26 | GLN |
| 1 | D | 30 | GLN |
| 1 | D | 34 | ASN |
| 1 | D | 38 | GLN |
| 1 | D | 110 | HIS |
| 1 | D | 148 | ASN |
| 1 | D | 159 | ASN |
| 1 | D | 190 | GLN |
| 1 | E | 26 | GLN |
| 1 | E | 30 | GLN |
| 1 | E | 34 | ASN |
| 1 | E | 159 | ASN |
| 1 | E | 190 | GLN |
| 1 | F | 26 | GLN |
| 1 | F | 30 | GLN |
| 1 | F | 34 | ASN |
| 1 | F | 38 | GLN |
| 1 | F | 110 | HIS |
| 1 | F | 148 | ASN |
| 1 | F | 159 | ASN |
| 1 | F | 190 | GLN |
| 1 | G | 15 | GLN |
| 1 | G | 26 | GLN |
| 1 | G | 30 | GLN |
| 1 | G | 38 | GLN |
| 1 | G | 53 | HIS |
| 1 | G | 148 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 159 | ASN |
| 1 | G | 190 | GLN |
| 1 | H | 26 | GLN |
| 1 | H | 30 | GLN |
| 1 | H | 34 | ASN |
| 1 | H | 38 | GLN |
| 1 | H | 159 | ASN |
| 1 | I | 26 | GLN |
| 1 | I | 30 | GLN |
| 1 | I | 34 | ASN |
| 1 | I | 38 | GLN |
| 1 | I | 51 | ASN |
| 1 | I | 122 | GLN |
| 1 | I | 141 | ASN |
| 1 | I | 148 | ASN |
| 1 | I | 159 | ASN |
| 1 | I | 190 | GLN |
| 1 | J | 30 | GLN |
| 1 | J | 34 | ASN |
| 1 | J | 98 | GLN |
| 1 | J | 148 | ASN |
| 1 | J | 159 | ASN |
| 1 | J | 190 | GLN |
| 1 | K | 17 | HIS |
| 1 | K | 30 | GLN |
| 1 | K | 38 | GLN |
| 1 | K | 122 | GLN |
| 1 | K | 159 | ASN |
| 1 | K | 179 | GLN |
| 1 | K | 190 | GLN |
| 1 | L | 26 | GLN |
| 1 | L | 30 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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 | 213/219 (97%) | -0.02 | 1 (0%) | 91 | 92 | 21, 34, 50, 57 | 0 |
| 1 | B | 216/219 (98%) | -0.05 | 2 (0%) | 85 | 88 | 23, 39, 59, 71 | 0 |
| 1 | C | 213/219 (97%) | 0.09 | 5 (2%) | 64 | 67 | 24, 38, 62, 76 | 0 |
| 1 | D | 213/219 (97%) | 0.12 | 3 (1%) | 78 | 80 | 27, 42, 60, 80 | 0 |
| 1 | E | 215/219 (98%) | 0.13 | 4 (1%) | 70 | 73 | 30, 45, 64, 84 | 0 |
| 1 | F | 212/219 (96%) | 0.17 | 5 (2%) | 62 | 66 | 29, 45, 62, 74 | 0 |
| 1 | G | 213/219 (97%) | 0.19 | 6 (2%) | 56 | 61 | 31, 41, 59, 69 | 0 |
| 1 | H | 216/219 (98%) | 0.14 | 10 (4%) | 36 | 41 | 19, 37, 52, 72 | 0 |
| 1 | I | 214/219 (97%) | 0.25 | 5 (2%) | 64 | 67 | 32, 44, 62, 72 | 0 |
| 1 | J | 211/219 (96%) | 0.72 | 31 (14%) | 3 | 3 | 38, 55, 77, 81 | 0 |
| 1 | K | 212/219 (96%) | 0.70 | 24 (11%) | 7 | 7 | 43, 59, 76, 88 | 0 |
| 1 | L | 210/219 (95%) | 0.82 | 33 (15%) | 3 | 2 | 40, 55, 74, 84 | 0 |
| All | All | 2558/2628 (97%) | 0.27 | 129 (5%) | 32 | 37 | 19, 44, 69, 88 | 0 |

All (129) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 124 | VAL | 6.3 |
| 1 | J | 125 | ALA | 5.8 |
| 1 | H | 5 | ILE | 5.0 |
| 1 | J | 6 | THR | 4.8 |
| 1 | L | 6 | THR | 4.8 |
| 1 | J | 46 | LYS | 4.1 |
| 1 | K | 158 | LEU | 4.1 |
| 1 | G | 15 | GLN | 4.0 |
| 1 | L | 15 | GLN | 3.9 |
| 1 | K | 215 | TRP | 3.9 |
| 1 | L | 115 | GLN | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 122 | GLN | 3.8 |
| 1 | H | 218 | GLY | 3.8 |
| 1 | F | 173 | MET | 3.7 |
| 1 | K | 114 | ARG | 3.7 |
| 1 | K | 98 | GLN | 3.7 |
| 1 | L | 125 | ALA | 3.6 |
| 1 | L | 113 | PHE | 3.6 |
| 1 | L | 181 | ASP | 3.6 |
| 1 | L | 131 | LEU | 3.5 |
| 1 | L | 118 | HIS | 3.4 |
| 1 | J | 43 | ALA | 3.4 |
| 1 | J | 181 | ASP | 3.3 |
| 1 | D | 46 | LYS | 3.3 |
| 1 | K | 50 | LYS | 3.3 |
| 1 | F | 77 | MET | 3.3 |
| 1 | L | 114 | ARG | 3.3 |
| 1 | L | 112 | ASP | 3.2 |
| 1 | I | 124 | VAL | 3.2 |
| 1 | H | 219 | ALA | 3.1 |
| 1 | G | 6 | THR | 3.1 |
| 1 | L | 122 | GLN | 3.1 |
| 1 | G | 98 | GLN | 3.0 |
| 1 | F | 211 | TYR | 2.9 |
| 1 | C | 118 | HIS | 2.9 |
| 1 | L | 71 | PRO | 2.9 |
| 1 | L | 23 | GLU | 2.8 |
| 1 | J | 50 | LYS | 2.8 |
| 1 | J | 14 | SER | 2.8 |
| 1 | K | 46 | LYS | 2.8 |
| 1 | J | 156 | PHE | 2.8 |
| 1 | L | 188 | ALA | 2.8 |
| 1 | K | 22 | PHE | 2.7 |
| 1 | L | 14 | SER | 2.7 |
| 1 | H | 6 | THR | 2.7 |
| 1 | L | 89 | HIS | 2.7 |
| 1 | K | 173 | MET | 2.7 |
| 1 | J | 15 | GLN | 2.7 |
| 1 | J | 180 | GLY | 2.6 |
| 1 | J | 34 | ASN | 2.6 |
| 1 | J | 97 | GLU | 2.6 |
| 1 | L | 77 | MET | 2.6 |
| 1 | I | 157 | ASP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | L | 179 | GLN | 2.6 |
| 1 | L | 45 | LEU | 2.6 |
| 1 | F | 181 | ASP | 2.6 |
| 1 | E | 155 | SER | 2.5 |
| 1 | K | 15 | GLN | 2.5 |
| 1 | H | 154 | THR | 2.5 |
| 1 | J | 51 | ASN | 2.5 |
| 1 | E | 12 | ASP | 2.5 |
| 1 | A | 181 | ASP | 2.5 |
| 1 | J | 138 | PHE | 2.5 |
| 1 | J | 99 | THR | 2.5 |
| 1 | J | 118 | HIS | 2.4 |
| 1 | L | 189 | ILE | 2.4 |
| 1 | J | 188 | ALA | 2.4 |
| 1 | J | 95 | PHE | 2.4 |
| 1 | J | 98 | GLN | 2.4 |
| 1 | K | 42 | THR | 2.4 |
| 1 | K | 180 | GLY | 2.4 |
| 1 | L | 130 | ASN | 2.4 |
| 1 | L | 180 | GLY | 2.4 |
| 1 | K | 36 | THR | 2.4 |
| 1 | K | 17 | HIS | 2.4 |
| 1 | K | 211 | TYR | 2.4 |
| 1 | L | 50 | LYS | 2.4 |
| 1 | B | 216 | GLN | 2.4 |
| 1 | H | 155 | SER | 2.4 |
| 1 | J | 130 | ASN | 2.3 |
| 1 | D | 217 | GLY | 2.3 |
| 1 | C | 115 | GLN | 2.3 |
| 1 | K | 44 | PHE | 2.3 |
| 1 | K | 110 | HIS | 2.3 |
| 1 | J | 13 | ILE | 2.3 |
| 1 | J | 121 | SER | 2.3 |
| 1 | D | 98 | GLN | 2.3 |
| 1 | K | 34 | ASN | 2.3 |
| 1 | K | 12 | ASP | 2.3 |
| 1 | E | 173 | MET | 2.3 |
| 1 | J | 126 | CYS | 2.3 |
| 1 | K | 127 | TYR | 2.2 |
| 1 | L | 172 | THR | 2.2 |
| 1 | L | 8 | TYR | 2.2 |
| 1 | L | 83 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 15 | GLN | 2.2 |
| 1 | K | 81 | GLU | 2.2 |
| 1 | J | 127 | TYR | 2.2 |
| 1 | C | 52 | LYS | 2.2 |
| 1 | G | 157 | ASP | 2.2 |
| 1 | J | 201 | VAL | 2.2 |
| 1 | K | 48 | VAL | 2.2 |
| 1 | F | 156 | PHE | 2.2 |
| 1 | K | 130 | ASN | 2.2 |
| 1 | L | 7 | GLY | 2.1 |
| 1 | L | 127 | TYR | 2.1 |
| 1 | K | 159 | ASN | 2.1 |
| 1 | L | 157 | ASP | 2.1 |
| 1 | J | 36 | THR | 2.1 |
| 1 | G | 173 | MET | 2.1 |
| 1 | B | 155 | SER | 2.1 |
| 1 | I | 52 | LYS | 2.1 |
| 1 | L | 11 | VAL | 2.1 |
| 1 | L | 123 | ASP | 2.1 |
| 1 | G | 188 | ALA | 2.1 |
| 1 | I | 129 | GLU | 2.1 |
| 1 | I | 155 | SER | 2.1 |
| 1 | J | 117 | LEU | 2.0 |
| 1 | K | 55 | PHE | 2.0 |
| 1 | C | 181 | ASP | 2.0 |
| 1 | J | 179 | GLN | 2.0 |
| 1 | J | 131 | LEU | 2.0 |
| 1 | E | 36 | THR | 2.0 |
| 1 | H | 156 | PHE | 2.0 |
| 1 | H | 4 | LYS | 2.0 |
| 1 | H | 34 | ASN | 2.0 |
| 1 | C | 180 | GLY | 2.0 |
| 1 | L | 135 | PRO | 2.0 |
| 1 | L | 34 | ASN | 2.0 |

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.