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

Aug 15, 2023 – 05:32 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1TWC |
| Title | : | RNA polymerase II complexed with GTP |
| Authors | : | Westover, K.D.; Bushnell, D.A.; Kornberg, R.D. |
| Deposited on | : | 2004-06-30 |
| Resolution | : | 3.00 Å(reported) |

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

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

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

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

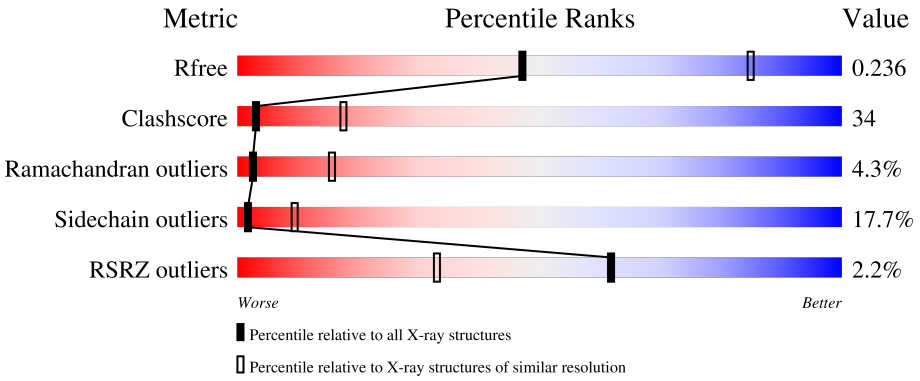
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1733 | .%<br>21% 32% 19% 6% 22% |
| 2 | B | 1224 | 3%<br>22% 39% 21% 7% 11% |
| 3 | C | 318 | .%<br>18% 36% 22% 7% 16% |
| 4 | E | 215 | 2%<br>20% 39% 31% 11% |
| 5 | F | 155 | 13% 22% 15% . 46% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | H | 146 | 3% 8% 31% 29% 23% 9% |
| 7 | I | 122 | % 12% 48% 30% 9% |
| 8 | J | 70 | 24% 43% 19% 6% 9% |
| 9 | K | 120 | 23% 39% 22% 10% 5% |
| 10 | L | 70 | 6% 19% 24% 20% 34% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 13 | GTP | B | 3008 | X | - | - | - |

# 2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 27772 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 DNA-directed RNA polymerase II largest subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1351 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10625 | 6704 | 1844 | 2019 | 58 | | | |

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 1091 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8690 | 5511 | 1516 | 1610 | 53 | | | |

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 266 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2095 | 1317 | 348 | 417 | 13 | | | |

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | E | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1760 | 1116 | 310 | 322 | 12 | | | |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | F | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 670 | 428 | 114 | 125 | 3 | | | |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | H | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1068 | 673 | 180 | 211 | 4 | | | |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | I | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 990 | 610 | 181 | 188 | 11 | | | |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | J | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 334 | 92 | 93 | 6 | | | |

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | K | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 919 | 590 | 156 | 171 | 2 | | | |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | L | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 364 | 224 | 72 | 64 | 4 | | | |

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 11 | A | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 11 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | C | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | I | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 11 | J | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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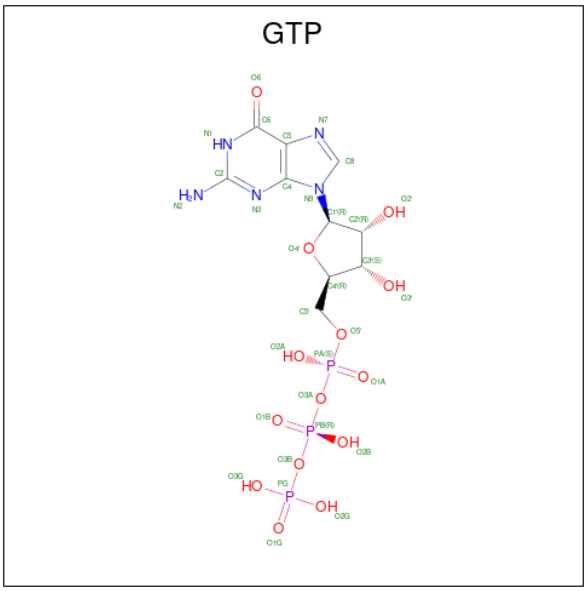
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 11 | L | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 12 | A | 2 | Total Mn<br>2 2 | 0 | 0 |

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 13 | B | 1 | Total C N O P<br>32 10 5 14 3 | 0 | 0 |

- Molecule 14 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 14 | A | 11 | Total O<br>11 11 | 0 | 0 |
| 14 | B | 11 | Total O<br>11 11 | 0 | 0 |
| 14 | F | 1 | Total O<br>1 1 | 0 | 0 |

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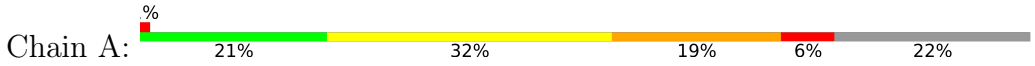
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 14 | L | 1 | Total O<br>1 1 | 0 | 0 |

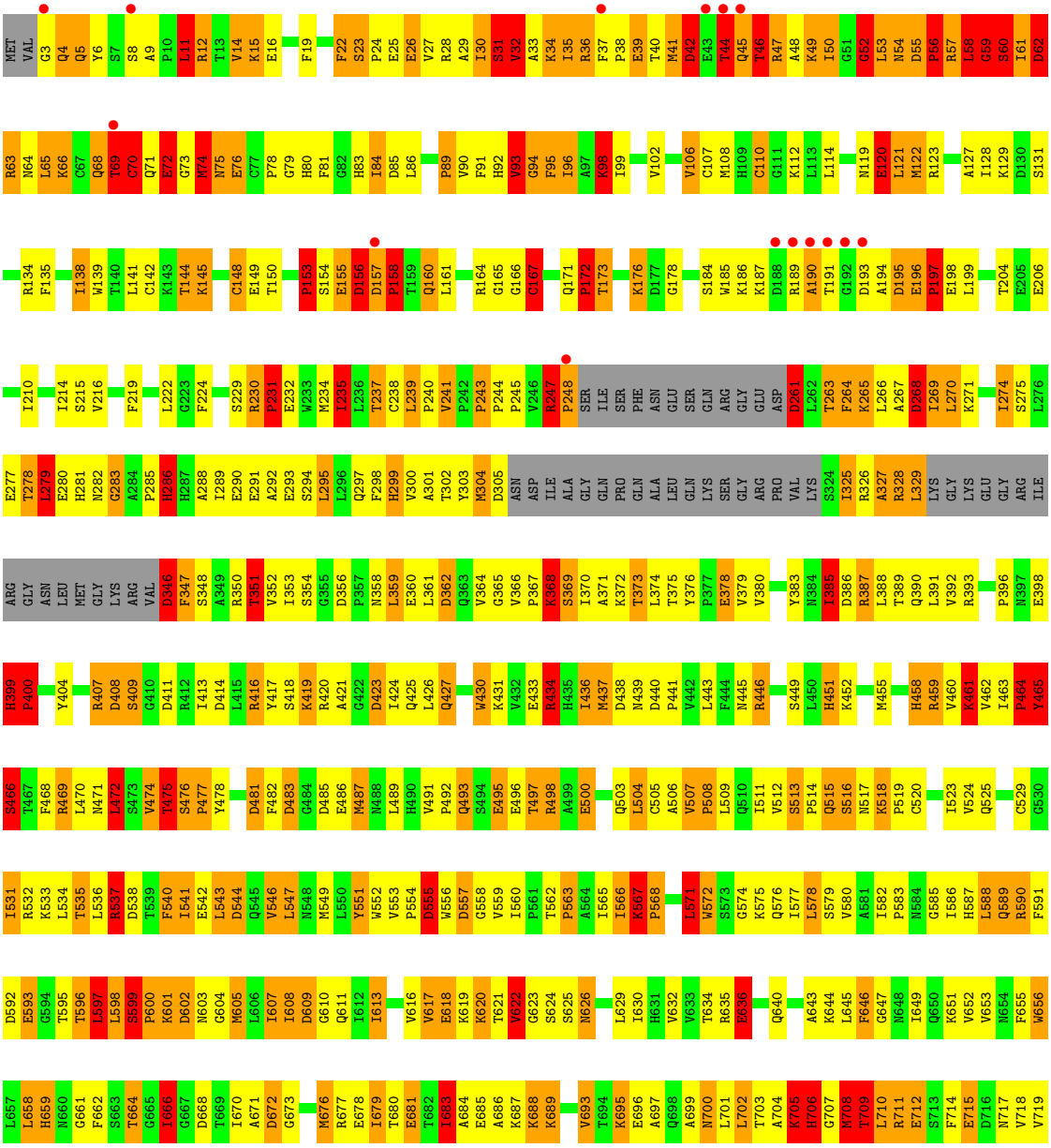
# 3 Residue-property plots (i)

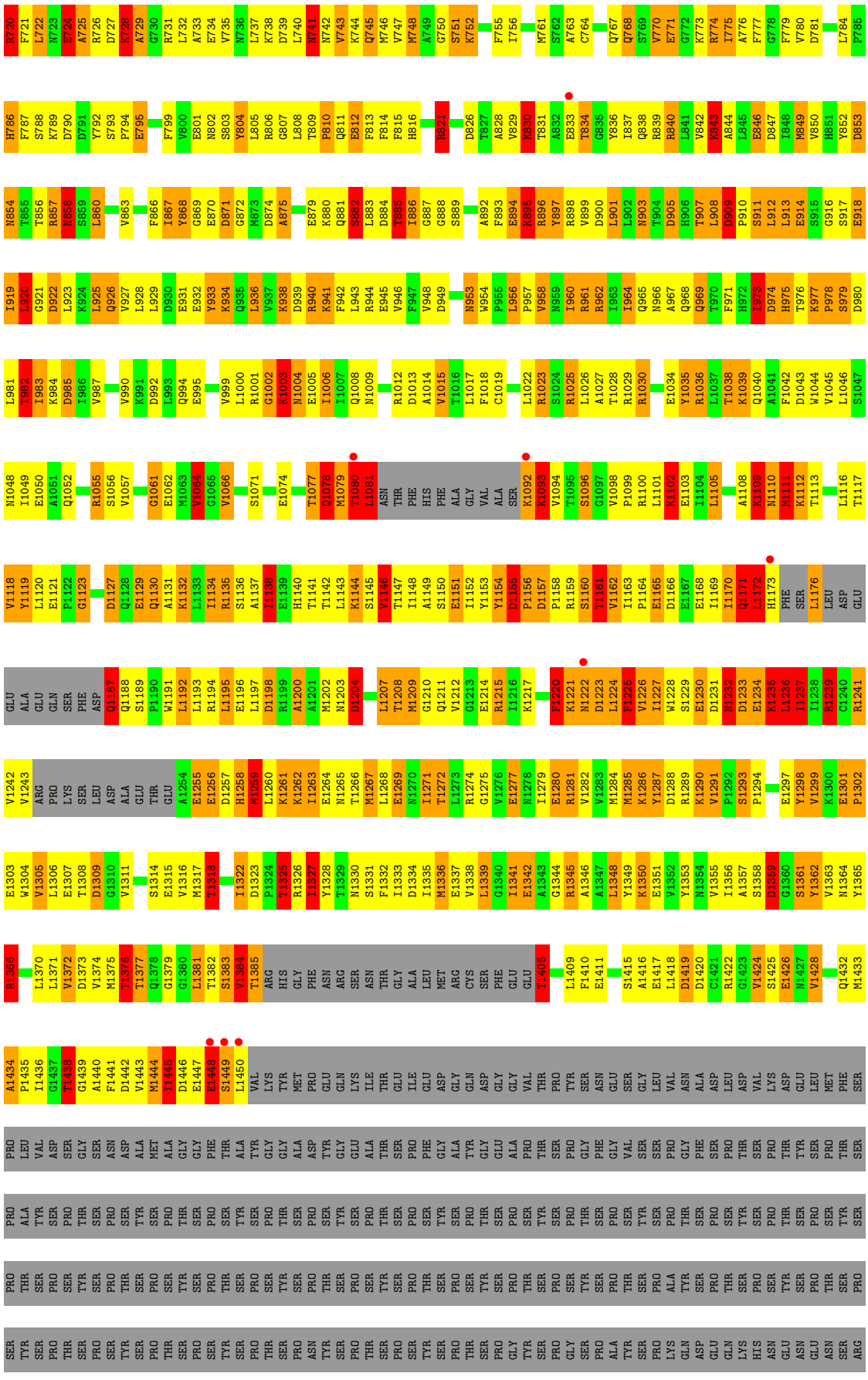
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II largest subunit

Chain A:

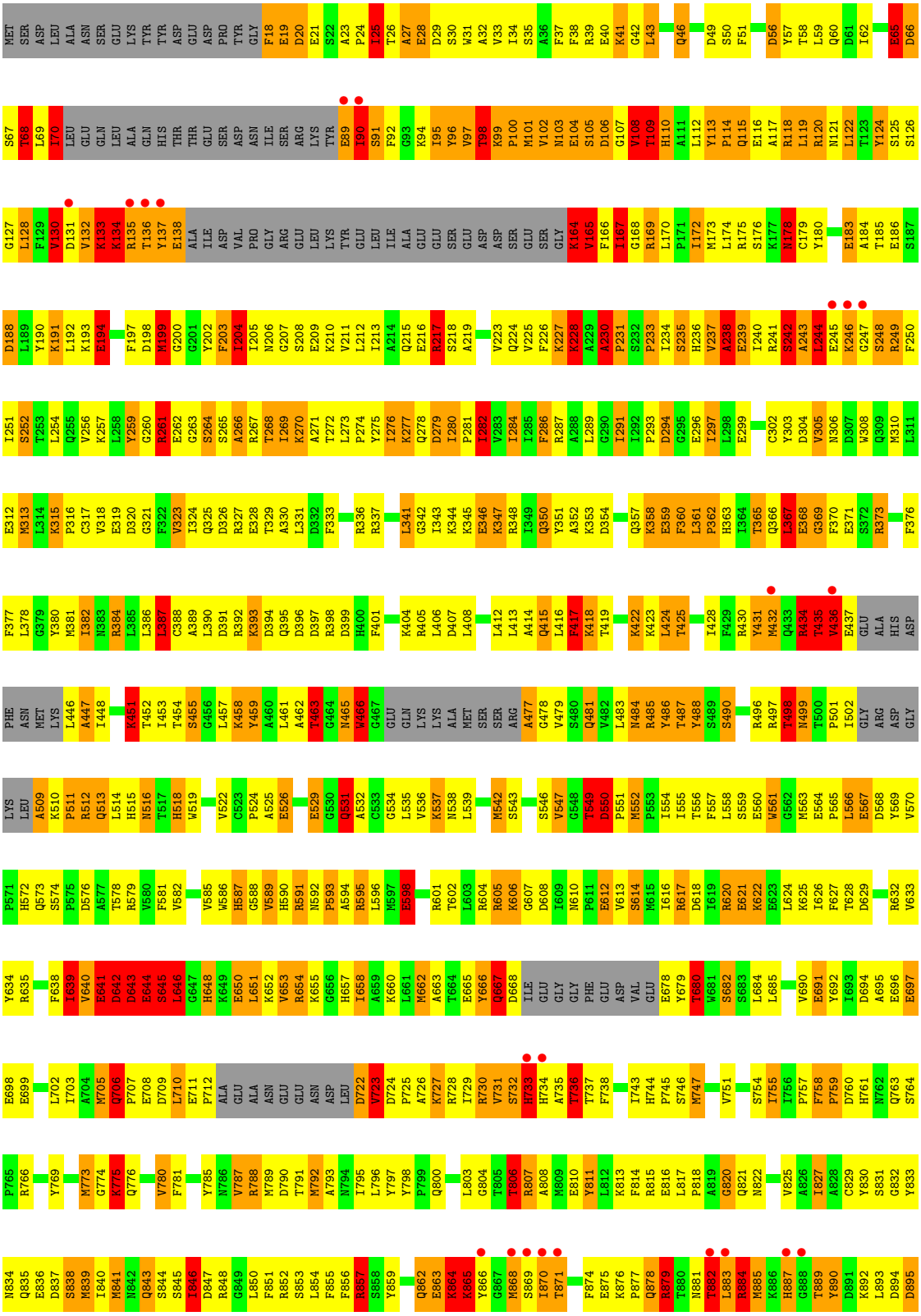


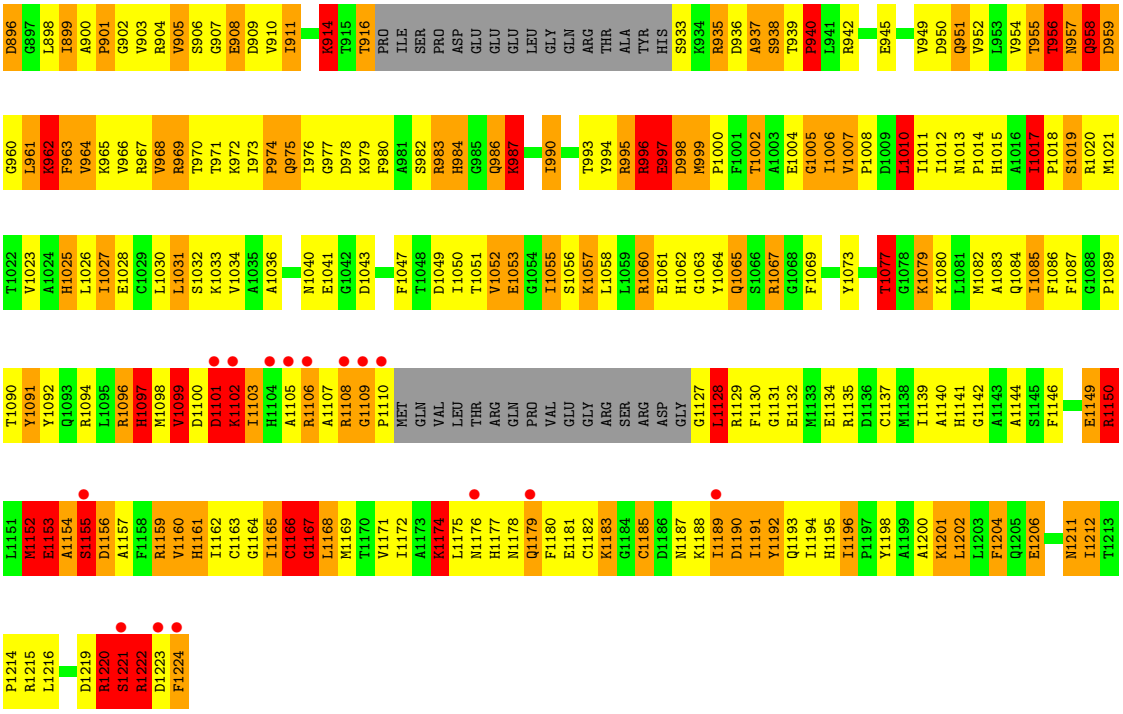





• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

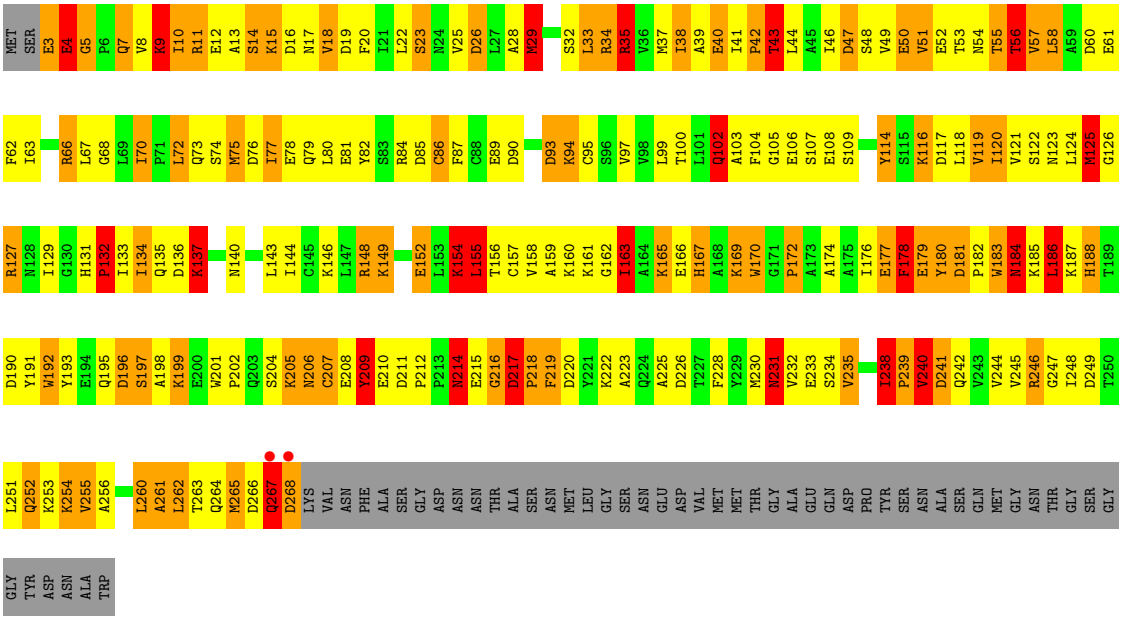
Chain B:



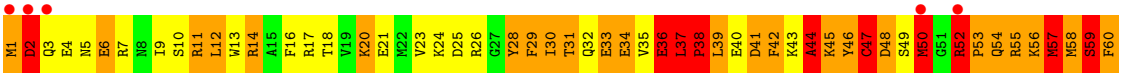
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

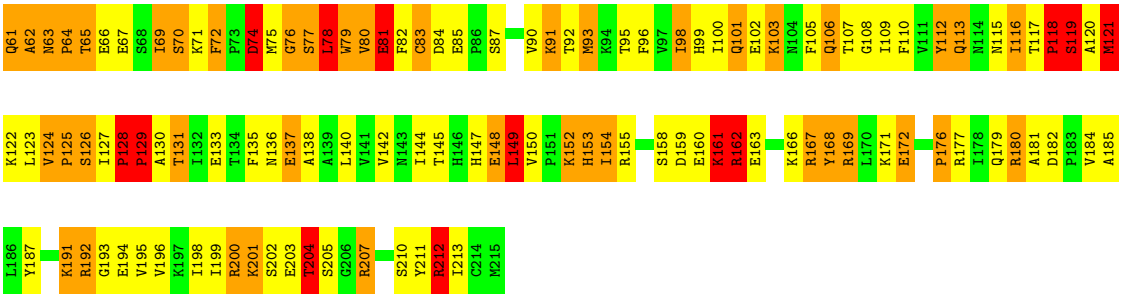
Chain C:

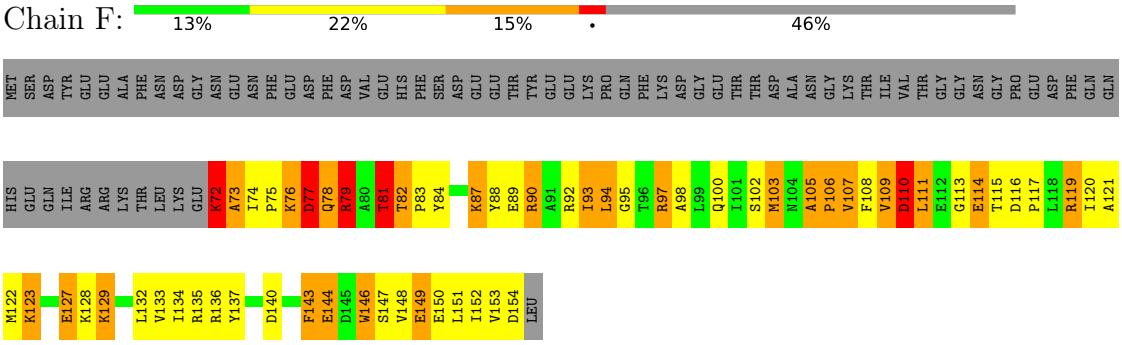
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:

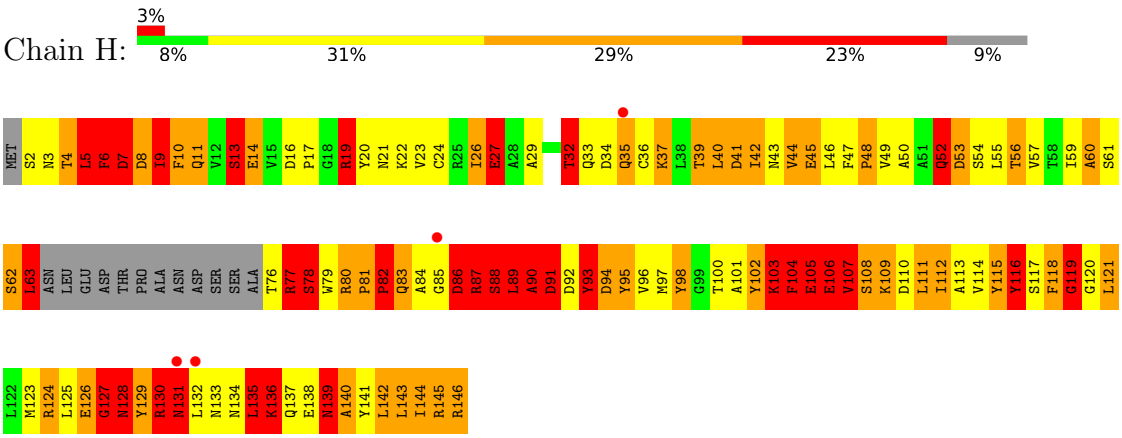





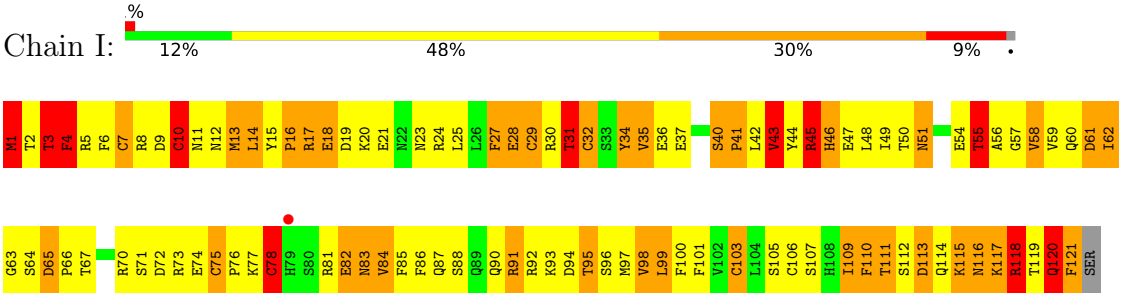
• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



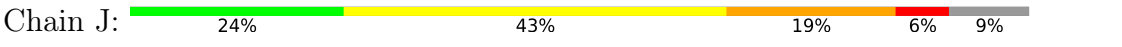

• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

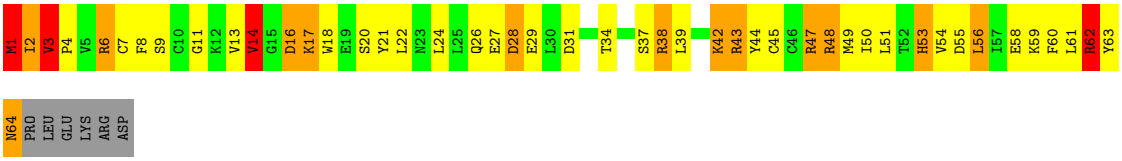



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

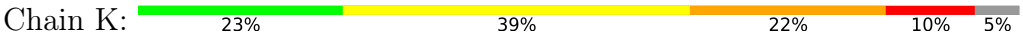


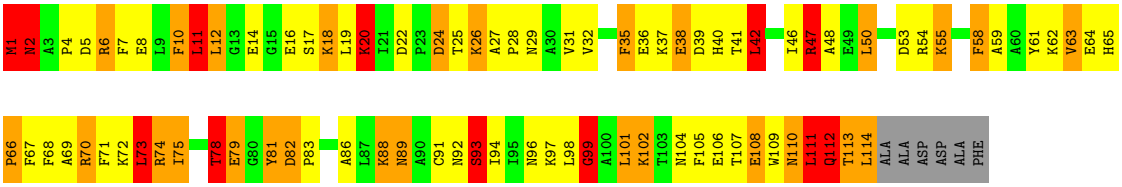

• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



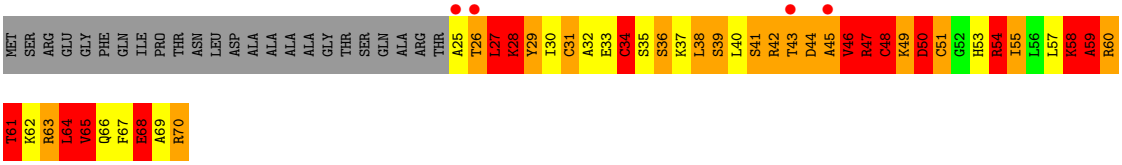



• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide




• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | I 2 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 123.23Å 223.61Å 374.61Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 3.00<br>39.76 – 2.90 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (40.00-3.00)<br>91.6 (39.76-2.90) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.19 (at 2.90Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.234 , 0.255<br>0.198 , 0.236 | Depositor<br>DCC |
| $R_{free}$ test set | 3424 reflections (2.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 56.3 | Xtriage |
| Anisotropy | 0.418 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 55.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 27772 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 56.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 3.17 | 1078/10811 (10.0%) | 2.44 | 610/14626 (4.2%) |
| 2 | B | 3.28 | 922/8860 (10.4%) | 2.47 | 497/11945 (4.2%) |
| 3 | C | 3.33 | 245/2133 (11.5%) | 2.58 | 122/2891 (4.2%) |
| 4 | E | 3.29 | 172/1796 (9.6%) | 2.31 | 92/2416 (3.8%) |
| 5 | F | 2.94 | 59/682 (8.7%) | 2.24 | 31/922 (3.4%) |
| 6 | H | 3.24 | 126/1086 (11.6%) | 2.37 | 58/1470 (3.9%) |
| 7 | I | 3.57 | 138/1009 (13.7%) | 2.46 | 75/1357 (5.5%) |
| 8 | J | 2.92 | 47/533 (8.8%) | 2.82 | 46/715 (6.4%) |
| 9 | K | 3.18 | 100/937 (10.7%) | 2.62 | 58/1265 (4.6%) |
| 10 | L | 3.58 | 46/366 (12.6%) | 2.81 | 36/485 (7.4%) |
| All | All | 3.24 | 2933/28213 (10.4%) | 2.46 | 1625/38092 (4.3%) |

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 | 28 |
| 2 | B | 0 | 32 |
| 3 | C | 0 | 13 |
| 4 | E | 1 | 7 |
| 6 | H | 0 | 13 |
| 7 | I | 0 | 3 |
| 9 | K | 0 | 2 |
| 10 | L | 0 | 4 |
| All | All | 1 | 102 |

All (2933) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 771 | GLU | CD-OE2 | 27.21 | 1.55 | 1.25 |
| 2 | B | 552 | MET | CG-SD | 25.82 | 2.48 | 1.81 |
| 1 | A | 728 | LYS | CD-CE | 23.14 | 2.09 | 1.51 |
| 10 | L | 68 | GLU | CG-CD | 22.53 | 1.85 | 1.51 |
| 1 | A | 1005 | GLU | CD-OE1 | 21.89 | 1.49 | 1.25 |
| 1 | A | 496 | GLU | CD-OE1 | 20.92 | 1.48 | 1.25 |
| 3 | C | 165 | LYS | CE-NZ | 20.84 | 2.01 | 1.49 |
| 2 | B | 1150 | ARG | CZ-NH1 | 20.35 | 1.59 | 1.33 |
| 4 | E | 162 | ARG | CG-CD | 19.89 | 2.01 | 1.51 |
| 2 | B | 529 | GLU | CD-OE2 | 19.69 | 1.47 | 1.25 |
| 2 | B | 194 | GLU | CD-OE1 | 19.69 | 1.47 | 1.25 |
| 1 | A | 1277 | GLU | CD-OE2 | 18.98 | 1.46 | 1.25 |
| 1 | A | 618 | GLU | CD-OE2 | 18.85 | 1.46 | 1.25 |
| 3 | C | 154 | LYS | CD-CE | 18.81 | 1.98 | 1.51 |
| 6 | H | 19 | ARG | CG-CD | 18.75 | 1.98 | 1.51 |
| 3 | C | 166 | GLU | CD-OE2 | 18.74 | 1.46 | 1.25 |
| 1 | A | 1015 | VAL | CB-CG2 | -18.32 | 1.14 | 1.52 |
| 2 | B | 299 | GLU | CD-OE1 | 18.25 | 1.45 | 1.25 |
| 2 | B | 641 | GLU | CG-CD | 18.22 | 1.79 | 1.51 |
| 7 | I | 28 | GLU | CD-OE2 | 17.97 | 1.45 | 1.25 |
| 1 | A | 16 | GLU | CD-OE1 | 17.84 | 1.45 | 1.25 |
| 2 | B | 1150 | ARG | CZ-NH2 | 17.75 | 1.56 | 1.33 |
| 1 | A | 466 | SER | CB-OG | -17.74 | 1.19 | 1.42 |
| 7 | I | 10 | CYS | CB-SG | -17.56 | 1.52 | 1.82 |
| 4 | E | 162 | ARG | NE-CZ | 17.53 | 1.55 | 1.33 |
| 1 | A | 938 | LYS | CD-CE | 17.52 | 1.95 | 1.51 |
| 2 | B | 945 | GLU | CD-OE1 | 17.36 | 1.44 | 1.25 |
| 9 | K | 108 | GLU | CD-OE2 | 17.29 | 1.44 | 1.25 |
| 2 | B | 963 | PHE | CE1-CZ | 17.12 | 1.69 | 1.37 |
| 2 | B | 346 | GLU | CG-CD | 17.05 | 1.77 | 1.51 |
| 3 | C | 50 | GLU | CG-CD | 17.00 | 1.77 | 1.51 |
| 1 | A | 801 | GLU | CD-OE1 | 16.93 | 1.44 | 1.25 |
| 1 | A | 1135 | ARG | CZ-NH2 | 16.91 | 1.55 | 1.33 |
| 1 | A | 1232 | ASN | CB-CG | 16.88 | 1.89 | 1.51 |
| 1 | A | 801 | GLU | CD-OE2 | 16.77 | 1.44 | 1.25 |
| 2 | B | 1154 | ALA | CA-CB | 16.70 | 1.87 | 1.52 |
| 1 | A | 346 | ASP | CB-CG | 16.61 | 1.86 | 1.51 |
| 1 | A | 1280 | GLU | CD-OE2 | 16.52 | 1.43 | 1.25 |
| 4 | E | 50 | MET | SD-CE | 16.51 | 2.70 | 1.77 |
| 1 | A | 1349 | TYR | CG-CD2 | -16.50 | 1.17 | 1.39 |
| 2 | B | 239 | GLU | CD-OE2 | 16.45 | 1.43 | 1.25 |
| 7 | I | 37 | GLU | CD-OE1 | 16.34 | 1.43 | 1.25 |
| 2 | B | 598 | GLU | CG-CD | 16.27 | 1.76 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | L | 68 | GLU | CD-OE1 | 16.26 | 1.43 | 1.25 |
| 2 | B | 650 | GLU | CD-OE2 | 16.21 | 1.43 | 1.25 |
| 2 | B | 531 | GLN | CG-CD | 16.18 | 1.88 | 1.51 |
| 2 | B | 275 | TYR | CE2-CZ | -16.08 | 1.17 | 1.38 |
| 1 | A | 795 | GLU | CG-CD | 16.08 | 1.76 | 1.51 |
| 7 | I | 55 | THR | CB-CG2 | 15.96 | 2.05 | 1.52 |
| 7 | I | 17 | ARG | CG-CD | 15.94 | 1.91 | 1.51 |
| 1 | A | 1196 | GLU | CD-OE1 | 15.93 | 1.43 | 1.25 |
| 1 | A | 16 | GLU | CD-OE2 | 15.82 | 1.43 | 1.25 |
| 1 | A | 734 | GLU | CD-OE2 | 15.79 | 1.43 | 1.25 |
| 2 | B | 477 | ALA | CA-CB | 15.76 | 1.85 | 1.52 |
| 1 | A | 496 | GLU | CD-OE2 | 15.71 | 1.43 | 1.25 |
| 1 | A | 751 | SER | CB-OG | 15.49 | 1.62 | 1.42 |
| 6 | H | 45 | GLU | CD-OE1 | 15.41 | 1.42 | 1.25 |
| 2 | B | 459 | TYR | CG-CD2 | 15.39 | 1.59 | 1.39 |
| 6 | H | 139 | ASN | CB-CG | 15.30 | 1.86 | 1.51 |
| 1 | A | 724 | GLU | CD-OE1 | 15.19 | 1.42 | 1.25 |
| 2 | B | 509 | ALA | CA-CB | 15.19 | 1.84 | 1.52 |
| 1 | A | 1119 | TYR | CE2-CZ | -15.19 | 1.18 | 1.38 |
| 2 | B | 211 | VAL | CB-CG1 | -15.19 | 1.21 | 1.52 |
| 2 | B | 1019 | SER | CB-OG | -15.12 | 1.22 | 1.42 |
| 2 | B | 620 | ARG | CZ-NH2 | 15.01 | 1.52 | 1.33 |
| 1 | A | 681 | GLU | CD-OE2 | 14.92 | 1.42 | 1.25 |
| 4 | E | 137 | GLU | CD-OE1 | 14.91 | 1.42 | 1.25 |
| 1 | A | 734 | GLU | CD-OE1 | 14.85 | 1.42 | 1.25 |
| 1 | A | 695 | LYS | CD-CE | 14.76 | 1.88 | 1.51 |
| 1 | A | 941 | LYS | CD-CE | 14.70 | 1.88 | 1.51 |
| 2 | B | 346 | GLU | CD-OE1 | 14.67 | 1.41 | 1.25 |
| 2 | B | 96 | TYR | CG-CD1 | 14.64 | 1.58 | 1.39 |
| 2 | B | 564 | GLU | CD-OE1 | 14.58 | 1.41 | 1.25 |
| 1 | A | 498 | ARG | NE-CZ | -14.54 | 1.14 | 1.33 |
| 2 | B | 529 | GLU | CD-OE1 | 14.39 | 1.41 | 1.25 |
| 4 | E | 180 | ARG | CG-CD | 14.39 | 1.88 | 1.51 |
| 1 | A | 620 | LYS | CE-NZ | 14.37 | 1.84 | 1.49 |
| 2 | B | 723 | VAL | CA-CB | 14.37 | 1.84 | 1.54 |
| 1 | A | 931 | GLU | CG-CD | 14.36 | 1.73 | 1.51 |
| 1 | A | 934 | LYS | CD-CE | 14.36 | 1.87 | 1.51 |
| 4 | E | 20 | LYS | CE-NZ | 14.33 | 1.84 | 1.49 |
| 2 | B | 723 | VAL | CB-CG1 | 14.30 | 1.82 | 1.52 |
| 1 | A | 653 | VAL | CB-CG2 | -14.26 | 1.23 | 1.52 |
| 1 | A | 931 | GLU | CD-OE2 | 14.24 | 1.41 | 1.25 |
| 4 | E | 131 | THR | CB-CG2 | 14.21 | 1.99 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 34 | GLU | CD-OE2 | 14.20 | 1.41 | 1.25 |
| 1 | A | 775 | ILE | CG1-CD1 | 14.15 | 2.48 | 1.50 |
| 1 | A | 620 | LYS | CD-CE | 14.13 | 1.86 | 1.51 |
| 2 | B | 870 | ILE | CA-CB | 14.11 | 1.87 | 1.54 |
| 1 | A | 705 | LYS | CB-CG | 14.05 | 1.90 | 1.52 |
| 1 | A | 618 | GLU | CD-OE1 | 14.00 | 1.41 | 1.25 |
| 4 | E | 152 | LYS | CD-CE | 13.98 | 1.86 | 1.51 |
| 2 | B | 758 | PHE | CE2-CZ | -13.95 | 1.10 | 1.37 |
| 1 | A | 1417 | GLU | CD-OE1 | 13.85 | 1.40 | 1.25 |
| 2 | B | 552 | MET | SD-CE | 13.79 | 2.55 | 1.77 |
| 2 | B | 764 | SER | CB-OG | -13.77 | 1.24 | 1.42 |
| 10 | L | 26 | THR | CA-CB | 13.76 | 1.89 | 1.53 |
| 1 | A | 1417 | GLU | CD-OE2 | 13.75 | 1.40 | 1.25 |
| 2 | B | 885 | MET | SD-CE | 13.71 | 2.54 | 1.77 |
| 1 | A | 290 | GLU | CD-OE2 | 13.66 | 1.40 | 1.25 |
| 2 | B | 239 | GLU | CG-CD | 13.65 | 1.72 | 1.51 |
| 1 | A | 681 | GLU | CD-OE1 | 13.65 | 1.40 | 1.25 |
| 4 | E | 66 | GLU | CD-OE2 | 13.63 | 1.40 | 1.25 |
| 1 | A | 895 | LYS | CD-CE | 13.60 | 1.85 | 1.51 |
| 1 | A | 795 | GLU | CD-OE2 | 13.50 | 1.40 | 1.25 |
| 1 | A | 1225 | PHE | CD1-CE1 | 13.43 | 1.66 | 1.39 |
| 2 | B | 347 | LYS | CG-CD | 13.41 | 1.98 | 1.52 |
| 1 | A | 1277 | GLU | CG-CD | 13.33 | 1.72 | 1.51 |
| 1 | A | 836 | TYR | CG-CD2 | 13.33 | 1.56 | 1.39 |
| 9 | K | 81 | TYR | CD2-CE2 | -13.31 | 1.19 | 1.39 |
| 3 | C | 23 | SER | CB-OG | 13.23 | 1.59 | 1.42 |
| 2 | B | 736 | THR | CB-CG2 | 13.22 | 1.96 | 1.52 |
| 1 | A | 995 | GLU | CD-OE2 | 13.22 | 1.40 | 1.25 |
| 1 | A | 1162 | VAL | CB-CG1 | 13.22 | 1.80 | 1.52 |
| 1 | A | 724 | GLU | CG-CD | 13.20 | 1.71 | 1.51 |
| 1 | A | 446 | ARG | CZ-NH1 | 13.20 | 1.50 | 1.33 |
| 2 | B | 194 | GLU | CD-OE2 | 13.13 | 1.40 | 1.25 |
| 3 | C | 78 | GLU | CD-OE2 | 13.14 | 1.40 | 1.25 |
| 1 | A | 1204 | ASP | CB-CG | 13.09 | 1.79 | 1.51 |
| 2 | B | 1206 | GLU | CD-OE1 | 13.09 | 1.40 | 1.25 |
| 3 | C | 104 | PHE | CD2-CE2 | 13.04 | 1.65 | 1.39 |
| 1 | A | 1415 | SER | CB-OG | -13.01 | 1.25 | 1.42 |
| 1 | A | 1214 | GLU | CD-OE1 | 12.98 | 1.40 | 1.25 |
| 2 | B | 987 | LYS | CE-NZ | 12.95 | 1.81 | 1.49 |
| 1 | A | 1372 | VAL | CB-CG1 | -12.93 | 1.25 | 1.52 |
| 2 | B | 1132 | GLU | CD-OE1 | 12.92 | 1.39 | 1.25 |
| 1 | A | 1234 | GLU | CD-OE1 | 12.89 | 1.39 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 653 | VAL | CB-CG2 | -12.88 | 1.25 | 1.52 |
| 3 | C | 197 | SER | CB-OG | 12.87 | 1.58 | 1.42 |
| 1 | A | 555 | ASP | CB-CG | 12.86 | 1.78 | 1.51 |
| 1 | A | 1074 | GLU | CD-OE2 | 12.85 | 1.39 | 1.25 |
| 9 | K | 32 | VAL | CB-CG2 | -12.83 | 1.25 | 1.52 |
| 1 | A | 264 | PHE | CB-CG | 12.83 | 1.73 | 1.51 |
| 7 | I | 32 | CYS | CB-SG | -12.82 | 1.60 | 1.82 |
| 2 | B | 838 | SER | CB-OG | -12.79 | 1.25 | 1.42 |
| 6 | H | 141 | TYR | CE1-CZ | -12.78 | 1.22 | 1.38 |
| 4 | E | 72 | PHE | CE2-CZ | 12.72 | 1.61 | 1.37 |
| 2 | B | 833 | TYR | CE1-CZ | -12.70 | 1.22 | 1.38 |
| 4 | E | 162 | ARG | CB-CG | 12.70 | 1.86 | 1.52 |
| 2 | B | 1007 | VAL | CB-CG1 | -12.69 | 1.26 | 1.52 |
| 2 | B | 305 | VAL | CB-CG1 | 12.68 | 1.79 | 1.52 |
| 2 | B | 226 | PHE | CE2-CZ | 12.66 | 1.61 | 1.37 |
| 3 | C | 12 | GLU | CD-OE2 | 12.65 | 1.39 | 1.25 |
| 7 | I | 28 | GLU | CD-OE1 | 12.65 | 1.39 | 1.25 |
| 3 | C | 177 | GLU | CD-OE2 | 12.62 | 1.39 | 1.25 |
| 1 | A | 1290 | LYS | CE-NZ | 12.61 | 1.80 | 1.49 |
| 2 | B | 621 | GLU | CD-OE2 | 12.60 | 1.39 | 1.25 |
| 7 | I | 1 | MET | CG-SD | 12.59 | 2.13 | 1.81 |
| 2 | B | 962 | LYS | CD-CE | 12.58 | 1.82 | 1.51 |
| 2 | B | 164 | LYS | CD-CE | 12.56 | 1.82 | 1.51 |
| 1 | A | 1411 | GLU | CG-CD | 12.56 | 1.70 | 1.51 |
| 2 | B | 319 | GLU | CG-CD | 12.55 | 1.70 | 1.51 |
| 4 | E | 106 | GLN | CG-CD | 12.53 | 1.79 | 1.51 |
| 4 | E | 57 | MET | SD-CE | 12.49 | 2.47 | 1.77 |
| 4 | E | 121 | MET | CG-SD | 12.48 | 2.13 | 1.81 |
| 2 | B | 459 | TYR | CE2-CZ | 12.47 | 1.54 | 1.38 |
| 2 | B | 371 | GLU | CD-OE1 | 12.44 | 1.39 | 1.25 |
| 7 | I | 45 | ARG | CG-CD | 12.38 | 1.82 | 1.51 |
| 1 | A | 601 | LYS | CD-CE | 12.35 | 1.82 | 1.51 |
| 2 | B | 1101 | ASP | CB-CG | 12.35 | 1.77 | 1.51 |
| 1 | A | 291 | GLU | CG-CD | 12.35 | 1.70 | 1.51 |
| 1 | A | 1154 | TYR | CE2-CZ | 12.34 | 1.54 | 1.38 |
| 4 | E | 192 | ARG | NE-CZ | 12.25 | 1.49 | 1.33 |
| 1 | A | 585 | GLY | C-O | 12.22 | 1.43 | 1.23 |
| 1 | A | 1285 | MET | SD-CE | 12.22 | 2.46 | 1.77 |
| 1 | A | 487 | MET | SD-CE | -12.20 | 1.09 | 1.77 |
| 4 | E | 201 | LYS | CG-CD | 12.19 | 1.93 | 1.52 |
| 2 | B | 785 | TYR | CE1-CZ | -12.11 | 1.22 | 1.38 |
| 1 | A | 544 | ASP | CB-CG | 12.11 | 1.77 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 239 | GLU | CD-OE1 | 12.04 | 1.38 | 1.25 |
| 2 | B | 328 | GLU | CD-OE1 | 12.02 | 1.38 | 1.25 |
| 4 | E | 41 | ASP | CB-CG | 12.02 | 1.76 | 1.51 |
| 9 | K | 61 | TYR | CE1-CZ | -12.01 | 1.23 | 1.38 |
| 3 | C | 192 | TRP | CE3-CZ3 | -11.98 | 1.18 | 1.38 |
| 1 | A | 830 | LYS | CD-CE | 11.96 | 1.81 | 1.51 |
| 1 | A | 1417 | GLU | CG-CD | 11.90 | 1.69 | 1.51 |
| 1 | A | 1230 | GLU | CD-OE1 | 11.88 | 1.38 | 1.25 |
| 1 | A | 728 | LYS | CG-CD | 11.87 | 1.92 | 1.52 |
| 2 | B | 598 | GLU | CD-OE2 | 11.87 | 1.38 | 1.25 |
| 2 | B | 706 | GLN | CB-CG | 11.87 | 1.84 | 1.52 |
| 2 | B | 968 | VAL | CB-CG2 | -11.85 | 1.27 | 1.52 |
| 2 | B | 296 | GLU | CD-OE1 | 11.82 | 1.38 | 1.25 |
| 2 | B | 115 | GLN | CG-CD | 11.80 | 1.78 | 1.51 |
| 2 | B | 1097 | HIS | CA-CB | 11.78 | 1.79 | 1.53 |
| 1 | A | 481 | ASP | CB-CG | 11.76 | 1.76 | 1.51 |
| 3 | C | 50 | GLU | CD-OE2 | 11.76 | 1.38 | 1.25 |
| 1 | A | 1187 | GLN | CB-CG | 11.75 | 1.84 | 1.52 |
| 1 | A | 1110 | ASN | CB-CG | 11.75 | 1.78 | 1.51 |
| 1 | A | 423 | ASP | CB-CG | 11.73 | 1.76 | 1.51 |
| 1 | A | 677 | ARG | NE-CZ | 11.71 | 1.48 | 1.33 |
| 2 | B | 230 | ALA | CA-CB | 11.68 | 1.76 | 1.52 |
| 2 | B | 31 | TRP | CZ3-CH2 | -11.67 | 1.21 | 1.40 |
| 2 | B | 1041 | GLU | CD-OE1 | 11.65 | 1.38 | 1.25 |
| 3 | C | 97 | VAL | C-O | -11.63 | 1.01 | 1.23 |
| 2 | B | 1041 | GLU | CD-OE2 | 11.60 | 1.38 | 1.25 |
| 1 | A | 879 | GLU | CD-OE1 | 11.59 | 1.38 | 1.25 |
| 9 | K | 61 | TYR | CG-CD2 | -11.54 | 1.24 | 1.39 |
| 6 | H | 104 | PHE | CA-C | 11.50 | 1.82 | 1.52 |
| 2 | B | 792 | MET | SD-CE | 11.50 | 2.42 | 1.77 |
| 6 | H | 19 | ARG | NE-CZ | 11.49 | 1.48 | 1.33 |
| 1 | A | 1419 | ASP | CB-CG | 11.48 | 1.75 | 1.51 |
| 1 | A | 464 | PRO | C-O | -11.47 | 1.00 | 1.23 |
| 3 | C | 180 | TYR | CG-CD1 | -11.44 | 1.24 | 1.39 |
| 3 | C | 116 | LYS | CD-CE | 11.42 | 1.79 | 1.51 |
| 1 | A | 593 | GLU | C-O | 11.41 | 1.45 | 1.23 |
| 1 | A | 496 | GLU | CG-CD | 11.39 | 1.69 | 1.51 |
| 1 | A | 681 | GLU | CG-CD | 11.39 | 1.69 | 1.51 |
| 2 | B | 303 | TYR | CG-CD2 | -11.38 | 1.24 | 1.39 |
| 1 | A | 833 | GLU | CG-CD | 11.38 | 1.69 | 1.51 |
| 1 | A | 404 | TYR | CG-CD1 | -11.36 | 1.24 | 1.39 |
| 1 | A | 945 | GLU | CD-OE2 | 11.36 | 1.38 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 719 | VAL | CB-CG1 | -11.30 | 1.29 | 1.52 |
| 4 | E | 66 | GLU | CD-OE1 | 11.29 | 1.38 | 1.25 |
| 2 | B | 975 | GLN | CD-NE2 | 11.26 | 1.61 | 1.32 |
| 2 | B | 594 | ALA | CA-CB | -11.26 | 1.28 | 1.52 |
| 1 | A | 948 | VAL | CB-CG1 | -11.25 | 1.29 | 1.52 |
| 1 | A | 507 | VAL | CB-CG2 | -11.24 | 1.29 | 1.52 |
| 9 | K | 61 | TYR | CE2-CZ | -11.24 | 1.24 | 1.38 |
| 3 | C | 40 | GLU | CD-OE2 | 11.23 | 1.38 | 1.25 |
| 1 | A | 1035 | TYR | CE2-CZ | -11.23 | 1.24 | 1.38 |
| 7 | I | 84 | VAL | CB-CG1 | -11.23 | 1.29 | 1.52 |
| 2 | B | 690 | VAL | CB-CG1 | -11.21 | 1.29 | 1.52 |
| 2 | B | 415 | GLN | CB-CG | 11.19 | 1.82 | 1.52 |
| 2 | B | 31 | TRP | CD2-CE2 | -11.18 | 1.27 | 1.41 |
| 1 | A | 37 | PHE | CD1-CE1 | 11.16 | 1.61 | 1.39 |
| 1 | A | 821 | ARG | CD-NE | -11.12 | 1.27 | 1.46 |
| 7 | I | 82 | GLU | CG-CD | 11.11 | 1.68 | 1.51 |
| 2 | B | 436 | VAL | CA-CB | 11.10 | 1.78 | 1.54 |
| 1 | A | 914 | GLU | CD-OE1 | 11.09 | 1.37 | 1.25 |
| 8 | J | 42 | LYS | CD-CE | 11.09 | 1.78 | 1.51 |
| 3 | C | 15 | LYS | CG-CD | 11.08 | 1.90 | 1.52 |
| 2 | B | 96 | TYR | CE1-CZ | 11.08 | 1.52 | 1.38 |
| 3 | C | 3 | GLU | CD-OE1 | 11.06 | 1.37 | 1.25 |
| 3 | C | 87 | PHE | CD2-CE2 | 11.06 | 1.61 | 1.39 |
| 1 | A | 1291 | VAL | CB-CG1 | -11.03 | 1.29 | 1.52 |
| 2 | B | 235 | SER | CB-OG | -11.02 | 1.27 | 1.42 |
| 2 | B | 370 | PHE | CD1-CE1 | 11.00 | 1.61 | 1.39 |
| 4 | E | 34 | GLU | CD-OE1 | 11.00 | 1.37 | 1.25 |
| 9 | K | 63 | VAL | CB-CG1 | -10.99 | 1.29 | 1.52 |
| 1 | A | 720 | ARG | CG-CD | 10.98 | 1.79 | 1.51 |
| 1 | A | 1171 | GLN | CG-CD | 10.97 | 1.76 | 1.51 |
| 2 | B | 660 | LYS | CD-CE | -10.97 | 1.23 | 1.51 |
| 1 | A | 291 | GLU | CD-OE1 | 10.95 | 1.37 | 1.25 |
| 4 | E | 211 | TYR | CE1-CZ | -10.93 | 1.24 | 1.38 |
| 1 | A | 1112 | LYS | CB-CG | 10.92 | 1.82 | 1.52 |
| 4 | E | 26 | ARG | CB-CG | -10.89 | 1.23 | 1.52 |
| 1 | A | 1222 | ASN | CB-CG | 10.89 | 1.76 | 1.51 |
| 3 | C | 12 | GLU | CD-OE1 | 10.89 | 1.37 | 1.25 |
| 2 | B | 226 | PHE | CD1-CE1 | 10.88 | 1.61 | 1.39 |
| 1 | A | 37 | PHE | CG-CD2 | 10.86 | 1.55 | 1.38 |
| 2 | B | 96 | TYR | CE2-CZ | 10.86 | 1.52 | 1.38 |
| 3 | C | 208 | GLU | CD-OE2 | 10.86 | 1.37 | 1.25 |
| 1 | A | 961 | ARG | CZ-NH2 | 10.85 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1259 | MET | CG-SD | 10.85 | 2.09 | 1.81 |
| 1 | A | 677 | ARG | CZ-NH2 | 10.84 | 1.47 | 1.33 |
| 2 | B | 959 | ASP | CB-CG | 10.83 | 1.74 | 1.51 |
| 2 | B | 18 | PHE | CB-CG | 10.80 | 1.69 | 1.51 |
| 2 | B | 137 | TYR | CG-CD1 | 10.78 | 1.53 | 1.39 |
| 2 | B | 434 | ARG | CG-CD | 10.76 | 1.78 | 1.51 |
| 3 | C | 191 | TYR | CB-CG | 10.76 | 1.67 | 1.51 |
| 7 | I | 72 | ASP | CB-CG | 10.76 | 1.74 | 1.51 |
| 9 | K | 7 | PHE | CB-CG | -10.74 | 1.33 | 1.51 |
| 2 | B | 775 | LYS | CB-CG | 10.72 | 1.81 | 1.52 |
| 1 | A | 1103 | GLU | CD-OE2 | 10.72 | 1.37 | 1.25 |
| 2 | B | 986 | GLN | CG-CD | 10.72 | 1.75 | 1.51 |
| 1 | A | 290 | GLU | CD-OE1 | 10.69 | 1.37 | 1.25 |
| 6 | H | 77 | ARG | CB-CG | 10.69 | 1.81 | 1.52 |
| 2 | B | 328 | GLU | CD-OE2 | 10.66 | 1.37 | 1.25 |
| 2 | B | 1153 | GLU | CD-OE2 | 10.62 | 1.37 | 1.25 |
| 1 | A | 708 | MET | SD-CE | 10.62 | 2.37 | 1.77 |
| 2 | B | 137 | TYR | CB-CG | 10.62 | 1.67 | 1.51 |
| 2 | B | 705 | MET | SD-CE | -10.61 | 1.18 | 1.77 |
| 4 | E | 162 | ARG | CZ-NH1 | 10.60 | 1.46 | 1.33 |
| 1 | A | 1102 | LYS | CD-CE | 10.59 | 1.77 | 1.51 |
| 1 | A | 1316 | VAL | CB-CG2 | -10.59 | 1.30 | 1.52 |
| 3 | C | 40 | GLU | CD-OE1 | 10.58 | 1.37 | 1.25 |
| 1 | A | 1350 | LYS | CE-NZ | 10.57 | 1.75 | 1.49 |
| 4 | E | 98 | ILE | CA-CB | 10.54 | 1.79 | 1.54 |
| 2 | B | 191 | LYS | CB-CG | 10.53 | 1.80 | 1.52 |
| 1 | A | 714 | PHE | CD2-CE2 | -10.52 | 1.18 | 1.39 |
| 3 | C | 220 | ASP | CB-CG | 10.52 | 1.73 | 1.51 |
| 1 | A | 518 | LYS | CD-CE | 10.51 | 1.77 | 1.51 |
| 5 | F | 127 | GLU | CD-OE1 | 10.49 | 1.37 | 1.25 |
| 2 | B | 519 | TRP | CD2-CE2 | -10.49 | 1.28 | 1.41 |
| 1 | A | 1064 | VAL | CB-CG1 | -10.48 | 1.30 | 1.52 |
| 1 | A | 1277 | GLU | CD-OE1 | 10.48 | 1.37 | 1.25 |
| 2 | B | 531 | GLN | CD-OE1 | 10.47 | 1.47 | 1.24 |
| 2 | B | 895 | ASP | CB-CG | 10.46 | 1.73 | 1.51 |
| 1 | A | 724 | GLU | CD-OE2 | 10.45 | 1.37 | 1.25 |
| 6 | H | 129 | TYR | CE1-CZ | 10.45 | 1.52 | 1.38 |
| 1 | A | 1135 | ARG | CG-CD | 10.44 | 1.78 | 1.51 |
| 1 | A | 830 | LYS | CG-CD | 10.44 | 1.88 | 1.52 |
| 1 | A | 1446 | ASP | CB-CG | 10.43 | 1.73 | 1.51 |
| 2 | B | 962 | LYS | CG-CD | 10.43 | 1.87 | 1.52 |
| 7 | I | 92 | ARG | C-O | 10.42 | 1.43 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 734 | GLU | CG-CD | 10.41 | 1.67 | 1.51 |
| 1 | A | 843 | LYS | CG-CD | 10.41 | 1.87 | 1.52 |
| 3 | C | 122 | SER | CB-OG | 10.41 | 1.55 | 1.42 |
| 1 | A | 1280 | GLU | CG-CD | 10.41 | 1.67 | 1.51 |
| 2 | B | 1219 | ASP | CB-CG | 10.39 | 1.73 | 1.51 |
| 2 | B | 101 | MET | SD-CE | 10.37 | 2.35 | 1.77 |
| 2 | B | 31 | TRP | CG-CD1 | -10.36 | 1.22 | 1.36 |
| 2 | B | 951 | GLN | CG-CD | 10.36 | 1.74 | 1.51 |
| 1 | A | 995 | GLU | CD-OE1 | 10.35 | 1.37 | 1.25 |
| 6 | H | 52 | GLN | CG-CD | 10.35 | 1.74 | 1.51 |
| 2 | B | 486 | TYR | CG-CD1 | 10.32 | 1.52 | 1.39 |
| 2 | B | 999 | MET | SD-CE | -10.31 | 1.20 | 1.77 |
| 3 | C | 3 | GLU | CD-OE2 | 10.30 | 1.36 | 1.25 |
| 7 | I | 83 | ASN | CB-CG | -10.28 | 1.27 | 1.51 |
| 1 | A | 839 | ARG | NE-CZ | 10.27 | 1.46 | 1.33 |
| 3 | C | 50 | GLU | CD-OE1 | 10.27 | 1.36 | 1.25 |
| 3 | C | 199 | LYS | CD-CE | 10.27 | 1.76 | 1.51 |
| 1 | A | 1130 | GLN | CG-CD | 10.26 | 1.74 | 1.51 |
| 2 | B | 853 | SER | CB-OG | 10.26 | 1.55 | 1.42 |
| 8 | J | 29 | GLU | CD-OE1 | 10.25 | 1.36 | 1.25 |
| 2 | B | 169 | ARG | NE-CZ | 10.25 | 1.46 | 1.33 |
| 4 | E | 72 | PHE | CG-CD1 | 10.24 | 1.54 | 1.38 |
| 9 | K | 1 | MET | SD-CE | 10.24 | 2.35 | 1.77 |
| 1 | A | 836 | TYR | CZ-OH | 10.23 | 1.55 | 1.37 |
| 1 | A | 1014 | ALA | CA-CB | -10.23 | 1.30 | 1.52 |
| 2 | B | 963 | PHE | CB-CG | -10.22 | 1.33 | 1.51 |
| 1 | A | 5 | GLN | CB-CG | 10.21 | 1.80 | 1.52 |
| 5 | F | 72 | LYS | CD-CE | 10.20 | 1.76 | 1.51 |
| 1 | A | 347 | PHE | N-CA | 10.20 | 1.66 | 1.46 |
| 1 | A | 987 | VAL | CB-CG1 | -10.19 | 1.31 | 1.52 |
| 2 | B | 620 | ARG | CG-CD | 10.19 | 1.77 | 1.51 |
| 1 | A | 1214 | GLU | C-O | 10.18 | 1.42 | 1.23 |
| 2 | B | 529 | GLU | CG-CD | 10.15 | 1.67 | 1.51 |
| 2 | B | 57 | TYR | CE2-CZ | -10.15 | 1.25 | 1.38 |
| 2 | B | 958 | GLN | CG-CD | 10.14 | 1.74 | 1.51 |
| 2 | B | 643 | ASP | CB-CG | 10.14 | 1.73 | 1.51 |
| 1 | A | 945 | GLU | CD-OE1 | 10.13 | 1.36 | 1.25 |
| 1 | A | 1132 | LYS | CE-NZ | 10.13 | 1.74 | 1.49 |
| 1 | A | 678 | GLU | CD-OE2 | 10.12 | 1.36 | 1.25 |
| 2 | B | 347 | LYS | CD-CE | 10.12 | 1.76 | 1.51 |
| 7 | I | 84 | VAL | CB-CG2 | -10.10 | 1.31 | 1.52 |
| 6 | H | 126 | GLU | CD-OE1 | 10.10 | 1.36 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 274 | ILE | CA-CB | 10.10 | 1.78 | 1.54 |
| 2 | B | 183 | GLU | CD-OE1 | 10.10 | 1.36 | 1.25 |
| 2 | B | 665 | GLU | CG-CD | 10.09 | 1.67 | 1.51 |
| 2 | B | 50 | SER | CB-OG | -10.08 | 1.29 | 1.42 |
| 1 | A | 1298 | TYR | CD2-CE2 | -10.07 | 1.24 | 1.39 |
| 7 | I | 47 | GLU | CG-CD | 10.06 | 1.67 | 1.51 |
| 7 | I | 47 | GLU | CD-OE2 | 10.06 | 1.36 | 1.25 |
| 9 | K | 111 | LEU | C-O | 10.04 | 1.42 | 1.23 |
| 1 | A | 1109 | LYS | CB-CG | 10.01 | 1.79 | 1.52 |
| 4 | E | 161 | LYS | CD-CE | 10.01 | 1.76 | 1.51 |
| 2 | B | 1069 | PHE | CE2-CZ | -10.00 | 1.18 | 1.37 |
| 2 | B | 781 | PHE | CB-CG | -9.99 | 1.34 | 1.51 |
| 5 | F | 103 | MET | SD-CE | 9.98 | 2.33 | 1.77 |
| 1 | A | 777 | PHE | CD1-CE1 | 9.98 | 1.59 | 1.39 |
| 2 | B | 963 | PHE | CD2-CE2 | 9.98 | 1.59 | 1.39 |
| 1 | A | 1035 | TYR | CG-CD1 | -9.98 | 1.26 | 1.39 |
| 6 | H | 45 | GLU | CD-OE2 | 9.98 | 1.36 | 1.25 |
| 2 | B | 519 | TRP | CB-CG | 9.97 | 1.68 | 1.50 |
| 1 | A | 792 | TYR | CD2-CE2 | -9.97 | 1.24 | 1.39 |
| 1 | A | 843 | LYS | CD-CE | 9.96 | 1.76 | 1.51 |
| 1 | A | 1336 | MET | C-O | -9.96 | 1.04 | 1.23 |
| 3 | C | 89 | GLU | C-O | 9.94 | 1.42 | 1.23 |
| 1 | A | 1055 | ARG | CG-CD | 9.93 | 1.76 | 1.51 |
| 1 | A | 1337 | GLU | CG-CD | 9.93 | 1.66 | 1.51 |
| 1 | A | 1419 | ASP | CG-OD1 | 9.93 | 1.48 | 1.25 |
| 1 | A | 376 | TYR | CD1-CE1 | -9.91 | 1.24 | 1.39 |
| 1 | A | 1261 | LYS | CD-CE | 9.91 | 1.76 | 1.51 |
| 1 | A | 1362 | TYR | CG-CD2 | -9.90 | 1.26 | 1.39 |
| 1 | A | 525 | GLN | CG-CD | 9.90 | 1.73 | 1.51 |
| 2 | B | 320 | ASP | CB-CG | 9.88 | 1.72 | 1.51 |
| 6 | H | 131 | ASN | CB-CG | 9.88 | 1.73 | 1.51 |
| 1 | A | 846 | GLU | CD-OE1 | 9.86 | 1.36 | 1.25 |
| 2 | B | 1134 | GLU | CD-OE1 | 9.87 | 1.36 | 1.25 |
| 1 | A | 542 | GLU | CD-OE1 | 9.85 | 1.36 | 1.25 |
| 3 | C | 209 | TYR | CD2-CE2 | 9.85 | 1.54 | 1.39 |
| 10 | L | 29 | TYR | CE1-CZ | -9.85 | 1.25 | 1.38 |
| 1 | A | 1074 | GLU | CG-CD | 9.82 | 1.66 | 1.51 |
| 2 | B | 370 | PHE | CE2-CZ | 9.82 | 1.56 | 1.37 |
| 1 | A | 792 | TYR | CE1-CZ | -9.82 | 1.25 | 1.38 |
| 1 | A | 1223 | ASP | CB-CG | 9.80 | 1.72 | 1.51 |
| 1 | A | 481 | ASP | CA-CB | -9.80 | 1.32 | 1.53 |
| 2 | B | 641 | GLU | CD-OE1 | 9.79 | 1.36 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1301 | GLU | CD-OE1 | 9.76 | 1.36 | 1.25 |
| 1 | A | 580 | VAL | CB-CG2 | -9.75 | 1.32 | 1.52 |
| 7 | I | 91 | ARG | CA-C | -9.73 | 1.27 | 1.52 |
| 1 | A | 1445 | ILE | CB-CG2 | 9.72 | 1.82 | 1.52 |
| 2 | B | 237 | VAL | CB-CG1 | -9.72 | 1.32 | 1.52 |
| 2 | B | 105 | SER | CA-CB | 9.71 | 1.67 | 1.52 |
| 4 | E | 54 | GLN | CB-CG | 9.70 | 1.78 | 1.52 |
| 8 | J | 3 | VAL | CA-CB | -9.69 | 1.34 | 1.54 |
| 1 | A | 552 | TRP | CG-CD1 | -9.69 | 1.23 | 1.36 |
| 3 | C | 166 | GLU | CD-OE1 | 9.69 | 1.36 | 1.25 |
| 10 | L | 54 | ARG | CG-CD | 9.69 | 1.76 | 1.51 |
| 3 | C | 180 | TYR | CD2-CE2 | 9.67 | 1.53 | 1.39 |
| 5 | F | 154 | ASP | CB-CG | 9.67 | 1.72 | 1.51 |
| 4 | E | 40 | GLU | CD-OE1 | 9.66 | 1.36 | 1.25 |
| 3 | C | 57 | VAL | CB-CG2 | -9.65 | 1.32 | 1.52 |
| 2 | B | 370 | PHE | CD2-CE2 | 9.64 | 1.58 | 1.39 |
| 1 | A | 684 | ALA | CA-CB | 9.64 | 1.72 | 1.52 |
| 2 | B | 665 | GLU | CD-OE2 | 9.63 | 1.36 | 1.25 |
| 4 | E | 133 | GLU | CD-OE1 | 9.63 | 1.36 | 1.25 |
| 1 | A | 1230 | GLU | CD-OE2 | 9.62 | 1.36 | 1.25 |
| 2 | B | 126 | SER | CA-CB | -9.61 | 1.38 | 1.52 |
| 2 | B | 434 | ARG | CB-CG | 9.61 | 1.78 | 1.52 |
| 1 | A | 520 | CYS | CB-SG | -9.61 | 1.66 | 1.82 |
| 2 | B | 486 | TYR | CE1-CZ | 9.61 | 1.51 | 1.38 |
| 2 | B | 607 | GLY | C-O | -9.61 | 1.08 | 1.23 |
| 3 | C | 66 | ARG | CZ-NH1 | -9.61 | 1.20 | 1.33 |
| 1 | A | 610 | GLY | C-O | 9.59 | 1.39 | 1.23 |
| 2 | B | 1155 | SER | CA-CB | 9.58 | 1.67 | 1.52 |
| 1 | A | 597 | LEU | CG-CD1 | 9.58 | 1.87 | 1.51 |
| 10 | L | 48 | CYS | CB-SG | -9.58 | 1.66 | 1.82 |
| 1 | A | 1003 | LYS | CB-CG | 9.57 | 1.78 | 1.52 |
| 2 | B | 994 | TYR | CD1-CE1 | -9.57 | 1.25 | 1.39 |
| 6 | H | 9 | ILE | CA-CB | 9.56 | 1.76 | 1.54 |
| 6 | H | 118 | PHE | CD2-CE2 | 9.56 | 1.58 | 1.39 |
| 2 | B | 315 | LYS | CE-NZ | 9.56 | 1.73 | 1.49 |
| 1 | A | 1232 | ASN | C-O | 9.54 | 1.41 | 1.23 |
| 2 | B | 662 | MET | SD-CE | 9.54 | 2.31 | 1.77 |
| 10 | L | 28 | LYS | CA-C | 9.53 | 1.77 | 1.52 |
| 9 | K | 2 | ASN | C-O | 9.52 | 1.41 | 1.23 |
| 9 | K | 36 | GLU | CD-OE1 | 9.52 | 1.36 | 1.25 |
| 2 | B | 202 | TYR | CE1-CZ | -9.52 | 1.26 | 1.38 |
| 1 | A | 398 | GLU | CG-CD | 9.51 | 1.66 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | K | 17 | SER | C-O | -9.51 | 1.05 | 1.23 |
| 2 | B | 1102 | LYS | CB-CG | 9.51 | 1.78 | 1.52 |
| 1 | A | 931 | GLU | CD-OE1 | 9.50 | 1.36 | 1.25 |
| 3 | C | 102 | GLN | CB-CG | 9.48 | 1.78 | 1.52 |
| 7 | I | 82 | GLU | CD-OE1 | 9.48 | 1.36 | 1.25 |
| 1 | A | 66 | LYS | CB-CG | 9.47 | 1.78 | 1.52 |
| 2 | B | 27 | ALA | CA-CB | -9.46 | 1.32 | 1.52 |
| 2 | B | 41 | LYS | CE-NZ | 9.46 | 1.72 | 1.49 |
| 2 | B | 497 | ARG | CZ-NH1 | 9.46 | 1.45 | 1.33 |
| 2 | B | 57 | TYR | CE1-CZ | -9.45 | 1.26 | 1.38 |
| 2 | B | 983 | ARG | CD-NE | -9.45 | 1.30 | 1.46 |
| 7 | I | 107 | SER | CB-OG | -9.45 | 1.29 | 1.42 |
| 4 | E | 46 | TYR | CD2-CE2 | 9.45 | 1.53 | 1.39 |
| 1 | A | 37 | PHE | CE1-CZ | 9.44 | 1.55 | 1.37 |
| 3 | C | 209 | TYR | CE2-CZ | 9.43 | 1.50 | 1.38 |
| 1 | A | 729 | ALA | CA-CB | -9.42 | 1.32 | 1.52 |
| 1 | A | 1287 | TYR | CG-CD1 | 9.42 | 1.51 | 1.39 |
| 2 | B | 833 | TYR | CG-CD2 | -9.42 | 1.26 | 1.39 |
| 2 | B | 399 | ASP | CB-CG | 9.41 | 1.71 | 1.51 |
| 2 | B | 1091 | TYR | CE1-CZ | -9.41 | 1.26 | 1.38 |
| 2 | B | 706 | GLN | CG-CD | 9.40 | 1.72 | 1.51 |
| 10 | L | 45 | ALA | CA-CB | 9.40 | 1.72 | 1.52 |
| 1 | A | 1214 | GLU | CG-CD | 9.38 | 1.66 | 1.51 |
| 5 | F | 129 | LYS | CE-NZ | 9.38 | 1.72 | 1.49 |
| 1 | A | 840 | ARG | CG-CD | 9.38 | 1.75 | 1.51 |
| 2 | B | 479 | VAL | CB-CG1 | -9.37 | 1.33 | 1.52 |
| 9 | K | 111 | LEU | CG-CD1 | 9.37 | 1.86 | 1.51 |
| 1 | A | 551 | TYR | CE1-CZ | -9.36 | 1.26 | 1.38 |
| 4 | E | 13 | TRP | CG-CD1 | 9.36 | 1.49 | 1.36 |
| 2 | B | 106 | ASP | CB-CG | 9.36 | 1.71 | 1.51 |
| 1 | A | 1297 | GLU | CD-OE1 | -9.35 | 1.15 | 1.25 |
| 4 | E | 191 | LYS | CE-NZ | 9.35 | 1.72 | 1.49 |
| 1 | A | 1111 | MET | CG-SD | 9.34 | 2.05 | 1.81 |
| 10 | L | 48 | CYS | CA-C | 9.34 | 1.77 | 1.52 |
| 8 | J | 58 | GLU | CG-CD | 9.34 | 1.66 | 1.51 |
| 1 | A | 1187 | GLN | CG-CD | 9.32 | 1.72 | 1.51 |
| 2 | B | 697 | GLU | CD-OE2 | 9.28 | 1.35 | 1.25 |
| 5 | F | 146 | TRP | CB-CG | -9.28 | 1.33 | 1.50 |
| 2 | B | 531 | GLN | CB-CG | 9.28 | 1.77 | 1.52 |
| 2 | B | 666 | TYR | CE1-CZ | 9.28 | 1.50 | 1.38 |
| 1 | A | 1438 | THR | CB-CG2 | -9.27 | 1.21 | 1.52 |
| 2 | B | 999 | MET | CG-SD | 9.27 | 2.05 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1291 | VAL | CB-CG2 | 9.26 | 1.72 | 1.52 |
| 7 | I | 100 | PHE | CE1-CZ | -9.26 | 1.19 | 1.37 |
| 2 | B | 766 | ARG | NE-CZ | 9.25 | 1.45 | 1.33 |
| 1 | A | 985 | ASP | CG-OD2 | 9.25 | 1.46 | 1.25 |
| 2 | B | 216 | GLU | CD-OE2 | 9.23 | 1.35 | 1.25 |
| 1 | A | 237 | THR | CB-CG2 | 9.23 | 1.82 | 1.52 |
| 1 | A | 478 | TYR | CD2-CE2 | -9.23 | 1.25 | 1.39 |
| 2 | B | 216 | GLU | CD-OE1 | 9.23 | 1.35 | 1.25 |
| 6 | H | 20 | TYR | CE2-CZ | -9.23 | 1.26 | 1.38 |
| 2 | B | 448 | ILE | N-CA | 9.22 | 1.64 | 1.46 |
| 3 | C | 114 | TYR | CE2-CZ | -9.22 | 1.26 | 1.38 |
| 1 | A | 44 | THR | CA-CB | 9.21 | 1.77 | 1.53 |
| 1 | A | 1129 | GLU | CG-CD | 9.21 | 1.65 | 1.51 |
| 2 | B | 249 | ARG | NE-CZ | 9.20 | 1.45 | 1.33 |
| 1 | A | 46 | THR | CA-CB | 9.19 | 1.77 | 1.53 |
| 2 | B | 30 | SER | CB-OG | -9.18 | 1.30 | 1.42 |
| 2 | B | 797 | TYR | CE1-CZ | -9.18 | 1.26 | 1.38 |
| 10 | L | 50 | ASP | CB-CG | 9.18 | 1.71 | 1.51 |
| 2 | B | 319 | GLU | CD-OE1 | 9.17 | 1.35 | 1.25 |
| 2 | B | 459 | TYR | CD1-CE1 | 9.17 | 1.53 | 1.39 |
| 2 | B | 581 | PHE | CG-CD1 | -9.16 | 1.25 | 1.38 |
| 2 | B | 359 | GLU | CD-OE1 | 9.16 | 1.35 | 1.25 |
| 3 | C | 89 | GLU | CD-OE2 | 9.16 | 1.35 | 1.25 |
| 1 | A | 16 | GLU | CG-CD | 9.15 | 1.65 | 1.51 |
| 2 | B | 124 | TYR | CE1-CZ | -9.15 | 1.26 | 1.38 |
| 1 | A | 1302 | PRO | CB-CG | 9.15 | 1.95 | 1.50 |
| 1 | A | 1405 | THR | CA-CB | 9.15 | 1.77 | 1.53 |
| 1 | A | 91 | PHE | CG-CD1 | -9.14 | 1.25 | 1.38 |
| 2 | B | 1149 | GLU | CD-OE1 | 9.14 | 1.35 | 1.25 |
| 3 | C | 170 | TRP | CZ3-CH2 | -9.14 | 1.25 | 1.40 |
| 4 | E | 67 | GLU | CD-OE1 | 9.12 | 1.35 | 1.25 |
| 1 | A | 1214 | GLU | CD-OE2 | 9.12 | 1.35 | 1.25 |
| 2 | B | 226 | PHE | CG-CD2 | 9.11 | 1.52 | 1.38 |
| 1 | A | 37 | PHE | CD2-CE2 | 9.11 | 1.57 | 1.39 |
| 1 | A | 1286 | LYS | CB-CG | 9.11 | 1.77 | 1.52 |
| 1 | A | 497 | THR | CB-CG2 | -9.10 | 1.22 | 1.52 |
| 1 | A | 678 | GLU | CG-CD | 9.10 | 1.65 | 1.51 |
| 10 | L | 62 | LYS | CD-CE | 9.09 | 1.74 | 1.51 |
| 2 | B | 975 | GLN | CB-CG | -9.09 | 1.28 | 1.52 |
| 1 | A | 932 | GLU | CD-OE2 | 9.05 | 1.35 | 1.25 |
| 3 | C | 195 | GLN | CG-CD | 9.05 | 1.71 | 1.51 |
| 2 | B | 65 | GLU | CG-CD | 9.05 | 1.65 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 7 | GLN | CB-CG | 9.04 | 1.76 | 1.52 |
| 1 | A | 771 | GLU | CD-OE1 | 9.04 | 1.35 | 1.25 |
| 1 | A | 787 | PHE | CD1-CE1 | 9.04 | 1.57 | 1.39 |
| 2 | B | 1156 | ASP | CB-CG | 9.03 | 1.70 | 1.51 |
| 1 | A | 676 | MET | CG-SD | 9.03 | 2.04 | 1.81 |
| 1 | A | 1342 | GLU | CD-OE1 | 9.02 | 1.35 | 1.25 |
| 2 | B | 875 | GLU | CG-CD | 9.02 | 1.65 | 1.51 |
| 1 | A | 662 | PHE | CE1-CZ | -9.02 | 1.20 | 1.37 |
| 1 | A | 626 | ASN | CG-ND2 | 9.01 | 1.55 | 1.32 |
| 1 | A | 373 | THR | CB-CG2 | -9.01 | 1.22 | 1.52 |
| 1 | A | 787 | PHE | CG-CD1 | -9.00 | 1.25 | 1.38 |
| 2 | B | 296 | GLU | CG-CD | 9.00 | 1.65 | 1.51 |
| 2 | B | 96 | TYR | CG-CD2 | 9.00 | 1.50 | 1.39 |
| 1 | A | 1005 | GLU | CG-CD | 8.98 | 1.65 | 1.51 |
| 1 | A | 971 | PHE | CE2-CZ | -8.97 | 1.20 | 1.37 |
| 1 | A | 1337 | GLU | CD-OE1 | 8.96 | 1.35 | 1.25 |
| 7 | I | 43 | VAL | CB-CG1 | -8.95 | 1.34 | 1.52 |
| 1 | A | 1093 | LYS | CB-CG | 8.95 | 1.76 | 1.52 |
| 2 | B | 373 | ARG | CZ-NH1 | 8.95 | 1.44 | 1.33 |
| 4 | E | 59 | SER | CB-OG | 8.95 | 1.53 | 1.42 |
| 4 | E | 66 | GLU | CG-CD | 8.94 | 1.65 | 1.51 |
| 1 | A | 777 | PHE | CD2-CE2 | 8.94 | 1.57 | 1.39 |
| 2 | B | 418 | LYS | CD-CE | 8.93 | 1.73 | 1.51 |
| 1 | A | 61 | ILE | CA-CB | 8.92 | 1.75 | 1.54 |
| 2 | B | 1057 | LYS | CD-CE | 8.92 | 1.73 | 1.51 |
| 3 | C | 154 | LYS | CG-CD | 8.92 | 1.82 | 1.52 |
| 2 | B | 723 | VAL | CB-CG2 | 8.91 | 1.71 | 1.52 |
| 1 | A | 672 | ASP | CB-CG | -8.90 | 1.33 | 1.51 |
| 9 | K | 61 | TYR | C-O | -8.90 | 1.06 | 1.23 |
| 1 | A | 1305 | VAL | CB-CG1 | -8.89 | 1.34 | 1.52 |
| 1 | A | 478 | TYR | CD1-CE1 | -8.88 | 1.26 | 1.39 |
| 1 | A | 1239 | ARG | CG-CD | 8.87 | 1.74 | 1.51 |
| 2 | B | 246 | LYS | CA-C | 8.87 | 1.76 | 1.52 |
| 3 | C | 125 | MET | SD-CE | 8.85 | 2.27 | 1.77 |
| 6 | H | 121 | LEU | C-O | 8.85 | 1.40 | 1.23 |
| 7 | I | 75 | CYS | CB-SG | -8.85 | 1.67 | 1.82 |
| 2 | B | 296 | GLU | CD-OE2 | 8.85 | 1.35 | 1.25 |
| 6 | H | 95 | TYR | CD2-CE2 | 8.85 | 1.52 | 1.39 |
| 6 | H | 129 | TYR | CG-CD2 | 8.84 | 1.50 | 1.39 |
| 1 | A | 833 | GLU | CD-OE1 | 8.84 | 1.35 | 1.25 |
| 3 | C | 28 | ALA | C-O | 8.84 | 1.40 | 1.23 |
| 6 | H | 98 | TYR | CE1-CZ | -8.84 | 1.27 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1315 | GLU | CD-OE2 | 8.83 | 1.35 | 1.25 |
| 1 | A | 1149 | ALA | CA-CB | -8.82 | 1.33 | 1.52 |
| 1 | A | 1078 | GLN | CG-CD | 8.82 | 1.71 | 1.51 |
| 2 | B | 275 | TYR | CG-CD1 | -8.81 | 1.27 | 1.39 |
| 7 | I | 36 | GLU | CG-CD | 8.81 | 1.65 | 1.51 |
| 6 | H | 41 | ASP | CB-CG | 8.81 | 1.70 | 1.51 |
| 2 | B | 137 | TYR | CE1-CZ | 8.79 | 1.50 | 1.38 |
| 2 | B | 103 | ASN | CB-CG | 8.79 | 1.71 | 1.51 |
| 2 | B | 1164 | GLY | C-O | 8.79 | 1.37 | 1.23 |
| 8 | J | 48 | ARG | CZ-NH1 | -8.79 | 1.21 | 1.33 |
| 2 | B | 21 | GLU | CD-OE2 | 8.78 | 1.35 | 1.25 |
| 4 | E | 152 | LYS | CG-CD | 8.78 | 1.82 | 1.52 |
| 7 | I | 98 | VAL | CB-CG2 | -8.78 | 1.34 | 1.52 |
| 2 | B | 245 | GLU | CG-CD | 8.77 | 1.65 | 1.51 |
| 3 | C | 66 | ARG | NE-CZ | -8.77 | 1.21 | 1.33 |
| 5 | F | 93 | ILE | C-O | -8.77 | 1.06 | 1.23 |
| 1 | A | 1426 | GLU | CD-OE2 | 8.75 | 1.35 | 1.25 |
| 3 | C | 9 | LYS | CG-CD | 8.74 | 1.82 | 1.52 |
| 2 | B | 958 | GLN | CB-CG | 8.73 | 1.76 | 1.52 |
| 3 | C | 18 | VAL | CB-CG2 | -8.73 | 1.34 | 1.52 |
| 3 | C | 177 | GLU | CG-CD | 8.73 | 1.65 | 1.51 |
| 4 | E | 196 | VAL | CB-CG1 | -8.73 | 1.34 | 1.52 |
| 2 | B | 184 | ALA | CA-CB | -8.73 | 1.34 | 1.52 |
| 2 | B | 595 | ARG | NE-CZ | 8.72 | 1.44 | 1.33 |
| 2 | B | 708 | GLU | CD-OE2 | 8.72 | 1.35 | 1.25 |
| 1 | A | 1121 | GLU | CD-OE1 | 8.72 | 1.35 | 1.25 |
| 1 | A | 1132 | LYS | CD-CE | 8.71 | 1.73 | 1.51 |
| 4 | E | 90 | VAL | CB-CG1 | 8.71 | 1.71 | 1.52 |
| 2 | B | 595 | ARG | CG-CD | 8.71 | 1.73 | 1.51 |
| 3 | C | 159 | ALA | C-O | -8.69 | 1.06 | 1.23 |
| 2 | B | 1221 | SER | CA-CB | 8.69 | 1.66 | 1.52 |
| 4 | E | 155 | ARG | NE-CZ | 8.69 | 1.44 | 1.33 |
| 2 | B | 815 | ARG | CZ-NH2 | 8.69 | 1.44 | 1.33 |
| 2 | B | 115 | GLN | CB-CG | 8.68 | 1.75 | 1.52 |
| 2 | B | 485 | ARG | NE-CZ | -8.68 | 1.21 | 1.33 |
| 2 | B | 1132 | GLU | CG-CD | 8.67 | 1.65 | 1.51 |
| 1 | A | 673 | GLY | C-O | -8.66 | 1.09 | 1.23 |
| 2 | B | 217 | ARG | CZ-NH1 | -8.66 | 1.21 | 1.33 |
| 1 | A | 1215 | ARG | CB-CG | 8.65 | 1.75 | 1.52 |
| 2 | B | 626 | ILE | C-O | -8.65 | 1.06 | 1.23 |
| 7 | I | 28 | GLU | CG-CD | 8.65 | 1.65 | 1.51 |
| 1 | A | 549 | MET | SD-CE | -8.64 | 1.29 | 1.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 478 | GLY | N-CA | 8.64 | 1.59 | 1.46 |
| 1 | A | 398 | GLU | CD-OE2 | 8.64 | 1.35 | 1.25 |
| 1 | A | 941 | LYS | CE-NZ | 8.63 | 1.70 | 1.49 |
| 3 | C | 198 | ALA | CA-CB | -8.63 | 1.34 | 1.52 |
| 1 | A | 673 | GLY | CA-C | -8.63 | 1.38 | 1.51 |
| 2 | B | 542 | MET | SD-CE | -8.62 | 1.29 | 1.77 |
| 1 | A | 1080 | THR | CA-CB | 8.61 | 1.75 | 1.53 |
| 1 | A | 1132 | LYS | CB-CG | 8.61 | 1.75 | 1.52 |
| 7 | I | 20 | LYS | CD-CE | 8.61 | 1.72 | 1.51 |
| 1 | A | 1337 | GLU | CD-OE2 | 8.60 | 1.35 | 1.25 |
| 3 | C | 196 | ASP | CB-CG | 8.60 | 1.69 | 1.51 |
| 3 | C | 178 | PHE | CG-CD2 | -8.60 | 1.25 | 1.38 |
| 4 | E | 33 | GLU | CD-OE1 | 8.59 | 1.35 | 1.25 |
| 2 | B | 118 | ARG | CZ-NH1 | -8.59 | 1.21 | 1.33 |
| 7 | I | 35 | VAL | CB-CG2 | -8.59 | 1.34 | 1.52 |
| 2 | B | 376 | PHE | CE2-CZ | -8.59 | 1.21 | 1.37 |
| 2 | B | 250 | PHE | CE1-CZ | 8.58 | 1.53 | 1.37 |
| 1 | A | 728 | LYS | CE-NZ | 8.57 | 1.70 | 1.49 |
| 3 | C | 134 | ILE | CA-CB | -8.57 | 1.35 | 1.54 |
| 2 | B | 266 | ALA | CA-CB | 8.57 | 1.70 | 1.52 |
| 2 | B | 186 | GLU | CD-OE2 | 8.56 | 1.35 | 1.25 |
| 2 | B | 219 | ALA | CA-CB | 8.56 | 1.70 | 1.52 |
| 2 | B | 330 | ALA | CA-CB | -8.55 | 1.34 | 1.52 |
| 2 | B | 459 | TYR | CD2-CE2 | 8.55 | 1.52 | 1.39 |
| 1 | A | 1411 | GLU | CD-OE1 | 8.55 | 1.35 | 1.25 |
| 3 | C | 180 | TYR | CD1-CE1 | 8.55 | 1.52 | 1.39 |
| 1 | A | 1159 | ARG | NE-CZ | 8.53 | 1.44 | 1.33 |
| 1 | A | 553 | VAL | CB-CG1 | -8.53 | 1.34 | 1.52 |
| 1 | A | 1355 | VAL | CA-CB | -8.53 | 1.36 | 1.54 |
| 2 | B | 138 | GLU | CD-OE2 | -8.53 | 1.16 | 1.25 |
| 1 | A | 304 | MET | SD-CE | 8.53 | 2.25 | 1.77 |
| 1 | A | 893 | PHE | CG-CD1 | -8.53 | 1.25 | 1.38 |
| 2 | B | 488 | TYR | CE1-CZ | -8.53 | 1.27 | 1.38 |
| 2 | B | 592 | ASN | CG-OD1 | 8.52 | 1.42 | 1.24 |
| 2 | B | 28 | GLU | CG-CD | 8.52 | 1.64 | 1.51 |
| 2 | B | 1135 | ARG | NE-CZ | -8.52 | 1.22 | 1.33 |
| 9 | K | 105 | PHE | CD1-CE1 | -8.51 | 1.22 | 1.39 |
| 3 | C | 108 | GLU | CG-CD | 8.51 | 1.64 | 1.51 |
| 2 | B | 389 | ALA | CA-CB | -8.51 | 1.34 | 1.52 |
| 1 | A | 498 | ARG | CZ-NH2 | -8.50 | 1.22 | 1.33 |
| 7 | I | 11 | ASN | CG-OD1 | -8.50 | 1.05 | 1.24 |
| 1 | A | 589 | GLN | CG-CD | 8.49 | 1.70 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1359 | ASP | CB-CG | 8.49 | 1.69 | 1.51 |
| 2 | B | 641 | GLU | CD-OE2 | 8.49 | 1.34 | 1.25 |
| 3 | C | 75 | MET | SD-CE | 8.49 | 2.25 | 1.77 |
| 1 | A | 481 | ASP | CG-OD2 | 8.48 | 1.44 | 1.25 |
| 2 | B | 569 | TYR | CG-CD2 | -8.48 | 1.28 | 1.39 |
| 2 | B | 797 | TYR | CD1-CE1 | 8.48 | 1.52 | 1.39 |
| 9 | K | 79 | GLU | CG-CD | 8.48 | 1.64 | 1.51 |
| 2 | B | 1092 | TYR | CG-CD1 | -8.48 | 1.28 | 1.39 |
| 1 | A | 1280 | GLU | CD-OE1 | 8.48 | 1.34 | 1.25 |
| 3 | C | 51 | VAL | CB-CG1 | -8.48 | 1.35 | 1.52 |
| 1 | A | 421 | ALA | CA-CB | -8.47 | 1.34 | 1.52 |
| 1 | A | 688 | LYS | CD-CE | 8.47 | 1.72 | 1.51 |
| 1 | A | 1234 | GLU | CG-CD | 8.47 | 1.64 | 1.51 |
| 1 | A | 404 | TYR | CE2-CZ | -8.45 | 1.27 | 1.38 |
| 2 | B | 531 | GLN | CD-NE2 | 8.44 | 1.53 | 1.32 |
| 1 | A | 69 | THR | CA-C | 8.43 | 1.74 | 1.52 |
| 3 | C | 106 | GLU | CD-OE1 | 8.43 | 1.34 | 1.25 |
| 6 | H | 126 | GLU | CG-CD | 8.43 | 1.64 | 1.51 |
| 7 | I | 34 | TYR | CG-CD2 | -8.43 | 1.28 | 1.39 |
| 2 | B | 883 | LEU | CA-CB | 8.43 | 1.73 | 1.53 |
| 3 | C | 135 | GLN | CG-CD | 8.43 | 1.70 | 1.51 |
| 2 | B | 462 | ALA | CA-CB | -8.43 | 1.34 | 1.52 |
| 1 | A | 1103 | GLU | CD-OE1 | 8.42 | 1.34 | 1.25 |
| 9 | K | 22 | ASP | CB-CG | 8.42 | 1.69 | 1.51 |
| 8 | J | 48 | ARG | CZ-NH2 | -8.41 | 1.22 | 1.33 |
| 2 | B | 319 | GLU | CD-OE2 | 8.40 | 1.34 | 1.25 |
| 1 | A | 836 | TYR | CE2-CZ | 8.40 | 1.49 | 1.38 |
| 2 | B | 622 | LYS | CE-NZ | 8.40 | 1.70 | 1.49 |
| 1 | A | 977 | LYS | CB-CG | 8.39 | 1.75 | 1.52 |
| 4 | E | 20 | LYS | CD-CE | 8.39 | 1.72 | 1.51 |
| 2 | B | 227 | LYS | CE-NZ | 8.38 | 1.70 | 1.49 |
| 2 | B | 108 | VAL | CB-CG2 | 8.38 | 1.70 | 1.52 |
| 10 | L | 25 | ALA | CA-CB | 8.38 | 1.70 | 1.52 |
| 2 | B | 668 | ASP | CB-CG | 8.38 | 1.69 | 1.51 |
| 9 | K | 47 | ARG | CZ-NH1 | 8.38 | 1.44 | 1.33 |
| 1 | A | 1349 | TYR | CE1-CZ | -8.38 | 1.27 | 1.38 |
| 2 | B | 1215 | ARG | CG-CD | 8.37 | 1.72 | 1.51 |
| 3 | C | 143 | LEU | C-O | -8.37 | 1.07 | 1.23 |
| 1 | A | 1280 | GLU | C-O | -8.37 | 1.07 | 1.23 |
| 1 | A | 1422 | ARG | NE-CZ | 8.37 | 1.44 | 1.33 |
| 4 | E | 28 | TYR | CE2-CZ | -8.37 | 1.27 | 1.38 |
| 2 | B | 485 | ARG | CG-CD | -8.36 | 1.31 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 379 | VAL | CB-CG1 | -8.36 | 1.35 | 1.52 |
| 4 | E | 42 | PHE | CD1-CE1 | 8.36 | 1.55 | 1.39 |
| 1 | A | 74 | MET | CB-CG | 8.36 | 1.78 | 1.51 |
| 2 | B | 797 | TYR | CG-CD1 | -8.35 | 1.28 | 1.39 |
| 1 | A | 49 | LYS | CD-CE | 8.35 | 1.72 | 1.51 |
| 1 | A | 1351 | GLU | CD-OE2 | 8.35 | 1.34 | 1.25 |
| 1 | A | 551 | TYR | CD2-CE2 | -8.34 | 1.26 | 1.39 |
| 2 | B | 769 | TYR | CE1-CZ | -8.34 | 1.27 | 1.38 |
| 1 | A | 1132 | LYS | CG-CD | 8.33 | 1.80 | 1.52 |
| 2 | B | 271 | ALA | CA-CB | -8.33 | 1.34 | 1.52 |
| 3 | C | 84 | ARG | C-O | -8.32 | 1.07 | 1.23 |
| 1 | A | 277 | GLU | CD-OE2 | 8.31 | 1.34 | 1.25 |
| 1 | A | 1363 | VAL | CB-CG1 | 8.31 | 1.70 | 1.52 |
| 1 | A | 897 | TYR | CG-CD2 | -8.31 | 1.28 | 1.39 |
| 5 | F | 137 | TYR | CD2-CE2 | -8.31 | 1.26 | 1.39 |
| 4 | E | 4 | GLU | CD-OE1 | -8.30 | 1.16 | 1.25 |
| 2 | B | 246 | LYS | N-CA | 8.30 | 1.62 | 1.46 |
| 7 | I | 91 | ARG | C-O | -8.29 | 1.07 | 1.23 |
| 1 | A | 1269 | GLU | CD-OE1 | 8.28 | 1.34 | 1.25 |
| 7 | I | 120 | GLN | CB-CG | 8.28 | 1.74 | 1.52 |
| 9 | K | 54 | ARG | NE-CZ | 8.27 | 1.43 | 1.33 |
| 2 | B | 459 | TYR | CE1-CZ | 8.27 | 1.49 | 1.38 |
| 1 | A | 1235 | LYS | CD-CE | 8.27 | 1.72 | 1.51 |
| 2 | B | 458 | LYS | C-O | -8.27 | 1.07 | 1.23 |
| 3 | C | 137 | LYS | CD-CE | 8.26 | 1.72 | 1.51 |
| 3 | C | 9 | LYS | CD-CE | 8.26 | 1.71 | 1.51 |
| 2 | B | 994 | TYR | CG-CD2 | -8.26 | 1.28 | 1.39 |
| 3 | C | 225 | ALA | CA-CB | -8.26 | 1.35 | 1.52 |
| 2 | B | 209 | GLU | CD-OE2 | -8.26 | 1.16 | 1.25 |
| 2 | B | 1061 | GLU | CD-OE1 | 8.25 | 1.34 | 1.25 |
| 1 | A | 419 | LYS | C-O | -8.24 | 1.07 | 1.23 |
| 2 | B | 404 | LYS | CE-NZ | -8.24 | 1.28 | 1.49 |
| 1 | A | 376 | TYR | CG-CD1 | -8.24 | 1.28 | 1.39 |
| 2 | B | 908 | GLU | CB-CG | 8.24 | 1.67 | 1.52 |
| 3 | C | 78 | GLU | C-O | -8.23 | 1.07 | 1.23 |
| 1 | A | 697 | ALA | CA-CB | -8.22 | 1.35 | 1.52 |
| 1 | A | 712 | GLU | CD-OE2 | 8.22 | 1.34 | 1.25 |
| 2 | B | 641 | GLU | CB-CG | 8.22 | 1.67 | 1.52 |
| 2 | B | 874 | PHE | CD2-CE2 | -8.22 | 1.22 | 1.39 |
| 7 | I | 93 | LYS | CD-CE | 8.22 | 1.71 | 1.51 |
| 1 | A | 1157 | ASP | CB-CG | 8.21 | 1.69 | 1.51 |
| 1 | A | 1281 | ARG | NE-CZ | 8.20 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 731 | VAL | CB-CG2 | 8.20 | 1.70 | 1.52 |
| 1 | A | 1345 | ARG | NE-CZ | -8.19 | 1.22 | 1.33 |
| 1 | A | 1196 | GLU | CD-OE2 | 8.19 | 1.34 | 1.25 |
| 1 | A | 567 | LYS | CD-CE | 8.18 | 1.71 | 1.51 |
| 3 | C | 20 | PHE | CB-CG | -8.18 | 1.37 | 1.51 |
| 1 | A | 1119 | TYR | CG-CD1 | -8.18 | 1.28 | 1.39 |
| 1 | A | 1235 | LYS | CE-NZ | 8.18 | 1.69 | 1.49 |
| 2 | B | 204 | ILE | CA-CB | -8.18 | 1.36 | 1.54 |
| 4 | E | 131 | THR | CA-CB | 8.17 | 1.74 | 1.53 |
| 4 | E | 211 | TYR | CE2-CZ | -8.17 | 1.27 | 1.38 |
| 3 | C | 34 | ARG | CD-NE | -8.16 | 1.32 | 1.46 |
| 1 | A | 868 | TYR | CE2-CZ | -8.15 | 1.27 | 1.38 |
| 6 | H | 88 | SER | CA-CB | 8.15 | 1.65 | 1.52 |
| 2 | B | 183 | GLU | CG-CD | 8.15 | 1.64 | 1.51 |
| 7 | I | 101 | PHE | CB-CG | -8.14 | 1.37 | 1.51 |
| 1 | A | 359 | LEU | CA-CB | -8.14 | 1.35 | 1.53 |
| 8 | J | 21 | TYR | CA-CB | 8.14 | 1.71 | 1.53 |
| 3 | C | 252 | GLN | CB-CG | 8.13 | 1.74 | 1.52 |
| 1 | A | 622 | VAL | CA-CB | -8.12 | 1.37 | 1.54 |
| 3 | C | 15 | LYS | CD-CE | 8.12 | 1.71 | 1.51 |
| 1 | A | 875 | ALA | CA-CB | -8.12 | 1.35 | 1.52 |
| 4 | E | 102 | GLU | CG-CD | 8.12 | 1.64 | 1.51 |
| 4 | E | 191 | LYS | CD-CE | 8.12 | 1.71 | 1.51 |
| 1 | A | 870 | GLU | CD-OE2 | 8.11 | 1.34 | 1.25 |
| 2 | B | 245 | GLU | CA-C | 8.10 | 1.74 | 1.52 |
| 1 | A | 839 | ARG | CG-CD | 8.10 | 1.72 | 1.51 |
| 1 | A | 1381 | LEU | C-O | -8.10 | 1.07 | 1.23 |
| 6 | H | 116 | TYR | CG-CD1 | 8.10 | 1.49 | 1.39 |
| 3 | C | 106 | GLU | CD-OE2 | 8.09 | 1.34 | 1.25 |
| 9 | K | 36 | GLU | CA-CB | -8.09 | 1.36 | 1.53 |
| 1 | A | 386 | ASP | CB-CG | 8.08 | 1.68 | 1.51 |
| 1 | A | 1287 | TYR | C-O | 8.08 | 1.38 | 1.23 |
| 1 | A | 1362 | TYR | CE2-CZ | 8.07 | 1.49 | 1.38 |
| 7 | I | 42 | LEU | C-O | -8.07 | 1.08 | 1.23 |
| 1 | A | 1109 | LYS | CG-CD | 8.07 | 1.79 | 1.52 |
| 9 | K | 64 | GLU | CD-OE2 | -8.06 | 1.16 | 1.25 |
| 1 | A | 685 | GLU | CD-OE1 | 8.06 | 1.34 | 1.25 |
| 1 | A | 836 | TYR | CG-CD1 | 8.06 | 1.49 | 1.39 |
| 6 | H | 105 | GLU | CG-CD | 8.06 | 1.64 | 1.51 |
| 2 | B | 1040 | ASN | CB-CG | -8.05 | 1.32 | 1.51 |
| 4 | E | 50 | MET | CG-SD | 8.05 | 2.02 | 1.81 |
| 2 | B | 89 | GLU | CA-C | 8.05 | 1.73 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 699 | GLU | CD-OE1 | 8.05 | 1.34 | 1.25 |
| 2 | B | 519 | TRP | CZ3-CH2 | -8.04 | 1.27 | 1.40 |
| 2 | B | 646 | LEU | CG-CD2 | 8.04 | 1.81 | 1.51 |
| 8 | J | 48 | ARG | CG-CD | -8.03 | 1.31 | 1.51 |
| 7 | I | 54 | GLU | CD-OE2 | 8.03 | 1.34 | 1.25 |
| 4 | E | 93 | MET | CG-SD | 8.03 | 2.02 | 1.81 |
| 9 | K | 36 | GLU | CD-OE2 | 8.03 | 1.34 | 1.25 |
| 2 | B | 191 | LYS | CD-CE | 8.03 | 1.71 | 1.51 |
| 8 | J | 6 | ARG | CZ-NH1 | -8.02 | 1.22 | 1.33 |
| 9 | K | 71 | PHE | C-O | 8.02 | 1.38 | 1.23 |
| 1 | A | 990 | VAL | CA-CB | -8.01 | 1.38 | 1.54 |
| 1 | A | 1029 | ARG | CB-CG | -8.01 | 1.30 | 1.52 |
| 3 | C | 87 | PHE | CB-CG | -8.01 | 1.37 | 1.51 |
| 4 | E | 200 | ARG | NE-CZ | -8.01 | 1.22 | 1.33 |
| 2 | B | 747 | MET | SD-CE | -8.01 | 1.33 | 1.77 |
| 1 | A | 1109 | LYS | CD-CE | 8.00 | 1.71 | 1.51 |
| 2 | B | 337 | ARG | CD-NE | -8.00 | 1.32 | 1.46 |
| 3 | C | 267 | GLN | CA-C | 8.00 | 1.73 | 1.52 |
| 1 | A | 1424 | VAL | C-O | 8.00 | 1.38 | 1.23 |
| 9 | K | 16 | GLU | CG-CD | 8.00 | 1.64 | 1.51 |
| 9 | K | 35 | PHE | CE1-CZ | -7.99 | 1.22 | 1.37 |
| 1 | A | 1061 | GLY | CA-C | 7.99 | 1.64 | 1.51 |
| 1 | A | 1424 | VAL | CB-CG1 | -7.98 | 1.36 | 1.52 |
| 2 | B | 1171 | VAL | C-O | 7.96 | 1.38 | 1.23 |
| 1 | A | 468 | PHE | CE2-CZ | -7.96 | 1.22 | 1.37 |
| 2 | B | 242 | SER | CB-OG | 7.96 | 1.52 | 1.42 |
| 4 | E | 36 | GLU | C-O | -7.96 | 1.08 | 1.23 |
| 5 | F | 97 | ARG | CB-CG | -7.95 | 1.31 | 1.52 |
| 4 | E | 103 | LYS | CD-CE | 7.95 | 1.71 | 1.51 |
| 2 | B | 262 | GLU | CD-OE1 | 7.95 | 1.34 | 1.25 |
| 1 | A | 52 | GLY | C-O | -7.95 | 1.10 | 1.23 |
| 2 | B | 855 | PHE | CG-CD2 | -7.95 | 1.26 | 1.38 |
| 7 | I | 34 | TYR | CD2-CE2 | 7.94 | 1.51 | 1.39 |
| 1 | A | 69 | THR | CA-CB | 7.94 | 1.74 | 1.53 |
| 9 | K | 91 | CYS | CB-SG | -7.94 | 1.68 | 1.82 |
| 1 | A | 714 | PHE | CD1-CE1 | -7.94 | 1.23 | 1.39 |
| 6 | H | 23 | VAL | CA-CB | -7.94 | 1.38 | 1.54 |
| 2 | B | 1155 | SER | N-CA | 7.93 | 1.62 | 1.46 |
| 2 | B | 130 | VAL | CB-CG2 | -7.93 | 1.36 | 1.52 |
| 1 | A | 469 | ARG | CD-NE | -7.93 | 1.32 | 1.46 |
| 2 | B | 32 | ALA | CA-CB | 7.93 | 1.69 | 1.52 |
| 2 | B | 1002 | THR | CA-C | 7.93 | 1.73 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 646 | LEU | CG-CD1 | 7.92 | 1.81 | 1.51 |
| 1 | A | 1338 | VAL | CB-CG2 | -7.92 | 1.36 | 1.52 |
| 9 | K | 79 | GLU | CD-OE1 | 7.92 | 1.34 | 1.25 |
| 4 | E | 37 | LEU | CG-CD1 | 7.92 | 1.81 | 1.51 |
| 2 | B | 512 | ARG | CZ-NH1 | 7.92 | 1.43 | 1.33 |
| 6 | H | 107 | VAL | CA-CB | 7.92 | 1.71 | 1.54 |
| 1 | A | 738 | LYS | C-O | -7.92 | 1.08 | 1.23 |
| 9 | K | 20 | LYS | CD-CE | 7.91 | 1.71 | 1.51 |
| 2 | B | 589 | VAL | CB-CG2 | -7.91 | 1.36 | 1.52 |
| 1 | A | 1362 | TYR | CE1-CZ | -7.91 | 1.28 | 1.38 |
| 2 | B | 337 | ARG | NE-CZ | -7.90 | 1.22 | 1.33 |
| 3 | C | 97 | VAL | CA-CB | -7.90 | 1.38 | 1.54 |
| 7 | I | 21 | GLU | C-O | -7.90 | 1.08 | 1.23 |
| 2 | B | 259 | TYR | CE1-CZ | -7.90 | 1.28 | 1.38 |
| 2 | B | 662 | MET | C-O | -7.90 | 1.08 | 1.23 |
| 2 | B | 1053 | GLU | CD-OE2 | 7.89 | 1.34 | 1.25 |
| 2 | B | 1086 | PHE | CG-CD1 | -7.89 | 1.26 | 1.38 |
| 4 | E | 102 | GLU | CD-OE2 | 7.89 | 1.34 | 1.25 |
| 1 | A | 733 | ALA | C-O | -7.89 | 1.08 | 1.23 |
| 1 | A | 558 | GLY | C-O | -7.88 | 1.11 | 1.23 |
| 1 | A | 940 | ARG | CD-NE | -7.88 | 1.33 | 1.46 |
| 1 | A | 1220 | PHE | CG-CD1 | -7.88 | 1.26 | 1.38 |
| 1 | A | 1336 | MET | CG-SD | -7.88 | 1.60 | 1.81 |
| 2 | B | 184 | ALA | C-O | -7.87 | 1.08 | 1.23 |
| 2 | B | 1101 | ASP | CA-C | 7.87 | 1.73 | 1.52 |
| 1 | A | 874 | ASP | CG-OD2 | 7.86 | 1.43 | 1.25 |
| 2 | B | 19 | GLU | CG-CD | 7.85 | 1.63 | 1.51 |
| 3 | C | 84 | ARG | NE-CZ | 7.85 | 1.43 | 1.33 |
| 2 | B | 176 | SER | CB-OG | -7.84 | 1.32 | 1.42 |
| 2 | B | 759 | PRO | C-O | 7.84 | 1.39 | 1.23 |
| 7 | I | 110 | PHE | CD1-CE1 | 7.84 | 1.54 | 1.39 |
| 7 | I | 34 | TYR | CE2-CZ | -7.84 | 1.28 | 1.38 |
| 1 | A | 1232 | ASN | CG-OD1 | 7.84 | 1.41 | 1.24 |
| 2 | B | 227 | LYS | CD-CE | 7.83 | 1.70 | 1.51 |
| 2 | B | 346 | GLU | CD-OE2 | 7.82 | 1.34 | 1.25 |
| 2 | B | 1097 | HIS | CA-C | 7.82 | 1.73 | 1.52 |
| 1 | A | 813 | PHE | CE1-CZ | -7.82 | 1.22 | 1.37 |
| 2 | B | 250 | PHE | CD2-CE2 | 7.82 | 1.54 | 1.39 |
| 1 | A | 478 | TYR | CE1-CZ | -7.81 | 1.28 | 1.38 |
| 7 | I | 101 | PHE | CD1-CE1 | 7.81 | 1.54 | 1.39 |
| 6 | H | 2 | SER | CA-C | 7.81 | 1.73 | 1.52 |
| 1 | A | 264 | PHE | CG-CD2 | 7.81 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 671 | ALA | CA-CB | -7.80 | 1.36 | 1.52 |
| 2 | B | 218 | SER | C-O | -7.80 | 1.08 | 1.23 |
| 5 | F | 77 | ASP | C-O | 7.80 | 1.38 | 1.23 |
| 2 | B | 856 | PHE | CE2-CZ | 7.79 | 1.52 | 1.37 |
| 1 | A | 1350 | LYS | CG-CD | 7.79 | 1.78 | 1.52 |
| 2 | B | 652 | LYS | CD-CE | 7.79 | 1.70 | 1.51 |
| 2 | B | 843 | GLN | CG-CD | -7.79 | 1.33 | 1.51 |
| 2 | B | 313 | MET | SD-CE | -7.79 | 1.34 | 1.77 |
| 2 | B | 1154 | ALA | CA-C | 7.78 | 1.73 | 1.52 |
| 1 | A | 25 | GLU | CG-CD | 7.78 | 1.63 | 1.51 |
| 1 | A | 685 | GLU | CG-CD | 7.78 | 1.63 | 1.51 |
| 9 | K | 110 | ASN | CB-CG | 7.78 | 1.69 | 1.51 |
| 2 | B | 459 | TYR | CG-CD1 | 7.78 | 1.49 | 1.39 |
| 6 | H | 95 | TYR | CD1-CE1 | 7.78 | 1.51 | 1.39 |
| 2 | B | 612 | GLU | CD-OE1 | 7.77 | 1.34 | 1.25 |
| 1 | A | 4 | GLN | CB-CG | 7.77 | 1.73 | 1.52 |
| 2 | B | 194 | GLU | CG-CD | 7.77 | 1.63 | 1.51 |
| 1 | A | 870 | GLU | CD-OE1 | 7.77 | 1.34 | 1.25 |
| 1 | A | 1112 | LYS | CD-CE | 7.77 | 1.70 | 1.51 |
| 1 | A | 1288 | ASP | CG-OD1 | 7.77 | 1.43 | 1.25 |
| 7 | I | 61 | ASP | C-O | -7.77 | 1.08 | 1.23 |
| 3 | C | 172 | PRO | CA-C | -7.76 | 1.37 | 1.52 |
| 2 | B | 250 | PHE | CB-CG | 7.76 | 1.64 | 1.51 |
| 1 | A | 1314 | SER | CA-CB | -7.75 | 1.41 | 1.52 |
| 1 | A | 806 | ARG | CZ-NH1 | 7.75 | 1.43 | 1.33 |
| 2 | B | 216 | GLU | CG-CD | 7.74 | 1.63 | 1.51 |
| 6 | H | 19 | ARG | CD-NE | 7.74 | 1.59 | 1.46 |
| 1 | A | 1044 | TRP | CB-CG | -7.74 | 1.36 | 1.50 |
| 2 | B | 733 | HIS | N-CA | 7.74 | 1.61 | 1.46 |
| 4 | E | 1 | MET | SD-CE | 7.73 | 2.21 | 1.77 |
| 1 | A | 98 | LYS | CD-CE | 7.73 | 1.70 | 1.51 |
| 1 | A | 1074 | GLU | CD-OE1 | 7.73 | 1.34 | 1.25 |
| 2 | B | 228 | LYS | CB-CG | 7.73 | 1.73 | 1.52 |
| 2 | B | 1102 | LYS | N-CA | 7.73 | 1.61 | 1.46 |
| 2 | B | 318 | VAL | CB-CG2 | -7.72 | 1.36 | 1.52 |
| 2 | B | 394 | ASP | CB-CG | 7.72 | 1.68 | 1.51 |
| 3 | C | 106 | GLU | CG-CD | 7.72 | 1.63 | 1.51 |
| 9 | K | 54 | ARG | CG-CD | 7.72 | 1.71 | 1.51 |
| 1 | A | 900 | ASP | C-O | 7.71 | 1.38 | 1.23 |
| 2 | B | 39 | ARG | NE-CZ | 7.71 | 1.43 | 1.33 |
| 1 | A | 71 | GLN | CG-CD | 7.71 | 1.68 | 1.51 |
| 1 | A | 1419 | ASP | CG-OD2 | 7.70 | 1.43 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | I | 15 | TYR | CG-CD2 | -7.70 | 1.29 | 1.39 |
| 1 | A | 747 | VAL | CB-CG1 | -7.69 | 1.36 | 1.52 |
| 6 | H | 3 | ASN | CB-CG | 7.69 | 1.68 | 1.51 |
| 1 | A | 792 | TYR | CG-CD1 | -7.69 | 1.29 | 1.39 |
| 3 | C | 117 | ASP | C-O | 7.69 | 1.38 | 1.23 |
| 4 | E | 207 | ARG | CG-CD | 7.68 | 1.71 | 1.51 |
| 1 | A | 933 | TYR | CG-CD1 | -7.68 | 1.29 | 1.39 |
| 2 | B | 188 | ASP | C-O | 7.68 | 1.38 | 1.23 |
| 1 | A | 1275 | GLY | C-O | 7.67 | 1.35 | 1.23 |
| 6 | H | 104 | PHE | CE2-CZ | 7.67 | 1.51 | 1.37 |
| 2 | B | 414 | ALA | CA-CB | -7.67 | 1.36 | 1.52 |
| 2 | B | 371 | GLU | CG-CD | 7.67 | 1.63 | 1.51 |
| 9 | K | 16 | GLU | CD-OE1 | 7.67 | 1.34 | 1.25 |
| 2 | B | 1092 | TYR | CE1-CZ | -7.67 | 1.28 | 1.38 |
| 2 | B | 1100 | ASP | CB-CG | 7.66 | 1.67 | 1.51 |
| 1 | A | 896 | ARG | CZ-NH1 | 7.66 | 1.43 | 1.33 |
| 1 | A | 897 | TYR | CE1-CZ | -7.66 | 1.28 | 1.38 |
| 1 | A | 1045 | VAL | CA-CB | -7.65 | 1.38 | 1.54 |
| 2 | B | 978 | ASP | CB-CG | 7.65 | 1.67 | 1.51 |
| 6 | H | 118 | PHE | CG-CD1 | 7.64 | 1.50 | 1.38 |
| 1 | A | 1264 | GLU | CD-OE1 | -7.64 | 1.17 | 1.25 |
| 3 | C | 252 | GLN | CD-OE1 | 7.64 | 1.40 | 1.24 |
| 6 | H | 102 | TYR | CG-CD2 | -7.64 | 1.29 | 1.39 |
| 1 | A | 1326 | ARG | C-O | -7.64 | 1.08 | 1.23 |
| 6 | H | 104 | PHE | CG-CD1 | 7.64 | 1.50 | 1.38 |
| 1 | A | 969 | GLN | CG-CD | 7.63 | 1.68 | 1.51 |
| 3 | C | 186 | LEU | CA-C | 7.63 | 1.72 | 1.52 |
| 4 | E | 179 | GLN | CD-OE1 | 7.63 | 1.40 | 1.24 |
| 1 | A | 603 | ASN | CB-CG | -7.63 | 1.33 | 1.51 |
| 1 | A | 774 | ARG | CD-NE | -7.63 | 1.33 | 1.46 |
| 4 | E | 212 | ARG | CZ-NH1 | -7.63 | 1.23 | 1.33 |
| 10 | L | 37 | LYS | C-O | -7.63 | 1.08 | 1.23 |
| 2 | B | 250 | PHE | CG-CD2 | 7.63 | 1.50 | 1.38 |
| 1 | A | 1101 | LEU | N-CA | -7.62 | 1.31 | 1.46 |
| 1 | A | 1129 | GLU | CD-OE1 | 7.62 | 1.34 | 1.25 |
| 5 | F | 88 | TYR | CD2-CE2 | -7.62 | 1.27 | 1.39 |
| 4 | E | 65 | THR | C-O | 7.61 | 1.37 | 1.23 |
| 1 | A | 644 | LYS | C-O | -7.61 | 1.08 | 1.23 |
| 4 | E | 45 | LYS | CD-CE | 7.60 | 1.70 | 1.51 |
| 3 | C | 163 | ILE | CA-CB | -7.60 | 1.37 | 1.54 |
| 1 | A | 1422 | ARG | CZ-NH1 | 7.60 | 1.43 | 1.33 |
| 2 | B | 1155 | SER | CB-OG | 7.60 | 1.52 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | J | 27 | GLU | CD-OE1 | 7.60 | 1.34 | 1.25 |
| 2 | B | 231 | PRO | CA-C | 7.59 | 1.68 | 1.52 |
| 2 | B | 848 | ARG | NE-CZ | -7.59 | 1.23 | 1.33 |
| 2 | B | 986 | GLN | CB-CG | 7.59 | 1.73 | 1.52 |
| 2 | B | 240 | ILE | C-O | -7.58 | 1.08 | 1.23 |
| 2 | B | 751 | VAL | CB-CG1 | -7.58 | 1.36 | 1.52 |
| 2 | B | 261 | ARG | NE-CZ | 7.58 | 1.43 | 1.33 |
| 1 | A | 1350 | LYS | CD-CE | 7.57 | 1.70 | 1.51 |
| 9 | K | 6 | ARG | CB-CG | -7.57 | 1.32 | 1.52 |
| 1 | A | 933 | TYR | CE2-CZ | -7.56 | 1.28 | 1.38 |
| 2 | B | 303 | TYR | CD2-CE2 | -7.56 | 1.28 | 1.39 |
| 3 | C | 50 | GLU | CB-CG | 7.56 | 1.66 | 1.52 |
| 5 | F | 100 | GLN | CG-CD | 7.56 | 1.68 | 1.51 |
| 5 | F | 143 | PHE | C-O | -7.56 | 1.08 | 1.23 |
| 1 | A | 1105 | LEU | C-O | -7.56 | 1.08 | 1.23 |
| 1 | A | 1358 | SER | CB-OG | 7.55 | 1.52 | 1.42 |
| 2 | B | 250 | PHE | CD1-CE1 | 7.55 | 1.54 | 1.39 |
| 1 | A | 1383 | SER | CA-CB | -7.55 | 1.41 | 1.52 |
| 4 | E | 71 | LYS | N-CA | 7.55 | 1.61 | 1.46 |
| 4 | E | 67 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | A | 364 | VAL | CB-CG1 | -7.54 | 1.37 | 1.52 |
| 2 | B | 33 | VAL | CB-CG1 | -7.54 | 1.37 | 1.52 |
| 2 | B | 245 | GLU | CB-CG | 7.54 | 1.66 | 1.52 |
| 2 | B | 810 | GLU | CG-CD | 7.54 | 1.63 | 1.51 |
| 1 | A | 908 | LEU | C-O | -7.54 | 1.09 | 1.23 |
| 4 | E | 85 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 9 | K | 81 | TYR | CD1-CE1 | -7.53 | 1.28 | 1.39 |
| 1 | A | 468 | PHE | CG-CD1 | -7.53 | 1.27 | 1.38 |
| 9 | K | 61 | TYR | CD2-CE2 | 7.53 | 1.50 | 1.39 |
| 1 | A | 1144 | LYS | CD-CE | 7.52 | 1.70 | 1.51 |
| 2 | B | 1091 | TYR | C-O | -7.52 | 1.09 | 1.23 |
| 1 | A | 366 | VAL | C-N | -7.51 | 1.20 | 1.34 |
| 1 | A | 1307 | GLU | CD-OE1 | 7.51 | 1.33 | 1.25 |
| 6 | H | 37 | LYS | C-O | 7.51 | 1.37 | 1.23 |
| 1 | A | 961 | ARG | NE-CZ | 7.51 | 1.42 | 1.33 |
| 1 | A | 451 | HIS | CA-CB | -7.51 | 1.37 | 1.53 |
| 4 | E | 112 | TYR | CD1-CE1 | 7.51 | 1.50 | 1.39 |
| 2 | B | 344 | LYS | CD-CE | 7.50 | 1.70 | 1.51 |
| 7 | I | 6 | PHE | CE1-CZ | -7.50 | 1.23 | 1.37 |
| 1 | A | 939 | ASP | CB-CG | 7.49 | 1.67 | 1.51 |
| 2 | B | 870 | ILE | N-CA | 7.49 | 1.61 | 1.46 |
| 5 | F | 76 | LYS | CD-CE | 7.49 | 1.70 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 836 | TYR | CE1-CZ | 7.49 | 1.48 | 1.38 |
| 1 | A | 647 | GLY | CA-C | 7.49 | 1.63 | 1.51 |
| 2 | B | 811 | TYR | CE2-CZ | -7.49 | 1.28 | 1.38 |
| 4 | E | 148 | GLU | CD-OE2 | 7.49 | 1.33 | 1.25 |
| 2 | B | 608 | ASP | C-O | -7.48 | 1.09 | 1.23 |
| 1 | A | 933 | TYR | CE1-CZ | -7.48 | 1.28 | 1.38 |
| 4 | E | 129 | PRO | CG-CD | 7.48 | 1.75 | 1.50 |
| 3 | C | 114 | TYR | CG-CD2 | -7.47 | 1.29 | 1.39 |
| 1 | A | 879 | GLU | CG-CD | 7.47 | 1.63 | 1.51 |
| 2 | B | 957 | ASN | CA-C | 7.46 | 1.72 | 1.52 |
| 9 | K | 94 | ILE | CA-CB | 7.46 | 1.72 | 1.54 |
| 1 | A | 486 | GLU | CD-OE2 | -7.46 | 1.17 | 1.25 |
| 1 | A | 1290 | LYS | CD-CE | 7.46 | 1.69 | 1.51 |
| 8 | J | 37 | SER | CA-CB | -7.45 | 1.41 | 1.52 |
| 9 | K | 26 | LYS | CG-CD | 7.45 | 1.77 | 1.52 |
| 10 | L | 43 | THR | CB-CG2 | 7.45 | 1.76 | 1.52 |
| 1 | A | 1434 | ALA | CA-CB | -7.45 | 1.36 | 1.52 |
| 3 | C | 94 | LYS | CE-NZ | 7.45 | 1.67 | 1.49 |
| 4 | E | 7 | ARG | NE-CZ | 7.45 | 1.42 | 1.33 |
| 2 | B | 1129 | ARG | NE-CZ | 7.44 | 1.42 | 1.33 |
| 2 | B | 1130 | PHE | CE1-CZ | -7.44 | 1.23 | 1.37 |
| 1 | A | 1256 | GLU | CG-CD | 7.44 | 1.63 | 1.51 |
| 3 | C | 179 | GLU | CD-OE1 | -7.44 | 1.17 | 1.25 |
| 4 | E | 192 | ARG | CZ-NH2 | 7.44 | 1.42 | 1.33 |
| 2 | B | 758 | PHE | CG-CD2 | -7.43 | 1.27 | 1.38 |
| 2 | B | 1080 | LYS | CD-CE | 7.43 | 1.69 | 1.51 |
| 2 | B | 567 | GLU | CD-OE2 | 7.43 | 1.33 | 1.25 |
| 5 | F | 153 | VAL | CB-CG2 | -7.43 | 1.37 | 1.52 |
| 1 | A | 894 | GLU | CG-CD | 7.42 | 1.63 | 1.51 |
| 1 | A | 469 | ARG | CZ-NH2 | -7.42 | 1.23 | 1.33 |
| 2 | B | 547 | VAL | CB-CG1 | -7.42 | 1.37 | 1.52 |
| 1 | A | 293 | GLU | CD-OE1 | 7.42 | 1.33 | 1.25 |
| 6 | H | 91 | ASP | CA-C | 7.42 | 1.72 | 1.52 |
| 9 | K | 86 | ALA | CA-CB | -7.42 | 1.36 | 1.52 |
| 1 | A | 1121 | GLU | CG-CD | 7.42 | 1.63 | 1.51 |
| 2 | B | 41 | LYS | CD-CE | 7.42 | 1.69 | 1.51 |
| 2 | B | 612 | GLU | CG-CD | 7.41 | 1.63 | 1.51 |
| 7 | I | 58 | VAL | CB-CG1 | -7.41 | 1.37 | 1.52 |
| 1 | A | 1152 | ILE | CA-CB | -7.41 | 1.37 | 1.54 |
| 4 | E | 192 | ARG | CD-NE | 7.40 | 1.59 | 1.46 |
| 5 | F | 123 | LYS | CE-NZ | 7.40 | 1.67 | 1.49 |
| 1 | A | 566 | ILE | CB-CG2 | 7.40 | 1.75 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 55 | THR | C-O | 7.39 | 1.37 | 1.23 |
| 2 | B | 692 | TYR | C-O | -7.39 | 1.09 | 1.23 |
| 2 | B | 377 | PHE | CB-CG | -7.39 | 1.38 | 1.51 |
| 1 | A | 392 | VAL | CA-CB | -7.38 | 1.39 | 1.54 |
| 2 | B | 327 | ARG | CB-CG | -7.38 | 1.32 | 1.52 |
| 1 | A | 842 | VAL | C-O | -7.38 | 1.09 | 1.23 |
| 1 | A | 1210 | GLY | C-O | 7.38 | 1.35 | 1.23 |
| 9 | K | 20 | LYS | CG-CD | 7.37 | 1.77 | 1.52 |
| 2 | B | 325 | GLN | CB-CG | -7.37 | 1.32 | 1.52 |
| 7 | I | 30 | ARG | CG-CD | 7.37 | 1.70 | 1.51 |
| 2 | B | 1188 | LYS | CD-CE | 7.36 | 1.69 | 1.51 |
| 1 | A | 1027 | ALA | C-O | 7.36 | 1.37 | 1.23 |
| 7 | I | 56 | ALA | C-O | -7.36 | 1.09 | 1.23 |
| 1 | A | 941 | LYS | CB-CG | -7.35 | 1.32 | 1.52 |
| 10 | L | 26 | THR | N-CA | 7.35 | 1.61 | 1.46 |
| 1 | A | 1285 | MET | CG-SD | 7.34 | 2.00 | 1.81 |
| 2 | B | 194 | GLU | CB-CG | 7.34 | 1.66 | 1.52 |
| 2 | B | 360 | PHE | CE2-CZ | -7.34 | 1.23 | 1.37 |
| 1 | A | 1420 | ASP | CG-OD2 | 7.33 | 1.42 | 1.25 |
| 5 | F | 149 | GLU | CG-CD | 7.33 | 1.62 | 1.51 |
| 2 | B | 1083 | ALA | CA-CB | -7.33 | 1.37 | 1.52 |
| 1 | A | 787 | PHE | CB-CG | -7.33 | 1.38 | 1.51 |
| 3 | C | 122 | SER | CA-CB | 7.32 | 1.64 | 1.52 |
| 1 | A | 1227 | ILE | C-O | -7.32 | 1.09 | 1.23 |
| 2 | B | 694 | ASP | CB-CG | 7.32 | 1.67 | 1.51 |
| 1 | A | 687 | LYS | CE-NZ | 7.31 | 1.67 | 1.49 |
| 2 | B | 38 | PHE | CD2-CE2 | -7.31 | 1.24 | 1.39 |
| 2 | B | 1036 | ALA | CA-CB | 7.31 | 1.67 | 1.52 |
| 3 | C | 161 | LYS | CD-CE | -7.31 | 1.32 | 1.51 |
| 7 | I | 99 | LEU | C-O | -7.31 | 1.09 | 1.23 |
| 1 | A | 644 | LYS | CD-CE | 7.31 | 1.69 | 1.51 |
| 1 | A | 1385 | THR | CA-C | 7.31 | 1.72 | 1.52 |
| 2 | B | 882 | THR | N-CA | 7.31 | 1.60 | 1.46 |
| 5 | F | 90 | ARG | NE-CZ | -7.31 | 1.23 | 1.33 |
| 2 | B | 614 | SER | CB-OG | -7.30 | 1.32 | 1.42 |
| 2 | B | 1052 | VAL | CB-CG2 | -7.30 | 1.37 | 1.52 |
| 3 | C | 154 | LYS | CB-CG | 7.30 | 1.72 | 1.52 |
| 1 | A | 788 | SER | CA-CB | 7.30 | 1.63 | 1.52 |
| 1 | A | 1298 | TYR | CG-CD1 | -7.30 | 1.29 | 1.39 |
| 1 | A | 1362 | TYR | CB-CG | -7.30 | 1.40 | 1.51 |
| 4 | E | 194 | GLU | CD-OE2 | -7.30 | 1.17 | 1.25 |
| 1 | A | 705 | LYS | CA-CB | 7.29 | 1.70 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1138 | ILE | C-O | 7.29 | 1.37 | 1.23 |
| 3 | C | 183 | TRP | CE2-CZ2 | -7.29 | 1.27 | 1.39 |
| 1 | A | 677 | ARG | CZ-NH1 | 7.29 | 1.42 | 1.33 |
| 2 | B | 1106 | ARG | CA-C | 7.29 | 1.72 | 1.52 |
| 6 | H | 93 | TYR | CG-CD1 | 7.29 | 1.48 | 1.39 |
| 2 | B | 208 | SER | CB-OG | -7.29 | 1.32 | 1.42 |
| 6 | H | 63 | LEU | C-O | 7.29 | 1.37 | 1.23 |
| 8 | J | 29 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | A | 268 | ASP | CB-CG | 7.28 | 1.67 | 1.51 |
| 1 | A | 1376 | THR | CB-CG2 | -7.28 | 1.28 | 1.52 |
| 1 | A | 1237 | ILE | N-CA | -7.28 | 1.31 | 1.46 |
| 2 | B | 564 | GLU | CD-OE2 | 7.28 | 1.33 | 1.25 |
| 1 | A | 352 | VAL | CB-CG2 | 7.28 | 1.68 | 1.52 |
| 1 | A | 1191 | TRP | CB-CG | -7.28 | 1.37 | 1.50 |
| 1 | A | 1299 | VAL | CB-CG1 | -7.28 | 1.37 | 1.52 |
| 2 | B | 593 | PRO | CB-CG | 7.28 | 1.86 | 1.50 |
| 6 | H | 104 | PHE | CE1-CZ | 7.27 | 1.51 | 1.37 |
| 9 | K | 55 | LYS | CB-CG | 7.27 | 1.72 | 1.52 |
| 1 | A | 1272 | THR | CB-CG2 | 7.27 | 1.76 | 1.52 |
| 6 | H | 48 | PRO | C-O | 7.27 | 1.37 | 1.23 |
| 2 | B | 200 | GLY | C-O | -7.27 | 1.12 | 1.23 |
| 1 | A | 509 | LEU | C-O | -7.26 | 1.09 | 1.23 |
| 3 | C | 114 | TYR | CD2-CE2 | -7.26 | 1.28 | 1.39 |
| 6 | H | 2 | SER | CA-CB | 7.26 | 1.63 | 1.52 |
| 1 | A | 551 | TYR | CE2-CZ | -7.26 | 1.29 | 1.38 |
| 1 | A | 1259 | MET | SD-CE | 7.26 | 2.18 | 1.77 |
| 1 | A | 811 | GLN | N-CA | -7.25 | 1.31 | 1.46 |
| 2 | B | 70 | ILE | CA-CB | 7.25 | 1.71 | 1.54 |
| 2 | B | 391 | ASP | C-O | -7.25 | 1.09 | 1.23 |
| 2 | B | 319 | GLU | CB-CG | 7.25 | 1.66 | 1.52 |
| 2 | B | 733 | HIS | CA-C | 7.25 | 1.71 | 1.52 |
| 1 | A | 756 | ILE | CB-CG2 | -7.25 | 1.30 | 1.52 |
| 3 | C | 70 | ILE | N-CA | 7.25 | 1.60 | 1.46 |
| 2 | B | 108 | VAL | CA-CB | 7.25 | 1.70 | 1.54 |
| 2 | B | 570 | VAL | CB-CG1 | -7.24 | 1.37 | 1.52 |
| 10 | L | 42 | ARG | NE-CZ | 7.24 | 1.42 | 1.33 |
| 1 | A | 506 | ALA | C-O | -7.24 | 1.09 | 1.23 |
| 9 | K | 58 | PHE | CB-CG | 7.24 | 1.63 | 1.51 |
| 1 | A | 1092 | LYS | CB-CG | 7.24 | 1.72 | 1.52 |
| 4 | E | 172 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 9 | K | 26 | LYS | CD-CE | 7.23 | 1.69 | 1.51 |
| 1 | A | 946 | VAL | CA-CB | -7.23 | 1.39 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 711 | GLU | CG-CD | 7.23 | 1.62 | 1.51 |
| 2 | B | 967 | ARG | N-CA | -7.23 | 1.31 | 1.46 |
| 1 | A | 437 | MET | SD-CE | 7.22 | 2.18 | 1.77 |
| 2 | B | 735 | ALA | N-CA | 7.22 | 1.60 | 1.46 |
| 1 | A | 973 | ILE | CB-CG2 | 7.21 | 1.75 | 1.52 |
| 2 | B | 875 | GLU | CD-OE1 | 7.21 | 1.33 | 1.25 |
| 1 | A | 1226 | VAL | CB-CG1 | -7.21 | 1.37 | 1.52 |
| 2 | B | 652 | LYS | CE-NZ | 7.20 | 1.67 | 1.49 |
| 4 | E | 1 | MET | CG-SD | 7.20 | 1.99 | 1.81 |
| 9 | K | 5 | ASP | CG-OD2 | 7.20 | 1.42 | 1.25 |
| 2 | B | 901 | PRO | C-O | -7.20 | 1.08 | 1.23 |
| 8 | J | 21 | TYR | CB-CG | 7.20 | 1.62 | 1.51 |
| 2 | B | 384 | ARG | CB-CG | 7.19 | 1.72 | 1.52 |
| 3 | C | 94 | LYS | CB-CG | 7.18 | 1.72 | 1.52 |
| 1 | A | 1154 | TYR | CG-CD2 | -7.18 | 1.29 | 1.39 |
| 2 | B | 572 | HIS | C-O | -7.18 | 1.09 | 1.23 |
| 1 | A | 1120 | LEU | C-O | -7.18 | 1.09 | 1.23 |
| 2 | B | 738 | PHE | CG-CD1 | -7.18 | 1.27 | 1.38 |
| 9 | K | 92 | ASN | N-CA | 7.18 | 1.60 | 1.46 |
| 3 | C | 191 | TYR | CG-CD2 | -7.18 | 1.29 | 1.39 |
| 6 | H | 124 | ARG | CB-CG | -7.17 | 1.33 | 1.52 |
| 1 | A | 1038 | THR | C-O | -7.17 | 1.09 | 1.23 |
| 4 | E | 26 | ARG | CD-NE | 7.17 | 1.58 | 1.46 |
| 4 | E | 52 | ARG | C-O | 7.17 | 1.36 | 1.23 |
| 1 | A | 571 | LEU | CG-CD2 | 7.17 | 1.78 | 1.51 |
| 7 | I | 94 | ASP | CB-CG | 7.17 | 1.66 | 1.51 |
| 1 | A | 1019 | CYS | CA-CB | -7.17 | 1.38 | 1.53 |
| 6 | H | 22 | LYS | CE-NZ | 7.17 | 1.67 | 1.49 |
| 2 | B | 855 | PHE | CD2-CE2 | 7.17 | 1.53 | 1.39 |
| 1 | A | 763 | ALA | CA-CB | -7.16 | 1.37 | 1.52 |
| 1 | A | 773 | LYS | CB-CG | -7.16 | 1.33 | 1.52 |
| 1 | A | 888 | GLY | CA-C | -7.16 | 1.40 | 1.51 |
| 1 | A | 1365 | TYR | CD2-CE2 | 7.16 | 1.50 | 1.39 |
| 2 | B | 980 | PHE | CG-CD1 | -7.15 | 1.28 | 1.38 |
| 4 | E | 13 | TRP | CB-CG | 7.15 | 1.63 | 1.50 |
| 1 | A | 14 | VAL | C-O | -7.15 | 1.09 | 1.23 |
| 2 | B | 39 | ARG | C-O | -7.15 | 1.09 | 1.23 |
| 1 | A | 847 | ASP | CG-OD1 | 7.15 | 1.41 | 1.25 |
| 2 | B | 498 | THR | CA-CB | 7.15 | 1.72 | 1.53 |
| 2 | B | 241 | ARG | NE-CZ | 7.14 | 1.42 | 1.33 |
| 3 | C | 253 | LYS | C-O | 7.14 | 1.36 | 1.23 |
| 3 | C | 17 | ASN | C-O | -7.14 | 1.09 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 233 | GLU | CD-OE1 | 7.13 | 1.33 | 1.25 |
| 1 | A | 905 | ASP | N-CA | -7.13 | 1.32 | 1.46 |
| 1 | A | 346 | ASP | CG-OD2 | 7.12 | 1.41 | 1.25 |
| 2 | B | 1061 | GLU | CB-CG | 7.12 | 1.65 | 1.52 |
| 4 | E | 28 | TYR | CG-CD1 | -7.12 | 1.29 | 1.39 |
| 1 | A | 1160 | SER | CB-OG | 7.12 | 1.51 | 1.42 |
| 1 | A | 1164 | PRO | CG-CD | 7.12 | 1.74 | 1.50 |
| 2 | B | 231 | PRO | CB-CG | 7.12 | 1.85 | 1.50 |
| 7 | I | 70 | ARG | NE-CZ | -7.12 | 1.23 | 1.33 |
| 3 | C | 23 | SER | CA-CB | 7.11 | 1.63 | 1.52 |
| 9 | K | 26 | LYS | CE-NZ | 7.11 | 1.66 | 1.49 |
| 1 | A | 767 | GLN | CA-CB | -7.11 | 1.38 | 1.53 |
| 2 | B | 1137 | CYS | CB-SG | -7.11 | 1.70 | 1.82 |
| 2 | B | 466 | TRP | CA-C | 7.11 | 1.71 | 1.52 |
| 2 | B | 19 | GLU | N-CA | 7.11 | 1.60 | 1.46 |
| 1 | A | 1229 | SER | C-O | 7.11 | 1.36 | 1.23 |
| 1 | A | 1094 | VAL | CB-CG2 | 7.10 | 1.67 | 1.52 |
| 2 | B | 119 | LEU | CA-CB | -7.10 | 1.37 | 1.53 |
| 10 | L | 68 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | A | 500 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 2 | B | 346 | GLU | CB-CG | 7.09 | 1.65 | 1.52 |
| 1 | A | 780 | VAL | C-O | 7.09 | 1.36 | 1.23 |
| 2 | B | 557 | PHE | CG-CD2 | 7.09 | 1.49 | 1.38 |
| 1 | A | 1268 | LEU | N-CA | -7.08 | 1.32 | 1.46 |
| 1 | A | 500 | GLU | CD-OE1 | 7.08 | 1.33 | 1.25 |
| 2 | B | 99 | LYS | CD-CE | 7.08 | 1.69 | 1.51 |
| 2 | B | 567 | GLU | C-O | -7.08 | 1.09 | 1.23 |
| 1 | A | 25 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 2 | B | 249 | ARG | C-O | 7.07 | 1.36 | 1.23 |
| 1 | A | 1359 | ASP | N-CA | 7.07 | 1.60 | 1.46 |
| 2 | B | 116 | GLU | CG-CD | 7.07 | 1.62 | 1.51 |
| 6 | H | 45 | GLU | CG-CD | 7.07 | 1.62 | 1.51 |
| 2 | B | 698 | GLU | CD-OE1 | -7.07 | 1.17 | 1.25 |
| 7 | I | 1 | MET | CB-CG | 7.07 | 1.74 | 1.51 |
| 5 | F | 114 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 2 | B | 1020 | ARG | CZ-NH2 | -7.06 | 1.23 | 1.33 |
| 2 | B | 18 | PHE | CG-CD2 | 7.06 | 1.49 | 1.38 |
| 3 | C | 179 | GLU | C-O | -7.06 | 1.09 | 1.23 |
| 4 | E | 78 | LEU | N-CA | -7.06 | 1.32 | 1.46 |
| 1 | A | 1382 | THR | C-O | 7.06 | 1.36 | 1.23 |
| 1 | A | 693 | VAL | CA-CB | -7.05 | 1.40 | 1.54 |
| 1 | A | 360 | GLU | CG-CD | 7.05 | 1.62 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 243 | ALA | CA-CB | 7.05 | 1.67 | 1.52 |
| 2 | B | 882 | THR | CA-CB | 7.05 | 1.71 | 1.53 |
| 3 | C | 49 | VAL | CB-CG2 | -7.05 | 1.38 | 1.52 |
| 5 | F | 146 | TRP | CG-CD1 | -7.05 | 1.26 | 1.36 |
| 1 | A | 1164 | PRO | CA-C | 7.05 | 1.67 | 1.52 |
| 1 | A | 1315 | GLU | CG-CD | 7.04 | 1.62 | 1.51 |
| 2 | B | 56 | ASP | C-O | -7.04 | 1.09 | 1.23 |
| 4 | E | 179 | GLN | CG-CD | -7.04 | 1.34 | 1.51 |
| 2 | B | 1092 | TYR | CE2-CZ | -7.03 | 1.29 | 1.38 |
| 5 | F | 98 | ALA | C-O | -7.03 | 1.09 | 1.23 |
| 1 | A | 1151 | GLU | CG-CD | 7.03 | 1.62 | 1.51 |
| 3 | C | 256 | ALA | CA-CB | -7.03 | 1.37 | 1.52 |
| 7 | I | 3 | THR | CB-CG2 | 7.02 | 1.75 | 1.52 |
| 1 | A | 390 | GLN | C-O | 7.02 | 1.36 | 1.23 |
| 1 | A | 264 | PHE | CE1-CZ | 7.02 | 1.50 | 1.37 |
| 2 | B | 422 | LYS | CB-CG | 7.02 | 1.71 | 1.52 |
| 1 | A | 420 | ARG | CB-CG | -7.02 | 1.33 | 1.52 |
| 7 | I | 56 | ALA | CA-CB | -7.01 | 1.37 | 1.52 |
| 8 | J | 18 | TRP | CE2-CZ2 | -7.01 | 1.27 | 1.39 |
| 2 | B | 903 | VAL | CB-CG1 | -7.01 | 1.38 | 1.52 |
| 1 | A | 1187 | GLN | C-O | 7.00 | 1.36 | 1.23 |
| 2 | B | 118 | ARG | CG-CD | 7.00 | 1.69 | 1.51 |
| 6 | H | 13 | SER | CA-CB | 7.00 | 1.63 | 1.52 |
| 6 | H | 11 | GLN | CA-C | -7.00 | 1.34 | 1.52 |
| 1 | A | 735 | VAL | CB-CG2 | 7.00 | 1.67 | 1.52 |
| 1 | A | 1264 | GLU | CD-OE2 | -6.99 | 1.18 | 1.25 |
| 6 | H | 32 | THR | CA-CB | 6.99 | 1.71 | 1.53 |
| 1 | A | 487 | MET | CG-SD | 6.99 | 1.99 | 1.81 |
| 1 | A | 551 | TYR | CD1-CE1 | -6.99 | 1.28 | 1.39 |
| 2 | B | 788 | ARG | CD-NE | -6.99 | 1.34 | 1.46 |
| 4 | E | 201 | LYS | CB-CG | 6.99 | 1.71 | 1.52 |
| 1 | A | 999 | VAL | CB-CG1 | -6.99 | 1.38 | 1.52 |
| 2 | B | 703 | ILE | C-O | 6.99 | 1.36 | 1.23 |
| 1 | A | 1385 | THR | CB-CG2 | 6.99 | 1.75 | 1.52 |
| 2 | B | 970 | THR | CA-CB | -6.99 | 1.35 | 1.53 |
| 2 | B | 259 | TYR | C-O | -6.98 | 1.10 | 1.23 |
| 2 | B | 692 | TYR | CG-CD2 | -6.98 | 1.30 | 1.39 |
| 10 | L | 59 | ALA | N-CA | 6.98 | 1.60 | 1.46 |
| 1 | A | 912 | LEU | CA-C | -6.98 | 1.34 | 1.52 |
| 1 | A | 1269 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | A | 843 | LYS | C-O | -6.98 | 1.10 | 1.23 |
| 2 | B | 1085 | ILE | CB-CG2 | -6.98 | 1.31 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 5 | GLY | CA-C | 6.97 | 1.63 | 1.51 |
| 7 | I | 34 | TYR | CE1-CZ | -6.97 | 1.29 | 1.38 |
| 2 | B | 865 | LYS | CA-CB | 6.97 | 1.69 | 1.53 |
| 2 | B | 982 | SER | CB-OG | -6.97 | 1.33 | 1.42 |
| 1 | A | 1036 | ARG | CZ-NH1 | 6.97 | 1.42 | 1.33 |
| 1 | A | 295 | LEU | CG-CD2 | 6.97 | 1.77 | 1.51 |
| 1 | A | 826 | ASP | CG-OD2 | 6.97 | 1.41 | 1.25 |
| 1 | A | 711 | ARG | C-O | -6.96 | 1.10 | 1.23 |
| 2 | B | 299 | GLU | CD-OE2 | 6.96 | 1.33 | 1.25 |
| 4 | E | 57 | MET | C-O | 6.96 | 1.36 | 1.23 |
| 6 | H | 137 | GLN | CB-CG | 6.96 | 1.71 | 1.52 |
| 7 | I | 8 | ARG | CZ-NH1 | 6.96 | 1.42 | 1.33 |
| 1 | A | 430 | TRP | CZ3-CH2 | -6.96 | 1.28 | 1.40 |
| 2 | B | 348 | ARG | NE-CZ | -6.96 | 1.24 | 1.33 |
| 2 | B | 1128 | LEU | N-CA | 6.96 | 1.60 | 1.46 |
| 3 | C | 219 | PHE | CE1-CZ | -6.96 | 1.24 | 1.37 |
| 1 | A | 608 | ILE | CB-CG2 | -6.96 | 1.31 | 1.52 |
| 10 | L | 26 | THR | CB-CG2 | 6.96 | 1.75 | 1.52 |
| 1 | A | 74 | MET | CG-SD | 6.96 | 1.99 | 1.81 |
| 1 | A | 446 | ARG | NE-CZ | -6.96 | 1.24 | 1.33 |
| 3 | C | 209 | TYR | CG-CD2 | 6.96 | 1.48 | 1.39 |
| 8 | J | 56 | LEU | N-CA | -6.96 | 1.32 | 1.46 |
| 1 | A | 1012 | ARG | CG-CD | 6.95 | 1.69 | 1.51 |
| 2 | B | 490 | SER | CB-OG | 6.95 | 1.51 | 1.42 |
| 2 | B | 589 | VAL | CB-CG1 | -6.95 | 1.38 | 1.52 |
| 6 | H | 132 | LEU | CA-CB | 6.95 | 1.69 | 1.53 |
| 3 | C | 26 | ASP | CG-OD1 | 6.95 | 1.41 | 1.25 |
| 10 | L | 61 | THR | CB-CG2 | 6.95 | 1.75 | 1.52 |
| 1 | A | 722 | LEU | C-O | -6.94 | 1.10 | 1.23 |
| 1 | A | 1135 | ARG | NE-CZ | 6.94 | 1.42 | 1.33 |
| 4 | E | 81 | GLU | CD-OE1 | 6.94 | 1.33 | 1.25 |
| 1 | A | 1146 | VAL | C-O | -6.93 | 1.10 | 1.23 |
| 2 | B | 436 | VAL | CA-C | 6.93 | 1.71 | 1.52 |
| 4 | E | 17 | ARG | CZ-NH2 | 6.93 | 1.42 | 1.33 |
| 1 | A | 1078 | GLN | CB-CG | 6.93 | 1.71 | 1.52 |
| 2 | B | 1204 | PHE | CD1-CE1 | 6.92 | 1.53 | 1.39 |
| 3 | C | 100 | THR | C-O | 6.92 | 1.36 | 1.23 |
| 4 | E | 185 | ALA | CA-CB | -6.92 | 1.38 | 1.52 |
| 1 | A | 711 | ARG | CB-CG | 6.92 | 1.71 | 1.52 |
| 2 | B | 798 | TYR | CE1-CZ | 6.92 | 1.47 | 1.38 |
| 1 | A | 24 | PRO | CG-CD | -6.92 | 1.27 | 1.50 |
| 5 | F | 103 | MET | C-O | -6.91 | 1.10 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1032 | SER | C-O | 6.91 | 1.36 | 1.23 |
| 6 | H | 27 | GLU | CA-C | 6.91 | 1.71 | 1.52 |
| 4 | E | 210 | SER | CB-OG | 6.91 | 1.51 | 1.42 |
| 4 | E | 110 | PHE | N-CA | -6.90 | 1.32 | 1.46 |
| 5 | F | 105 | ALA | CA-CB | -6.90 | 1.38 | 1.52 |
| 4 | E | 200 | ARG | CB-CG | -6.90 | 1.33 | 1.52 |
| 2 | B | 265 | SER | CA-CB | 6.89 | 1.63 | 1.52 |
| 1 | A | 264 | PHE | CG-CD1 | 6.89 | 1.49 | 1.38 |
| 1 | A | 725 | ALA | CA-CB | -6.89 | 1.38 | 1.52 |
| 4 | E | 52 | ARG | CB-CG | 6.89 | 1.71 | 1.52 |
| 2 | B | 512 | ARG | CA-C | 6.89 | 1.70 | 1.52 |
| 3 | C | 107 | SER | CB-OG | -6.88 | 1.33 | 1.42 |
| 9 | K | 55 | LYS | CD-CE | 6.88 | 1.68 | 1.51 |
| 2 | B | 266 | ALA | C-O | 6.88 | 1.36 | 1.23 |
| 2 | B | 983 | ARG | NE-CZ | -6.88 | 1.24 | 1.33 |
| 1 | A | 892 | ALA | CA-CB | -6.87 | 1.38 | 1.52 |
| 6 | H | 19 | ARG | CB-CG | 6.87 | 1.71 | 1.52 |
| 1 | A | 1056 | SER | CA-CB | -6.86 | 1.42 | 1.52 |
| 1 | A | 1005 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 2 | B | 579 | ARG | NE-CZ | -6.86 | 1.24 | 1.33 |
| 5 | F | 122 | MET | SD-CE | -6.86 | 1.39 | 1.77 |
| 2 | B | 904 | ARG | C-O | -6.86 | 1.10 | 1.23 |
| 1 | A | 1289 | ARG | NE-CZ | -6.86 | 1.24 | 1.33 |
| 2 | B | 113 | TYR | CD2-CE2 | -6.86 | 1.29 | 1.39 |
| 2 | B | 567 | GLU | CB-CG | 6.86 | 1.65 | 1.52 |
| 7 | I | 15 | TYR | CD2-CE2 | 6.86 | 1.49 | 1.39 |
| 1 | A | 1287 | TYR | CD1-CE1 | 6.85 | 1.49 | 1.39 |
| 2 | B | 209 | GLU | CD-OE1 | -6.84 | 1.18 | 1.25 |
| 2 | B | 352 | ALA | CA-CB | -6.84 | 1.38 | 1.52 |
| 6 | H | 127 | GLY | N-CA | 6.84 | 1.56 | 1.46 |
| 2 | B | 574 | SER | CB-OG | -6.83 | 1.33 | 1.42 |
| 1 | A | 1302 | PRO | C-O | 6.83 | 1.36 | 1.23 |
| 4 | E | 7 | ARG | CD-NE | 6.83 | 1.58 | 1.46 |
| 3 | C | 261 | ALA | C-O | -6.83 | 1.10 | 1.23 |
| 6 | H | 27 | GLU | CG-CD | 6.83 | 1.62 | 1.51 |
| 2 | B | 174 | LEU | C-O | -6.82 | 1.10 | 1.23 |
| 1 | A | 954 | TRP | CG-CD1 | -6.82 | 1.27 | 1.36 |
| 2 | B | 172 | ILE | CA-CB | -6.82 | 1.39 | 1.54 |
| 5 | F | 107 | VAL | CB-CG2 | -6.82 | 1.38 | 1.52 |
| 2 | B | 959 | ASP | CA-CB | 6.81 | 1.69 | 1.53 |
| 1 | A | 1003 | LYS | CD-CE | 6.81 | 1.68 | 1.51 |
| 2 | B | 875 | GLU | CD-OE2 | 6.81 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 201 | TRP | CD2-CE3 | -6.81 | 1.30 | 1.40 |
| 8 | J | 42 | LYS | C-O | 6.81 | 1.36 | 1.23 |
| 2 | B | 995 | ARG | CD-NE | -6.80 | 1.34 | 1.46 |
| 1 | A | 373 | THR | C-O | -6.80 | 1.10 | 1.23 |
| 1 | A | 572 | TRP | CE2-CZ2 | -6.80 | 1.28 | 1.39 |
| 1 | A | 1050 | GLU | CG-CD | 6.80 | 1.62 | 1.51 |
| 2 | B | 25 | ILE | CA-CB | 6.80 | 1.70 | 1.54 |
| 1 | A | 792 | TYR | CD1-CE1 | -6.80 | 1.29 | 1.39 |
| 9 | K | 7 | PHE | CE2-CZ | 6.79 | 1.50 | 1.37 |
| 7 | I | 107 | SER | CA-CB | -6.79 | 1.42 | 1.52 |
| 2 | B | 1200 | ALA | C-O | -6.79 | 1.10 | 1.23 |
| 3 | C | 158 | VAL | CA-CB | -6.79 | 1.40 | 1.54 |
| 1 | A | 1123 | GLY | CA-C | 6.78 | 1.62 | 1.51 |
| 1 | A | 1171 | GLN | CB-CG | 6.78 | 1.70 | 1.52 |
| 4 | E | 26 | ARG | CG-CD | -6.78 | 1.34 | 1.51 |
| 1 | A | 1081 | LEU | CG-CD2 | 6.78 | 1.76 | 1.51 |
| 2 | B | 361 | LEU | C-N | -6.78 | 1.21 | 1.34 |
| 1 | A | 1225 | PHE | C-O | -6.78 | 1.10 | 1.23 |
| 2 | B | 592 | ASN | CB-CG | 6.78 | 1.66 | 1.51 |
| 7 | I | 78 | CYS | CB-SG | 6.78 | 1.93 | 1.82 |
| 1 | A | 849 | MET | SD-CE | -6.77 | 1.40 | 1.77 |
| 1 | A | 1239 | ARG | CZ-NH2 | -6.77 | 1.24 | 1.33 |
| 2 | B | 173 | MET | C-O | -6.77 | 1.10 | 1.23 |
| 1 | A | 830 | LYS | CE-NZ | 6.76 | 1.66 | 1.49 |
| 2 | B | 114 | PRO | CG-CD | -6.76 | 1.28 | 1.50 |
| 1 | A | 298 | PHE | CG-CD2 | 6.76 | 1.48 | 1.38 |
| 7 | I | 6 | PHE | C-O | -6.76 | 1.10 | 1.23 |
| 4 | E | 142 | VAL | C-O | 6.76 | 1.36 | 1.23 |
| 6 | H | 141 | TYR | CZ-OH | -6.76 | 1.26 | 1.37 |
| 6 | H | 79 | TRP | CB-CG | -6.75 | 1.38 | 1.50 |
| 1 | A | 750 | GLY | C-O | -6.75 | 1.12 | 1.23 |
| 1 | A | 958 | VAL | CA-CB | -6.75 | 1.40 | 1.54 |
| 2 | B | 1192 | TYR | CE1-CZ | -6.75 | 1.29 | 1.38 |
| 1 | A | 689 | LYS | CD-CE | 6.75 | 1.68 | 1.51 |
| 9 | K | 26 | LYS | CB-CG | 6.75 | 1.70 | 1.52 |
| 1 | A | 1141 | THR | C-O | 6.75 | 1.36 | 1.23 |
| 8 | J | 13 | VAL | CB-CG2 | -6.75 | 1.38 | 1.52 |
| 1 | A | 1338 | VAL | CA-CB | -6.74 | 1.40 | 1.54 |
| 4 | E | 67 | GLU | CG-CD | 6.74 | 1.62 | 1.51 |
| 2 | B | 587 | HIS | C-O | -6.74 | 1.10 | 1.23 |
| 2 | B | 278 | GLN | CB-CG | -6.73 | 1.34 | 1.52 |
| 1 | A | 828 | ALA | CA-CB | -6.73 | 1.38 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 829 | VAL | CB-CG2 | 6.73 | 1.67 | 1.52 |
| 2 | B | 617 | ARG | C-O | -6.73 | 1.10 | 1.23 |
| 2 | B | 592 | ASN | CG-ND2 | 6.72 | 1.49 | 1.32 |
| 2 | B | 875 | GLU | CB-CG | 6.72 | 1.65 | 1.52 |
| 1 | A | 604 | GLY | CA-C | -6.72 | 1.41 | 1.51 |
| 1 | A | 1061 | GLY | N-CA | -6.72 | 1.35 | 1.46 |
| 2 | B | 618 | ASP | CG-OD1 | 6.72 | 1.40 | 1.25 |
| 2 | B | 662 | MET | CG-SD | -6.72 | 1.63 | 1.81 |
| 1 | A | 368 | LYS | CG-CD | 6.72 | 1.75 | 1.52 |
| 1 | A | 1141 | THR | CB-CG2 | -6.72 | 1.30 | 1.52 |
| 1 | A | 1416 | ALA | C-O | -6.71 | 1.10 | 1.23 |
| 7 | I | 48 | LEU | C-O | -6.71 | 1.10 | 1.23 |
| 10 | L | 29 | TYR | CG-CD2 | -6.71 | 1.30 | 1.39 |
| 1 | A | 383 | TYR | CE1-CZ | 6.71 | 1.47 | 1.38 |
| 8 | J | 7 | CYS | CB-SG | -6.71 | 1.70 | 1.82 |
| 6 | H | 139 | ASN | CA-CB | 6.70 | 1.70 | 1.53 |
| 1 | A | 1118 | VAL | CB-CG2 | -6.70 | 1.38 | 1.52 |
| 8 | J | 38 | ARG | CB-CG | 6.70 | 1.70 | 1.52 |
| 9 | K | 1 | MET | N-CA | 6.69 | 1.59 | 1.46 |
| 3 | C | 228 | PHE | CG-CD2 | -6.69 | 1.28 | 1.38 |
| 1 | A | 1191 | TRP | CE2-CZ2 | -6.68 | 1.28 | 1.39 |
| 2 | B | 267 | ARG | C-O | -6.68 | 1.10 | 1.23 |
| 2 | B | 1004 | GLU | CG-CD | 6.68 | 1.61 | 1.51 |
| 1 | A | 661 | GLY | CA-C | 6.68 | 1.62 | 1.51 |
| 1 | A | 518 | LYS | CE-NZ | -6.67 | 1.32 | 1.49 |
| 1 | A | 795 | GLU | CD-OE1 | 6.67 | 1.32 | 1.25 |
| 3 | C | 95 | CYS | CB-SG | -6.67 | 1.71 | 1.82 |
| 9 | K | 64 | GLU | C-O | -6.67 | 1.10 | 1.23 |
| 2 | B | 465 | ASN | CB-CG | 6.66 | 1.66 | 1.51 |
| 3 | C | 192 | TRP | CB-CG | 6.66 | 1.62 | 1.50 |
| 1 | A | 709 | THR | CB-CG2 | -6.66 | 1.30 | 1.52 |
| 1 | A | 427 | GLN | CG-CD | 6.66 | 1.66 | 1.51 |
| 1 | A | 414 | ASP | C-O | -6.66 | 1.10 | 1.23 |
| 1 | A | 361 | LEU | C-O | -6.66 | 1.10 | 1.23 |
| 2 | B | 397 | ASP | CG-OD1 | 6.66 | 1.40 | 1.25 |
| 6 | H | 129 | TYR | CE2-CZ | 6.66 | 1.47 | 1.38 |
| 1 | A | 599 | SER | CA-CB | 6.65 | 1.62 | 1.52 |
| 1 | A | 1146 | VAL | CB-CG1 | -6.65 | 1.38 | 1.52 |
| 1 | A | 291 | GLU | C-O | -6.65 | 1.10 | 1.23 |
| 1 | A | 1239 | ARG | CB-CG | -6.65 | 1.34 | 1.52 |
| 2 | B | 525 | ALA | C-O | 6.65 | 1.35 | 1.23 |
| 8 | J | 24 | LEU | CA-CB | -6.65 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 711 | GLU | CA-CB | -6.65 | 1.39 | 1.53 |
| 2 | B | 728 | ARG | CZ-NH1 | -6.64 | 1.24 | 1.33 |
| 1 | A | 1093 | LYS | N-CA | 6.64 | 1.59 | 1.46 |
| 2 | B | 90 | ILE | N-CA | 6.64 | 1.59 | 1.46 |
| 2 | B | 729 | ILE | C-O | -6.64 | 1.10 | 1.23 |
| 4 | E | 160 | GLU | CD-OE1 | 6.64 | 1.32 | 1.25 |
| 1 | A | 1045 | VAL | CB-CG1 | -6.64 | 1.39 | 1.52 |
| 2 | B | 604 | ARG | N-CA | 6.64 | 1.59 | 1.46 |
| 2 | B | 1221 | SER | N-CA | 6.64 | 1.59 | 1.46 |
| 1 | A | 53 | LEU | N-CA | 6.63 | 1.59 | 1.46 |
| 1 | A | 1228 | TRP | CE2-CZ2 | -6.63 | 1.28 | 1.39 |
| 2 | B | 105 | SER | CB-OG | 6.63 | 1.50 | 1.42 |
| 2 | B | 559 | SER | CB-OG | -6.63 | 1.33 | 1.42 |
| 2 | B | 816 | GLU | CD-OE1 | 6.63 | 1.32 | 1.25 |
| 4 | E | 79 | TRP | CD2-CE3 | 6.63 | 1.50 | 1.40 |
| 1 | A | 965 | GLN | CD-NE2 | 6.63 | 1.49 | 1.32 |
| 6 | H | 91 | ASP | C-O | 6.63 | 1.35 | 1.23 |
| 6 | H | 116 | TYR | CE1-CZ | 6.63 | 1.47 | 1.38 |
| 2 | B | 651 | LEU | CG-CD2 | -6.63 | 1.27 | 1.51 |
| 1 | A | 806 | ARG | CZ-NH2 | 6.62 | 1.41 | 1.33 |
| 1 | A | 1262 | LYS | CG-CD | 6.62 | 1.75 | 1.52 |
| 4 | E | 205 | SER | C-O | -6.62 | 1.10 | 1.23 |
| 1 | A | 1042 | PHE | CE2-CZ | 6.62 | 1.50 | 1.37 |
| 2 | B | 60 | GLN | CB-CG | -6.62 | 1.34 | 1.52 |
| 2 | B | 1057 | LYS | CG-CD | 6.62 | 1.75 | 1.52 |
| 7 | I | 63 | GLY | C-O | -6.62 | 1.13 | 1.23 |
| 2 | B | 227 | LYS | CG-CD | 6.61 | 1.75 | 1.52 |
| 1 | A | 838 | GLN | CG-CD | 6.61 | 1.66 | 1.51 |
| 2 | B | 851 | PHE | CB-CG | 6.61 | 1.62 | 1.51 |
| 1 | A | 1444 | MET | SD-CE | 6.61 | 2.14 | 1.77 |
| 2 | B | 586 | TRP | CE3-CZ3 | -6.61 | 1.27 | 1.38 |
| 7 | I | 14 | LEU | C-O | -6.61 | 1.10 | 1.23 |
| 1 | A | 1001 | ARG | NE-CZ | -6.61 | 1.24 | 1.33 |
| 1 | A | 1221 | LYS | CB-CG | 6.61 | 1.70 | 1.52 |
| 2 | B | 417 | PHE | CE1-CZ | -6.60 | 1.24 | 1.37 |
| 2 | B | 249 | ARG | CG-CD | 6.60 | 1.68 | 1.51 |
| 2 | B | 1079 | LYS | CE-NZ | -6.60 | 1.32 | 1.49 |
| 2 | B | 1096 | ARG | C-O | -6.60 | 1.10 | 1.23 |
| 1 | A | 1418 | LEU | C-O | -6.60 | 1.10 | 1.23 |
| 2 | B | 124 | TYR | CE2-CZ | -6.60 | 1.29 | 1.38 |
| 4 | E | 112 | TYR | CG-CD1 | -6.60 | 1.30 | 1.39 |
| 3 | C | 215 | GLU | CD-OE1 | 6.59 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 256 | VAL | CB-CG1 | -6.59 | 1.39 | 1.52 |
| 3 | C | 174 | ALA | CA-CB | -6.59 | 1.38 | 1.52 |
| 2 | B | 434 | ARG | NE-CZ | 6.59 | 1.41 | 1.33 |
| 2 | B | 874 | PHE | CD1-CE1 | -6.59 | 1.26 | 1.39 |
| 6 | H | 43 | ASN | CB-CG | 6.59 | 1.66 | 1.51 |
| 2 | B | 916 | THR | CB-CG2 | 6.59 | 1.74 | 1.52 |
| 2 | B | 97 | VAL | CB-CG1 | -6.59 | 1.39 | 1.52 |
| 1 | A | 591 | PHE | CB-CG | 6.58 | 1.62 | 1.51 |
| 1 | A | 919 | ILE | CA-CB | 6.58 | 1.70 | 1.54 |
| 3 | C | 216 | GLY | C-O | 6.58 | 1.34 | 1.23 |
| 1 | A | 802 | ASN | CB-CG | 6.58 | 1.66 | 1.51 |
| 6 | H | 6 | PHE | CA-C | -6.58 | 1.35 | 1.52 |
| 9 | K | 54 | ARG | CD-NE | 6.58 | 1.57 | 1.46 |
| 2 | B | 37 | PHE | CE2-CZ | -6.58 | 1.24 | 1.37 |
| 9 | K | 61 | TYR | CD1-CE1 | 6.58 | 1.49 | 1.39 |
| 6 | H | 27 | GLU | CD-OE1 | 6.57 | 1.32 | 1.25 |
| 1 | A | 624 | SER | CA-CB | 6.57 | 1.62 | 1.52 |
| 2 | B | 573 | GLN | C-O | -6.57 | 1.10 | 1.23 |
| 1 | A | 348 | SER | CA-CB | -6.57 | 1.43 | 1.52 |
| 3 | C | 61 | GLU | N-CA | 6.57 | 1.59 | 1.46 |
| 1 | A | 1057 | VAL | CB-CG2 | -6.57 | 1.39 | 1.52 |
| 2 | B | 238 | ALA | CA-CB | 6.57 | 1.66 | 1.52 |
| 6 | H | 131 | ASN | CA-CB | 6.56 | 1.70 | 1.53 |
| 2 | B | 608 | ASP | CB-CG | 6.56 | 1.65 | 1.51 |
| 5 | F | 127 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | A | 1442 | ASP | CA-C | -6.56 | 1.35 | 1.52 |
| 2 | B | 57 | TYR | CG-CD1 | -6.56 | 1.30 | 1.39 |
| 2 | B | 710 | LEU | CG-CD1 | -6.56 | 1.27 | 1.51 |
| 7 | I | 62 | ILE | C-O | -6.56 | 1.10 | 1.23 |
| 1 | A | 866 | PHE | CB-CG | -6.55 | 1.40 | 1.51 |
| 1 | A | 1448 | GLU | CA-C | 6.55 | 1.70 | 1.52 |
| 2 | B | 857 | ARG | NE-CZ | 6.55 | 1.41 | 1.33 |
| 3 | C | 49 | VAL | CB-CG1 | 6.55 | 1.66 | 1.52 |
| 3 | C | 39 | ALA | CA-CB | -6.55 | 1.38 | 1.52 |
| 1 | A | 1012 | ARG | NE-CZ | 6.55 | 1.41 | 1.33 |
| 2 | B | 479 | VAL | C-O | -6.55 | 1.10 | 1.23 |
| 2 | B | 627 | PHE | CD2-CE2 | -6.55 | 1.26 | 1.39 |
| 2 | B | 89 | GLU | C-O | 6.54 | 1.35 | 1.23 |
| 1 | A | 1428 | VAL | CB-CG2 | 6.54 | 1.66 | 1.52 |
| 2 | B | 382 | ILE | CG1-CD1 | 6.54 | 1.95 | 1.50 |
| 2 | B | 605 | ARG | CZ-NH1 | -6.54 | 1.24 | 1.33 |
| 10 | L | 65 | VAL | CB-CG2 | 6.54 | 1.66 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 679 | TYR | CE2-CZ | -6.54 | 1.30 | 1.38 |
| 7 | I | 54 | GLU | CD-OE1 | 6.53 | 1.32 | 1.25 |
| 2 | B | 1178 | ASN | CB-CG | -6.53 | 1.36 | 1.51 |
| 4 | E | 128 | PRO | CA-C | 6.53 | 1.66 | 1.52 |
| 1 | A | 941 | LYS | CG-CD | 6.53 | 1.74 | 1.52 |
| 7 | I | 86 | PHE | CE1-CZ | 6.53 | 1.49 | 1.37 |
| 4 | E | 185 | ALA | N-CA | -6.53 | 1.33 | 1.46 |
| 1 | A | 871 | ASP | C-O | -6.53 | 1.10 | 1.23 |
| 2 | B | 1224 | PHE | CG-CD2 | 6.53 | 1.48 | 1.38 |
| 1 | A | 31 | SER | C-O | 6.53 | 1.35 | 1.23 |
| 1 | A | 423 | ASP | CG-OD1 | 6.53 | 1.40 | 1.25 |
| 3 | C | 108 | GLU | CD-OE1 | 6.52 | 1.32 | 1.25 |
| 7 | I | 118 | ARG | NE-CZ | 6.52 | 1.41 | 1.33 |
| 9 | K | 68 | PHE | CG-CD1 | -6.52 | 1.28 | 1.38 |
| 2 | B | 1224 | PHE | CG-CD1 | 6.51 | 1.48 | 1.38 |
| 9 | K | 37 | LYS | CA-CB | -6.51 | 1.39 | 1.53 |
| 6 | H | 21 | ASN | C-O | -6.51 | 1.10 | 1.23 |
| 4 | E | 74 | ASP | CB-CG | -6.51 | 1.38 | 1.51 |
| 10 | L | 34 | CYS | CB-SG | -6.51 | 1.71 | 1.82 |
| 2 | B | 536 | VAL | CB-CG1 | -6.50 | 1.39 | 1.52 |
| 2 | B | 1073 | TYR | CD2-CE2 | -6.50 | 1.29 | 1.39 |
| 1 | A | 718 | VAL | CA-CB | -6.49 | 1.41 | 1.54 |
| 1 | A | 1080 | THR | CA-C | 6.49 | 1.69 | 1.52 |
| 1 | A | 1279 | ILE | N-CA | -6.49 | 1.33 | 1.46 |
| 2 | B | 905 | VAL | CB-CG1 | -6.49 | 1.39 | 1.52 |
| 1 | A | 298 | PHE | CD2-CE2 | 6.49 | 1.52 | 1.39 |
| 1 | A | 1108 | ALA | N-CA | -6.49 | 1.33 | 1.46 |
| 7 | I | 31 | THR | N-CA | -6.49 | 1.33 | 1.46 |
| 2 | B | 28 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 9 | K | 108 | GLU | CD-OE1 | 6.49 | 1.32 | 1.25 |
| 1 | A | 854 | ASN | CB-CG | 6.49 | 1.66 | 1.51 |
| 1 | A | 1018 | PHE | CE2-CZ | 6.49 | 1.49 | 1.37 |
| 2 | B | 1063 | GLY | C-O | -6.48 | 1.13 | 1.23 |
| 6 | H | 116 | TYR | N-CA | 6.48 | 1.59 | 1.46 |
| 1 | A | 1330 | ASN | C-O | -6.48 | 1.11 | 1.23 |
| 4 | E | 198 | ILE | CB-CG2 | -6.48 | 1.32 | 1.52 |
| 3 | C | 119 | VAL | CA-CB | 6.48 | 1.68 | 1.54 |
| 1 | A | 1119 | TYR | CD2-CE2 | -6.47 | 1.29 | 1.39 |
| 3 | C | 57 | VAL | CA-CB | -6.47 | 1.41 | 1.54 |
| 3 | C | 210 | GLU | CD-OE1 | 6.47 | 1.32 | 1.25 |
| 1 | A | 517 | ASN | CB-CG | 6.47 | 1.66 | 1.51 |
| 8 | J | 26 | GLN | CB-CG | 6.47 | 1.70 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 695 | ALA | CA-CB | -6.47 | 1.38 | 1.52 |
| 7 | I | 105 | SER | CB-OG | 6.46 | 1.50 | 1.42 |
| 2 | B | 643 | ASP | CA-CB | 6.46 | 1.68 | 1.53 |
| 6 | H | 115 | TYR | CE1-CZ | 6.46 | 1.47 | 1.38 |
| 2 | B | 197 | PHE | CG-CD1 | -6.46 | 1.29 | 1.38 |
| 2 | B | 1224 | PHE | CD1-CE1 | 6.46 | 1.52 | 1.39 |
| 3 | C | 114 | TYR | CD1-CE1 | -6.46 | 1.29 | 1.39 |
| 2 | B | 1132 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 3 | C | 181 | ASP | C-O | -6.46 | 1.11 | 1.23 |
| 4 | E | 168 | TYR | CG-CD1 | -6.46 | 1.30 | 1.39 |
| 6 | H | 102 | TYR | CD1-CE1 | -6.45 | 1.29 | 1.39 |
| 2 | B | 851 | PHE | CE1-CZ | 6.45 | 1.49 | 1.37 |
| 4 | E | 14 | ARG | CZ-NH2 | -6.45 | 1.24 | 1.33 |
| 2 | B | 969 | ARG | NE-CZ | -6.44 | 1.24 | 1.33 |
| 2 | B | 34 | ILE | CB-CG2 | -6.44 | 1.32 | 1.52 |
| 2 | B | 282 | ILE | CA-CB | -6.44 | 1.40 | 1.54 |
| 1 | A | 777 | PHE | CG-CD1 | -6.44 | 1.29 | 1.38 |
| 2 | B | 1183 | LYS | CA-CB | 6.44 | 1.68 | 1.53 |
| 3 | C | 191 | TYR | CE1-CZ | -6.44 | 1.30 | 1.38 |
| 6 | H | 104 | PHE | C-O | 6.44 | 1.35 | 1.23 |
| 2 | B | 1224 | PHE | CD2-CE2 | 6.44 | 1.52 | 1.39 |
| 1 | A | 678 | GLU | CD-OE1 | 6.43 | 1.32 | 1.25 |
| 3 | C | 81 | GLU | C-O | 6.43 | 1.35 | 1.23 |
| 2 | B | 366 | GLN | C-O | -6.43 | 1.11 | 1.23 |
| 1 | A | 1003 | LYS | CE-NZ | 6.43 | 1.65 | 1.49 |
| 8 | J | 9 | SER | CB-OG | 6.43 | 1.50 | 1.42 |
| 1 | A | 264 | PHE | CA-CB | 6.42 | 1.68 | 1.53 |
| 1 | A | 895 | LYS | CG-CD | 6.42 | 1.74 | 1.52 |
| 1 | A | 1044 | TRP | CE3-CZ3 | 6.42 | 1.49 | 1.38 |
| 2 | B | 732 | SER | CA-CB | 6.42 | 1.62 | 1.52 |
| 1 | A | 1093 | LYS | CG-CD | 6.42 | 1.74 | 1.52 |
| 2 | B | 1220 | ARG | NE-CZ | 6.42 | 1.41 | 1.33 |
| 1 | A | 971 | PHE | CG-CD1 | -6.41 | 1.29 | 1.38 |
| 3 | C | 254 | LYS | CA-C | -6.41 | 1.36 | 1.52 |
| 9 | K | 81 | TYR | C-O | -6.41 | 1.11 | 1.23 |
| 1 | A | 923 | LEU | C-O | 6.41 | 1.35 | 1.23 |
| 9 | K | 73 | LEU | C-O | 6.41 | 1.35 | 1.23 |
| 2 | B | 106 | ASP | CA-C | 6.40 | 1.69 | 1.52 |
| 1 | A | 469 | ARG | NE-CZ | -6.40 | 1.24 | 1.33 |
| 2 | B | 1091 | TYR | CD2-CE2 | 6.40 | 1.49 | 1.39 |
| 1 | A | 22 | PHE | CB-CG | -6.40 | 1.40 | 1.51 |
| 5 | F | 148 | VAL | C-O | 6.40 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | J | 44 | TYR | CE1-CZ | -6.40 | 1.30 | 1.38 |
| 1 | A | 617 | VAL | CA-CB | -6.39 | 1.41 | 1.54 |
| 2 | B | 1087 | PHE | CD2-CE2 | -6.39 | 1.26 | 1.39 |
| 2 | B | 369 | GLY | CA-C | 6.39 | 1.62 | 1.51 |
| 2 | B | 1134 | GLU | CB-CG | 6.39 | 1.64 | 1.52 |
| 1 | A | 1262 | LYS | CB-CG | 6.39 | 1.69 | 1.52 |
| 5 | F | 102 | SER | CB-OG | -6.39 | 1.33 | 1.42 |
| 2 | B | 851 | PHE | CD1-CE1 | -6.39 | 1.26 | 1.39 |
| 7 | I | 45 | ARG | CD-NE | 6.38 | 1.57 | 1.46 |
| 1 | A | 288 | ALA | CA-CB | 6.38 | 1.65 | 1.52 |
| 3 | C | 208 | GLU | CG-CD | 6.38 | 1.61 | 1.51 |
| 4 | E | 40 | GLU | CB-CG | 6.38 | 1.64 | 1.52 |
| 1 | A | 975 | HIS | CA-C | 6.38 | 1.69 | 1.52 |
| 3 | C | 267 | GLN | N-CA | 6.38 | 1.59 | 1.46 |
| 1 | A | 739 | ASP | CB-CG | 6.37 | 1.65 | 1.51 |
| 1 | A | 1433 | MET | SD-CE | -6.37 | 1.42 | 1.77 |
| 1 | A | 461 | LYS | CD-CE | 6.37 | 1.67 | 1.51 |
| 5 | F | 97 | ARG | CA-CB | -6.37 | 1.40 | 1.53 |
| 1 | A | 1009 | ASN | CG-OD1 | 6.37 | 1.38 | 1.24 |
| 2 | B | 279 | ASP | CB-CG | 6.37 | 1.65 | 1.51 |
| 3 | C | 215 | GLU | CG-CD | 6.37 | 1.61 | 1.51 |
| 1 | A | 568 | PRO | CB-CG | -6.37 | 1.18 | 1.50 |
| 2 | B | 996 | ARG | NE-CZ | -6.37 | 1.24 | 1.33 |
| 3 | C | 47 | ASP | CG-OD2 | 6.37 | 1.40 | 1.25 |
| 7 | I | 90 | GLN | C-O | -6.37 | 1.11 | 1.23 |
| 2 | B | 138 | GLU | N-CA | 6.36 | 1.59 | 1.46 |
| 1 | A | 934 | LYS | CG-CD | 6.36 | 1.74 | 1.52 |
| 1 | A | 1145 | SER | C-O | -6.36 | 1.11 | 1.23 |
| 9 | K | 66 | PRO | N-CD | -6.36 | 1.39 | 1.47 |
| 7 | I | 11 | ASN | CB-CG | -6.36 | 1.36 | 1.51 |
| 10 | L | 66 | GLN | CD-NE2 | 6.36 | 1.48 | 1.32 |
| 1 | A | 593 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | A | 1372 | VAL | CB-CG2 | -6.36 | 1.39 | 1.52 |
| 1 | A | 514 | PRO | CA-C | -6.36 | 1.40 | 1.52 |
| 2 | B | 252 | SER | CA-CB | 6.35 | 1.62 | 1.52 |
| 4 | E | 99 | HIS | N-CA | 6.35 | 1.59 | 1.46 |
| 1 | A | 618 | GLU | CG-CD | 6.35 | 1.61 | 1.51 |
| 1 | A | 393 | ARG | CZ-NH2 | 6.35 | 1.41 | 1.33 |
| 9 | K | 96 | ASN | CB-CG | 6.35 | 1.65 | 1.51 |
| 6 | H | 117 | SER | C-O | 6.34 | 1.35 | 1.23 |
| 1 | A | 593 | GLU | CB-CG | 6.34 | 1.64 | 1.52 |
| 2 | B | 166 | PHE | CB-CG | -6.34 | 1.40 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1362 | TYR | CD1-CE1 | 6.34 | 1.48 | 1.39 |
| 4 | E | 79 | TRP | CB-CG | 6.34 | 1.61 | 1.50 |
| 1 | A | 551 | TYR | CG-CD2 | -6.33 | 1.30 | 1.39 |
| 1 | A | 1008 | GLN | CB-CG | 6.33 | 1.69 | 1.52 |
| 2 | B | 1064 | TYR | CG-CD1 | -6.33 | 1.30 | 1.39 |
| 1 | A | 792 | TYR | CA-C | -6.33 | 1.36 | 1.52 |
| 10 | L | 67 | PHE | CG-CD2 | -6.33 | 1.29 | 1.38 |
| 1 | A | 461 | LYS | CA-CB | -6.33 | 1.40 | 1.53 |
| 2 | B | 312 | GLU | CG-CD | 6.33 | 1.61 | 1.51 |
| 10 | L | 65 | VAL | CA-C | -6.32 | 1.36 | 1.52 |
| 2 | B | 908 | GLU | CG-CD | 6.32 | 1.61 | 1.51 |
| 2 | B | 1047 | PHE | CD2-CE2 | 6.32 | 1.51 | 1.39 |
| 2 | B | 1106 | ARG | NE-CZ | 6.32 | 1.41 | 1.33 |
| 3 | C | 148 | ARG | CZ-NH1 | 6.32 | 1.41 | 1.33 |
| 7 | I | 72 | ASP | CG-OD2 | 6.32 | 1.39 | 1.25 |
| 2 | B | 962 | LYS | CE-NZ | 6.32 | 1.64 | 1.49 |
| 2 | B | 1018 | PRO | CA-C | -6.32 | 1.40 | 1.52 |
| 2 | B | 397 | ASP | CG-OD2 | 6.32 | 1.39 | 1.25 |
| 5 | F | 87 | LYS | CG-CD | 6.32 | 1.74 | 1.52 |
| 1 | A | 911 | SER | C-O | 6.31 | 1.35 | 1.23 |
| 2 | B | 526 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 2 | B | 336 | ARG | CZ-NH1 | 6.31 | 1.41 | 1.33 |
| 2 | B | 396 | ASP | C-O | 6.31 | 1.35 | 1.23 |
| 2 | B | 358 | LYS | CB-CG | 6.31 | 1.69 | 1.52 |
| 3 | C | 108 | GLU | C-O | 6.31 | 1.35 | 1.23 |
| 7 | I | 36 | GLU | CA-CB | -6.31 | 1.40 | 1.53 |
| 1 | A | 274 | ILE | CB-CG2 | 6.30 | 1.72 | 1.52 |
| 9 | K | 70 | ARG | CZ-NH1 | -6.30 | 1.24 | 1.33 |
| 2 | B | 343 | ILE | CB-CG2 | -6.30 | 1.33 | 1.52 |
| 6 | H | 136 | LYS | CA-CB | 6.30 | 1.67 | 1.53 |
| 1 | A | 1287 | TYR | CD2-CE2 | 6.30 | 1.48 | 1.39 |
| 3 | C | 199 | LYS | CG-CD | 6.30 | 1.73 | 1.52 |
| 10 | L | 27 | LEU | CA-CB | 6.29 | 1.68 | 1.53 |
| 3 | C | 22 | LEU | C-O | -6.29 | 1.11 | 1.23 |
| 1 | A | 292 | ALA | CA-CB | 6.29 | 1.65 | 1.52 |
| 9 | K | 16 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | A | 1157 | ASP | C-O | 6.29 | 1.35 | 1.23 |
| 9 | K | 38 | GLU | CD-OE2 | -6.29 | 1.18 | 1.25 |
| 2 | B | 691 | GLU | CG-CD | 6.28 | 1.61 | 1.51 |
| 1 | A | 551 | TYR | CB-CG | 6.28 | 1.61 | 1.51 |
| 2 | B | 706 | GLN | CD-NE2 | 6.28 | 1.48 | 1.32 |
| 2 | B | 249 | ARG | CB-CG | 6.28 | 1.69 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 792 | TYR | CE2-CZ | -6.28 | 1.30 | 1.38 |
| 5 | F | 87 | LYS | CE-NZ | 6.28 | 1.64 | 1.49 |
| 6 | H | 20 | TYR | CD2-CE2 | -6.28 | 1.29 | 1.39 |
| 6 | H | 115 | TYR | CD1-CE1 | 6.28 | 1.48 | 1.39 |
| 1 | A | 1332 | PHE | CE1-CZ | -6.27 | 1.25 | 1.37 |
| 2 | B | 351 | TYR | C-O | 6.27 | 1.35 | 1.23 |
| 1 | A | 1318 | THR | C-O | -6.27 | 1.11 | 1.23 |
| 2 | B | 792 | MET | C-O | -6.26 | 1.11 | 1.23 |
| 2 | B | 846 | ILE | CA-CB | 6.26 | 1.69 | 1.54 |
| 2 | B | 1108 | ARG | N-CA | 6.26 | 1.58 | 1.46 |
| 1 | A | 852 | TYR | CZ-OH | -6.26 | 1.27 | 1.37 |
| 1 | A | 880 | LYS | C-O | -6.26 | 1.11 | 1.23 |
| 2 | B | 384 | ARG | CG-CD | 6.26 | 1.67 | 1.51 |
| 1 | A | 967 | ALA | CA-CB | -6.26 | 1.39 | 1.52 |
| 2 | B | 1087 | PHE | C-O | -6.26 | 1.11 | 1.23 |
| 1 | A | 622 | VAL | CB-CG1 | -6.26 | 1.39 | 1.52 |
| 1 | A | 1189 | SER | C-O | -6.26 | 1.11 | 1.23 |
| 2 | B | 579 | ARG | CG-CD | 6.26 | 1.67 | 1.51 |
| 4 | E | 35 | VAL | CB-CG1 | -6.25 | 1.39 | 1.52 |
| 1 | A | 469 | ARG | CG-CD | 6.25 | 1.67 | 1.51 |
| 1 | A | 1002 | GLY | CA-C | 6.25 | 1.61 | 1.51 |
| 3 | C | 160 | LYS | CG-CD | 6.25 | 1.73 | 1.52 |
| 4 | E | 21 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 1 | A | 1225 | PHE | CB-CG | 6.24 | 1.61 | 1.51 |
| 1 | A | 94 | GLY | CA-C | 6.24 | 1.61 | 1.51 |
| 2 | B | 937 | ALA | CA-CB | 6.24 | 1.65 | 1.52 |
| 4 | E | 191 | LYS | C-O | -6.24 | 1.11 | 1.23 |
| 2 | B | 626 | ILE | CA-CB | -6.24 | 1.40 | 1.54 |
| 2 | B | 870 | ILE | C-O | 6.24 | 1.35 | 1.23 |
| 1 | A | 885 | THR | N-CA | -6.23 | 1.33 | 1.46 |
| 3 | C | 75 | MET | CB-CG | -6.23 | 1.31 | 1.51 |
| 1 | A | 76 | GLU | CD-OE1 | 6.22 | 1.32 | 1.25 |
| 9 | K | 88 | LYS | CG-CD | 6.22 | 1.73 | 1.52 |
| 1 | A | 95 | PHE | CD1-CE1 | 6.22 | 1.51 | 1.39 |
| 1 | A | 1026 | LEU | C-O | -6.22 | 1.11 | 1.23 |
| 1 | A | 1034 | GLU | CG-CD | 6.22 | 1.61 | 1.51 |
| 10 | L | 47 | ARG | CG-CD | 6.22 | 1.67 | 1.51 |
| 2 | B | 353 | LYS | CG-CD | 6.22 | 1.73 | 1.52 |
| 2 | B | 1108 | ARG | CA-C | 6.22 | 1.69 | 1.52 |
| 5 | F | 98 | ALA | CA-CB | -6.22 | 1.39 | 1.52 |
| 1 | A | 640 | GLN | CD-OE1 | 6.21 | 1.37 | 1.24 |
| 2 | B | 972 | LYS | CA-CB | -6.21 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1001 | ARG | C-O | 6.21 | 1.35 | 1.23 |
| 1 | A | 1092 | LYS | CA-C | 6.21 | 1.69 | 1.52 |
| 1 | A | 368 | LYS | CE-NZ | 6.21 | 1.64 | 1.49 |
| 1 | A | 787 | PHE | CE2-CZ | -6.21 | 1.25 | 1.37 |
| 2 | B | 865 | LYS | CB-CG | 6.21 | 1.69 | 1.52 |
| 1 | A | 1315 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 2 | B | 186 | GLU | C-O | 6.21 | 1.35 | 1.23 |
| 3 | C | 127 | ARG | N-CA | 6.21 | 1.58 | 1.46 |
| 6 | H | 130 | ARG | NE-CZ | -6.20 | 1.25 | 1.33 |
| 2 | B | 780 | VAL | CB-CG2 | -6.20 | 1.39 | 1.52 |
| 1 | A | 852 | TYR | CE1-CZ | -6.20 | 1.30 | 1.38 |
| 4 | E | 23 | VAL | C-O | 6.20 | 1.35 | 1.23 |
| 4 | E | 145 | THR | CA-CB | -6.20 | 1.37 | 1.53 |
| 2 | B | 624 | LEU | CA-CB | -6.20 | 1.39 | 1.53 |
| 3 | C | 78 | GLU | CD-OE1 | 6.20 | 1.32 | 1.25 |
| 1 | A | 347 | PHE | CG-CD2 | 6.19 | 1.48 | 1.38 |
| 1 | A | 572 | TRP | CZ3-CH2 | -6.19 | 1.30 | 1.40 |
| 1 | A | 1025 | ARG | CG-CD | -6.19 | 1.36 | 1.51 |
| 2 | B | 910 | VAL | C-O | -6.19 | 1.11 | 1.23 |
| 1 | A | 1417 | GLU | CA-CB | 6.19 | 1.67 | 1.53 |
| 2 | B | 1087 | PHE | CD1-CE1 | -6.19 | 1.26 | 1.39 |
| 3 | C | 63 | ILE | CA-CB | 6.19 | 1.69 | 1.54 |
| 1 | A | 1349 | TYR | C-O | -6.19 | 1.11 | 1.23 |
| 2 | B | 763 | GLN | CB-CG | -6.18 | 1.35 | 1.52 |
| 2 | B | 803 | LEU | CA-CB | -6.18 | 1.39 | 1.53 |
| 1 | A | 15 | LYS | CB-CG | 6.18 | 1.69 | 1.52 |
| 1 | A | 1208 | THR | C-O | 6.18 | 1.35 | 1.23 |
| 2 | B | 666 | TYR | CG-CD2 | 6.18 | 1.47 | 1.39 |
| 2 | B | 263 | GLY | C-O | 6.18 | 1.33 | 1.23 |
| 3 | C | 165 | LYS | CD-CE | 6.18 | 1.66 | 1.51 |
| 2 | B | 832 | GLY | CA-C | -6.18 | 1.42 | 1.51 |
| 4 | E | 187 | TYR | CD2-CE2 | 6.18 | 1.48 | 1.39 |
| 6 | H | 118 | PHE | CE2-CZ | 6.18 | 1.49 | 1.37 |
| 1 | A | 24 | PRO | CA-C | 6.17 | 1.65 | 1.52 |
| 1 | A | 681 | GLU | CB-CG | 6.17 | 1.63 | 1.52 |
| 1 | A | 814 | PHE | CE1-CZ | -6.17 | 1.25 | 1.37 |
| 5 | F | 144 | GLU | CD-OE1 | 6.17 | 1.32 | 1.25 |
| 10 | L | 62 | LYS | CE-NZ | 6.17 | 1.64 | 1.49 |
| 2 | B | 855 | PHE | CE2-CZ | -6.17 | 1.25 | 1.37 |
| 7 | I | 28 | GLU | C-O | -6.17 | 1.11 | 1.23 |
| 1 | A | 491 | VAL | C-O | -6.17 | 1.11 | 1.23 |
| 1 | A | 1417 | GLU | CB-CG | 6.17 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 194 | GLU | C-O | -6.16 | 1.11 | 1.23 |
| 1 | A | 346 | ASP | CA-CB | 6.16 | 1.67 | 1.53 |
| 4 | E | 42 | PHE | CD2-CE2 | 6.16 | 1.51 | 1.39 |
| 2 | B | 49 | ASP | CB-CG | 6.16 | 1.64 | 1.51 |
| 1 | A | 1151 | GLU | CD-OE1 | 6.16 | 1.32 | 1.25 |
| 2 | B | 109 | THR | CA-CB | 6.16 | 1.69 | 1.53 |
| 10 | L | 67 | PHE | C-O | -6.16 | 1.11 | 1.23 |
| 1 | A | 592 | ASP | CG-OD1 | 6.15 | 1.39 | 1.25 |
| 1 | A | 22 | PHE | CE1-CZ | 6.15 | 1.49 | 1.37 |
| 1 | A | 1420 | ASP | CG-OD1 | 6.15 | 1.39 | 1.25 |
| 7 | I | 120 | GLN | CG-CD | 6.15 | 1.65 | 1.51 |
| 6 | H | 105 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 6 | H | 14 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 3 | C | 148 | ARG | CD-NE | 6.15 | 1.56 | 1.46 |
| 2 | B | 550 | ASP | C-O | 6.14 | 1.35 | 1.23 |
| 3 | C | 241 | ASP | CA-CB | 6.14 | 1.67 | 1.53 |
| 1 | A | 808 | LEU | N-CA | -6.14 | 1.34 | 1.46 |
| 2 | B | 224 | GLN | CB-CG | 6.14 | 1.69 | 1.52 |
| 2 | B | 602 | THR | CB-CG2 | -6.14 | 1.32 | 1.52 |
| 4 | E | 138 | ALA | C-O | -6.13 | 1.11 | 1.23 |
| 1 | A | 1030 | ARG | CZ-NH2 | -6.13 | 1.25 | 1.33 |
| 2 | B | 793 | ALA | C-O | -6.13 | 1.11 | 1.23 |
| 1 | A | 696 | GLU | CD-OE2 | -6.13 | 1.19 | 1.25 |
| 2 | B | 38 | PHE | CD1-CE1 | -6.13 | 1.26 | 1.39 |
| 2 | B | 137 | TYR | CG-CD2 | 6.13 | 1.47 | 1.39 |
| 1 | A | 1202 | MET | CG-SD | -6.13 | 1.65 | 1.81 |
| 2 | B | 268 | THR | C-O | -6.13 | 1.11 | 1.23 |
| 2 | B | 368 | GLU | CA-CB | 6.13 | 1.67 | 1.53 |
| 2 | B | 1060 | ARG | CB-CG | -6.12 | 1.36 | 1.52 |
| 3 | C | 37 | MET | CA-CB | -6.12 | 1.40 | 1.53 |
| 1 | A | 286 | HIS | CB-CG | 6.12 | 1.61 | 1.50 |
| 1 | A | 445 | ASN | C-O | 6.12 | 1.34 | 1.23 |
| 1 | A | 1349 | TYR | CE2-CZ | -6.12 | 1.30 | 1.38 |
| 1 | A | 1376 | THR | C-O | -6.12 | 1.11 | 1.23 |
| 1 | A | 900 | ASP | N-CA | 6.12 | 1.58 | 1.46 |
| 2 | B | 1224 | PHE | CB-CG | 6.12 | 1.61 | 1.51 |
| 2 | B | 1168 | LEU | CA-C | -6.11 | 1.37 | 1.52 |
| 2 | B | 256 | VAL | CB-CG2 | -6.11 | 1.40 | 1.52 |
| 1 | A | 590 | ARG | CZ-NH2 | -6.11 | 1.25 | 1.33 |
| 2 | B | 638 | PHE | CD2-CE2 | -6.11 | 1.27 | 1.39 |
| 3 | C | 205 | LYS | N-CA | 6.11 | 1.58 | 1.46 |
| 3 | C | 180 | TYR | CB-CG | -6.11 | 1.42 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 476 | SER | C-O | -6.11 | 1.11 | 1.23 |
| 2 | B | 797 | TYR | CE2-CZ | -6.11 | 1.30 | 1.38 |
| 1 | A | 396 | PRO | CA-C | -6.11 | 1.40 | 1.52 |
| 2 | B | 466 | TRP | C-N | 6.11 | 1.44 | 1.33 |
| 2 | B | 1181 | GLU | CD-OE2 | -6.11 | 1.19 | 1.25 |
| 2 | B | 138 | GLU | CD-OE1 | -6.10 | 1.19 | 1.25 |
| 2 | B | 1156 | ASP | CA-CB | 6.10 | 1.67 | 1.53 |
| 1 | A | 1328 | TYR | C-O | -6.10 | 1.11 | 1.23 |
| 3 | C | 214 | ASN | C-O | 6.10 | 1.34 | 1.23 |
| 2 | B | 91 | SER | C-O | 6.10 | 1.34 | 1.23 |
| 2 | B | 974 | PRO | C-O | -6.10 | 1.11 | 1.23 |
| 1 | A | 360 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 8 | J | 1 | MET | CG-SD | -6.09 | 1.65 | 1.81 |
| 1 | A | 238 | CYS | C-O | -6.09 | 1.11 | 1.23 |
| 2 | B | 169 | ARG | CZ-NH2 | 6.09 | 1.41 | 1.33 |
| 8 | J | 44 | TYR | CG-CD2 | -6.09 | 1.31 | 1.39 |
| 10 | L | 46 | VAL | CB-CG2 | 6.09 | 1.65 | 1.52 |
| 4 | E | 37 | LEU | CG-CD2 | 6.09 | 1.74 | 1.51 |
| 2 | B | 1028 | GLU | CG-CD | 6.08 | 1.61 | 1.51 |
| 3 | C | 55 | THR | CB-OG1 | -6.08 | 1.31 | 1.43 |
| 2 | B | 984 | HIS | C-O | -6.08 | 1.11 | 1.23 |
| 3 | C | 87 | PHE | CE1-CZ | 6.08 | 1.49 | 1.37 |
| 4 | E | 77 | SER | N-CA | -6.08 | 1.34 | 1.46 |
| 2 | B | 680 | THR | CB-CG2 | -6.08 | 1.32 | 1.52 |
| 2 | B | 646 | LEU | CB-CG | 6.08 | 1.70 | 1.52 |
| 7 | I | 118 | ARG | CD-NE | 6.08 | 1.56 | 1.46 |
| 1 | A | 630 | ILE | CB-CG2 | -6.07 | 1.34 | 1.52 |
| 2 | B | 650 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 |
| 3 | C | 231 | ASN | CB-CG | 6.07 | 1.65 | 1.51 |
| 2 | B | 945 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 2 | B | 1050 | ILE | C-O | -6.07 | 1.11 | 1.23 |
| 1 | A | 768 | GLN | C-O | -6.07 | 1.11 | 1.23 |
| 1 | A | 1018 | PHE | CB-CG | -6.07 | 1.41 | 1.51 |
| 1 | A | 247 | ARG | C-O | 6.06 | 1.34 | 1.23 |
| 1 | A | 1222 | ASN | CA-CB | 6.06 | 1.69 | 1.53 |
| 1 | A | 387 | ARG | CG-CD | 6.06 | 1.67 | 1.51 |
| 1 | A | 880 | LYS | N-CA | -6.06 | 1.34 | 1.46 |
| 2 | B | 24 | PRO | CA-CB | -6.06 | 1.41 | 1.53 |
| 3 | C | 255 | VAL | CA-CB | -6.06 | 1.42 | 1.54 |
| 4 | E | 7 | ARG | CG-CD | 6.06 | 1.67 | 1.51 |
| 7 | I | 44 | TYR | CG-CD2 | 6.06 | 1.47 | 1.39 |
| 2 | B | 682 | SER | CA-C | -6.06 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | I | 65 | ASP | N-CA | 6.05 | 1.58 | 1.46 |
| 2 | B | 589 | VAL | CA-CB | -6.05 | 1.42 | 1.54 |
| 3 | C | 157 | CYS | CB-SG | -6.05 | 1.72 | 1.82 |
| 3 | C | 222 | LYS | CG-CD | 6.05 | 1.73 | 1.52 |
| 1 | A | 714 | PHE | CE1-CZ | -6.05 | 1.25 | 1.37 |
| 8 | J | 45 | CYS | CB-SG | 6.05 | 1.92 | 1.82 |
| 1 | A | 53 | LEU | CG-CD1 | 6.05 | 1.74 | 1.51 |
| 3 | C | 177 | GLU | CD-OE1 | 6.05 | 1.32 | 1.25 |
| 1 | A | 893 | PHE | CD2-CE2 | 6.04 | 1.51 | 1.39 |
| 7 | I | 101 | PHE | CD2-CE2 | 6.04 | 1.51 | 1.39 |
| 2 | B | 797 | TYR | CG-CD2 | -6.04 | 1.31 | 1.39 |
| 1 | A | 668 | ASP | CA-CB | -6.04 | 1.40 | 1.53 |
| 1 | A | 76 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 2 | B | 951 | GLN | N-CA | -6.04 | 1.34 | 1.46 |
| 2 | B | 977 | GLY | C-O | -6.04 | 1.14 | 1.23 |
| 3 | C | 120 | ILE | CA-CB | -6.04 | 1.41 | 1.54 |
| 1 | A | 540 | PHE | C-O | -6.03 | 1.11 | 1.23 |
| 1 | A | 969 | GLN | CD-OE1 | 6.03 | 1.37 | 1.24 |
| 1 | A | 1013 | ASP | CG-OD2 | 6.03 | 1.39 | 1.25 |
| 9 | K | 66 | PRO | CB-CG | -6.03 | 1.19 | 1.50 |
| 1 | A | 894 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | A | 1062 | GLU | CG-CD | -6.03 | 1.43 | 1.51 |
| 1 | A | 1322 | ILE | CB-CG2 | -6.03 | 1.34 | 1.52 |
| 2 | B | 560 | GLU | CG-CD | 6.03 | 1.60 | 1.51 |
| 1 | A | 1281 | ARG | CG-CD | 6.03 | 1.67 | 1.51 |
| 2 | B | 983 | ARG | CG-CD | 6.03 | 1.67 | 1.51 |
| 4 | E | 176 | PRO | N-CD | -6.03 | 1.39 | 1.47 |
| 1 | A | 1425 | SER | CB-OG | 6.02 | 1.50 | 1.42 |
| 6 | H | 115 | TYR | CB-CG | -6.02 | 1.42 | 1.51 |
| 2 | B | 585 | VAL | CB-CG2 | -6.02 | 1.40 | 1.52 |
| 2 | B | 775 | LYS | CE-NZ | 6.02 | 1.64 | 1.49 |
| 3 | C | 211 | ASP | CG-OD2 | 6.02 | 1.39 | 1.25 |
| 1 | A | 994 | GLN | CA-C | -6.02 | 1.37 | 1.52 |
| 1 | A | 1118 | VAL | N-CA | -6.02 | 1.34 | 1.46 |
| 2 | B | 190 | TYR | CD1-CE1 | 6.02 | 1.48 | 1.39 |
| 1 | A | 1256 | GLU | CA-CB | 6.01 | 1.67 | 1.53 |
| 7 | I | 85 | PHE | C-O | -6.01 | 1.11 | 1.23 |
| 3 | C | 49 | VAL | C-O | -6.01 | 1.11 | 1.23 |
| 2 | B | 401 | PHE | CB-CG | -6.01 | 1.41 | 1.51 |
| 1 | A | 702 | LEU | N-CA | -6.01 | 1.34 | 1.46 |
| 1 | A | 866 | PHE | CD2-CE2 | 6.01 | 1.51 | 1.39 |
| 1 | A | 656 | TRP | CG-CD2 | -6.00 | 1.33 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1103 | GLU | CB-CG | -6.00 | 1.40 | 1.52 |
| 2 | B | 18 | PHE | CA-CB | 6.00 | 1.67 | 1.53 |
| 2 | B | 708 | GLU | CD-OE1 | 6.00 | 1.32 | 1.25 |
| 5 | F | 92 | ARG | CA-CB | -6.00 | 1.40 | 1.53 |
| 1 | A | 408 | ASP | C-O | 6.00 | 1.34 | 1.23 |
| 7 | I | 121 | PHE | CG-CD1 | -6.00 | 1.29 | 1.38 |
| 1 | A | 264 | PHE | CE2-CZ | 6.00 | 1.48 | 1.37 |
| 2 | B | 1132 | GLU | CB-CG | 6.00 | 1.63 | 1.52 |
| 1 | A | 1103 | GLU | CG-CD | 6.00 | 1.60 | 1.51 |
| 8 | J | 26 | GLN | CG-CD | 6.00 | 1.64 | 1.51 |
| 3 | C | 209 | TYR | CG-CD1 | 5.99 | 1.47 | 1.39 |
| 3 | C | 260 | LEU | CG-CD2 | 5.99 | 1.74 | 1.51 |
| 1 | A | 1071 | SER | CA-CB | -5.99 | 1.44 | 1.52 |
| 5 | F | 149 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | A | 409 | SER | CA-CB | 5.99 | 1.61 | 1.52 |
| 1 | A | 954 | TRP | CD2-CE2 | -5.99 | 1.34 | 1.41 |
| 2 | B | 613 | VAL | CA-CB | 5.99 | 1.67 | 1.54 |
| 1 | A | 801 | GLU | CA-CB | -5.99 | 1.40 | 1.53 |
| 7 | I | 67 | THR | C-O | -5.99 | 1.11 | 1.23 |
| 1 | A | 1303 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 2 | B | 691 | GLU | CD-OE1 | 5.99 | 1.32 | 1.25 |
| 1 | A | 350 | ARG | C-O | -5.98 | 1.11 | 1.23 |
| 2 | B | 203 | PHE | CE2-CZ | -5.98 | 1.25 | 1.37 |
| 10 | L | 29 | TYR | CE2-CZ | -5.98 | 1.30 | 1.38 |
| 1 | A | 715 | GLU | CB-CG | 5.98 | 1.63 | 1.52 |
| 6 | H | 109 | LYS | CB-CG | 5.98 | 1.68 | 1.52 |
| 2 | B | 1183 | LYS | CA-C | 5.98 | 1.68 | 1.52 |
| 2 | B | 892 | LYS | CE-NZ | 5.98 | 1.64 | 1.49 |
| 1 | A | 839 | ARG | CZ-NH1 | 5.98 | 1.40 | 1.33 |
| 2 | B | 1180 | PHE | CE1-CZ | 5.98 | 1.48 | 1.37 |
| 1 | A | 1443 | VAL | CB-CG1 | -5.97 | 1.40 | 1.52 |
| 2 | B | 46 | GLN | CG-CD | -5.97 | 1.37 | 1.51 |
| 7 | I | 72 | ASP | CG-OD1 | 5.97 | 1.39 | 1.25 |
| 1 | A | 1325 | THR | CB-CG2 | -5.97 | 1.32 | 1.52 |
| 10 | L | 68 | GLU | CB-CG | 5.97 | 1.63 | 1.52 |
| 1 | A | 1159 | ARG | CB-CG | 5.97 | 1.68 | 1.52 |
| 1 | A | 1359 | ASP | CG-OD1 | 5.97 | 1.39 | 1.25 |
| 2 | B | 654 | ARG | CZ-NH1 | -5.97 | 1.25 | 1.33 |
| 2 | B | 312 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 5 | F | 108 | PHE | N-CA | -5.96 | 1.34 | 1.46 |
| 1 | A | 572 | TRP | CB-CG | -5.96 | 1.39 | 1.50 |
| 1 | A | 367 | PRO | CA-C | -5.96 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 857 | ARG | C-O | -5.96 | 1.12 | 1.23 |
| 3 | C | 205 | LYS | CB-CG | 5.96 | 1.68 | 1.52 |
| 1 | A | 1284 | MET | CA-C | -5.96 | 1.37 | 1.52 |
| 2 | B | 835 | GLN | CB-CG | 5.96 | 1.68 | 1.52 |
| 1 | A | 299 | HIS | C-O | -5.96 | 1.12 | 1.23 |
| 2 | B | 734 | HIS | C-N | 5.95 | 1.47 | 1.34 |
| 1 | A | 505 | CYS | C-O | -5.95 | 1.12 | 1.23 |
| 1 | A | 1285 | MET | CB-CG | 5.95 | 1.70 | 1.51 |
| 2 | B | 96 | TYR | CD1-CE1 | 5.95 | 1.48 | 1.39 |
| 2 | B | 262 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 2 | B | 486 | TYR | CG-CD2 | 5.95 | 1.46 | 1.39 |
| 3 | C | 169 | LYS | CD-CE | 5.95 | 1.66 | 1.51 |
| 1 | A | 655 | PHE | CB-CG | -5.95 | 1.41 | 1.51 |
| 1 | A | 485 | ASP | C-O | -5.95 | 1.12 | 1.23 |
| 1 | A | 1256 | GLU | N-CA | 5.95 | 1.58 | 1.46 |
| 2 | B | 582 | VAL | C-O | -5.95 | 1.12 | 1.23 |
| 5 | F | 76 | LYS | CE-NZ | 5.95 | 1.64 | 1.49 |
| 2 | B | 702 | LEU | CG-CD2 | -5.94 | 1.29 | 1.51 |
| 2 | B | 866 | TYR | CE1-CZ | 5.94 | 1.46 | 1.38 |
| 3 | C | 158 | VAL | C-O | -5.94 | 1.12 | 1.23 |
| 3 | C | 222 | LYS | CB-CG | 5.94 | 1.68 | 1.52 |
| 6 | H | 22 | LYS | CB-CG | 5.94 | 1.68 | 1.52 |
| 1 | A | 666 | ILE | CA-CB | -5.93 | 1.41 | 1.54 |
| 2 | B | 866 | TYR | CG-CD1 | 5.93 | 1.46 | 1.39 |
| 1 | A | 398 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |
| 1 | A | 1289 | ARG | CB-CG | -5.93 | 1.36 | 1.52 |
| 1 | A | 672 | ASP | CA-CB | 5.93 | 1.67 | 1.53 |
| 1 | A | 1289 | ARG | CZ-NH2 | -5.93 | 1.25 | 1.33 |
| 2 | B | 1180 | PHE | CD1-CE1 | -5.93 | 1.27 | 1.39 |
| 6 | H | 90 | ALA | CA-CB | -5.93 | 1.40 | 1.52 |
| 2 | B | 876 | LYS | C-O | -5.93 | 1.12 | 1.23 |
| 1 | A | 858 | ASN | CB-CG | -5.93 | 1.37 | 1.51 |
| 7 | I | 5 | ARG | C-O | 5.92 | 1.34 | 1.23 |
| 9 | K | 48 | ALA | CA-CB | -5.92 | 1.40 | 1.52 |
| 4 | E | 44 | ALA | C-O | 5.92 | 1.34 | 1.23 |
| 1 | A | 1153 | TYR | CG-CD1 | -5.92 | 1.31 | 1.39 |
| 2 | B | 370 | PHE | CG-CD1 | 5.92 | 1.47 | 1.38 |
| 1 | A | 1038 | THR | CA-C | -5.91 | 1.37 | 1.52 |
| 2 | B | 466 | TRP | C-O | 5.91 | 1.34 | 1.23 |
| 2 | B | 125 | SER | CA-CB | 5.91 | 1.61 | 1.52 |
| 2 | B | 822 | ASN | C-O | -5.91 | 1.12 | 1.23 |
| 7 | I | 24 | ARG | CG-CD | 5.91 | 1.66 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | I | 82 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | A | 489 | LEU | C-O | -5.91 | 1.12 | 1.23 |
| 10 | L | 40 | LEU | CB-CG | 5.91 | 1.69 | 1.52 |
| 1 | A | 867 | ILE | CB-CG1 | -5.90 | 1.37 | 1.54 |
| 2 | B | 304 | ASP | N-CA | 5.90 | 1.58 | 1.46 |
| 1 | A | 1023 | ARG | CA-C | -5.90 | 1.37 | 1.52 |
| 3 | C | 181 | ASP | CA-C | -5.90 | 1.37 | 1.52 |
| 6 | H | 131 | ASN | N-CA | 5.90 | 1.58 | 1.46 |
| 2 | B | 358 | LYS | CE-NZ | 5.90 | 1.63 | 1.49 |
| 2 | B | 1100 | ASP | CA-CB | 5.90 | 1.67 | 1.53 |
| 3 | C | 68 | GLY | N-CA | 5.90 | 1.54 | 1.46 |
| 1 | A | 466 | SER | N-CA | 5.90 | 1.58 | 1.46 |
| 4 | E | 113 | GLN | CG-CD | 5.90 | 1.64 | 1.51 |
| 7 | I | 59 | VAL | CB-CG1 | -5.90 | 1.40 | 1.52 |
| 6 | H | 19 | ARG | N-CA | 5.89 | 1.58 | 1.46 |
| 1 | A | 717 | ASN | CG-OD1 | 5.89 | 1.36 | 1.24 |
| 2 | B | 958 | GLN | N-CA | 5.89 | 1.58 | 1.46 |
| 1 | A | 803 | SER | CB-OG | 5.89 | 1.50 | 1.42 |
| 1 | A | 897 | TYR | CD1-CE1 | -5.89 | 1.30 | 1.39 |
| 1 | A | 1077 | THR | CB-CG2 | 5.89 | 1.71 | 1.52 |
| 3 | C | 15 | LYS | CB-CG | 5.88 | 1.68 | 1.52 |
| 3 | C | 79 | GLN | CD-OE1 | 5.88 | 1.36 | 1.24 |
| 1 | A | 962 | ARG | CG-CD | 5.88 | 1.66 | 1.51 |
| 2 | B | 103 | ASN | CA-CB | 5.88 | 1.68 | 1.53 |
| 2 | B | 132 | VAL | CB-CG1 | -5.88 | 1.40 | 1.52 |
| 6 | H | 88 | SER | N-CA | 5.88 | 1.58 | 1.46 |
| 6 | H | 93 | TYR | CE2-CZ | 5.88 | 1.46 | 1.38 |
| 7 | I | 121 | PHE | CD1-CE1 | -5.88 | 1.27 | 1.39 |
| 2 | B | 323 | VAL | C-O | -5.88 | 1.12 | 1.23 |
| 7 | I | 115 | LYS | CD-CE | 5.88 | 1.66 | 1.51 |
| 10 | L | 27 | LEU | CG-CD1 | 5.87 | 1.73 | 1.51 |
| 2 | B | 25 | ILE | C-O | -5.87 | 1.12 | 1.23 |
| 2 | B | 1150 | ARG | CG-CD | -5.87 | 1.37 | 1.51 |
| 2 | B | 303 | TYR | CG-CD1 | 5.87 | 1.46 | 1.39 |
| 1 | A | 1239 | ARG | N-CA | -5.87 | 1.34 | 1.46 |
| 10 | L | 47 | ARG | CB-CG | 5.87 | 1.68 | 1.52 |
| 2 | B | 265 | SER | CB-OG | 5.86 | 1.49 | 1.42 |
| 2 | B | 737 | THR | C-O | -5.86 | 1.12 | 1.23 |
| 1 | A | 393 | ARG | NE-CZ | 5.86 | 1.40 | 1.33 |
| 1 | A | 507 | VAL | CA-CB | 5.86 | 1.67 | 1.54 |
| 1 | A | 1311 | VAL | N-CA | -5.86 | 1.34 | 1.46 |
| 5 | F | 121 | ALA | CA-CB | -5.86 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | F | 137 | TYR | CE1-CZ | -5.86 | 1.30 | 1.38 |
| 2 | B | 625 | LYS | CD-CE | 5.86 | 1.65 | 1.51 |
| 1 | A | 619 | LYS | CE-NZ | 5.86 | 1.63 | 1.49 |
| 1 | A | 830 | LYS | N-CA | 5.85 | 1.58 | 1.46 |
| 2 | B | 546 | SER | C-O | -5.85 | 1.12 | 1.23 |
| 3 | C | 56 | THR | CB-CG2 | -5.85 | 1.33 | 1.52 |
| 6 | H | 78 | SER | C-O | -5.85 | 1.12 | 1.23 |
| 7 | I | 44 | TYR | CD2-CE2 | 5.85 | 1.48 | 1.39 |
| 1 | A | 1154 | TYR | CZ-OH | 5.84 | 1.47 | 1.37 |
| 2 | B | 466 | TRP | CG-CD1 | 5.84 | 1.45 | 1.36 |
| 2 | B | 1043 | ASP | CG-OD2 | 5.84 | 1.38 | 1.25 |
| 1 | A | 918 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 3 | C | 127 | ARG | CG-CD | -5.84 | 1.37 | 1.51 |
| 2 | B | 120 | ARG | CG-CD | 5.84 | 1.66 | 1.51 |
| 2 | B | 818 | PRO | CG-CD | -5.84 | 1.31 | 1.50 |
| 3 | C | 102 | GLN | C-O | 5.84 | 1.34 | 1.23 |
| 3 | C | 146 | LYS | CE-NZ | -5.84 | 1.34 | 1.49 |
| 6 | H | 78 | SER | CB-OG | -5.84 | 1.34 | 1.42 |
| 8 | J | 6 | ARG | CB-CG | 5.84 | 1.68 | 1.52 |
| 2 | B | 165 | VAL | N-CA | 5.84 | 1.58 | 1.46 |
| 7 | I | 112 | SER | CA-CB | -5.84 | 1.44 | 1.52 |
| 1 | A | 44 | THR | N-CA | 5.84 | 1.58 | 1.46 |
| 3 | C | 78 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 5 | F | 129 | LYS | CD-CE | 5.84 | 1.65 | 1.51 |
| 1 | A | 19 | PHE | CG-CD1 | 5.83 | 1.47 | 1.38 |
| 2 | B | 430 | ARG | NE-CZ | 5.82 | 1.40 | 1.33 |
| 2 | B | 529 | GLU | N-CA | 5.82 | 1.57 | 1.46 |
| 8 | J | 18 | TRP | CA-CB | -5.82 | 1.41 | 1.53 |
| 1 | A | 12 | ARG | CZ-NH1 | 5.82 | 1.40 | 1.33 |
| 7 | I | 27 | PHE | CG-CD2 | 5.82 | 1.47 | 1.38 |
| 7 | I | 37 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 9 | K | 10 | PHE | CE1-CZ | -5.82 | 1.26 | 1.37 |
| 1 | A | 372 | LYS | CE-NZ | -5.82 | 1.34 | 1.49 |
| 2 | B | 327 | ARG | NE-CZ | -5.82 | 1.25 | 1.33 |
| 8 | J | 59 | LYS | C-O | 5.82 | 1.34 | 1.23 |
| 2 | B | 535 | LEU | CG-CD1 | -5.81 | 1.30 | 1.51 |
| 2 | B | 1146 | PHE | C-O | -5.81 | 1.12 | 1.23 |
| 2 | B | 640 | VAL | CB-CG1 | -5.81 | 1.40 | 1.52 |
| 2 | B | 1027 | ILE | CA-CB | -5.81 | 1.41 | 1.54 |
| 2 | B | 1027 | ILE | N-CA | -5.81 | 1.34 | 1.46 |
| 3 | C | 42 | PRO | CA-CB | -5.81 | 1.42 | 1.53 |
| 1 | A | 1140 | HIS | CB-CG | -5.81 | 1.39 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 155 | ARG | CZ-NH1 | 5.81 | 1.40 | 1.33 |
| 1 | A | 1001 | ARG | N-CA | -5.80 | 1.34 | 1.46 |
| 2 | B | 360 | PHE | CG-CD2 | -5.80 | 1.30 | 1.38 |
| 3 | C | 29 | MET | SD-CE | 5.80 | 2.10 | 1.77 |
| 4 | E | 195 | VAL | CA-CB | -5.80 | 1.42 | 1.54 |
| 1 | A | 555 | ASP | CA-CB | 5.80 | 1.66 | 1.53 |
| 1 | A | 847 | ASP | CG-OD2 | 5.80 | 1.38 | 1.25 |
| 3 | C | 20 | PHE | CE1-CZ | 5.80 | 1.48 | 1.37 |
| 4 | E | 154 | ILE | CB-CG2 | -5.80 | 1.34 | 1.52 |
| 1 | A | 518 | LYS | CB-CG | -5.80 | 1.36 | 1.52 |
| 2 | B | 315 | LYS | CB-CG | -5.80 | 1.36 | 1.52 |
| 2 | B | 1154 | ALA | N-CA | 5.80 | 1.57 | 1.46 |
| 1 | A | 439 | ASN | CG-ND2 | -5.79 | 1.18 | 1.32 |
| 2 | B | 845 | SER | C-O | 5.79 | 1.34 | 1.23 |
| 9 | K | 68 | PHE | CB-CG | -5.79 | 1.41 | 1.51 |
| 1 | A | 1202 | MET | C-O | 5.79 | 1.34 | 1.23 |
| 1 | A | 241 | VAL | CB-CG1 | 5.79 | 1.65 | 1.52 |
| 1 | A | 799 | PHE | CG-CD1 | 5.79 | 1.47 | 1.38 |
| 6 | H | 117 | SER | N-CA | 5.79 | 1.57 | 1.46 |
| 1 | A | 1301 | GLU | CG-CD | 5.78 | 1.60 | 1.51 |
| 6 | H | 135 | LEU | CA-CB | 5.78 | 1.67 | 1.53 |
| 1 | A | 917 | SER | CA-C | -5.78 | 1.38 | 1.52 |
| 2 | B | 608 | ASP | CG-OD2 | 5.78 | 1.38 | 1.25 |
| 1 | A | 434 | ARG | CD-NE | -5.78 | 1.36 | 1.46 |
| 4 | E | 136 | ASN | CG-ND2 | 5.78 | 1.47 | 1.32 |
| 1 | A | 1450 | LEU | N-CA | 5.78 | 1.57 | 1.46 |
| 7 | I | 83 | ASN | C-O | 5.78 | 1.34 | 1.23 |
| 7 | I | 57 | GLY | C-O | -5.78 | 1.14 | 1.23 |
| 1 | A | 699 | ALA | C-O | -5.77 | 1.12 | 1.23 |
| 2 | B | 800 | GLN | CG-CD | 5.77 | 1.64 | 1.51 |
| 2 | B | 839 | MET | CG-SD | 5.77 | 1.96 | 1.81 |
| 6 | H | 77 | ARG | NE-CZ | 5.77 | 1.40 | 1.33 |
| 6 | H | 129 | TYR | CG-CD1 | 5.77 | 1.46 | 1.39 |
| 9 | K | 40 | HIS | CA-CB | 5.77 | 1.66 | 1.53 |
| 1 | A | 603 | ASN | N-CA | -5.77 | 1.34 | 1.46 |
| 2 | B | 1008 | PRO | CG-CD | -5.77 | 1.31 | 1.50 |
| 2 | B | 1034 | VAL | CB-CG1 | -5.77 | 1.40 | 1.52 |
| 1 | A | 685 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | A | 894 | GLU | CB-CG | 5.77 | 1.63 | 1.52 |
| 2 | B | 353 | LYS | C-O | -5.77 | 1.12 | 1.23 |
| 3 | C | 26 | ASP | CB-CG | 5.77 | 1.63 | 1.51 |
| 2 | B | 178 | ASN | CG-OD1 | 5.76 | 1.36 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 745 | PRO | CA-CB | -5.76 | 1.42 | 1.53 |
| 2 | B | 882 | THR | CB-CG2 | 5.76 | 1.71 | 1.52 |
| 2 | B | 763 | GLN | CG-CD | 5.76 | 1.64 | 1.51 |
| 1 | A | 700 | ASN | CG-ND2 | -5.76 | 1.18 | 1.32 |
| 3 | C | 7 | GLN | CD-OE1 | 5.76 | 1.36 | 1.24 |
| 3 | C | 212 | PRO | C-O | -5.76 | 1.11 | 1.23 |
| 5 | F | 152 | ILE | N-CA | -5.76 | 1.34 | 1.46 |
| 2 | B | 481 | GLN | C-O | 5.76 | 1.34 | 1.23 |
| 4 | E | 212 | ARG | CG-CD | 5.76 | 1.66 | 1.51 |
| 8 | J | 63 | TYR | CE2-CZ | -5.76 | 1.31 | 1.38 |
| 1 | A | 609 | ASP | CB-CG | 5.76 | 1.63 | 1.51 |
| 1 | A | 1287 | TYR | CE2-CZ | 5.76 | 1.46 | 1.38 |
| 7 | I | 96 | SER | CA-CB | -5.76 | 1.44 | 1.52 |
| 1 | A | 554 | PRO | N-CD | -5.76 | 1.39 | 1.47 |
| 1 | A | 1355 | VAL | CB-CG2 | -5.76 | 1.40 | 1.52 |
| 1 | A | 1328 | TYR | CD2-CE2 | -5.75 | 1.30 | 1.39 |
| 2 | B | 644 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 1 | A | 346 | ASP | CG-OD1 | 5.75 | 1.38 | 1.25 |
| 1 | A | 1112 | LYS | CG-CD | 5.75 | 1.72 | 1.52 |
| 2 | B | 1181 | GLU | N-CA | 5.75 | 1.57 | 1.46 |
| 2 | B | 1224 | PHE | CE1-CZ | 5.75 | 1.48 | 1.37 |
| 7 | I | 29 | CYS | C-O | 5.75 | 1.34 | 1.23 |
| 1 | A | 293 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | A | 1136 | SER | CB-OG | 5.74 | 1.49 | 1.42 |
| 1 | A | 553 | VAL | C-N | -5.74 | 1.23 | 1.34 |
| 1 | A | 874 | ASP | CA-C | -5.74 | 1.38 | 1.52 |
| 2 | B | 488 | TYR | CG-CD1 | 5.74 | 1.46 | 1.39 |
| 3 | C | 97 | VAL | CB-CG2 | 5.74 | 1.65 | 1.52 |
| 9 | K | 58 | PHE | CD2-CE2 | -5.74 | 1.27 | 1.39 |
| 1 | A | 371 | ALA | CA-CB | -5.74 | 1.40 | 1.52 |
| 1 | A | 1188 | GLN | CG-CD | 5.74 | 1.64 | 1.51 |
| 1 | A | 662 | PHE | CG-CD1 | -5.74 | 1.30 | 1.38 |
| 2 | B | 581 | PHE | CE2-CZ | -5.74 | 1.26 | 1.37 |
| 4 | E | 155 | ARG | CD-NE | 5.74 | 1.56 | 1.46 |
| 6 | H | 98 | TYR | CD1-CE1 | 5.74 | 1.48 | 1.39 |
| 7 | I | 4 | PHE | CE2-CZ | 5.74 | 1.48 | 1.37 |
| 1 | A | 774 | ARG | CZ-NH1 | -5.73 | 1.25 | 1.33 |
| 8 | J | 49 | MET | SD-CE | -5.73 | 1.45 | 1.77 |
| 2 | B | 727 | LYS | CE-NZ | -5.73 | 1.34 | 1.49 |
| 3 | C | 89 | GLU | CG-CD | 5.73 | 1.60 | 1.51 |
| 2 | B | 1069 | PHE | CB-CG | -5.73 | 1.41 | 1.51 |
| 2 | B | 1137 | CYS | C-O | -5.73 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 184 | ASN | N-CA | 5.73 | 1.57 | 1.46 |
| 1 | A | 240 | PRO | C-O | 5.72 | 1.34 | 1.23 |
| 6 | H | 102 | TYR | CE1-CZ | -5.72 | 1.31 | 1.38 |
| 1 | A | 362 | ASP | CB-CG | -5.72 | 1.39 | 1.51 |
| 1 | A | 779 | PHE | CE1-CZ | -5.72 | 1.26 | 1.37 |
| 2 | B | 916 | THR | CA-C | 5.72 | 1.67 | 1.52 |
| 3 | C | 108 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 4 | E | 6 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 9 | K | 102 | LYS | CD-CE | 5.72 | 1.65 | 1.51 |
| 1 | A | 1001 | ARG | CZ-NH2 | 5.72 | 1.40 | 1.33 |
| 1 | A | 1290 | LYS | CB-CG | 5.72 | 1.68 | 1.52 |
| 1 | A | 839 | ARG | CZ-NH2 | 5.72 | 1.40 | 1.33 |
| 2 | B | 250 | PHE | CG-CD1 | 5.72 | 1.47 | 1.38 |
| 2 | B | 425 | THR | CB-CG2 | 5.72 | 1.71 | 1.52 |
| 1 | A | 74 | MET | SD-CE | 5.71 | 2.09 | 1.77 |
| 2 | B | 1033 | LYS | CB-CG | -5.71 | 1.37 | 1.52 |
| 1 | A | 264 | PHE | CD2-CE2 | 5.71 | 1.50 | 1.39 |
| 2 | B | 604 | ARG | CD-NE | -5.71 | 1.36 | 1.46 |
| 4 | E | 57 | MET | CG-SD | 5.71 | 1.96 | 1.81 |
| 3 | C | 228 | PHE | C-O | -5.71 | 1.12 | 1.23 |
| 2 | B | 448 | ILE | CA-CB | 5.70 | 1.68 | 1.54 |
| 2 | B | 604 | ARG | C-O | -5.70 | 1.12 | 1.23 |
| 1 | A | 771 | GLU | CG-CD | 5.70 | 1.60 | 1.51 |
| 1 | A | 1096 | SER | CB-OG | 5.70 | 1.49 | 1.42 |
| 7 | I | 48 | LEU | CG-CD2 | -5.70 | 1.30 | 1.51 |
| 1 | A | 860 | LEU | C-O | -5.70 | 1.12 | 1.23 |
| 2 | B | 19 | GLU | CA-CB | 5.70 | 1.66 | 1.53 |
| 2 | B | 547 | VAL | N-CA | 5.70 | 1.57 | 1.46 |
| 1 | A | 1129 | GLU | CB-CG | 5.70 | 1.62 | 1.52 |
| 2 | B | 1031 | LEU | CA-CB | -5.70 | 1.40 | 1.53 |
| 7 | I | 111 | THR | CA-CB | -5.70 | 1.38 | 1.53 |
| 4 | E | 150 | VAL | CB-CG2 | -5.69 | 1.40 | 1.52 |
| 1 | A | 45 | GLN | CA-C | 5.69 | 1.67 | 1.52 |
| 1 | A | 546 | VAL | CA-CB | -5.69 | 1.42 | 1.54 |
| 8 | J | 63 | TYR | CG-CD2 | -5.69 | 1.31 | 1.39 |
| 2 | B | 883 | LEU | CG-CD2 | 5.69 | 1.73 | 1.51 |
| 6 | H | 87 | ARG | CG-CD | 5.69 | 1.66 | 1.51 |
| 2 | B | 734 | HIS | C-O | 5.69 | 1.34 | 1.23 |
| 6 | H | 24 | CYS | CB-SG | -5.69 | 1.72 | 1.81 |
| 1 | A | 63 | ARG | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | A | 274 | ILE | N-CA | 5.68 | 1.57 | 1.46 |
| 1 | A | 980 | ASP | C-O | 5.68 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | I | 75 | CYS | CA-C | -5.68 | 1.38 | 1.52 |
| 2 | B | 569 | TYR | CD1-CE1 | -5.68 | 1.30 | 1.39 |
| 1 | A | 893 | PHE | CB-CG | -5.68 | 1.41 | 1.51 |
| 1 | A | 1342 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 2 | B | 866 | TYR | CG-CD2 | 5.68 | 1.46 | 1.39 |
| 1 | A | 16 | GLU | N-CA | 5.68 | 1.57 | 1.46 |
| 3 | C | 234 | SER | C-O | 5.68 | 1.34 | 1.23 |
| 1 | A | 712 | GLU | C-O | -5.68 | 1.12 | 1.23 |
| 2 | B | 1101 | ASP | CA-CB | 5.68 | 1.66 | 1.53 |
| 2 | B | 1153 | GLU | CG-CD | 5.68 | 1.60 | 1.51 |
| 3 | C | 267 | GLN | C-O | 5.68 | 1.34 | 1.23 |
| 9 | K | 112 | GLN | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | A | 813 | PHE | CD2-CE2 | 5.67 | 1.50 | 1.39 |
| 1 | A | 1366 | ARG | CD-NE | -5.67 | 1.36 | 1.46 |
| 4 | E | 195 | VAL | CB-CG2 | 5.67 | 1.64 | 1.52 |
| 1 | A | 1223 | ASP | CG-OD1 | 5.67 | 1.38 | 1.25 |
| 2 | B | 70 | ILE | CB-CG2 | 5.67 | 1.70 | 1.52 |
| 2 | B | 120 | ARG | CZ-NH2 | 5.67 | 1.40 | 1.33 |
| 3 | C | 167 | HIS | CA-C | -5.67 | 1.38 | 1.52 |
| 8 | J | 1 | MET | CA-CB | -5.67 | 1.41 | 1.53 |
| 1 | A | 1131 | ALA | CA-CB | -5.67 | 1.40 | 1.52 |
| 2 | B | 198 | ASP | CB-CG | -5.67 | 1.39 | 1.51 |
| 1 | A | 1450 | LEU | CA-CB | 5.67 | 1.66 | 1.53 |
| 6 | H | 13 | SER | CB-OG | 5.67 | 1.49 | 1.42 |
| 7 | I | 6 | PHE | CE2-CZ | 5.67 | 1.48 | 1.37 |
| 7 | I | 98 | VAL | C-O | -5.67 | 1.12 | 1.23 |
| 1 | A | 486 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 1 | A | 839 | ARG | C-O | -5.67 | 1.12 | 1.23 |
| 1 | A | 358 | ASN | CA-C | -5.67 | 1.38 | 1.52 |
| 1 | A | 625 | SER | CB-OG | 5.67 | 1.49 | 1.42 |
| 1 | A | 656 | TRP | CE3-CZ3 | 5.67 | 1.48 | 1.38 |
| 1 | A | 942 | PHE | C-O | -5.67 | 1.12 | 1.23 |
| 2 | B | 18 | PHE | CG-CD1 | 5.67 | 1.47 | 1.38 |
| 4 | E | 162 | ARG | CA-CB | 5.66 | 1.66 | 1.53 |
| 6 | H | 119 | GLY | C-O | 5.66 | 1.32 | 1.23 |
| 2 | B | 883 | LEU | CB-CG | 5.66 | 1.69 | 1.52 |
| 6 | H | 146 | ARG | CZ-NH2 | 5.66 | 1.40 | 1.33 |
| 1 | A | 1212 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 6 | H | 44 | VAL | CB-CG1 | 5.65 | 1.64 | 1.52 |
| 1 | A | 1023 | ARG | CZ-NH1 | -5.65 | 1.25 | 1.33 |
| 1 | A | 1287 | TYR | CE1-CZ | 5.65 | 1.45 | 1.38 |
| 2 | B | 479 | VAL | CA-CB | -5.65 | 1.42 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | K | 16 | GLU | CB-CG | 5.65 | 1.62 | 1.52 |
| 1 | A | 913 | LEU | CA-CB | 5.65 | 1.66 | 1.53 |
| 2 | B | 286 | PHE | CE2-CZ | -5.65 | 1.26 | 1.37 |
| 4 | E | 38 | PRO | CA-C | -5.65 | 1.41 | 1.52 |
| 1 | A | 688 | LYS | CE-NZ | 5.65 | 1.63 | 1.49 |
| 1 | A | 1027 | ALA | N-CA | -5.65 | 1.35 | 1.46 |
| 2 | B | 1176 | ASN | CB-CG | 5.65 | 1.64 | 1.51 |
| 3 | C | 235 | VAL | CB-CG1 | -5.65 | 1.41 | 1.52 |
| 2 | B | 190 | TYR | CA-CB | -5.65 | 1.41 | 1.53 |
| 8 | J | 58 | GLU | CB-CG | 5.65 | 1.62 | 1.52 |
| 2 | B | 370 | PHE | CE1-CZ | 5.64 | 1.48 | 1.37 |
| 1 | A | 474 | VAL | CB-CG1 | -5.64 | 1.41 | 1.52 |
| 1 | A | 978 | PRO | CB-CG | 5.64 | 1.78 | 1.50 |
| 2 | B | 856 | PHE | CD1-CE1 | 5.64 | 1.50 | 1.39 |
| 3 | C | 201 | TRP | CE3-CZ3 | -5.64 | 1.28 | 1.38 |
| 4 | E | 135 | PHE | CE2-CZ | 5.64 | 1.48 | 1.37 |
| 1 | A | 895 | LYS | CE-NZ | 5.63 | 1.63 | 1.49 |
| 2 | B | 1129 | ARG | CZ-NH1 | 5.63 | 1.40 | 1.33 |
| 1 | A | 1225 | PHE | CD2-CE2 | 5.63 | 1.50 | 1.39 |
| 2 | B | 287 | ARG | CG-CD | 5.63 | 1.66 | 1.51 |
| 9 | K | 8 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 10 | L | 63 | ARG | NE-CZ | 5.63 | 1.40 | 1.33 |
| 2 | B | 208 | SER | C-O | 5.63 | 1.34 | 1.23 |
| 1 | A | 536 | LEU | CA-C | 5.63 | 1.67 | 1.52 |
| 1 | A | 601 | LYS | C-O | -5.63 | 1.12 | 1.23 |
| 4 | E | 23 | VAL | N-CA | -5.63 | 1.35 | 1.46 |
| 4 | E | 72 | PHE | CD2-CE2 | -5.63 | 1.27 | 1.39 |
| 1 | A | 711 | ARG | CA-C | -5.62 | 1.38 | 1.52 |
| 2 | B | 617 | ARG | CA-CB | -5.62 | 1.41 | 1.53 |
| 5 | F | 109 | VAL | CB-CG1 | -5.62 | 1.41 | 1.52 |
| 1 | A | 1441 | PHE | CG-CD1 | -5.62 | 1.30 | 1.38 |
| 3 | C | 48 | SER | CB-OG | 5.62 | 1.49 | 1.42 |
| 6 | H | 146 | ARG | CZ-NH1 | 5.62 | 1.40 | 1.33 |
| 7 | I | 74 | GLU | CB-CG | 5.62 | 1.62 | 1.52 |
| 1 | A | 95 | PHE | CG-CD1 | 5.62 | 1.47 | 1.38 |
| 1 | A | 248 | PRO | CB-CG | 5.62 | 1.78 | 1.50 |
| 1 | A | 37 | PHE | C-O | -5.62 | 1.12 | 1.23 |
| 1 | A | 789 | LYS | CG-CD | -5.62 | 1.33 | 1.52 |
| 7 | I | 25 | LEU | CG-CD2 | -5.62 | 1.31 | 1.51 |
| 1 | A | 724 | GLU | CB-CG | 5.61 | 1.62 | 1.52 |
| 1 | A | 516 | SER | CB-OG | 5.61 | 1.49 | 1.42 |
| 2 | B | 1097 | HIS | CB-CG | -5.61 | 1.40 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 122 | LYS | CA-CB | 5.61 | 1.66 | 1.53 |
| 7 | I | 100 | PHE | CD2-CE2 | 5.61 | 1.50 | 1.39 |
| 2 | B | 380 | TYR | CE1-CZ | -5.61 | 1.31 | 1.38 |
| 1 | A | 346 | ASP | C-O | -5.61 | 1.12 | 1.23 |
| 1 | A | 431 | LYS | CD-CE | 5.61 | 1.65 | 1.51 |
| 2 | B | 660 | LYS | CG-CD | 5.61 | 1.71 | 1.52 |
| 1 | A | 1034 | GLU | CA-CB | -5.60 | 1.41 | 1.53 |
| 1 | A | 458 | HIS | C-O | 5.60 | 1.33 | 1.23 |
| 1 | A | 589 | GLN | CA-C | -5.60 | 1.38 | 1.52 |
| 2 | B | 486 | TYR | CD2-CE2 | 5.60 | 1.47 | 1.39 |
| 7 | I | 87 | GLN | CB-CG | 5.60 | 1.67 | 1.52 |
| 2 | B | 1102 | LYS | CA-CB | 5.60 | 1.66 | 1.53 |
| 4 | E | 207 | ARG | NE-CZ | 5.60 | 1.40 | 1.33 |
| 1 | A | 572 | TRP | CG-CD1 | -5.60 | 1.28 | 1.36 |
| 2 | B | 397 | ASP | C-O | 5.60 | 1.33 | 1.23 |
| 7 | I | 70 | ARG | CZ-NH2 | -5.60 | 1.25 | 1.33 |
| 1 | A | 926 | GLN | CD-OE1 | 5.59 | 1.36 | 1.24 |
| 4 | E | 91 | LYS | CB-CG | 5.59 | 1.67 | 1.52 |
| 7 | I | 45 | ARG | CA-CB | -5.59 | 1.41 | 1.53 |
| 1 | A | 1080 | THR | N-CA | 5.59 | 1.57 | 1.46 |
| 1 | A | 285 | PRO | CB-CG | -5.59 | 1.22 | 1.50 |
| 1 | A | 386 | ASP | CG-OD1 | 5.59 | 1.38 | 1.25 |
| 2 | B | 997 | GLU | N-CA | 5.59 | 1.57 | 1.46 |
| 9 | K | 50 | LEU | CG-CD2 | -5.59 | 1.31 | 1.51 |
| 2 | B | 100 | PRO | CB-CG | -5.59 | 1.22 | 1.50 |
| 1 | A | 880 | LYS | CB-CG | 5.59 | 1.67 | 1.52 |
| 2 | B | 269 | ILE | CA-CB | -5.59 | 1.42 | 1.54 |
| 2 | B | 667 | GLN | CD-OE1 | 5.59 | 1.36 | 1.24 |
| 2 | B | 787 | VAL | N-CA | -5.59 | 1.35 | 1.46 |
| 3 | C | 10 | ILE | CA-CB | -5.59 | 1.42 | 1.54 |
| 7 | I | 27 | PHE | C-O | -5.59 | 1.12 | 1.23 |
| 1 | A | 853 | ASP | CB-CG | 5.58 | 1.63 | 1.51 |
| 3 | C | 155 | LEU | C-O | 5.58 | 1.33 | 1.23 |
| 1 | A | 776 | ALA | CA-CB | -5.58 | 1.40 | 1.52 |
| 1 | A | 1304 | TRP | CD2-CE2 | -5.58 | 1.34 | 1.41 |
| 2 | B | 612 | GLU | C-O | -5.58 | 1.12 | 1.23 |
| 3 | C | 192 | TRP | CE2-CZ2 | -5.58 | 1.30 | 1.39 |
| 6 | H | 111 | LEU | CA-C | 5.58 | 1.67 | 1.52 |
| 2 | B | 971 | THR | N-CA | -5.58 | 1.35 | 1.46 |
| 4 | E | 16 | PHE | CE1-CZ | -5.58 | 1.26 | 1.37 |
| 6 | H | 93 | TYR | CE1-CZ | 5.58 | 1.45 | 1.38 |
| 2 | B | 855 | PHE | CE1-CZ | 5.58 | 1.48 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 32 | SER | C-O | 5.58 | 1.33 | 1.23 |
| 1 | A | 801 | GLU | CG-CD | 5.58 | 1.60 | 1.51 |
| 2 | B | 1130 | PHE | N-CA | -5.58 | 1.35 | 1.46 |
| 4 | E | 122 | LYS | CD-CE | 5.58 | 1.65 | 1.51 |
| 3 | C | 125 | MET | CG-SD | 5.57 | 1.95 | 1.81 |
| 6 | H | 136 | LYS | CA-C | 5.57 | 1.67 | 1.52 |
| 8 | J | 53 | HIS | CG-CD2 | -5.57 | 1.26 | 1.35 |
| 2 | B | 979 | LYS | CB-CG | -5.57 | 1.37 | 1.52 |
| 3 | C | 119 | VAL | CB-CG1 | -5.57 | 1.41 | 1.52 |
| 2 | B | 1149 | GLU | CG-CD | 5.57 | 1.60 | 1.51 |
| 2 | B | 304 | ASP | CB-CG | 5.56 | 1.63 | 1.51 |
| 2 | B | 499 | ASN | C-O | -5.56 | 1.12 | 1.23 |
| 3 | C | 143 | LEU | CA-CB | -5.56 | 1.41 | 1.53 |
| 1 | A | 1309 | ASP | CA-C | -5.56 | 1.38 | 1.52 |
| 4 | E | 169 | ARG | CG-CD | 5.56 | 1.65 | 1.51 |
| 10 | L | 27 | LEU | CB-CG | 5.56 | 1.68 | 1.52 |
| 1 | A | 264 | PHE | CA-C | 5.56 | 1.67 | 1.52 |
| 2 | B | 279 | ASP | CG-OD1 | 5.56 | 1.38 | 1.25 |
| 6 | H | 19 | ARG | CZ-NH2 | 5.56 | 1.40 | 1.33 |
| 3 | C | 209 | TYR | CD1-CE1 | 5.56 | 1.47 | 1.39 |
| 3 | C | 211 | ASP | CB-CG | 5.56 | 1.63 | 1.51 |
| 1 | A | 655 | PHE | CG-CD2 | -5.55 | 1.30 | 1.38 |
| 3 | C | 214 | ASN | N-CA | 5.55 | 1.57 | 1.46 |
| 1 | A | 358 | ASN | C-O | -5.55 | 1.12 | 1.23 |
| 1 | A | 411 | ASP | C-O | -5.55 | 1.12 | 1.23 |
| 1 | A | 632 | VAL | CB-CG1 | -5.55 | 1.41 | 1.52 |
| 1 | A | 882 | SER | C-O | -5.55 | 1.12 | 1.23 |
| 1 | A | 983 | ILE | C-N | -5.55 | 1.21 | 1.34 |
| 1 | A | 686 | ALA | C-O | -5.55 | 1.12 | 1.23 |
| 1 | A | 1002 | GLY | C-O | 5.55 | 1.32 | 1.23 |
| 3 | C | 187 | LYS | CD-CE | 5.55 | 1.65 | 1.51 |
| 9 | K | 72 | LYS | C-O | -5.55 | 1.12 | 1.23 |
| 2 | B | 57 | TYR | CD2-CE2 | 5.54 | 1.47 | 1.39 |
| 5 | F | 79 | ARG | CZ-NH2 | -5.54 | 1.25 | 1.33 |
| 1 | A | 449 | SER | CB-OG | 5.54 | 1.49 | 1.42 |
| 7 | I | 51 | ASN | CB-CG | 5.54 | 1.63 | 1.51 |
| 1 | A | 1411 | GLU | CB-CG | 5.54 | 1.62 | 1.52 |
| 2 | B | 499 | ASN | CG-ND2 | 5.54 | 1.46 | 1.32 |
| 2 | B | 1196 | ILE | CA-CB | -5.54 | 1.42 | 1.54 |
| 10 | L | 27 | LEU | CG-CD2 | 5.54 | 1.72 | 1.51 |
| 1 | A | 836 | TYR | CA-C | 5.53 | 1.67 | 1.52 |
| 2 | B | 42 | GLY | C-O | 5.53 | 1.32 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 954 | VAL | CB-CG2 | 5.53 | 1.64 | 1.52 |
| 1 | A | 623 | GLY | C-O | 5.53 | 1.32 | 1.23 |
| 1 | A | 400 | PRO | C-O | -5.53 | 1.12 | 1.23 |
| 1 | A | 576 | GLN | CA-C | -5.53 | 1.38 | 1.52 |
| 2 | B | 259 | TYR | CD2-CE2 | -5.53 | 1.31 | 1.39 |
| 1 | A | 881 | GLN | CB-CG | -5.53 | 1.37 | 1.52 |
| 1 | A | 1339 | LEU | CA-CB | -5.53 | 1.41 | 1.53 |
| 2 | B | 422 | LYS | CG-CD | 5.52 | 1.71 | 1.52 |
| 1 | A | 726 | ARG | CZ-NH2 | 5.52 | 1.40 | 1.33 |
| 1 | A | 1303 | GLU | C-O | -5.52 | 1.12 | 1.23 |
| 4 | E | 93 | MET | SD-CE | 5.52 | 2.08 | 1.77 |
| 1 | A | 383 | TYR | CD1-CE1 | 5.52 | 1.47 | 1.39 |
| 1 | A | 770 | VAL | C-O | -5.52 | 1.12 | 1.23 |
| 3 | C | 165 | LYS | N-CA | 5.52 | 1.57 | 1.46 |
| 4 | E | 48 | ASP | CB-CG | 5.52 | 1.63 | 1.51 |
| 1 | A | 643 | ALA | CA-CB | -5.52 | 1.40 | 1.52 |
| 2 | B | 1023 | VAL | CB-CG2 | -5.52 | 1.41 | 1.52 |
| 6 | H | 140 | ALA | CA-CB | -5.52 | 1.40 | 1.52 |
| 2 | B | 371 | GLU | C-O | -5.52 | 1.12 | 1.23 |
| 7 | I | 103 | CYS | C-O | -5.52 | 1.12 | 1.23 |
| 2 | B | 174 | LEU | CG-CD1 | 5.52 | 1.72 | 1.51 |
| 6 | H | 120 | GLY | C-O | 5.52 | 1.32 | 1.23 |
| 2 | B | 271 | ALA | C-O | -5.51 | 1.12 | 1.23 |
| 2 | B | 635 | ARG | CZ-NH2 | -5.51 | 1.25 | 1.33 |
| 1 | A | 969 | GLN | CD-NE2 | 5.51 | 1.46 | 1.32 |
| 1 | A | 420 | ARG | CZ-NH2 | -5.51 | 1.25 | 1.33 |
| 1 | A | 39 | GLU | CA-C | 5.51 | 1.67 | 1.52 |
| 1 | A | 731 | ARG | CZ-NH1 | 5.51 | 1.40 | 1.33 |
| 3 | C | 188 | HIS | C-O | 5.51 | 1.33 | 1.23 |
| 1 | A | 478 | TYR | CG-CD1 | -5.51 | 1.31 | 1.39 |
| 1 | A | 811 | GLN | CB-CG | -5.51 | 1.37 | 1.52 |
| 2 | B | 610 | ASN | C-O | 5.51 | 1.33 | 1.23 |
| 6 | H | 50 | ALA | N-CA | 5.51 | 1.57 | 1.46 |
| 1 | A | 1311 | VAL | CB-CG2 | -5.50 | 1.41 | 1.52 |
| 2 | B | 994 | TYR | CE2-CZ | -5.50 | 1.31 | 1.38 |
| 3 | C | 239 | PRO | C-N | -5.50 | 1.21 | 1.34 |
| 7 | I | 74 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 9 | K | 108 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 5 | F | 78 | GLN | C-O | -5.50 | 1.12 | 1.23 |
| 1 | A | 6 | TYR | CD1-CE1 | 5.49 | 1.47 | 1.39 |
| 2 | B | 1004 | GLU | C-O | 5.49 | 1.33 | 1.23 |
| 1 | A | 41 | MET | CG-SD | 5.49 | 1.95 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 788 | SER | C-O | -5.49 | 1.12 | 1.23 |
| 4 | E | 71 | LYS | CE-NZ | -5.49 | 1.35 | 1.49 |
| 5 | F | 147 | SER | CB-OG | 5.49 | 1.49 | 1.42 |
| 1 | A | 984 | LYS | CE-NZ | 5.49 | 1.62 | 1.49 |
| 6 | H | 85 | GLY | CA-C | 5.49 | 1.60 | 1.51 |
| 7 | I | 8 | ARG | CB-CG | 5.49 | 1.67 | 1.52 |
| 2 | B | 1096 | ARG | CB-CG | -5.49 | 1.37 | 1.52 |
| 2 | B | 401 | PHE | C-O | -5.49 | 1.12 | 1.23 |
| 2 | B | 458 | LYS | CD-CE | 5.49 | 1.65 | 1.51 |
| 3 | C | 228 | PHE | CG-CD1 | -5.48 | 1.30 | 1.38 |
| 2 | B | 893 | LEU | CG-CD2 | -5.48 | 1.31 | 1.51 |
| 7 | I | 7 | CYS | CB-SG | -5.48 | 1.72 | 1.81 |
| 1 | A | 500 | GLU | CB-CG | -5.48 | 1.41 | 1.52 |
| 2 | B | 193 | LYS | CD-CE | 5.48 | 1.65 | 1.51 |
| 2 | B | 755 | ILE | C-O | 5.48 | 1.33 | 1.23 |
| 2 | B | 1215 | ARG | NE-CZ | -5.48 | 1.25 | 1.33 |
| 4 | E | 162 | ARG | CD-NE | 5.47 | 1.55 | 1.46 |
| 1 | A | 425 | GLN | CG-CD | 5.47 | 1.63 | 1.51 |
| 7 | I | 50 | THR | CA-C | -5.47 | 1.38 | 1.52 |
| 2 | B | 685 | LEU | CG-CD1 | -5.47 | 1.31 | 1.51 |
| 1 | A | 956 | LEU | C-N | -5.47 | 1.23 | 1.34 |
| 2 | B | 333 | PHE | CG-CD2 | -5.47 | 1.30 | 1.38 |
| 7 | I | 73 | ARG | CA-CB | -5.47 | 1.42 | 1.53 |
| 1 | A | 1328 | TYR | CE2-CZ | 5.46 | 1.45 | 1.38 |
| 2 | B | 110 | HIS | CA-C | 5.46 | 1.67 | 1.52 |
| 2 | B | 629 | ASP | CB-CG | 5.46 | 1.63 | 1.51 |
| 4 | E | 44 | ALA | CA-CB | 5.46 | 1.64 | 1.52 |
| 1 | A | 368 | LYS | CD-CE | 5.46 | 1.65 | 1.51 |
| 1 | A | 486 | GLU | CG-CD | 5.46 | 1.60 | 1.51 |
| 1 | A | 1280 | GLU | CB-CG | 5.46 | 1.62 | 1.52 |
| 2 | B | 202 | TYR | CG-CD1 | -5.46 | 1.32 | 1.39 |
| 2 | B | 557 | PHE | CD2-CE2 | -5.46 | 1.28 | 1.39 |
| 9 | K | 19 | LEU | CA-CB | -5.46 | 1.41 | 1.53 |
| 9 | K | 55 | LYS | CE-NZ | 5.45 | 1.62 | 1.49 |
| 2 | B | 250 | PHE | N-CA | 5.45 | 1.57 | 1.46 |
| 2 | B | 972 | LYS | CE-NZ | 5.45 | 1.62 | 1.49 |
| 1 | A | 563 | PRO | CG-CD | 5.45 | 1.68 | 1.50 |
| 3 | C | 9 | LYS | CE-NZ | 5.45 | 1.62 | 1.49 |
| 1 | A | 293 | GLU | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | A | 565 | ILE | CB-CG2 | -5.45 | 1.35 | 1.52 |
| 2 | B | 49 | ASP | C-O | -5.45 | 1.13 | 1.23 |
| 2 | B | 486 | TYR | CB-CG | -5.45 | 1.43 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | H | 9 | ILE | C-O | 5.45 | 1.33 | 1.23 |
| 2 | B | 942 | ARG | CZ-NH2 | 5.44 | 1.40 | 1.33 |
| 9 | K | 35 | PHE | CD1-CE1 | -5.44 | 1.28 | 1.39 |
| 1 | A | 1373 | ASP | CG-OD2 | 5.44 | 1.37 | 1.25 |
| 2 | B | 225 | VAL | CB-CG2 | -5.44 | 1.41 | 1.52 |
| 2 | B | 780 | VAL | C-O | -5.44 | 1.13 | 1.23 |
| 8 | J | 8 | PHE | CD2-CE2 | 5.44 | 1.50 | 1.39 |
| 2 | B | 348 | ARG | CZ-NH1 | -5.44 | 1.25 | 1.33 |
| 3 | C | 43 | THR | C-O | 5.44 | 1.33 | 1.23 |
| 6 | H | 127 | GLY | CA-C | 5.44 | 1.60 | 1.51 |
| 4 | E | 137 | GLU | CG-CD | 5.44 | 1.60 | 1.51 |
| 10 | L | 64 | LEU | CG-CD1 | 5.44 | 1.72 | 1.51 |
| 10 | L | 44 | ASP | C-O | 5.44 | 1.33 | 1.23 |
| 2 | B | 935 | ARG | NE-CZ | 5.43 | 1.40 | 1.33 |
| 4 | E | 121 | MET | SD-CE | 5.43 | 2.08 | 1.77 |
| 7 | I | 121 | PHE | CE2-CZ | -5.43 | 1.27 | 1.37 |
| 1 | A | 11 | LEU | C-O | -5.43 | 1.13 | 1.23 |
| 1 | A | 393 | ARG | CG-CD | 5.43 | 1.65 | 1.51 |
| 2 | B | 173 | MET | CB-CG | 5.43 | 1.68 | 1.51 |
| 10 | L | 66 | GLN | CD-OE1 | 5.43 | 1.35 | 1.24 |
| 1 | A | 799 | PHE | CE2-CZ | 5.43 | 1.47 | 1.37 |
| 1 | A | 1117 | THR | CA-CB | -5.43 | 1.39 | 1.53 |
| 1 | A | 468 | PHE | CD2-CE2 | -5.43 | 1.28 | 1.39 |
| 1 | A | 1418 | LEU | CG-CD1 | 5.43 | 1.72 | 1.51 |
| 2 | B | 223 | VAL | C-O | -5.43 | 1.13 | 1.23 |
| 4 | E | 35 | VAL | CA-CB | -5.43 | 1.43 | 1.54 |
| 1 | A | 992 | ASP | CB-CG | 5.43 | 1.63 | 1.51 |
| 2 | B | 732 | SER | CA-C | 5.42 | 1.67 | 1.52 |
| 2 | B | 890 | TYR | CD1-CE1 | 5.42 | 1.47 | 1.39 |
| 6 | H | 141 | TYR | CG-CD2 | -5.42 | 1.32 | 1.39 |
| 1 | A | 1156 | PRO | C-O | 5.42 | 1.34 | 1.23 |
| 9 | K | 25 | THR | CB-CG2 | 5.42 | 1.70 | 1.52 |
| 4 | E | 34 | GLU | CG-CD | 5.42 | 1.60 | 1.51 |
| 3 | C | 196 | ASP | CG-OD1 | 5.42 | 1.37 | 1.25 |
| 2 | B | 958 | GLN | CA-CB | 5.42 | 1.65 | 1.53 |
| 1 | A | 905 | ASP | CA-CB | -5.41 | 1.42 | 1.53 |
| 1 | A | 271 | LYS | CD-CE | 5.41 | 1.64 | 1.51 |
| 2 | B | 658 | ILE | CB-CG2 | -5.41 | 1.36 | 1.52 |
| 2 | B | 743 | ILE | CB-CG2 | -5.41 | 1.36 | 1.52 |
| 2 | B | 790 | ASP | CA-C | -5.41 | 1.38 | 1.52 |
| 3 | C | 193 | TYR | CG-CD2 | 5.41 | 1.46 | 1.39 |
| 9 | K | 54 | ARG | CZ-NH1 | 5.41 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 863 | VAL | CB-CG1 | 5.41 | 1.64 | 1.52 |
| 1 | A | 1200 | ALA | C-O | 5.41 | 1.33 | 1.23 |
| 1 | A | 417 | TYR | CD2-CE2 | 5.41 | 1.47 | 1.39 |
| 1 | A | 892 | ALA | C-O | -5.41 | 1.13 | 1.23 |
| 2 | B | 578 | THR | CB-CG2 | -5.41 | 1.34 | 1.52 |
| 2 | B | 1109 | GLY | CA-C | 5.41 | 1.60 | 1.51 |
| 7 | I | 111 | THR | C-O | -5.41 | 1.13 | 1.23 |
| 9 | K | 63 | VAL | CB-CG2 | 5.40 | 1.64 | 1.52 |
| 1 | A | 899 | VAL | CB-CG1 | -5.40 | 1.41 | 1.52 |
| 2 | B | 105 | SER | CA-C | 5.40 | 1.67 | 1.52 |
| 2 | B | 367 | LEU | CA-CB | 5.40 | 1.66 | 1.53 |
| 2 | B | 632 | ARG | NE-CZ | -5.40 | 1.26 | 1.33 |
| 6 | H | 136 | LYS | N-CA | 5.40 | 1.57 | 1.46 |
| 7 | I | 86 | PHE | CG-CD2 | 5.40 | 1.46 | 1.38 |
| 4 | E | 202 | SER | CB-OG | -5.40 | 1.35 | 1.42 |
| 1 | A | 1356 | ILE | CA-CB | -5.40 | 1.42 | 1.54 |
| 1 | A | 1361 | SER | CB-OG | 5.40 | 1.49 | 1.42 |
| 9 | K | 29 | ASN | CG-ND2 | 5.40 | 1.46 | 1.32 |
| 1 | A | 745 | GLN | CD-OE1 | 5.40 | 1.35 | 1.24 |
| 1 | A | 833 | GLU | CB-CG | 5.39 | 1.62 | 1.52 |
| 2 | B | 949 | VAL | CA-CB | -5.39 | 1.43 | 1.54 |
| 7 | I | 97 | MET | N-CA | -5.39 | 1.35 | 1.46 |
| 1 | A | 50 | ILE | N-CA | 5.39 | 1.57 | 1.46 |
| 1 | A | 737 | LEU | CG-CD2 | 5.39 | 1.71 | 1.51 |
| 1 | A | 6 | TYR | CE1-CZ | 5.39 | 1.45 | 1.38 |
| 9 | K | 82 | ASP | C-O | -5.38 | 1.13 | 1.23 |
| 1 | A | 1042 | PHE | CG-CD1 | 5.38 | 1.46 | 1.38 |
| 1 | A | 1426 | GLU | CG-CD | 5.38 | 1.60 | 1.51 |
| 2 | B | 227 | LYS | C-O | -5.38 | 1.13 | 1.23 |
| 1 | A | 1036 | ARG | C-O | -5.38 | 1.13 | 1.23 |
| 2 | B | 413 | LEU | C-O | -5.38 | 1.13 | 1.23 |
| 2 | B | 901 | PRO | CG-CD | 5.38 | 1.68 | 1.50 |
| 1 | A | 61 | ILE | CB-CG2 | 5.38 | 1.69 | 1.52 |
| 1 | A | 929 | LEU | N-CA | -5.38 | 1.35 | 1.46 |
| 1 | A | 56 | PRO | C-O | 5.38 | 1.34 | 1.23 |
| 3 | C | 9 | LYS | C-O | -5.38 | 1.13 | 1.23 |
| 6 | H | 143 | LEU | CA-C | -5.38 | 1.39 | 1.52 |
| 8 | J | 47 | ARG | CZ-NH1 | -5.38 | 1.26 | 1.33 |
| 9 | K | 102 | LYS | CB-CG | 5.38 | 1.67 | 1.52 |
| 1 | A | 1236 | LEU | CG-CD2 | 5.38 | 1.71 | 1.51 |
| 4 | E | 31 | THR | CA-CB | 5.38 | 1.67 | 1.53 |
| 2 | B | 830 | TYR | CG-CD1 | -5.37 | 1.32 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 804 | GLY | N-CA | 5.37 | 1.54 | 1.46 |
| 1 | A | 724 | GLU | N-CA | -5.37 | 1.35 | 1.46 |
| 2 | B | 488 | TYR | C-O | 5.37 | 1.33 | 1.23 |
| 1 | A | 815 | PHE | CG-CD2 | -5.37 | 1.30 | 1.38 |
| 3 | C | 204 | SER | C-O | 5.37 | 1.33 | 1.23 |
| 5 | F | 84 | TYR | CE2-CZ | 5.37 | 1.45 | 1.38 |
| 9 | K | 2 | ASN | CA-C | 5.36 | 1.66 | 1.52 |
| 7 | I | 24 | ARG | C-O | 5.36 | 1.33 | 1.23 |
| 1 | A | 1341 | ILE | CB-CG2 | -5.36 | 1.36 | 1.52 |
| 1 | A | 536 | LEU | C-O | 5.36 | 1.33 | 1.23 |
| 1 | A | 872 | GLY | CA-C | -5.36 | 1.43 | 1.51 |
| 1 | A | 1079 | MET | C-O | 5.36 | 1.33 | 1.23 |
| 2 | B | 360 | PHE | C-O | 5.36 | 1.33 | 1.23 |
| 4 | E | 79 | TRP | C-O | -5.36 | 1.13 | 1.23 |
| 1 | A | 1129 | GLU | CA-CB | 5.35 | 1.65 | 1.53 |
| 3 | C | 62 | PHE | CE1-CZ | 5.35 | 1.47 | 1.37 |
| 1 | A | 370 | ILE | C-O | -5.35 | 1.13 | 1.23 |
| 1 | A | 813 | PHE | CG-CD2 | -5.35 | 1.30 | 1.38 |
| 1 | A | 1327 | ILE | N-CA | -5.35 | 1.35 | 1.46 |
| 7 | I | 6 | PHE | CD1-CE1 | 5.35 | 1.50 | 1.39 |
| 4 | E | 47 | CYS | CA-C | 5.35 | 1.66 | 1.52 |
| 2 | B | 1135 | ARG | CD-NE | -5.35 | 1.37 | 1.46 |
| 1 | A | 1237 | ILE | CA-CB | -5.35 | 1.42 | 1.54 |
| 6 | H | 79 | TRP | CA-CB | -5.35 | 1.42 | 1.53 |
| 2 | B | 1204 | PHE | CB-CG | 5.34 | 1.60 | 1.51 |
| 5 | F | 72 | LYS | CG-CD | 5.34 | 1.70 | 1.52 |
| 1 | A | 720 | ARG | CD-NE | 5.34 | 1.55 | 1.46 |
| 2 | B | 35 | SER | CA-CB | -5.34 | 1.45 | 1.52 |
| 8 | J | 1 | MET | SD-CE | 5.34 | 2.07 | 1.77 |
| 2 | B | 1008 | PRO | CA-CB | -5.34 | 1.42 | 1.53 |
| 3 | C | 159 | ALA | N-CA | -5.34 | 1.35 | 1.46 |
| 1 | A | 462 | VAL | CA-CB | -5.33 | 1.43 | 1.54 |
| 4 | E | 203 | GLU | CA-CB | -5.33 | 1.42 | 1.53 |
| 1 | A | 387 | ARG | CD-NE | 5.33 | 1.55 | 1.46 |
| 1 | A | 925 | LEU | N-CA | -5.33 | 1.35 | 1.46 |
| 2 | B | 199 | MET | C-O | -5.33 | 1.13 | 1.23 |
| 2 | B | 224 | GLN | N-CA | -5.33 | 1.35 | 1.46 |
| 1 | A | 1426 | GLU | CB-CG | 5.33 | 1.62 | 1.52 |
| 7 | I | 18 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 5 | F | 149 | GLU | C-O | 5.33 | 1.33 | 1.23 |
| 1 | A | 1447 | GLU | CB-CG | 5.33 | 1.62 | 1.52 |
| 1 | A | 409 | SER | CB-OG | 5.32 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 620 | LYS | CB-CG | 5.32 | 1.67 | 1.52 |
| 1 | A | 857 | ARG | CZ-NH2 | 5.32 | 1.40 | 1.33 |
| 2 | B | 367 | LEU | CG-CD2 | 5.32 | 1.71 | 1.51 |
| 2 | B | 1073 | TYR | CG-CD2 | -5.32 | 1.32 | 1.39 |
| 2 | B | 1220 | ARG | CG-CD | 5.32 | 1.65 | 1.51 |
| 2 | B | 549 | THR | C-O | 5.32 | 1.33 | 1.23 |
| 2 | B | 798 | TYR | CG-CD2 | 5.32 | 1.46 | 1.39 |
| 1 | A | 500 | GLU | C-O | -5.32 | 1.13 | 1.23 |
| 1 | A | 1450 | LEU | CA-C | 5.32 | 1.66 | 1.52 |
| 2 | B | 224 | GLN | C-O | -5.32 | 1.13 | 1.23 |
| 2 | B | 233 | PRO | CB-CG | 5.32 | 1.76 | 1.50 |
| 3 | C | 226 | ASP | C-O | -5.32 | 1.13 | 1.23 |
| 4 | E | 83 | CYS | CB-SG | 5.32 | 1.91 | 1.82 |
| 7 | I | 1 | MET | CA-CB | 5.32 | 1.65 | 1.53 |
| 1 | A | 1298 | TYR | CG-CD2 | -5.32 | 1.32 | 1.39 |
| 2 | B | 1060 | ARG | CZ-NH2 | -5.32 | 1.26 | 1.33 |
| 2 | B | 810 | GLU | CD-OE2 | 5.32 | 1.31 | 1.25 |
| 3 | C | 244 | VAL | CA-CB | -5.32 | 1.43 | 1.54 |
| 10 | L | 47 | ARG | NE-CZ | 5.32 | 1.40 | 1.33 |
| 2 | B | 351 | TYR | CD1-CE1 | 5.32 | 1.47 | 1.39 |
| 2 | B | 1191 | ILE | CA-CB | -5.32 | 1.42 | 1.54 |
| 2 | B | 239 | GLU | C-O | 5.31 | 1.33 | 1.23 |
| 2 | B | 993 | THR | CA-C | -5.31 | 1.39 | 1.52 |
| 4 | E | 40 | GLU | CG-CD | 5.31 | 1.59 | 1.51 |
| 1 | A | 1194 | ARG | CD-NE | -5.31 | 1.37 | 1.46 |
| 2 | B | 280 | ILE | CB-CG2 | -5.31 | 1.36 | 1.52 |
| 2 | B | 887 | HIS | CA-CB | 5.31 | 1.65 | 1.53 |
| 3 | C | 268 | ASP | CB-CG | 5.31 | 1.62 | 1.51 |
| 7 | I | 87 | GLN | C-O | -5.31 | 1.13 | 1.23 |
| 1 | A | 1362 | TYR | CD2-CE2 | -5.31 | 1.31 | 1.39 |
| 2 | B | 785 | TYR | CZ-OH | -5.31 | 1.28 | 1.37 |
| 1 | A | 826 | ASP | CB-CG | 5.30 | 1.62 | 1.51 |
| 2 | B | 337 | ARG | CZ-NH2 | -5.30 | 1.26 | 1.33 |
| 1 | A | 32 | VAL | CA-C | 5.30 | 1.66 | 1.52 |
| 1 | A | 974 | ASP | N-CA | 5.30 | 1.56 | 1.46 |
| 2 | B | 643 | ASP | C-O | -5.30 | 1.13 | 1.23 |
| 2 | B | 1087 | PHE | CE1-CZ | -5.30 | 1.27 | 1.37 |
| 3 | C | 214 | ASN | CB-CG | 5.30 | 1.63 | 1.51 |
| 7 | I | 60 | GLN | CG-CD | 5.30 | 1.63 | 1.51 |
| 7 | I | 93 | LYS | CG-CD | 5.30 | 1.70 | 1.52 |
| 9 | K | 26 | LYS | CA-C | 5.30 | 1.66 | 1.52 |
| 8 | J | 38 | ARG | CG-CD | -5.30 | 1.38 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 393 | ARG | CD-NE | 5.30 | 1.55 | 1.46 |
| 2 | B | 37 | PHE | CA-CB | -5.30 | 1.42 | 1.53 |
| 3 | C | 3 | GLU | CG-CD | 5.30 | 1.59 | 1.51 |
| 3 | C | 4 | GLU | CD-OE1 | 5.30 | 1.31 | 1.25 |
| 1 | A | 464 | PRO | C-N | -5.29 | 1.21 | 1.34 |
| 1 | A | 14 | VAL | CB-CG1 | -5.29 | 1.41 | 1.52 |
| 1 | A | 838 | GLN | CD-OE1 | 5.29 | 1.35 | 1.24 |
| 1 | A | 1127 | ASP | CG-OD2 | 5.29 | 1.37 | 1.25 |
| 1 | A | 590 | ARG | CB-CG | 5.29 | 1.66 | 1.52 |
| 2 | B | 351 | TYR | CD2-CE2 | 5.29 | 1.47 | 1.39 |
| 6 | H | 2 | SER | N-CA | 5.29 | 1.56 | 1.46 |
| 1 | A | 941 | LYS | CA-CB | 5.29 | 1.65 | 1.53 |
| 1 | A | 1225 | PHE | CG-CD2 | 5.29 | 1.46 | 1.38 |
| 2 | B | 20 | ASP | CB-CG | 5.29 | 1.62 | 1.51 |
| 1 | A | 529 | CYS | C-O | -5.29 | 1.13 | 1.23 |
| 1 | A | 1326 | ARG | CZ-NH1 | -5.29 | 1.26 | 1.33 |
| 5 | F | 135 | ARG | CG-CD | 5.29 | 1.65 | 1.51 |
| 6 | H | 22 | LYS | C-O | 5.29 | 1.33 | 1.23 |
| 6 | H | 104 | PHE | CG-CD2 | 5.29 | 1.46 | 1.38 |
| 2 | B | 781 | PHE | CE2-CZ | 5.29 | 1.47 | 1.37 |
| 2 | B | 815 | ARG | CD-NE | -5.29 | 1.37 | 1.46 |
| 2 | B | 371 | GLU | CA-C | -5.29 | 1.39 | 1.52 |
| 2 | B | 904 | ARG | CG-CD | -5.29 | 1.38 | 1.51 |
| 2 | B | 1021 | MET | CG-SD | -5.28 | 1.67 | 1.81 |
| 1 | A | 1256 | GLU | CB-CG | 5.28 | 1.62 | 1.52 |
| 1 | A | 1308 | THR | N-CA | -5.28 | 1.35 | 1.46 |
| 1 | A | 515 | GLN | CG-CD | 5.28 | 1.63 | 1.51 |
| 3 | C | 123 | ASN | CB-CG | 5.28 | 1.63 | 1.51 |
| 2 | B | 945 | GLU | CG-CD | 5.28 | 1.59 | 1.51 |
| 4 | E | 23 | VAL | CB-CG1 | 5.28 | 1.64 | 1.52 |
| 7 | I | 1 | MET | SD-CE | 5.28 | 2.07 | 1.77 |
| 1 | A | 1224 | LEU | C-O | -5.28 | 1.13 | 1.23 |
| 2 | B | 235 | SER | N-CA | -5.28 | 1.35 | 1.46 |
| 2 | B | 328 | GLU | CB-CG | 5.28 | 1.62 | 1.52 |
| 2 | B | 606 | LYS | CB-CG | -5.27 | 1.38 | 1.52 |
| 2 | B | 275 | TYR | CD1-CE1 | -5.27 | 1.31 | 1.39 |
| 2 | B | 561 | TRP | CE3-CZ3 | 5.27 | 1.47 | 1.38 |
| 2 | B | 1211 | ASN | CB-CG | -5.27 | 1.39 | 1.51 |
| 3 | C | 13 | ALA | C-O | -5.27 | 1.13 | 1.23 |
| 2 | B | 165 | VAL | CA-CB | 5.27 | 1.65 | 1.54 |
| 2 | B | 1135 | ARG | CG-CD | -5.27 | 1.38 | 1.51 |
| 1 | A | 821 | ARG | NE-CZ | -5.26 | 1.26 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | K | 35 | PHE | CG-CD1 | -5.26 | 1.30 | 1.38 |
| 1 | A | 469 | ARG | CB-CG | 5.26 | 1.66 | 1.52 |
| 1 | A | 598 | LEU | CG-CD1 | 5.26 | 1.71 | 1.51 |
| 2 | B | 350 | GLN | CA-CB | -5.26 | 1.42 | 1.53 |
| 3 | C | 240 | VAL | CA-C | -5.26 | 1.39 | 1.52 |
| 1 | A | 303 | TYR | CG-CD2 | -5.26 | 1.32 | 1.39 |
| 2 | B | 776 | GLN | CG-CD | 5.26 | 1.63 | 1.51 |
| 3 | C | 154 | LYS | CE-NZ | 5.26 | 1.62 | 1.49 |
| 4 | E | 21 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 4 | E | 30 | ILE | CA-CB | 5.26 | 1.67 | 1.54 |
| 1 | A | 556 | TRP | CB-CG | -5.25 | 1.40 | 1.50 |
| 1 | A | 1040 | GLN | CD-OE1 | 5.25 | 1.35 | 1.24 |
| 1 | A | 1353 | TYR | CD1-CE1 | 5.25 | 1.47 | 1.39 |
| 2 | B | 199 | MET | CG-SD | 5.25 | 1.94 | 1.81 |
| 1 | A | 98 | LYS | CB-CG | -5.25 | 1.38 | 1.52 |
| 5 | F | 108 | PHE | CE2-CZ | 5.25 | 1.47 | 1.37 |
| 2 | B | 315 | LYS | CA-CB | -5.25 | 1.42 | 1.53 |
| 2 | B | 567 | GLU | CG-CD | 5.25 | 1.59 | 1.51 |
| 2 | B | 1021 | MET | CB-CG | 5.25 | 1.68 | 1.51 |
| 2 | B | 1174 | LYS | CB-CG | 5.25 | 1.66 | 1.52 |
| 1 | A | 889 | SER | C-O | -5.24 | 1.13 | 1.23 |
| 1 | A | 927 | VAL | CB-CG1 | -5.24 | 1.41 | 1.52 |
| 2 | B | 483 | LEU | C-O | -5.24 | 1.13 | 1.23 |
| 2 | B | 1155 | SER | C-O | 5.24 | 1.33 | 1.23 |
| 9 | K | 69 | ALA | N-CA | 5.24 | 1.56 | 1.46 |
| 3 | C | 104 | PHE | CB-CG | -5.24 | 1.42 | 1.51 |
| 2 | B | 973 | ILE | N-CA | -5.24 | 1.35 | 1.46 |
| 1 | A | 8 | SER | CA-CB | 5.24 | 1.60 | 1.52 |
| 4 | E | 169 | ARG | C-O | 5.24 | 1.33 | 1.23 |
| 1 | A | 1346 | ALA | CA-CB | -5.24 | 1.41 | 1.52 |
| 2 | B | 404 | LYS | N-CA | -5.24 | 1.35 | 1.46 |
| 3 | C | 90 | ASP | N-CA | 5.24 | 1.56 | 1.46 |
| 5 | F | 88 | TYR | CG-CD1 | -5.24 | 1.32 | 1.39 |
| 2 | B | 60 | GLN | C-O | -5.23 | 1.13 | 1.23 |
| 2 | B | 333 | PHE | CE1-CZ | -5.23 | 1.27 | 1.37 |
| 5 | F | 79 | ARG | CD-NE | -5.23 | 1.37 | 1.46 |
| 5 | F | 95 | GLY | C-O | -5.23 | 1.15 | 1.23 |
| 5 | F | 110 | ASP | CG-OD1 | 5.23 | 1.37 | 1.25 |
| 3 | C | 60 | ASP | CA-C | -5.23 | 1.39 | 1.52 |
| 1 | A | 944 | ARG | CZ-NH2 | -5.23 | 1.26 | 1.33 |
| 2 | B | 816 | GLU | CG-CD | 5.23 | 1.59 | 1.51 |
| 2 | B | 862 | GLN | CD-OE1 | 5.23 | 1.35 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | K | 113 | THR | CB-CG2 | 5.23 | 1.69 | 1.52 |
| 1 | A | 646 | PHE | CG-CD1 | -5.23 | 1.30 | 1.38 |
| 7 | I | 87 | GLN | CA-C | -5.23 | 1.39 | 1.52 |
| 1 | A | 961 | ARG | CG-CD | 5.22 | 1.65 | 1.51 |
| 2 | B | 455 | SER | CB-OG | 5.22 | 1.49 | 1.42 |
| 2 | B | 1005 | GLY | C-O | 5.22 | 1.32 | 1.23 |
| 5 | F | 106 | PRO | CG-CD | -5.22 | 1.33 | 1.50 |
| 7 | I | 30 | ARG | CA-CB | -5.22 | 1.42 | 1.53 |
| 1 | A | 1274 | ARG | CZ-NH2 | 5.22 | 1.39 | 1.33 |
| 2 | B | 610 | ASN | CG-ND2 | -5.22 | 1.19 | 1.32 |
| 3 | C | 193 | TYR | CD2-CE2 | 5.22 | 1.47 | 1.39 |
| 7 | I | 18 | GLU | CG-CD | -5.22 | 1.44 | 1.51 |
| 1 | A | 411 | ASP | CG-OD1 | 5.22 | 1.37 | 1.25 |
| 1 | A | 1127 | ASP | CB-CG | 5.22 | 1.62 | 1.51 |
| 4 | E | 29 | PHE | CD2-CE2 | -5.22 | 1.28 | 1.39 |
| 1 | A | 1235 | LYS | CB-CG | 5.21 | 1.66 | 1.52 |
| 9 | K | 38 | GLU | CG-CD | 5.21 | 1.59 | 1.51 |
| 4 | E | 6 | GLU | CG-CD | 5.21 | 1.59 | 1.51 |
| 1 | A | 653 | VAL | C-O | -5.21 | 1.13 | 1.23 |
| 1 | A | 1308 | THR | CB-CG2 | -5.21 | 1.35 | 1.52 |
| 2 | B | 230 | ALA | N-CA | 5.21 | 1.56 | 1.46 |
| 9 | K | 99 | GLY | C-O | 5.21 | 1.31 | 1.23 |
| 1 | A | 652 | VAL | CB-CG1 | -5.21 | 1.42 | 1.52 |
| 1 | A | 973 | ILE | C-O | 5.21 | 1.33 | 1.23 |
| 2 | B | 1094 | ARG | NE-CZ | -5.21 | 1.26 | 1.33 |
| 1 | A | 351 | THR | CB-CG2 | -5.21 | 1.35 | 1.52 |
| 1 | A | 567 | LYS | CB-CG | -5.21 | 1.38 | 1.52 |
| 2 | B | 556 | THR | C-O | 5.21 | 1.33 | 1.23 |
| 1 | A | 905 | ASP | CG-OD2 | 5.20 | 1.37 | 1.25 |
| 2 | B | 89 | GLU | CG-CD | 5.20 | 1.59 | 1.51 |
| 2 | B | 650 | GLU | CG-CD | 5.20 | 1.59 | 1.51 |
| 2 | B | 728 | ARG | CG-CD | 5.20 | 1.65 | 1.51 |
| 1 | A | 493 | GLN | CB-CG | -5.20 | 1.38 | 1.52 |
| 2 | B | 627 | PHE | CE1-CZ | 5.20 | 1.47 | 1.37 |
| 2 | B | 892 | LYS | C-O | -5.20 | 1.13 | 1.23 |
| 6 | H | 103 | LYS | CA-C | -5.20 | 1.39 | 1.52 |
| 1 | A | 1142 | THR | C-O | 5.20 | 1.33 | 1.23 |
| 4 | E | 90 | VAL | CA-CB | 5.20 | 1.65 | 1.54 |
| 4 | E | 70 | SER | CB-OG | -5.19 | 1.35 | 1.42 |
| 4 | E | 78 | LEU | C-O | 5.19 | 1.33 | 1.23 |
| 6 | H | 112 | ILE | CB-CG2 | -5.19 | 1.36 | 1.52 |
| 2 | B | 678 | GLU | CG-CD | 5.19 | 1.59 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | J | 3 | VAL | CB-CG1 | -5.19 | 1.42 | 1.52 |
| 1 | A | 987 | VAL | CB-CG2 | -5.19 | 1.42 | 1.52 |
| 2 | B | 995 | ARG | NE-CZ | -5.19 | 1.26 | 1.33 |
| 1 | A | 857 | ARG | C-O | 5.19 | 1.33 | 1.23 |
| 1 | A | 1303 | GLU | N-CA | -5.19 | 1.35 | 1.46 |
| 2 | B | 730 | ARG | CZ-NH1 | -5.19 | 1.26 | 1.33 |
| 1 | A | 532 | ARG | CB-CG | -5.18 | 1.38 | 1.52 |
| 1 | A | 1304 | TRP | CG-CD1 | -5.18 | 1.29 | 1.36 |
| 2 | B | 534 | GLY | C-O | 5.18 | 1.31 | 1.23 |
| 3 | C | 10 | ILE | C-O | -5.18 | 1.13 | 1.23 |
| 1 | A | 1228 | TRP | CZ3-CH2 | -5.18 | 1.31 | 1.40 |
| 6 | H | 111 | LEU | N-CA | 5.18 | 1.56 | 1.46 |
| 1 | A | 380 | VAL | C-O | 5.18 | 1.33 | 1.23 |
| 1 | A | 463 | ILE | CB-CG2 | -5.18 | 1.36 | 1.52 |
| 2 | B | 820 | GLY | N-CA | -5.17 | 1.38 | 1.46 |
| 2 | B | 1183 | LYS | CB-CG | 5.17 | 1.66 | 1.52 |
| 1 | A | 1048 | ASN | N-CA | -5.17 | 1.36 | 1.46 |
| 2 | B | 899 | ILE | CA-CB | -5.17 | 1.43 | 1.54 |
| 2 | B | 958 | GLN | CD-NE2 | 5.17 | 1.45 | 1.32 |
| 9 | K | 89 | ASN | CB-CG | 5.17 | 1.62 | 1.51 |
| 9 | K | 107 | THR | C-O | 5.17 | 1.33 | 1.23 |
| 1 | A | 1255 | GLU | CG-CD | 5.17 | 1.59 | 1.51 |
| 2 | B | 1077 | THR | C-O | -5.17 | 1.13 | 1.23 |
| 3 | C | 20 | PHE | C-O | -5.17 | 1.13 | 1.23 |
| 9 | K | 16 | GLU | C-O | -5.17 | 1.13 | 1.23 |
| 1 | A | 23 | SER | C-O | 5.17 | 1.33 | 1.23 |
| 1 | A | 248 | PRO | N-CD | 5.17 | 1.55 | 1.47 |
| 1 | A | 992 | ASP | C-O | -5.17 | 1.13 | 1.23 |
| 2 | B | 654 | ARG | CA-CB | -5.17 | 1.42 | 1.53 |
| 1 | A | 387 | ARG | NE-CZ | 5.17 | 1.39 | 1.33 |
| 1 | A | 965 | GLN | CD-OE1 | 5.17 | 1.35 | 1.24 |
| 2 | B | 136 | THR | C-O | 5.17 | 1.33 | 1.23 |
| 1 | A | 513 | SER | CB-OG | -5.16 | 1.35 | 1.42 |
| 2 | B | 265 | SER | CA-C | 5.16 | 1.66 | 1.52 |
| 1 | A | 431 | LYS | CE-NZ | 5.16 | 1.61 | 1.49 |
| 9 | K | 50 | LEU | C-O | -5.16 | 1.13 | 1.23 |
| 1 | A | 25 | GLU | CB-CG | 5.16 | 1.61 | 1.52 |
| 1 | A | 994 | GLN | CG-CD | -5.16 | 1.39 | 1.51 |
| 1 | A | 1209 | MET | N-CA | -5.16 | 1.36 | 1.46 |
| 4 | E | 212 | ARG | CD-NE | -5.16 | 1.37 | 1.46 |
| 1 | A | 894 | GLU | CD-OE1 | 5.16 | 1.31 | 1.25 |
| 2 | B | 678 | GLU | CD-OE1 | 5.16 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 855 | PHE | CG-CD1 | -5.16 | 1.31 | 1.38 |
| 2 | B | 395 | GLN | CB-CG | -5.16 | 1.38 | 1.52 |
| 2 | B | 1139 | ILE | C-O | -5.16 | 1.13 | 1.23 |
| 1 | A | 15 | LYS | CD-CE | 5.15 | 1.64 | 1.51 |
| 1 | A | 821 | ARG | CG-CD | 5.15 | 1.64 | 1.51 |
| 2 | B | 49 | ASP | CG-OD2 | 5.15 | 1.37 | 1.25 |
| 2 | B | 394 | ASP | CG-OD2 | 5.15 | 1.37 | 1.25 |
| 1 | A | 779 | PHE | CG-CD2 | -5.15 | 1.31 | 1.38 |
| 3 | C | 109 | SER | CA-CB | 5.15 | 1.60 | 1.52 |
| 2 | B | 23 | ALA | CA-CB | -5.15 | 1.41 | 1.52 |
| 3 | C | 199 | LYS | CA-C | -5.15 | 1.39 | 1.52 |
| 1 | A | 1446 | ASP | N-CA | 5.15 | 1.56 | 1.46 |
| 2 | B | 807 | ARG | NE-CZ | -5.15 | 1.26 | 1.33 |
| 1 | A | 933 | TYR | CG-CD2 | -5.14 | 1.32 | 1.39 |
| 2 | B | 1157 | ALA | CA-CB | 5.14 | 1.63 | 1.52 |
| 9 | K | 2 | ASN | CB-CG | 5.14 | 1.62 | 1.51 |
| 2 | B | 306 | ASN | CB-CG | 5.14 | 1.62 | 1.51 |
| 1 | A | 404 | TYR | CZ-OH | -5.14 | 1.29 | 1.37 |
| 8 | J | 18 | TRP | CE3-CZ3 | -5.14 | 1.29 | 1.38 |
| 2 | B | 452 | THR | CA-CB | 5.14 | 1.66 | 1.53 |
| 1 | A | 350 | ARG | CG-CD | -5.14 | 1.39 | 1.51 |
| 1 | A | 711 | ARG | N-CA | -5.14 | 1.36 | 1.46 |
| 1 | A | 911 | SER | CA-CB | 5.14 | 1.60 | 1.52 |
| 1 | A | 1137 | ALA | C-O | 5.14 | 1.33 | 1.23 |
| 8 | J | 31 | ASP | CG-OD1 | 5.14 | 1.37 | 1.25 |
| 1 | A | 786 | HIS | CA-CB | -5.13 | 1.42 | 1.53 |
| 1 | A | 1030 | ARG | CB-CG | -5.13 | 1.38 | 1.52 |
| 2 | B | 722 | ASP | CB-CG | 5.13 | 1.62 | 1.51 |
| 1 | A | 1170 | ILE | CA-CB | 5.13 | 1.66 | 1.54 |
| 1 | A | 976 | THR | CA-CB | 5.13 | 1.66 | 1.53 |
| 1 | A | 303 | TYR | CG-CD1 | -5.13 | 1.32 | 1.39 |
| 1 | A | 977 | LYS | CG-CD | 5.13 | 1.69 | 1.52 |
| 1 | A | 1304 | TRP | CE2-CZ2 | -5.13 | 1.31 | 1.39 |
| 6 | H | 141 | TYR | CE2-CZ | -5.13 | 1.31 | 1.38 |
| 1 | A | 607 | ILE | CB-CG1 | -5.13 | 1.39 | 1.54 |
| 1 | A | 1191 | TRP | C-O | 5.13 | 1.33 | 1.23 |
| 2 | B | 106 | ASP | CA-CB | 5.13 | 1.65 | 1.53 |
| 8 | J | 42 | LYS | CG-CD | 5.13 | 1.69 | 1.52 |
| 2 | B | 37 | PHE | CD1-CE1 | -5.12 | 1.29 | 1.39 |
| 1 | A | 1220 | PHE | CD2-CE2 | 5.12 | 1.49 | 1.39 |
| 6 | H | 10 | PHE | CD2-CE2 | 5.12 | 1.49 | 1.39 |
| 2 | B | 605 | ARG | NE-CZ | -5.12 | 1.26 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1243 | VAL | CA-CB | 5.12 | 1.65 | 1.54 |
| 3 | C | 158 | VAL | CB-CG1 | -5.12 | 1.42 | 1.52 |
| 6 | H | 115 | TYR | CD2-CE2 | 5.12 | 1.47 | 1.39 |
| 1 | A | 942 | PHE | CB-CG | -5.12 | 1.42 | 1.51 |
| 2 | B | 1079 | LYS | CA-C | -5.12 | 1.39 | 1.52 |
| 2 | B | 137 | TYR | CD1-CE1 | 5.11 | 1.47 | 1.39 |
| 1 | A | 549 | MET | C-O | -5.11 | 1.13 | 1.23 |
| 1 | A | 664 | THR | CB-CG2 | -5.11 | 1.35 | 1.52 |
| 2 | B | 758 | PHE | CD2-CE2 | 5.11 | 1.49 | 1.39 |
| 1 | A | 971 | PHE | CB-CG | -5.11 | 1.42 | 1.51 |
| 1 | A | 1003 | LYS | C-O | 5.11 | 1.33 | 1.23 |
| 7 | I | 41 | PRO | CA-CB | -5.11 | 1.43 | 1.53 |
| 8 | J | 24 | LEU | CG-CD2 | -5.11 | 1.32 | 1.51 |
| 1 | A | 833 | GLU | C-O | 5.11 | 1.33 | 1.23 |
| 5 | F | 77 | ASP | CG-OD1 | 5.11 | 1.37 | 1.25 |
| 1 | A | 940 | ARG | CZ-NH1 | -5.10 | 1.26 | 1.33 |
| 1 | A | 1029 | ARG | CA-CB | -5.10 | 1.42 | 1.53 |
| 2 | B | 294 | ASP | CB-CG | 5.10 | 1.62 | 1.51 |
| 2 | B | 627 | PHE | CE2-CZ | -5.10 | 1.27 | 1.37 |
| 2 | B | 889 | THR | N-CA | 5.10 | 1.56 | 1.46 |
| 4 | E | 42 | PHE | CE1-CZ | -5.10 | 1.27 | 1.37 |
| 1 | A | 776 | ALA | C-O | -5.10 | 1.13 | 1.23 |
| 1 | A | 1195 | LEU | N-CA | 5.10 | 1.56 | 1.46 |
| 2 | B | 869 | SER | CA-C | 5.10 | 1.66 | 1.52 |
| 1 | A | 1151 | GLU | CB-CG | -5.10 | 1.42 | 1.52 |
| 1 | A | 1344 | GLY | C-O | -5.09 | 1.15 | 1.23 |
| 2 | B | 565 | PRO | CG-CD | -5.09 | 1.33 | 1.50 |
| 10 | L | 63 | ARG | CD-NE | 5.09 | 1.55 | 1.46 |
| 1 | A | 1077 | THR | C-O | -5.09 | 1.13 | 1.23 |
| 3 | C | 223 | ALA | CA-CB | -5.09 | 1.41 | 1.52 |
| 3 | C | 247 | GLY | N-CA | -5.09 | 1.38 | 1.46 |
| 1 | A | 1052 | GLN | N-CA | -5.09 | 1.36 | 1.46 |
| 2 | B | 57 | TYR | CA-CB | 5.09 | 1.65 | 1.53 |
| 2 | B | 68 | THR | CA-CB | 5.09 | 1.66 | 1.53 |
| 7 | I | 114 | GLN | C-O | -5.09 | 1.13 | 1.23 |
| 1 | A | 1195 | LEU | C-N | -5.09 | 1.22 | 1.34 |
| 3 | C | 218 | PRO | CG-CD | 5.09 | 1.67 | 1.50 |
| 1 | A | 244 | PRO | C-O | 5.08 | 1.33 | 1.23 |
| 1 | A | 459 | ARG | CD-NE | -5.08 | 1.37 | 1.46 |
| 3 | C | 82 | TYR | CD1-CE1 | -5.08 | 1.31 | 1.39 |
| 1 | A | 635 | ARG | C-O | -5.08 | 1.13 | 1.23 |
| 2 | B | 344 | LYS | CG-CD | 5.08 | 1.69 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 561 | TRP | CZ3-CH2 | 5.08 | 1.48 | 1.40 |
| 1 | A | 446 | ARG | CZ-NH2 | 5.08 | 1.39 | 1.33 |
| 4 | E | 67 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 4 | E | 124 | VAL | CB-CG2 | -5.08 | 1.42 | 1.52 |
| 1 | A | 677 | ARG | CD-NE | 5.08 | 1.55 | 1.46 |
| 1 | A | 74 | MET | CA-CB | 5.08 | 1.65 | 1.53 |
| 2 | B | 694 | ASP | CG-OD2 | 5.08 | 1.37 | 1.25 |
| 4 | E | 211 | TYR | C-O | 5.08 | 1.32 | 1.23 |
| 2 | B | 275 | TYR | CZ-OH | -5.08 | 1.29 | 1.37 |
| 2 | B | 852 | ARG | CZ-NH2 | -5.08 | 1.26 | 1.33 |
| 2 | B | 1128 | LEU | CA-C | 5.08 | 1.66 | 1.52 |
| 1 | A | 593 | GLU | C-N | 5.08 | 1.42 | 1.33 |
| 2 | B | 308 | TRP | CA-C | -5.08 | 1.39 | 1.52 |
| 4 | E | 126 | SER | CA-CB | 5.08 | 1.60 | 1.52 |
| 7 | I | 15 | TYR | C-O | -5.08 | 1.13 | 1.23 |
| 1 | A | 89 | PRO | CA-C | -5.07 | 1.42 | 1.52 |
| 1 | A | 556 | TRP | CD2-CE3 | -5.07 | 1.32 | 1.40 |
| 1 | A | 1049 | ILE | CA-CB | -5.07 | 1.43 | 1.54 |
| 1 | A | 1286 | LYS | C-O | -5.07 | 1.13 | 1.23 |
| 2 | B | 217 | ARG | CD-NE | -5.07 | 1.37 | 1.46 |
| 2 | B | 643 | ASP | CA-C | -5.07 | 1.39 | 1.52 |
| 2 | B | 827 | ILE | CB-CG2 | -5.07 | 1.37 | 1.52 |
| 2 | B | 1091 | TYR | CB-CG | -5.07 | 1.44 | 1.51 |
| 2 | B | 310 | MET | C-O | 5.07 | 1.32 | 1.23 |
| 1 | A | 285 | PRO | C-O | -5.07 | 1.13 | 1.23 |
| 3 | C | 211 | ASP | CG-OD1 | 5.07 | 1.37 | 1.25 |
| 1 | A | 805 | LEU | CG-CD1 | -5.07 | 1.33 | 1.51 |
| 2 | B | 451 | LYS | CG-CD | 5.07 | 1.69 | 1.52 |
| 1 | A | 920 | LEU | CA-CB | -5.07 | 1.42 | 1.53 |
| 1 | A | 1274 | ARG | CB-CG | -5.07 | 1.38 | 1.52 |
| 1 | A | 1298 | TYR | CE1-CZ | -5.07 | 1.31 | 1.38 |
| 10 | L | 42 | ARG | CD-NE | 5.07 | 1.55 | 1.46 |
| 1 | A | 1446 | ASP | CA-CB | 5.07 | 1.65 | 1.53 |
| 2 | B | 106 | ASP | CG-OD2 | 5.07 | 1.37 | 1.25 |
| 3 | C | 117 | ASP | CG-OD1 | 5.07 | 1.37 | 1.25 |
| 10 | L | 63 | ARG | CG-CD | 5.07 | 1.64 | 1.51 |
| 1 | A | 404 | TYR | CE1-CZ | -5.06 | 1.31 | 1.38 |
| 3 | C | 79 | GLN | CG-CD | 5.06 | 1.62 | 1.51 |
| 9 | K | 78 | THR | CA-CB | -5.06 | 1.40 | 1.53 |
| 1 | A | 621 | THR | CB-CG2 | -5.06 | 1.35 | 1.52 |
| 1 | A | 803 | SER | CA-CB | 5.06 | 1.60 | 1.52 |
| 1 | A | 360 | GLU | CD-OE1 | 5.06 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 378 | GLU | CG-CD | -5.06 | 1.44 | 1.51 |
| 2 | B | 745 | PRO | N-CD | -5.06 | 1.40 | 1.47 |
| 1 | A | 367 | PRO | N-CD | -5.06 | 1.40 | 1.47 |
| 3 | C | 191 | TYR | CD1-CE1 | 5.06 | 1.47 | 1.39 |
| 6 | H | 56 | THR | CA-CB | 5.06 | 1.66 | 1.53 |
| 2 | B | 226 | PHE | CE1-CZ | 5.05 | 1.47 | 1.37 |
| 2 | B | 552 | MET | CA-CB | -5.05 | 1.42 | 1.53 |
| 2 | B | 1223 | ASP | CA-C | 5.05 | 1.66 | 1.52 |
| 1 | A | 982 | THR | CB-OG1 | -5.05 | 1.33 | 1.43 |
| 3 | C | 191 | TYR | N-CA | -5.05 | 1.36 | 1.46 |
| 7 | I | 117 | LYS | CE-NZ | 5.05 | 1.61 | 1.49 |
| 1 | A | 781 | ASP | C-O | 5.05 | 1.32 | 1.23 |
| 2 | B | 1082 | MET | CA-C | -5.05 | 1.39 | 1.52 |
| 4 | E | 110 | PHE | CG-CD2 | -5.05 | 1.31 | 1.38 |
| 5 | F | 84 | TYR | CZ-OH | 5.05 | 1.46 | 1.37 |
| 1 | A | 1228 | TRP | CA-C | -5.05 | 1.39 | 1.52 |
| 2 | B | 388 | CYS | CB-SG | -5.05 | 1.73 | 1.81 |
| 2 | B | 735 | ALA | CA-CB | -5.05 | 1.41 | 1.52 |
| 6 | H | 37 | LYS | CA-C | 5.05 | 1.66 | 1.52 |
| 2 | B | 660 | LYS | CB-CG | 5.05 | 1.66 | 1.52 |
| 2 | B | 30 | SER | C-O | -5.05 | 1.13 | 1.23 |
| 7 | I | 20 | LYS | CG-CD | 5.05 | 1.69 | 1.52 |
| 1 | A | 297 | GLN | C-O | -5.04 | 1.13 | 1.23 |
| 1 | A | 359 | LEU | CG-CD2 | -5.04 | 1.33 | 1.51 |
| 2 | B | 257 | LYS | C-O | -5.04 | 1.13 | 1.23 |
| 2 | B | 1188 | LYS | CG-CD | 5.04 | 1.69 | 1.52 |
| 1 | A | 1116 | LEU | CA-CB | -5.04 | 1.42 | 1.53 |
| 6 | H | 130 | ARG | CA-C | 5.04 | 1.66 | 1.52 |
| 1 | A | 626 | ASN | CG-OD1 | 5.04 | 1.35 | 1.24 |
| 2 | B | 96 | TYR | CD2-CE2 | 5.04 | 1.47 | 1.39 |
| 1 | A | 568 | PRO | N-CD | -5.04 | 1.40 | 1.47 |
| 1 | A | 656 | TRP | CD2-CE3 | -5.04 | 1.32 | 1.40 |
| 3 | C | 167 | HIS | CA-CB | -5.04 | 1.42 | 1.53 |
| 5 | F | 148 | VAL | CA-CB | -5.04 | 1.44 | 1.54 |
| 8 | J | 1 | MET | CB-CG | -5.04 | 1.35 | 1.51 |
| 1 | A | 883 | LEU | C-O | 5.04 | 1.32 | 1.23 |
| 1 | A | 1282 | VAL | CA-CB | -5.04 | 1.44 | 1.54 |
| 1 | A | 712 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 1 | A | 897 | TYR | N-CA | 5.04 | 1.56 | 1.46 |
| 2 | B | 513 | GLN | CD-NE2 | 5.03 | 1.45 | 1.32 |
| 2 | B | 854 | LEU | CA-C | -5.03 | 1.39 | 1.52 |
| 2 | B | 964 | VAL | CA-CB | -5.03 | 1.44 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 39 | ALA | C-O | 5.03 | 1.32 | 1.23 |
| 7 | I | 27 | PHE | CE1-CZ | -5.03 | 1.27 | 1.37 |
| 3 | C | 158 | VAL | N-CA | -5.03 | 1.36 | 1.46 |
| 3 | C | 244 | VAL | CB-CG1 | -5.03 | 1.42 | 1.52 |
| 1 | A | 93 | VAL | CB-CG1 | 5.03 | 1.63 | 1.52 |
| 1 | A | 586 | ILE | CB-CG2 | -5.03 | 1.37 | 1.52 |
| 2 | B | 398 | ARG | CZ-NH1 | 5.03 | 1.39 | 1.33 |
| 1 | A | 537 | ARG | CZ-NH1 | 5.03 | 1.39 | 1.33 |
| 2 | B | 1140 | ALA | C-O | 5.03 | 1.32 | 1.23 |
| 1 | A | 953 | ASN | CG-OD1 | 5.02 | 1.35 | 1.24 |
| 5 | F | 153 | VAL | CA-C | -5.02 | 1.39 | 1.52 |
| 1 | A | 477 | PRO | CG-CD | 5.02 | 1.67 | 1.50 |
| 1 | A | 578 | LEU | N-CA | 5.02 | 1.56 | 1.46 |
| 9 | K | 61 | TYR | CZ-OH | -5.02 | 1.29 | 1.37 |
| 2 | B | 291 | ILE | CB-CG2 | -5.02 | 1.37 | 1.52 |
| 2 | B | 829 | CYS | CB-SG | 5.02 | 1.90 | 1.82 |
| 1 | A | 1050 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 8 | J | 38 | ARG | N-CA | -5.02 | 1.36 | 1.46 |
| 1 | A | 661 | GLY | C-O | 5.02 | 1.31 | 1.23 |
| 9 | K | 66 | PRO | C-O | -5.01 | 1.13 | 1.23 |
| 1 | A | 471 | ASN | CA-C | -5.01 | 1.40 | 1.52 |
| 1 | A | 944 | ARG | CZ-NH1 | -5.01 | 1.26 | 1.33 |
| 1 | A | 601 | LYS | CE-NZ | 5.01 | 1.61 | 1.49 |
| 1 | A | 940 | ARG | CZ-NH2 | -5.01 | 1.26 | 1.33 |
| 1 | A | 994 | GLN | CD-OE1 | -5.01 | 1.12 | 1.24 |
| 2 | B | 231 | PRO | N-CA | 5.01 | 1.55 | 1.47 |
| 2 | B | 1154 | ALA | C-N | 5.01 | 1.45 | 1.34 |
| 6 | H | 14 | GLU | CD-OE1 | 5.01 | 1.31 | 1.25 |
| 2 | B | 1130 | PHE | C-O | -5.01 | 1.13 | 1.23 |
| 2 | B | 130 | VAL | CA-C | 5.00 | 1.66 | 1.52 |
| 1 | A | 611 | GLN | CD-NE2 | 5.00 | 1.45 | 1.32 |
| 2 | B | 660 | LYS | N-CA | -5.00 | 1.36 | 1.46 |
| 1 | A | 1168 | GLU | CB-CG | 5.00 | 1.61 | 1.52 |
| 3 | C | 58 | LEU | CG-CD2 | -5.00 | 1.33 | 1.51 |

All (1625) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1366 | ARG | NE-CZ-NH2 | -34.23 | 103.18 | 120.30 |
| 1 | A | 774 | ARG | NE-CZ-NH1 | 32.19 | 136.39 | 120.30 |
| 3 | C | 34 | ARG | NE-CZ-NH2 | -31.55 | 104.53 | 120.30 |
| 2 | B | 995 | ARG | NE-CZ-NH2 | -30.46 | 105.07 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1366 | ARG | NE-CZ-NH1 | 28.94 | 134.77 | 120.30 |
| 9 | K | 47 | ARG | NE-CZ-NH2 | -27.69 | 106.45 | 120.30 |
| 1 | A | 469 | ARG | NE-CZ-NH2 | -26.96 | 106.82 | 120.30 |
| 3 | C | 35 | ARG | NE-CZ-NH2 | -24.26 | 108.17 | 120.30 |
| 2 | B | 496 | ARG | NE-CZ-NH1 | 24.02 | 132.31 | 120.30 |
| 1 | A | 940 | ARG | NE-CZ-NH1 | 23.85 | 132.22 | 120.30 |
| 1 | A | 469 | ARG | NE-CZ-NH1 | 23.64 | 132.12 | 120.30 |
| 2 | B | 995 | ARG | NE-CZ-NH1 | 23.07 | 131.83 | 120.30 |
| 2 | B | 1135 | ARG | NE-CZ-NH2 | -22.80 | 108.90 | 120.30 |
| 1 | A | 446 | ARG | NE-CZ-NH2 | -22.60 | 109.00 | 120.30 |
| 2 | B | 604 | ARG | NE-CZ-NH1 | 21.98 | 131.29 | 120.30 |
| 1 | A | 459 | ARG | NE-CZ-NH2 | -21.91 | 109.35 | 120.30 |
| 3 | C | 35 | ARG | NE-CZ-NH1 | 20.90 | 130.75 | 120.30 |
| 3 | C | 34 | ARG | NE-CZ-NH1 | 20.81 | 130.70 | 120.30 |
| 2 | B | 620 | ARG | NE-CZ-NH1 | -20.38 | 110.11 | 120.30 |
| 2 | B | 496 | ARG | NE-CZ-NH2 | -19.91 | 110.35 | 120.30 |
| 3 | C | 66 | ARG | NE-CZ-NH1 | -19.84 | 110.38 | 120.30 |
| 1 | A | 1336 | MET | CG-SD-CE | 19.29 | 131.07 | 100.20 |
| 2 | B | 807 | ARG | NE-CZ-NH2 | -19.12 | 110.74 | 120.30 |
| 2 | B | 106 | ASP | CB-CG-OD2 | 19.06 | 135.46 | 118.30 |
| 3 | C | 66 | ARG | NE-CZ-NH2 | 18.64 | 129.62 | 120.30 |
| 1 | A | 434 | ARG | NE-CZ-NH2 | -18.48 | 111.06 | 120.30 |
| 1 | A | 896 | ARG | NE-CZ-NH2 | -18.46 | 111.07 | 120.30 |
| 1 | A | 590 | ARG | NE-CZ-NH2 | -18.33 | 111.13 | 120.30 |
| 3 | C | 16 | ASP | CB-CG-OD2 | 18.08 | 134.57 | 118.30 |
| 1 | A | 821 | ARG | NE-CZ-NH2 | -17.81 | 111.39 | 120.30 |
| 2 | B | 996 | ARG | NE-CZ-NH1 | -17.48 | 111.56 | 120.30 |
| 2 | B | 983 | ARG | NE-CZ-NH2 | -17.00 | 111.80 | 120.30 |
| 1 | A | 1135 | ARG | NE-CZ-NH1 | -17.00 | 111.80 | 120.30 |
| 2 | B | 287 | ARG | NE-CZ-NH2 | -16.82 | 111.89 | 120.30 |
| 2 | B | 909 | ASP | CB-CG-OD2 | 16.77 | 133.39 | 118.30 |
| 1 | A | 434 | ARG | NE-CZ-NH1 | 16.72 | 128.66 | 120.30 |
| 1 | A | 1100 | ARG | NE-CZ-NH2 | -16.55 | 112.02 | 120.30 |
| 2 | B | 839 | MET | CG-SD-CE | -16.26 | 74.18 | 100.20 |
| 2 | B | 1150 | ARG | NE-CZ-NH1 | -16.25 | 112.17 | 120.30 |
| 1 | A | 1241 | ARG | NE-CZ-NH2 | -16.21 | 112.19 | 120.30 |
| 2 | B | 405 | ARG | NE-CZ-NH1 | 16.13 | 128.37 | 120.30 |
| 1 | A | 962 | ARG | NE-CZ-NH2 | -15.84 | 112.38 | 120.30 |
| 2 | B | 394 | ASP | CB-CG-OD2 | 15.79 | 132.51 | 118.30 |
| 2 | B | 604 | ARG | NE-CZ-NH2 | -15.76 | 112.42 | 120.30 |
| 1 | A | 949 | ASP | CB-CG-OD2 | 15.73 | 132.46 | 118.30 |
| 1 | A | 985 | ASP | CB-CG-OD1 | -15.64 | 104.23 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 249 | ARG | NE-CZ-NH1 | 15.62 | 128.11 | 120.30 |
| 9 | K | 22 | ASP | CB-CG-OD1 | 15.50 | 132.25 | 118.30 |
| 1 | A | 1100 | ARG | NE-CZ-NH1 | 15.46 | 128.03 | 120.30 |
| 1 | A | 940 | ARG | NE-CZ-NH2 | -15.45 | 112.57 | 120.30 |
| 1 | A | 481 | ASP | CB-CG-OD1 | 15.40 | 132.16 | 118.30 |
| 8 | J | 43 | ARG | NE-CZ-NH1 | -15.31 | 112.64 | 120.30 |
| 1 | A | 1422 | ARG | NE-CZ-NH1 | 15.27 | 127.93 | 120.30 |
| 1 | A | 774 | ARG | NE-CZ-NH2 | -15.26 | 112.67 | 120.30 |
| 10 | L | 70 | ARG | NE-CZ-NH1 | 15.21 | 127.90 | 120.30 |
| 2 | B | 497 | ARG | NE-CZ-NH2 | -15.14 | 112.73 | 120.30 |
| 10 | L | 68 | GLU | OE1-CD-OE2 | -15.11 | 105.17 | 123.30 |
| 3 | C | 220 | ASP | CB-CG-OD1 | 15.00 | 131.80 | 118.30 |
| 1 | A | 1036 | ARG | NE-CZ-NH2 | -14.99 | 112.81 | 120.30 |
| 8 | J | 6 | ARG | NE-CZ-NH2 | 14.95 | 127.77 | 120.30 |
| 7 | I | 61 | ASP | CB-CG-OD2 | 14.93 | 131.74 | 118.30 |
| 1 | A | 1241 | ARG | NE-CZ-NH1 | 14.90 | 127.75 | 120.30 |
| 2 | B | 1043 | ASP | CB-CG-OD2 | 14.90 | 131.71 | 118.30 |
| 2 | B | 983 | ARG | NE-CZ-NH1 | 14.89 | 127.75 | 120.30 |
| 9 | K | 47 | ARG | NE-CZ-NH1 | 14.85 | 127.72 | 120.30 |
| 2 | B | 39 | ARG | NE-CZ-NH1 | 14.83 | 127.71 | 120.30 |
| 2 | B | 287 | ARG | NE-CZ-NH1 | 14.78 | 127.69 | 120.30 |
| 9 | K | 5 | ASP | CB-CG-OD1 | -14.74 | 105.04 | 118.30 |
| 1 | A | 420 | ARG | NE-CZ-NH1 | 14.59 | 127.59 | 120.30 |
| 1 | A | 1442 | ASP | CB-CG-OD2 | 14.53 | 131.38 | 118.30 |
| 1 | A | 961 | ARG | NE-CZ-NH1 | -14.45 | 113.07 | 120.30 |
| 1 | A | 172 | PRO | CA-N-CD | -14.41 | 91.33 | 111.50 |
| 3 | C | 84 | ARG | NE-CZ-NH2 | 14.39 | 127.50 | 120.30 |
| 2 | B | 998 | ASP | CB-CG-OD2 | 14.39 | 131.25 | 118.30 |
| 2 | B | 326 | ASP | CB-CG-OD2 | 14.34 | 131.20 | 118.30 |
| 2 | B | 620 | ARG | NH1-CZ-NH2 | 14.20 | 135.02 | 119.40 |
| 8 | J | 48 | ARG | NE-CZ-NH1 | 14.20 | 127.40 | 120.30 |
| 9 | K | 114 | LEU | CB-CG-CD2 | 14.19 | 135.12 | 111.00 |
| 8 | J | 38 | ARG | NE-CZ-NH1 | 14.17 | 127.39 | 120.30 |
| 2 | B | 373 | ARG | NE-CZ-NH2 | -14.04 | 113.28 | 120.30 |
| 8 | J | 43 | ARG | NE-CZ-NH2 | 14.03 | 127.31 | 120.30 |
| 4 | E | 14 | ARG | NE-CZ-NH1 | 13.95 | 127.27 | 120.30 |
| 3 | C | 93 | ASP | CB-CG-OD2 | 13.81 | 130.73 | 118.30 |
| 1 | A | 483 | ASP | CB-CG-OD2 | 13.69 | 130.62 | 118.30 |
| 1 | A | 483 | ASP | CB-CG-OD1 | -13.65 | 106.01 | 118.30 |
| 1 | A | 407 | ARG | NE-CZ-NH2 | -13.55 | 113.52 | 120.30 |
| 8 | J | 49 | MET | CG-SD-CE | -13.51 | 78.58 | 100.20 |
| 5 | F | 92 | ARG | NE-CZ-NH1 | 13.48 | 127.04 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 591 | ARG | NE-CZ-NH1 | 13.48 | 127.04 | 120.30 |
| 1 | A | 1006 | ILE | CG1-CB-CG2 | -13.45 | 81.80 | 111.40 |
| 6 | H | 77 | ARG | NE-CZ-NH1 | 13.29 | 126.94 | 120.30 |
| 2 | B | 1019 | SER | CB-CA-C | -13.21 | 84.99 | 110.10 |
| 4 | E | 11 | ARG | NE-CZ-NH1 | -13.18 | 113.71 | 120.30 |
| 3 | C | 268 | ASP | CB-CG-OD2 | 13.11 | 130.09 | 118.30 |
| 1 | A | 153 | PRO | CA-N-CD | -13.06 | 93.21 | 111.50 |
| 2 | B | 790 | ASP | CB-CG-OD2 | -13.06 | 106.55 | 118.30 |
| 1 | A | 884 | ASP | CB-CG-OD1 | -13.01 | 106.59 | 118.30 |
| 2 | B | 642 | ASP | CB-CG-OD1 | 12.94 | 129.95 | 118.30 |
| 1 | A | 806 | ARG | NE-CZ-NH1 | -12.84 | 113.88 | 120.30 |
| 2 | B | 790 | ASP | CB-CG-OD1 | 12.79 | 129.81 | 118.30 |
| 1 | A | 538 | ASP | CB-CA-C | -12.79 | 84.83 | 110.40 |
| 2 | B | 241 | ARG | NE-CZ-NH1 | 12.74 | 126.67 | 120.30 |
| 4 | E | 212 | ARG | NE-CZ-NH2 | -12.66 | 113.97 | 120.30 |
| 9 | K | 5 | ASP | CB-CG-OD2 | 12.65 | 129.69 | 118.30 |
| 5 | F | 81 | THR | N-CA-CB | -12.61 | 86.34 | 110.30 |
| 4 | E | 207 | ARG | NE-CZ-NH1 | 12.59 | 126.60 | 120.30 |
| 1 | A | 826 | ASP | CB-CG-OD2 | 12.54 | 129.59 | 118.30 |
| 2 | B | 348 | ARG | NE-CZ-NH2 | -12.52 | 114.04 | 120.30 |
| 4 | E | 212 | ARG | CD-NE-CZ | 12.49 | 141.09 | 123.60 |
| 2 | B | 106 | ASP | CB-CG-OD1 | -12.36 | 107.17 | 118.30 |
| 9 | K | 114 | LEU | CA-CB-CG | 12.33 | 143.65 | 115.30 |
| 2 | B | 807 | ARG | NE-CZ-NH1 | 12.32 | 126.46 | 120.30 |
| 10 | L | 68 | GLU | CG-CD-OE1 | 12.31 | 142.93 | 118.30 |
| 2 | B | 49 | ASP | CB-CG-OD2 | 12.13 | 129.22 | 118.30 |
| 2 | B | 391 | ASP | CB-CG-OD2 | 12.13 | 129.22 | 118.30 |
| 2 | B | 883 | LEU | CA-CB-CG | 12.13 | 143.20 | 115.30 |
| 1 | A | 446 | ARG | NH1-CZ-NH2 | 12.12 | 132.74 | 119.40 |
| 2 | B | 294 | ASP | CB-CG-OD2 | 12.12 | 129.21 | 118.30 |
| 4 | E | 200 | ARG | NE-CZ-NH1 | -12.12 | 114.24 | 120.30 |
| 2 | B | 188 | ASP | CB-CG-OD2 | 12.07 | 129.17 | 118.30 |
| 2 | B | 1150 | ARG | NH1-CZ-NH2 | 12.01 | 132.61 | 119.40 |
| 2 | B | 120 | ARG | NE-CZ-NH1 | -11.95 | 114.33 | 120.30 |
| 4 | E | 204 | THR | CA-CB-CG2 | 11.94 | 129.12 | 112.40 |
| 7 | I | 70 | ARG | NE-CZ-NH2 | -11.93 | 114.33 | 120.30 |
| 1 | A | 557 | ASP | CB-CG-OD2 | 11.81 | 128.93 | 118.30 |
| 2 | B | 635 | ARG | NE-CZ-NH1 | 11.80 | 126.20 | 120.30 |
| 10 | L | 34 | CYS | CA-CB-SG | -11.78 | 92.79 | 114.00 |
| 1 | A | 1269 | GLU | OE1-CD-OE2 | 11.74 | 137.38 | 123.30 |
| 1 | A | 423 | ASP | CB-CG-OD1 | 11.70 | 128.83 | 118.30 |
| 2 | B | 1043 | ASP | CB-CG-OD1 | -11.70 | 107.77 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1062 | GLU | CB-CA-C | -11.67 | 87.05 | 110.40 |
| 1 | A | 518 | LYS | CD-CE-NZ | -11.63 | 84.96 | 111.70 |
| 1 | A | 1196 | GLU | OE1-CD-OE2 | 11.62 | 137.24 | 123.30 |
| 2 | B | 1220 | ARG | NE-CZ-NH2 | 11.62 | 126.11 | 120.30 |
| 1 | A | 944 | ARG | NE-CZ-NH2 | 11.62 | 126.11 | 120.30 |
| 1 | A | 459 | ARG | NE-CZ-NH1 | 11.59 | 126.09 | 120.30 |
| 6 | H | 130 | ARG | NE-CZ-NH1 | -11.52 | 114.54 | 120.30 |
| 3 | C | 86 | CYS | CA-CB-SG | 11.45 | 134.61 | 114.00 |
| 1 | A | 884 | ASP | CB-CG-OD2 | 11.41 | 128.57 | 118.30 |
| 4 | E | 24 | LYS | CD-CE-NZ | -11.39 | 85.49 | 111.70 |
| 1 | A | 42 | ASP | CB-CG-OD2 | 11.37 | 128.53 | 118.30 |
| 9 | K | 42 | LEU | CB-CG-CD1 | -11.36 | 91.68 | 111.00 |
| 1 | A | 857 | ARG | NE-CZ-NH1 | -11.34 | 114.63 | 120.30 |
| 1 | A | 728 | LYS | CD-CE-NZ | 11.30 | 137.69 | 111.70 |
| 2 | B | 747 | MET | CG-SD-CE | -11.30 | 82.12 | 100.20 |
| 1 | A | 801 | GLU | OE1-CD-OE2 | 11.29 | 136.84 | 123.30 |
| 2 | B | 1219 | ASP | CB-CG-OD2 | 11.23 | 128.41 | 118.30 |
| 6 | H | 135 | LEU | CA-CB-CG | 11.14 | 140.92 | 115.30 |
| 2 | B | 485 | ARG | NE-CZ-NH2 | -11.13 | 114.73 | 120.30 |
| 1 | A | 740 | LEU | CB-CG-CD1 | 11.12 | 129.90 | 111.00 |
| 7 | I | 45 | ARG | NE-CZ-NH1 | -11.11 | 114.74 | 120.30 |
| 1 | A | 609 | ASP | CB-CG-OD2 | 11.04 | 128.24 | 118.30 |
| 1 | A | 416 | ARG | NE-CZ-NH2 | -11.03 | 114.78 | 120.30 |
| 2 | B | 568 | ASP | CB-CG-OD2 | 11.02 | 128.22 | 118.30 |
| 1 | A | 372 | LYS | CD-CE-NZ | -11.00 | 86.40 | 111.70 |
| 1 | A | 544 | ASP | CB-CG-OD1 | 10.99 | 128.19 | 118.30 |
| 2 | B | 1135 | ARG | NH1-CZ-NH2 | 10.97 | 131.47 | 119.40 |
| 1 | A | 197 | PRO | CA-N-CD | -10.94 | 96.18 | 111.50 |
| 1 | A | 748 | MET | CG-SD-CE | 10.91 | 117.66 | 100.20 |
| 2 | B | 579 | ARG | NE-CZ-NH1 | -10.88 | 114.86 | 120.30 |
| 1 | A | 1043 | ASP | CB-CG-OD2 | 10.87 | 128.08 | 118.30 |
| 2 | B | 620 | ARG | NE-CZ-NH2 | -10.87 | 114.87 | 120.30 |
| 1 | A | 36 | ARG | NE-CZ-NH1 | 10.84 | 125.72 | 120.30 |
| 3 | C | 246 | ARG | NE-CZ-NH1 | 10.83 | 125.71 | 120.30 |
| 1 | A | 949 | ASP | N-CA-CB | -10.80 | 91.16 | 110.60 |
| 7 | I | 81 | ARG | NE-CZ-NH1 | 10.77 | 125.68 | 120.30 |
| 2 | B | 552 | MET | CG-SD-CE | 10.76 | 117.41 | 100.20 |
| 1 | A | 93 | VAL | CB-CA-C | -10.75 | 90.97 | 111.40 |
| 1 | A | 537 | ARG | NE-CZ-NH1 | 10.73 | 125.67 | 120.30 |
| 6 | H | 110 | ASP | CB-CG-OD2 | 10.70 | 127.93 | 118.30 |
| 9 | K | 6 | ARG | NE-CZ-NH2 | -10.66 | 114.97 | 120.30 |
| 2 | B | 326 | ASP | CB-CG-OD1 | -10.66 | 108.70 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 941 | LYS | CD-CE-NZ | -10.59 | 87.34 | 111.70 |
| 1 | A | 1055 | ARG | NE-CZ-NH1 | 10.56 | 125.58 | 120.30 |
| 1 | A | 857 | ARG | NE-CZ-NH2 | 10.56 | 125.58 | 120.30 |
| 1 | A | 352 | VAL | CG1-CB-CG2 | -10.55 | 94.02 | 110.90 |
| 1 | A | 592 | ASP | CB-CG-OD2 | -10.54 | 108.81 | 118.30 |
| 1 | A | 537 | ARG | NE-CZ-NH2 | -10.46 | 115.07 | 120.30 |
| 2 | B | 1097 | HIS | CB-CA-C | 10.40 | 131.21 | 110.40 |
| 2 | B | 56 | ASP | CB-CG-OD2 | 10.40 | 127.66 | 118.30 |
| 1 | A | 771 | GLU | OE1-CD-OE2 | 10.38 | 135.75 | 123.30 |
| 1 | A | 1284 | MET | CA-CB-CG | -10.36 | 95.69 | 113.30 |
| 1 | A | 771 | GLU | CG-CD-OE1 | -10.36 | 97.58 | 118.30 |
| 2 | B | 1006 | ILE | CG1-CB-CG2 | -10.34 | 88.65 | 111.40 |
| 4 | E | 25 | ASP | CB-CG-OD2 | 10.32 | 127.59 | 118.30 |
| 1 | A | 605 | MET | CG-SD-CE | -10.31 | 83.70 | 100.20 |
| 1 | A | 961 | ARG | NE-CZ-NH2 | 10.27 | 125.44 | 120.30 |
| 1 | A | 1207 | LEU | CB-CG-CD1 | -10.26 | 93.57 | 111.00 |
| 1 | A | 1422 | ARG | NE-CZ-NH2 | -10.23 | 115.19 | 120.30 |
| 4 | E | 50 | MET | CG-SD-CE | 10.20 | 116.52 | 100.20 |
| 1 | A | 53 | LEU | CA-CB-CG | 10.18 | 138.72 | 115.30 |
| 8 | J | 1 | MET | CG-SD-CE | -10.18 | 83.91 | 100.20 |
| 2 | B | 1150 | ARG | NE-CZ-NH2 | -10.17 | 115.22 | 120.30 |
| 2 | B | 652 | LYS | CD-CE-NZ | 10.14 | 135.03 | 111.70 |
| 1 | A | 853 | ASP | CB-CG-OD2 | 10.11 | 127.40 | 118.30 |
| 2 | B | 337 | ARG | CG-CD-NE | -10.04 | 90.72 | 111.80 |
| 1 | A | 455 | MET | CG-SD-CE | -10.01 | 84.18 | 100.20 |
| 1 | A | 28 | ARG | NE-CZ-NH1 | 10.01 | 125.30 | 120.30 |
| 3 | C | 172 | PRO | N-CD-CG | 9.98 | 118.17 | 103.20 |
| 1 | A | 1366 | ARG | CD-NE-CZ | 9.97 | 137.55 | 123.60 |
| 3 | C | 160 | LYS | CD-CE-NZ | 9.96 | 134.61 | 111.70 |
| 2 | B | 1160 | VAL | CB-CA-C | -9.93 | 92.53 | 111.40 |
| 7 | I | 81 | ARG | NE-CZ-NH2 | -9.92 | 115.34 | 120.30 |
| 2 | B | 605 | ARG | NE-CZ-NH1 | -9.91 | 115.34 | 120.30 |
| 1 | A | 620 | LYS | CD-CE-NZ | 9.90 | 134.47 | 111.70 |
| 2 | B | 547 | VAL | CG1-CB-CG2 | 9.86 | 126.67 | 110.90 |
| 1 | A | 466 | SER | CB-CA-C | -9.86 | 91.38 | 110.10 |
| 2 | B | 408 | LEU | CB-CG-CD2 | -9.84 | 94.27 | 111.00 |
| 4 | E | 14 | ARG | NE-CZ-NH2 | -9.83 | 115.39 | 120.30 |
| 3 | C | 163 | ILE | CA-CB-CG2 | 9.82 | 130.54 | 110.90 |
| 4 | E | 162 | ARG | NE-CZ-NH1 | 9.80 | 125.20 | 120.30 |
| 2 | B | 598 | GLU | OE1-CD-OE2 | -9.78 | 111.56 | 123.30 |
| 1 | A | 974 | ASP | N-CA-CB | 9.77 | 128.19 | 110.60 |
| 1 | A | 1228 | TRP | CB-CA-C | -9.77 | 90.86 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | J | 51 | LEU | CB-CG-CD1 | 9.75 | 127.58 | 111.00 |
| 1 | A | 1376 | THR | N-CA-CB | -9.74 | 91.78 | 110.30 |
| 2 | B | 24 | PRO | N-CD-CG | -9.74 | 88.59 | 103.20 |
| 1 | A | 1157 | ASP | CB-CG-OD2 | 9.74 | 127.06 | 118.30 |
| 7 | I | 113 | ASP | CB-CG-OD2 | 9.74 | 127.06 | 118.30 |
| 2 | B | 996 | ARG | NH1-CZ-NH2 | 9.73 | 130.11 | 119.40 |
| 2 | B | 188 | ASP | CB-CG-OD1 | -9.73 | 109.55 | 118.30 |
| 1 | A | 438 | ASP | CB-CG-OD2 | 9.72 | 127.05 | 118.30 |
| 3 | C | 18 | VAL | CB-CA-C | -9.71 | 92.94 | 111.40 |
| 1 | A | 16 | GLU | OE1-CD-OE2 | 9.69 | 134.92 | 123.30 |
| 4 | E | 182 | ASP | CB-CG-OD1 | 9.67 | 127.00 | 118.30 |
| 1 | A | 1062 | GLU | OE1-CD-OE2 | 9.66 | 134.89 | 123.30 |
| 2 | B | 1097 | HIS | CB-CG-ND1 | -9.65 | 99.07 | 123.20 |
| 1 | A | 305 | ASP | CB-CG-OD2 | 9.64 | 126.98 | 118.30 |
| 5 | F | 119 | ARG | NE-CZ-NH2 | -9.64 | 115.48 | 120.30 |
| 1 | A | 1204 | ASP | CB-CG-OD2 | 9.63 | 126.97 | 118.30 |
| 2 | B | 337 | ARG | NE-CZ-NH2 | -9.62 | 115.49 | 120.30 |
| 2 | B | 118 | ARG | NE-CZ-NH1 | 9.61 | 125.11 | 120.30 |
| 2 | B | 563 | MET | CG-SD-CE | 9.61 | 115.57 | 100.20 |
| 3 | C | 93 | ASP | CB-CG-OD1 | -9.58 | 109.67 | 118.30 |
| 1 | A | 1420 | ASP | CB-CG-OD1 | -9.55 | 109.71 | 118.30 |
| 2 | B | 348 | ARG | NE-CZ-NH1 | 9.53 | 125.06 | 120.30 |
| 8 | J | 6 | ARG | NE-CZ-NH1 | -9.51 | 115.54 | 120.30 |
| 7 | I | 109 | ILE | CG1-CB-CG2 | -9.50 | 90.49 | 111.40 |
| 1 | A | 982 | THR | CA-CB-CG2 | 9.48 | 125.68 | 112.40 |
| 3 | C | 136 | ASP | CB-CG-OD2 | 9.48 | 126.83 | 118.30 |
| 1 | A | 291 | GLU | OE1-CD-OE2 | -9.46 | 111.94 | 123.30 |
| 8 | J | 3 | VAL | CB-CA-C | -9.46 | 93.43 | 111.40 |
| 2 | B | 760 | ASP | CB-CG-OD2 | 9.44 | 126.80 | 118.30 |
| 1 | A | 1081 | LEU | CB-CG-CD2 | 9.44 | 127.05 | 111.00 |
| 3 | C | 85 | ASP | CB-CG-OD2 | 9.40 | 126.76 | 118.30 |
| 1 | A | 549 | MET | CG-SD-CE | 9.38 | 115.22 | 100.20 |
| 1 | A | 1055 | ARG | CG-CD-NE | -9.38 | 92.09 | 111.80 |
| 1 | A | 962 | ARG | NE-CZ-NH1 | 9.38 | 124.99 | 120.30 |
| 1 | A | 28 | ARG | NE-CZ-NH2 | -9.38 | 115.61 | 120.30 |
| 7 | I | 43 | VAL | N-CA-CB | -9.36 | 90.90 | 111.50 |
| 7 | I | 54 | GLU | OE1-CD-OE2 | 9.35 | 134.52 | 123.30 |
| 1 | A | 1285 | MET | CG-SD-CE | 9.35 | 115.15 | 100.20 |
| 2 | B | 564 | GLU | OE1-CD-OE2 | 9.34 | 134.50 | 123.30 |
| 1 | A | 486 | GLU | OE1-CD-OE2 | -9.33 | 112.10 | 123.30 |
| 2 | B | 137 | TYR | CA-CB-CG | 9.32 | 131.12 | 113.40 |
| 2 | B | 384 | ARG | NE-CZ-NH1 | 9.32 | 124.96 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | I | 113 | ASP | CB-CG-OD1 | 9.32 | 126.69 | 118.30 |
| 9 | K | 82 | ASP | CB-CG-OD2 | 9.30 | 126.67 | 118.30 |
| 1 | A | 472 | LEU | CA-CB-CG | -9.27 | 93.98 | 115.30 |
| 1 | A | 389 | THR | OG1-CB-CG2 | -9.24 | 88.76 | 110.00 |
| 2 | B | 791 | THR | OG1-CB-CG2 | -9.23 | 88.76 | 110.00 |
| 2 | B | 837 | ASP | CB-CG-OD1 | 9.23 | 126.61 | 118.30 |
| 2 | B | 1159 | ARG | NE-CZ-NH2 | -9.23 | 115.68 | 120.30 |
| 1 | A | 346 | ASP | CB-CG-OD1 | 9.23 | 126.61 | 118.30 |
| 1 | A | 982 | THR | N-CA-CB | -9.22 | 92.78 | 110.30 |
| 1 | A | 726 | ARG | NE-CZ-NH1 | -9.21 | 115.69 | 120.30 |
| 2 | B | 629 | ASP | CB-CG-OD2 | 9.20 | 126.58 | 118.30 |
| 1 | A | 909 | ASP | CB-CG-OD1 | 9.18 | 126.56 | 118.30 |
| 4 | E | 201 | LYS | CD-CE-NZ | -9.18 | 90.59 | 111.70 |
| 2 | B | 391 | ASP | OD1-CG-OD2 | -9.14 | 105.94 | 123.30 |
| 2 | B | 788 | ARG | NE-CZ-NH1 | 9.13 | 124.86 | 120.30 |
| 2 | B | 1050 | ILE | CG1-CB-CG2 | -9.10 | 91.38 | 111.40 |
| 2 | B | 367 | LEU | CB-CG-CD2 | 9.10 | 126.47 | 111.00 |
| 1 | A | 944 | ARG | NH1-CZ-NH2 | -9.10 | 109.40 | 119.40 |
| 1 | A | 85 | ASP | CB-CG-OD1 | -9.09 | 110.12 | 118.30 |
| 1 | A | 1326 | ARG | NE-CZ-NH1 | 9.09 | 124.84 | 120.30 |
| 1 | A | 596 | THR | CA-CB-CG2 | -9.04 | 99.74 | 112.40 |
| 1 | A | 1198 | ASP | CB-CG-OD1 | 9.04 | 126.44 | 118.30 |
| 6 | H | 132 | LEU | CA-CB-CG | 9.03 | 136.06 | 115.30 |
| 3 | C | 125 | MET | CG-SD-CE | 8.98 | 114.58 | 100.20 |
| 7 | I | 113 | ASP | OD1-CG-OD2 | -8.98 | 106.23 | 123.30 |
| 10 | L | 48 | CYS | N-CA-CB | -8.98 | 94.44 | 110.60 |
| 3 | C | 155 | LEU | CB-CA-C | -8.98 | 93.15 | 110.20 |
| 10 | L | 27 | LEU | CA-CB-CG | 8.97 | 135.94 | 115.30 |
| 9 | K | 73 | LEU | CB-CG-CD1 | -8.97 | 95.75 | 111.00 |
| 2 | B | 567 | GLU | O-C-N | -8.96 | 108.37 | 122.70 |
| 3 | C | 165 | LYS | CD-CE-NZ | 8.94 | 132.26 | 111.70 |
| 8 | J | 61 | LEU | CB-CG-CD2 | 8.93 | 126.18 | 111.00 |
| 2 | B | 1041 | GLU | OE1-CD-OE2 | 8.92 | 134.01 | 123.30 |
| 2 | B | 857 | ARG | NE-CZ-NH1 | 8.91 | 124.76 | 120.30 |
| 2 | B | 484 | ASN | CB-CA-C | -8.91 | 92.58 | 110.40 |
| 1 | A | 821 | ARG | CG-CD-NE | -8.90 | 93.11 | 111.80 |
| 2 | B | 316 | PRO | N-CD-CG | -8.90 | 89.85 | 103.20 |
| 2 | B | 680 | THR | N-CA-CB | -8.90 | 93.39 | 110.30 |
| 1 | A | 1373 | ASP | CB-CG-OD2 | 8.89 | 126.30 | 118.30 |
| 9 | K | 24 | ASP | CB-CG-OD2 | 8.89 | 126.30 | 118.30 |
| 1 | A | 53 | LEU | CB-CG-CD1 | 8.89 | 126.11 | 111.00 |
| 1 | A | 557 | ASP | OD1-CG-OD2 | -8.89 | 106.41 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1176 | LEU | N-CA-C | -8.89 | 87.00 | 111.00 |
| 9 | K | 78 | THR | CA-CB-CG2 | -8.86 | 99.99 | 112.40 |
| 8 | J | 48 | ARG | NE-CZ-NH2 | -8.85 | 115.87 | 120.30 |
| 1 | A | 360 | GLU | OE1-CD-OE2 | -8.84 | 112.69 | 123.30 |
| 3 | C | 76 | ASP | CB-CG-OD1 | 8.84 | 126.26 | 118.30 |
| 2 | B | 405 | ARG | NE-CZ-NH2 | -8.83 | 115.89 | 120.30 |
| 2 | B | 552 | MET | CA-CB-CG | 8.81 | 128.28 | 113.30 |
| 1 | A | 231 | PRO | CA-N-CD | -8.81 | 99.17 | 111.50 |
| 2 | B | 963 | PHE | CB-CA-C | -8.78 | 92.84 | 110.40 |
| 1 | A | 787 | PHE | CB-CG-CD2 | 8.77 | 126.94 | 120.80 |
| 2 | B | 95 | ILE | CG1-CB-CG2 | -8.77 | 92.11 | 111.40 |
| 2 | B | 601 | ARG | NE-CZ-NH2 | -8.75 | 115.92 | 120.30 |
| 2 | B | 964 | VAL | CA-CB-CG2 | -8.74 | 97.79 | 110.90 |
| 9 | K | 36 | GLU | OE1-CD-OE2 | 8.74 | 133.78 | 123.30 |
| 1 | A | 590 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 2 | B | 642 | ASP | N-CA-C | -8.72 | 87.45 | 111.00 |
| 2 | B | 1067 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 2 | B | 1010 | LEU | CB-CG-CD1 | -8.71 | 96.19 | 111.00 |
| 1 | A | 1064 | VAL | N-CA-CB | -8.71 | 92.34 | 111.50 |
| 4 | E | 25 | ASP | OD1-CG-OD2 | -8.71 | 106.75 | 123.30 |
| 1 | A | 1271 | ILE | CG1-CB-CG2 | -8.71 | 92.25 | 111.40 |
| 2 | B | 416 | LEU | CB-CA-C | -8.70 | 93.67 | 110.20 |
| 2 | B | 710 | LEU | CB-CG-CD2 | 8.68 | 125.76 | 111.00 |
| 2 | B | 336 | ARG | CB-CA-C | -8.68 | 93.05 | 110.40 |
| 5 | F | 135 | ARG | NE-CZ-NH1 | -8.68 | 115.96 | 120.30 |
| 1 | A | 261 | ASP | CB-CG-OD2 | 8.66 | 126.09 | 118.30 |
| 1 | A | 821 | ARG | NE-CZ-NH1 | 8.66 | 124.63 | 120.30 |
| 1 | A | 1195 | LEU | CB-CG-CD1 | -8.66 | 96.28 | 111.00 |
| 1 | A | 672 | ASP | CB-CG-OD1 | 8.65 | 126.09 | 118.30 |
| 2 | B | 101 | MET | CG-SD-CE | 8.65 | 114.05 | 100.20 |
| 2 | B | 582 | VAL | CG1-CB-CG2 | -8.65 | 97.05 | 110.90 |
| 4 | E | 1 | MET | CG-SD-CE | 8.65 | 114.05 | 100.20 |
| 1 | A | 1289 | ARG | NE-CZ-NH1 | -8.65 | 115.97 | 120.30 |
| 1 | A | 1442 | ASP | CB-CG-OD1 | -8.65 | 110.52 | 118.30 |
| 2 | B | 1098 | MET | CG-SD-CE | 8.65 | 114.04 | 100.20 |
| 1 | A | 913 | LEU | CB-CG-CD1 | -8.64 | 96.32 | 111.00 |
| 8 | J | 62 | ARG | NE-CZ-NH1 | 8.63 | 124.61 | 120.30 |
| 3 | C | 9 | LYS | CD-CE-NZ | 8.63 | 131.54 | 111.70 |
| 1 | A | 992 | ASP | CB-CG-OD2 | 8.63 | 126.06 | 118.30 |
| 5 | F | 150 | GLU | N-CA-CB | -8.62 | 95.08 | 110.60 |
| 1 | A | 414 | ASP | CB-CG-OD2 | 8.60 | 126.04 | 118.30 |
| 2 | B | 118 | ARG | CD-NE-CZ | 8.59 | 135.63 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 245 | GLU | OE1-CD-OE2 | -8.59 | 113.00 | 123.30 |
| 2 | B | 513 | GLN | CA-CB-CG | 8.59 | 132.29 | 113.40 |
| 1 | A | 720 | ARG | NE-CZ-NH2 | 8.57 | 124.59 | 120.30 |
| 9 | K | 1 | MET | CG-SD-CE | 8.54 | 113.86 | 100.20 |
| 2 | B | 1020 | ARG | NE-CZ-NH2 | 8.53 | 124.56 | 120.30 |
| 4 | E | 20 | LYS | CA-CB-CG | 8.53 | 132.16 | 113.40 |
| 7 | I | 61 | ASP | CB-CG-OD1 | -8.53 | 110.63 | 118.30 |
| 1 | A | 495 | GLU | N-CA-CB | -8.52 | 95.26 | 110.60 |
| 2 | B | 730 | ARG | NE-CZ-NH2 | 8.51 | 124.55 | 120.30 |
| 7 | I | 5 | ARG | NE-CZ-NH2 | 8.50 | 124.55 | 120.30 |
| 1 | A | 481 | ASP | CB-CG-OD2 | -8.50 | 110.65 | 118.30 |
| 1 | A | 555 | ASP | CB-CG-OD1 | 8.49 | 125.94 | 118.30 |
| 1 | A | 1257 | ASP | CB-CG-OD2 | 8.49 | 125.94 | 118.30 |
| 2 | B | 559 | SER | CA-CB-OG | -8.46 | 88.35 | 111.20 |
| 6 | H | 89 | LEU | CA-CB-CG | 8.43 | 134.69 | 115.30 |
| 2 | B | 368 | GLU | C-N-CA | -8.43 | 104.60 | 122.30 |
| 2 | B | 668 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 1 | A | 740 | LEU | CB-CG-CD2 | -8.40 | 96.72 | 111.00 |
| 2 | B | 120 | ARG | NE-CZ-NH2 | 8.39 | 124.50 | 120.30 |
| 1 | A | 652 | VAL | CG1-CB-CG2 | -8.39 | 97.48 | 110.90 |
| 3 | C | 235 | VAL | CG1-CB-CG2 | -8.39 | 97.48 | 110.90 |
| 1 | A | 268 | ASP | CB-CG-OD2 | 8.38 | 125.84 | 118.30 |
| 1 | A | 618 | GLU | OE1-CD-OE2 | 8.38 | 133.36 | 123.30 |
| 10 | L | 60 | ARG | NE-CZ-NH1 | -8.37 | 116.11 | 120.30 |
| 1 | A | 909 | ASP | CB-CG-OD2 | -8.37 | 110.77 | 118.30 |
| 3 | C | 11 | ARG | NE-CZ-NH1 | 8.36 | 124.48 | 120.30 |
| 1 | A | 726 | ARG | NE-CZ-NH2 | 8.36 | 124.48 | 120.30 |
| 7 | I | 13 | MET | CG-SD-CE | -8.35 | 86.83 | 100.20 |
| 1 | A | 1226 | VAL | CB-CA-C | -8.34 | 95.55 | 111.40 |
| 3 | C | 149 | LYS | CD-CE-NZ | -8.34 | 92.52 | 111.70 |
| 5 | F | 119 | ARG | NE-CZ-NH1 | 8.34 | 124.47 | 120.30 |
| 1 | A | 856 | THR | OG1-CB-CG2 | -8.31 | 90.89 | 110.00 |
| 1 | A | 96 | ILE | CG1-CB-CG2 | -8.31 | 93.12 | 111.40 |
| 1 | A | 283 | GLY | N-CA-C | -8.30 | 92.34 | 113.10 |
| 1 | A | 419 | LYS | CD-CE-NZ | -8.29 | 92.62 | 111.70 |
| 2 | B | 56 | ASP | CB-CG-OD1 | -8.29 | 110.83 | 118.30 |
| 1 | A | 12 | ARG | NE-CZ-NH2 | -8.29 | 116.16 | 120.30 |
| 2 | B | 1077 | THR | N-CA-CB | -8.28 | 94.57 | 110.30 |
| 8 | J | 38 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |
| 2 | B | 605 | ARG | NE-CZ-NH2 | 8.27 | 124.43 | 120.30 |
| 2 | B | 542 | MET | CG-SD-CE | -8.23 | 87.04 | 100.20 |
| 7 | I | 32 | CYS | CB-CA-C | -8.23 | 93.94 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 399 | HIS | C-N-CD | -8.22 | 102.51 | 120.60 |
| 2 | B | 398 | ARG | CB-CA-C | -8.22 | 93.96 | 110.40 |
| 2 | B | 722 | ASP | CB-CG-OD1 | 8.22 | 125.70 | 118.30 |
| 1 | A | 50 | ILE | CB-CA-C | -8.20 | 95.21 | 111.60 |
| 2 | B | 169 | ARG | NE-CZ-NH1 | 8.19 | 124.39 | 120.30 |
| 1 | A | 1281 | ARG | NE-CZ-NH1 | 8.19 | 124.39 | 120.30 |
| 2 | B | 304 | ASP | CB-CG-OD1 | 8.18 | 125.66 | 118.30 |
| 3 | C | 183 | TRP | C-N-CA | -8.17 | 101.28 | 121.70 |
| 10 | L | 50 | ASP | CB-CG-OD1 | 8.17 | 125.65 | 118.30 |
| 4 | E | 41 | ASP | CB-CG-OD1 | 8.16 | 125.65 | 118.30 |
| 2 | B | 633 | VAL | CG1-CB-CG2 | -8.16 | 97.85 | 110.90 |
| 2 | B | 641 | GLU | OE1-CD-OE2 | -8.14 | 113.53 | 123.30 |
| 9 | K | 53 | ASP | CB-CG-OD2 | 8.14 | 125.63 | 118.30 |
| 1 | A | 1135 | ARG | NE-CZ-NH2 | 8.12 | 124.36 | 120.30 |
| 2 | B | 297 | ILE | CA-CB-CG1 | 8.12 | 126.42 | 111.00 |
| 1 | A | 1161 | THR | OG1-CB-CG2 | -8.12 | 91.33 | 110.00 |
| 1 | A | 266 | LEU | CA-CB-CG | 8.10 | 133.93 | 115.30 |
| 2 | B | 654 | ARG | NE-CZ-NH1 | -8.10 | 116.25 | 120.30 |
| 1 | A | 32 | VAL | CG1-CB-CG2 | -8.08 | 97.97 | 110.90 |
| 2 | B | 89 | GLU | N-CA-C | 8.07 | 132.80 | 111.00 |
| 10 | L | 47 | ARG | NE-CZ-NH2 | 8.07 | 124.34 | 120.30 |
| 3 | C | 143 | LEU | CB-CG-CD2 | -8.05 | 97.31 | 111.00 |
| 1 | A | 475 | THR | CA-CB-CG2 | 8.05 | 123.67 | 112.40 |
| 2 | B | 942 | ARG | NE-CZ-NH1 | -8.05 | 116.28 | 120.30 |
| 3 | C | 226 | ASP | CB-CG-OD2 | 8.03 | 125.52 | 118.30 |
| 2 | B | 622 | LYS | CA-CB-CG | 8.02 | 131.04 | 113.40 |
| 1 | A | 1438 | THR | N-CA-CB | -8.02 | 95.07 | 110.30 |
| 1 | A | 645 | LEU | CB-CG-CD1 | -8.00 | 97.40 | 111.00 |
| 7 | I | 31 | THR | N-CA-CB | -8.00 | 95.10 | 110.30 |
| 2 | B | 137 | TYR | CB-CG-CD1 | 7.99 | 125.79 | 121.00 |
| 1 | A | 914 | GLU | CG-CD-OE2 | -7.98 | 102.34 | 118.30 |
| 4 | E | 167 | ARG | NE-CZ-NH1 | -7.98 | 116.31 | 120.30 |
| 1 | A | 731 | ARG | NE-CZ-NH1 | -7.97 | 116.32 | 120.30 |
| 2 | B | 711 | GLU | OE1-CD-OE2 | -7.95 | 113.76 | 123.30 |
| 1 | A | 1151 | GLU | OE1-CD-OE2 | -7.92 | 113.80 | 123.30 |
| 1 | A | 1005 | GLU | CG-CD-OE1 | 7.92 | 134.13 | 118.30 |
| 2 | B | 1167 | GLY | N-CA-C | 7.91 | 132.88 | 113.10 |
| 2 | B | 477 | ALA | N-CA-CB | 7.91 | 121.18 | 110.10 |
| 4 | E | 81 | GLU | OE1-CD-OE2 | 7.91 | 132.79 | 123.30 |
| 1 | A | 905 | ASP | CB-CG-OD1 | -7.90 | 111.19 | 118.30 |
| 1 | A | 898 | ARG | NE-CZ-NH1 | 7.90 | 124.25 | 120.30 |
| 2 | B | 46 | GLN | CA-CB-CG | -7.88 | 96.06 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1034 | GLU | OE1-CD-OE2 | -7.88 | 113.84 | 123.30 |
| 6 | H | 91 | ASP | CB-CG-OD2 | 7.87 | 125.38 | 118.30 |
| 1 | A | 74 | MET | CG-SD-CE | 7.86 | 112.77 | 100.20 |
| 1 | A | 1136 | SER | CB-CA-C | 7.86 | 125.03 | 110.10 |
| 2 | B | 259 | TYR | CB-CG-CD2 | 7.86 | 125.72 | 121.00 |
| 1 | A | 498 | ARG | NE-CZ-NH1 | -7.85 | 116.38 | 120.30 |
| 4 | E | 163 | GLU | OE1-CD-OE2 | -7.83 | 113.91 | 123.30 |
| 2 | B | 394 | ASP | CB-CG-OD1 | -7.82 | 111.26 | 118.30 |
| 3 | C | 26 | ASP | CB-CG-OD1 | 7.82 | 125.33 | 118.30 |
| 8 | J | 17 | LYS | CD-CE-NZ | -7.82 | 93.72 | 111.70 |
| 9 | K | 61 | TYR | CB-CG-CD1 | 7.81 | 125.69 | 121.00 |
| 1 | A | 928 | LEU | CB-CG-CD1 | -7.80 | 97.74 | 111.00 |
| 1 | A | 1239 | ARG | CB-CA-C | 7.80 | 126.00 | 110.40 |
| 4 | E | 25 | ASP | CB-CG-OD1 | 7.80 | 125.32 | 118.30 |
| 1 | A | 1012 | ARG | CG-CD-NE | -7.79 | 95.44 | 111.80 |
| 1 | A | 942 | PHE | CB-CG-CD2 | -7.79 | 115.35 | 120.80 |
| 2 | B | 303 | TYR | CB-CG-CD1 | 7.79 | 125.67 | 121.00 |
| 2 | B | 390 | LEU | CB-CG-CD1 | -7.78 | 97.77 | 111.00 |
| 2 | B | 620 | ARG | CG-CD-NE | -7.78 | 95.45 | 111.80 |
| 1 | A | 547 | LEU | CB-CG-CD2 | -7.78 | 97.78 | 111.00 |
| 1 | A | 774 | ARG | NH1-CZ-NH2 | -7.76 | 110.86 | 119.40 |
| 2 | B | 320 | ASP | CB-CG-OD1 | 7.76 | 125.28 | 118.30 |
| 7 | I | 35 | VAL | CA-CB-CG2 | -7.76 | 99.26 | 110.90 |
| 1 | A | 708 | MET | N-CA-CB | -7.76 | 96.64 | 110.60 |
| 1 | A | 1005 | GLU | CG-CD-OE2 | -7.75 | 102.79 | 118.30 |
| 2 | B | 387 | LEU | CB-CG-CD1 | -7.75 | 97.82 | 111.00 |
| 2 | B | 1101 | ASP | CB-CG-OD2 | 7.75 | 125.27 | 118.30 |
| 1 | A | 1196 | GLU | CG-CD-OE2 | -7.74 | 102.81 | 118.30 |
| 2 | B | 764 | SER | N-CA-CB | -7.74 | 98.88 | 110.50 |
| 4 | E | 198 | ILE | CG1-CB-CG2 | -7.74 | 94.37 | 111.40 |
| 1 | A | 22 | PHE | CB-CG-CD1 | -7.74 | 115.38 | 120.80 |
| 1 | A | 949 | ASP | CB-CG-OD1 | -7.73 | 111.34 | 118.30 |
| 1 | A | 361 | LEU | CB-CG-CD2 | -7.72 | 97.87 | 111.00 |
| 3 | C | 11 | ARG | NE-CZ-NH2 | -7.71 | 116.45 | 120.30 |
| 3 | C | 90 | ASP | CB-CG-OD2 | -7.71 | 111.37 | 118.30 |
| 1 | A | 571 | LEU | CB-CG-CD1 | -7.70 | 97.91 | 111.00 |
| 9 | K | 22 | ASP | OD1-CG-OD2 | -7.70 | 108.67 | 123.30 |
| 2 | B | 598 | GLU | N-CA-CB | 7.70 | 124.46 | 110.60 |
| 2 | B | 498 | THR | N-CA-CB | -7.69 | 95.68 | 110.30 |
| 3 | C | 124 | LEU | CB-CG-CD1 | -7.69 | 97.92 | 111.00 |
| 2 | B | 959 | ASP | CB-CG-OD2 | 7.67 | 125.20 | 118.30 |
| 6 | H | 87 | ARG | NE-CZ-NH2 | -7.67 | 116.46 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 944 | ARG | NE-CZ-NH1 | 7.66 | 124.13 | 120.30 |
| 1 | A | 567 | LYS | CD-CE-NZ | 7.66 | 129.31 | 111.70 |
| 1 | A | 709 | THR | N-CA-CB | -7.66 | 95.75 | 110.30 |
| 2 | B | 653 | VAL | CB-CA-C | -7.66 | 96.86 | 111.40 |
| 2 | B | 1129 | ARG | NE-CZ-NH1 | 7.65 | 124.13 | 120.30 |
| 3 | C | 254 | LYS | CD-CE-NZ | -7.65 | 94.11 | 111.70 |
| 1 | A | 1415 | SER | CB-CA-C | -7.62 | 95.61 | 110.10 |
| 1 | A | 1280 | GLU | CG-CD-OE2 | 7.61 | 133.52 | 118.30 |
| 2 | B | 654 | ARG | NE-CZ-NH2 | 7.61 | 124.10 | 120.30 |
| 1 | A | 1036 | ARG | NH1-CZ-NH2 | 7.61 | 127.77 | 119.40 |
| 2 | B | 329 | THR | OG1-CB-CG2 | -7.59 | 92.53 | 110.00 |
| 2 | B | 404 | LYS | CD-CE-NZ | -7.59 | 94.24 | 111.70 |
| 2 | B | 967 | ARG | NE-CZ-NH1 | -7.59 | 116.50 | 120.30 |
| 2 | B | 766 | ARG | NE-CZ-NH2 | 7.58 | 124.09 | 120.30 |
| 2 | B | 303 | TYR | CD1-CE1-CZ | -7.56 | 112.99 | 119.80 |
| 2 | B | 90 | ILE | CB-CA-C | -7.56 | 96.48 | 111.60 |
| 4 | E | 17 | ARG | NE-CZ-NH2 | 7.56 | 124.08 | 120.30 |
| 6 | H | 19 | ARG | CD-NE-CZ | 7.54 | 134.16 | 123.60 |
| 1 | A | 830 | LYS | CB-CA-C | -7.54 | 95.32 | 110.40 |
| 4 | E | 142 | VAL | CG1-CB-CG2 | -7.54 | 98.84 | 110.90 |
| 3 | C | 11 | ARG | CB-CA-C | -7.54 | 95.33 | 110.40 |
| 1 | A | 1259 | MET | CG-SD-CE | 7.53 | 112.25 | 100.20 |
| 1 | A | 1318 | THR | CA-CB-CG2 | 7.53 | 122.94 | 112.40 |
| 2 | B | 305 | VAL | CG1-CB-CG2 | 7.52 | 122.93 | 110.90 |
| 2 | B | 618 | ASP | CB-CG-OD2 | -7.51 | 111.54 | 118.30 |
| 2 | B | 662 | MET | CA-CB-CG | -7.51 | 100.53 | 113.30 |
| 4 | E | 58 | MET | CG-SD-CE | -7.50 | 88.20 | 100.20 |
| 3 | C | 118 | LEU | CB-CG-CD2 | 7.50 | 123.75 | 111.00 |
| 1 | A | 469 | ARG | CG-CD-NE | -7.49 | 96.06 | 111.80 |
| 2 | B | 1129 | ARG | NE-CZ-NH2 | -7.48 | 116.56 | 120.30 |
| 2 | B | 346 | GLU | OE1-CD-OE2 | -7.48 | 114.33 | 123.30 |
| 1 | A | 600 | PRO | N-CD-CG | -7.47 | 91.99 | 103.20 |
| 1 | A | 537 | ARG | CB-CG-CD | 7.47 | 131.02 | 111.60 |
| 6 | H | 135 | LEU | CB-CG-CD2 | 7.47 | 123.70 | 111.00 |
| 8 | J | 62 | ARG | CG-CD-NE | -7.46 | 96.12 | 111.80 |
| 2 | B | 595 | ARG | NE-CZ-NH2 | 7.46 | 124.03 | 120.30 |
| 2 | B | 1096 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 1 | A | 1274 | ARG | NE-CZ-NH1 | -7.46 | 116.57 | 120.30 |
| 2 | B | 539 | LEU | CB-CG-CD2 | 7.45 | 123.67 | 111.00 |
| 2 | B | 910 | VAL | CG1-CB-CG2 | -7.45 | 98.97 | 110.90 |
| 7 | I | 30 | ARG | NE-CZ-NH1 | -7.45 | 116.57 | 120.30 |
| 1 | A | 158 | PRO | CA-N-CD | -7.45 | 101.07 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | F | 116 | ASP | CB-CG-OD2 | 7.44 | 125.00 | 118.30 |
| 8 | J | 44 | TYR | CB-CG-CD1 | 7.44 | 125.47 | 121.00 |
| 2 | B | 550 | ASP | CB-CG-OD1 | 7.43 | 124.99 | 118.30 |
| 1 | A | 706 | HIS | N-CA-CB | 7.43 | 123.97 | 110.60 |
| 1 | A | 636 | GLU | OE1-CD-OE2 | -7.42 | 114.40 | 123.30 |
| 2 | B | 1129 | ARG | CG-CD-NE | -7.42 | 96.23 | 111.80 |
| 1 | A | 12 | ARG | CG-CD-NE | -7.41 | 96.23 | 111.80 |
| 1 | A | 1385 | THR | N-CA-CB | -7.41 | 96.22 | 110.30 |
| 1 | A | 1349 | TYR | CZ-CE2-CD2 | 7.41 | 126.47 | 119.80 |
| 6 | H | 111 | LEU | CA-CB-CG | 7.40 | 132.31 | 115.30 |
| 1 | A | 895 | LYS | N-CA-CB | 7.39 | 123.91 | 110.60 |
| 1 | A | 1385 | THR | N-CA-C | 7.39 | 130.96 | 111.00 |
| 3 | C | 230 | MET | CG-SD-CE | 7.39 | 112.03 | 100.20 |
| 1 | A | 1418 | LEU | CB-CG-CD1 | 7.39 | 123.56 | 111.00 |
| 1 | A | 1055 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 9 | K | 24 | ASP | CB-CG-OD1 | -7.38 | 111.65 | 118.30 |
| 1 | A | 918 | GLU | OE1-CD-OE2 | -7.38 | 114.44 | 123.30 |
| 2 | B | 241 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 1 | A | 440 | ASP | CB-CG-OD1 | 7.37 | 124.93 | 118.30 |
| 1 | A | 65 | LEU | CA-CB-CG | 7.37 | 132.24 | 115.30 |
| 1 | A | 655 | PHE | CB-CG-CD2 | -7.36 | 115.65 | 120.80 |
| 1 | A | 1012 | ARG | NE-CZ-NH1 | 7.36 | 123.98 | 120.30 |
| 1 | A | 629 | LEU | CB-CG-CD2 | -7.36 | 98.49 | 111.00 |
| 3 | C | 217 | ASP | CB-CG-OD2 | 7.36 | 124.92 | 118.30 |
| 2 | B | 397 | ASP | CB-CG-OD1 | -7.34 | 111.69 | 118.30 |
| 1 | A | 557 | ASP | C-N-CA | -7.33 | 106.91 | 122.30 |
| 1 | A | 61 | ILE | N-CA-C | -7.31 | 91.26 | 111.00 |
| 2 | B | 57 | TYR | CB-CG-CD2 | 7.31 | 125.39 | 121.00 |
| 1 | A | 424 | ILE | CG1-CB-CG2 | -7.31 | 95.32 | 111.40 |
| 2 | B | 1223 | ASP | CB-CG-OD2 | 7.31 | 124.88 | 118.30 |
| 4 | E | 148 | GLU | CG-CD-OE2 | 7.30 | 132.90 | 118.30 |
| 8 | J | 43 | ARG | CG-CD-NE | -7.30 | 96.47 | 111.80 |
| 3 | C | 252 | GLN | CA-CB-CG | 7.29 | 129.44 | 113.40 |
| 6 | H | 102 | TYR | CG-CD1-CE1 | 7.29 | 127.13 | 121.30 |
| 1 | A | 1057 | VAL | CA-CB-CG2 | -7.29 | 99.97 | 110.90 |
| 1 | A | 592 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | A | 1286 | LYS | CD-CE-NZ | -7.26 | 94.99 | 111.70 |
| 2 | B | 997 | GLU | CA-CB-CG | -7.26 | 97.42 | 113.40 |
| 2 | B | 825 | VAL | CG1-CB-CG2 | -7.26 | 99.29 | 110.90 |
| 2 | B | 39 | ARG | NH1-CZ-NH2 | -7.25 | 111.42 | 119.40 |
| 1 | A | 1298 | TYR | CG-CD2-CE2 | 7.25 | 127.10 | 121.30 |
| 4 | E | 98 | ILE | CG1-CB-CG2 | -7.25 | 95.45 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 29 | MET | CG-SD-CE | 7.24 | 111.79 | 100.20 |
| 1 | A | 737 | LEU | CB-CG-CD1 | -7.23 | 98.70 | 111.00 |
| 2 | B | 694 | ASP | CB-CG-OD2 | 7.23 | 124.81 | 118.30 |
| 8 | J | 48 | ARG | CA-CB-CG | 7.22 | 129.29 | 113.40 |
| 2 | B | 601 | ARG | NH1-CZ-NH2 | 7.21 | 127.34 | 119.40 |
| 1 | A | 464 | PRO | O-C-N | -7.21 | 111.16 | 122.70 |
| 2 | B | 252 | SER | N-CA-CB | 7.21 | 121.32 | 110.50 |
| 6 | H | 41 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 1 | A | 59 | GLY | N-CA-C | 7.21 | 131.12 | 113.10 |
| 1 | A | 1223 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 7 | I | 73 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 7 | I | 19 | ASP | CB-CG-OD2 | 7.20 | 124.78 | 118.30 |
| 1 | A | 414 | ASP | OD1-CG-OD2 | -7.20 | 109.62 | 123.30 |
| 3 | C | 57 | VAL | CG1-CB-CG2 | 7.20 | 122.42 | 110.90 |
| 1 | A | 850 | VAL | CG1-CB-CG2 | -7.19 | 99.40 | 110.90 |
| 3 | C | 84 | ARG | NH1-CZ-NH2 | -7.19 | 111.50 | 119.40 |
| 1 | A | 1301 | GLU | OE1-CD-OE2 | 7.18 | 131.91 | 123.30 |
| 8 | J | 1 | MET | CA-CB-CG | 7.18 | 125.50 | 113.30 |
| 2 | B | 796 | LEU | CA-CB-CG | 7.17 | 131.80 | 115.30 |
| 2 | B | 601 | ARG | NE-CZ-NH1 | -7.17 | 116.71 | 120.30 |
| 5 | F | 82 | THR | CB-CA-C | -7.17 | 92.24 | 111.60 |
| 7 | I | 75 | CYS | CB-CA-C | -7.17 | 96.06 | 110.40 |
| 10 | L | 70 | ARG | NH1-CZ-NH2 | -7.17 | 111.52 | 119.40 |
| 1 | A | 1119 | TYR | CG-CD2-CE2 | 7.16 | 127.03 | 121.30 |
| 2 | B | 942 | ARG | CB-CA-C | -7.16 | 96.08 | 110.40 |
| 1 | A | 1334 | ASP | CB-CG-OD1 | 7.16 | 124.74 | 118.30 |
| 1 | A | 1305 | VAL | CG1-CB-CG2 | -7.14 | 99.47 | 110.90 |
| 1 | A | 1042 | PHE | CB-CG-CD2 | -7.14 | 115.80 | 120.80 |
| 2 | B | 983 | ARG | CA-CB-CG | 7.13 | 129.09 | 113.40 |
| 1 | A | 487 | MET | CG-SD-CE | -7.12 | 88.80 | 100.20 |
| 8 | J | 22 | LEU | CA-CB-CG | 7.12 | 131.69 | 115.30 |
| 9 | K | 39 | ASP | CB-CG-OD1 | 7.12 | 124.71 | 118.30 |
| 2 | B | 1166 | CYS | O-C-N | -7.11 | 111.12 | 123.20 |
| 4 | E | 128 | PRO | N-CD-CG | 7.11 | 113.86 | 103.20 |
| 1 | A | 408 | ASP | CB-CG-OD2 | 7.11 | 124.69 | 118.30 |
| 6 | H | 143 | LEU | CB-CG-CD1 | 7.10 | 123.08 | 111.00 |
| 2 | B | 1026 | LEU | CB-CG-CD1 | -7.09 | 98.94 | 111.00 |
| 6 | H | 86 | ASP | CB-CA-C | 7.09 | 124.58 | 110.40 |
| 7 | I | 45 | ARG | CD-NE-CZ | -7.08 | 113.68 | 123.60 |
| 3 | C | 210 | GLU | CG-CD-OE2 | -7.06 | 104.17 | 118.30 |
| 2 | B | 999 | MET | CG-SD-CE | -7.05 | 88.92 | 100.20 |
| 1 | A | 557 | ASP | O-C-N | -7.05 | 111.22 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 249 | ARG | CD-NE-CZ | 7.05 | 133.47 | 123.60 |
| 3 | C | 117 | ASP | CB-CG-OD1 | 7.05 | 124.64 | 118.30 |
| 2 | B | 1004 | GLU | OE1-CD-OE2 | -7.05 | 114.84 | 123.30 |
| 1 | A | 630 | ILE | CG1-CB-CG2 | -7.04 | 95.91 | 111.40 |
| 3 | C | 121 | VAL | CA-CB-CG1 | 7.03 | 121.45 | 110.90 |
| 1 | A | 460 | VAL | CG1-CB-CG2 | -7.03 | 99.65 | 110.90 |
| 1 | A | 907 | THR | CB-CA-C | -7.03 | 92.62 | 111.60 |
| 2 | B | 165 | VAL | CB-CA-C | -7.03 | 98.05 | 111.40 |
| 2 | B | 558 | LEU | CB-CG-CD1 | -7.03 | 99.05 | 111.00 |
| 2 | B | 122 | LEU | CB-CG-CD1 | -7.02 | 99.06 | 111.00 |
| 1 | A | 983 | ILE | CG1-CB-CG2 | -7.02 | 95.96 | 111.40 |
| 2 | B | 40 | GLU | OE1-CD-OE2 | 7.02 | 131.72 | 123.30 |
| 8 | J | 22 | LEU | N-CA-CB | -7.01 | 96.38 | 110.40 |
| 1 | A | 929 | LEU | CB-CG-CD2 | -6.99 | 99.12 | 111.00 |
| 5 | F | 72 | LYS | C-N-CA | 6.98 | 139.15 | 121.70 |
| 9 | K | 64 | GLU | OE1-CD-OE2 | -6.97 | 114.94 | 123.30 |
| 1 | A | 1198 | ASP | OD1-CG-OD2 | -6.96 | 110.07 | 123.30 |
| 5 | F | 72 | LYS | N-CA-C | 6.96 | 129.80 | 111.00 |
| 1 | A | 833 | GLU | CG-CD-OE1 | 6.96 | 132.22 | 118.30 |
| 7 | I | 111 | THR | CB-CA-C | -6.96 | 92.82 | 111.60 |
| 1 | A | 1280 | GLU | CA-C-N | 6.95 | 132.48 | 117.20 |
| 5 | F | 77 | ASP | C-N-CA | -6.95 | 104.34 | 121.70 |
| 5 | F | 79 | ARG | CB-CG-CD | -6.95 | 93.54 | 111.60 |
| 2 | B | 1185 | CYS | CA-CB-SG | 6.94 | 126.50 | 114.00 |
| 3 | C | 100 | THR | OG1-CB-CG2 | -6.94 | 94.03 | 110.00 |
| 10 | L | 27 | LEU | CB-CG-CD2 | 6.93 | 122.78 | 111.00 |
| 1 | A | 940 | ARG | CG-CD-NE | -6.93 | 97.25 | 111.80 |
| 1 | A | 603 | ASN | N-CA-CB | -6.93 | 98.13 | 110.60 |
| 3 | C | 53 | THR | OG1-CB-CG2 | -6.92 | 94.08 | 110.00 |
| 8 | J | 1 | MET | N-CA-CB | -6.92 | 98.14 | 110.60 |
| 1 | A | 555 | ASP | OD1-CG-OD2 | -6.92 | 110.15 | 123.30 |
| 2 | B | 691 | GLU | CA-CB-CG | 6.91 | 128.61 | 113.40 |
| 1 | A | 557 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 1 | A | 649 | ILE | CA-CB-CG1 | 6.90 | 124.11 | 111.00 |
| 2 | B | 587 | HIS | CA-C-N | 6.89 | 129.98 | 116.20 |
| 9 | K | 6 | ARG | CG-CD-NE | -6.89 | 97.34 | 111.80 |
| 1 | A | 291 | GLU | CA-CB-CG | 6.88 | 128.55 | 113.40 |
| 2 | B | 435 | THR | OG1-CB-CG2 | -6.88 | 94.17 | 110.00 |
| 1 | A | 1411 | GLU | OE1-CD-OE2 | -6.88 | 115.04 | 123.30 |
| 7 | I | 5 | ARG | NH1-CZ-NH2 | -6.88 | 111.83 | 119.40 |
| 1 | A | 1111 | MET | CG-SD-CE | -6.88 | 89.19 | 100.20 |
| 4 | E | 2 | ASP | CB-CG-OD2 | 6.88 | 124.49 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 676 | MET | CG-SD-CE | 6.87 | 111.19 | 100.20 |
| 1 | A | 727 | ASP | CB-CG-OD1 | 6.87 | 124.48 | 118.30 |
| 8 | J | 3 | VAL | CG1-CB-CG2 | 6.87 | 121.89 | 110.90 |
| 2 | B | 227 | LYS | CD-CE-NZ | 6.86 | 127.49 | 111.70 |
| 2 | B | 175 | ARG | NE-CZ-NH2 | 6.85 | 123.73 | 120.30 |
| 2 | B | 137 | TYR | CB-CG-CD2 | -6.85 | 116.89 | 121.00 |
| 2 | B | 393 | LYS | N-CA-CB | 6.85 | 122.92 | 110.60 |
| 2 | B | 960 | GLY | N-CA-C | 6.85 | 130.21 | 113.10 |
| 2 | B | 591 | ARG | NE-CZ-NH2 | -6.84 | 116.88 | 120.30 |
| 2 | B | 712 | PRO | N-CD-CG | -6.83 | 92.95 | 103.20 |
| 2 | B | 1019 | SER | N-CA-CB | 6.83 | 120.74 | 110.50 |
| 2 | B | 125 | SER | CB-CA-C | 6.83 | 123.07 | 110.10 |
| 4 | E | 162 | ARG | CB-CG-CD | 6.83 | 129.35 | 111.60 |
| 2 | B | 327 | ARG | NE-CZ-NH1 | -6.82 | 116.89 | 120.30 |
| 1 | A | 374 | LEU | CB-CG-CD1 | 6.81 | 122.58 | 111.00 |
| 5 | F | 123 | LYS | CD-CE-NZ | -6.81 | 96.03 | 111.70 |
| 1 | A | 1409 | LEU | CB-CG-CD2 | -6.81 | 99.42 | 111.00 |
| 2 | B | 391 | ASP | CB-CG-OD1 | 6.81 | 124.43 | 118.30 |
| 2 | B | 722 | ASP | OD1-CG-OD2 | -6.81 | 110.37 | 123.30 |
| 1 | A | 86 | LEU | CB-CG-CD1 | -6.79 | 99.45 | 111.00 |
| 1 | A | 1176 | LEU | CA-CB-CG | 6.79 | 130.92 | 115.30 |
| 2 | B | 399 | ASP | N-CA-CB | -6.79 | 98.37 | 110.60 |
| 2 | B | 170 | LEU | CB-CG-CD1 | -6.79 | 99.47 | 111.00 |
| 7 | I | 91 | ARG | NE-CZ-NH2 | -6.78 | 116.91 | 120.30 |
| 1 | A | 504 | LEU | CA-CB-CG | 6.78 | 130.90 | 115.30 |
| 1 | A | 960 | ILE | CG1-CB-CG2 | -6.77 | 96.51 | 111.40 |
| 1 | A | 565 | ILE | CG1-CB-CG2 | -6.76 | 96.52 | 111.40 |
| 2 | B | 303 | TYR | CZ-CE2-CD2 | 6.76 | 125.89 | 119.80 |
| 8 | J | 16 | ASP | CB-CG-OD2 | 6.76 | 124.39 | 118.30 |
| 8 | J | 59 | LYS | CD-CE-NZ | -6.76 | 96.15 | 111.70 |
| 1 | A | 1280 | GLU | O-C-N | -6.76 | 111.89 | 122.70 |
| 4 | E | 148 | GLU | OE1-CD-OE2 | -6.75 | 115.20 | 123.30 |
| 2 | B | 972 | LYS | CD-CE-NZ | -6.75 | 96.19 | 111.70 |
| 1 | A | 464 | PRO | CA-C-N | 6.74 | 132.04 | 117.20 |
| 9 | K | 12 | LEU | CA-CB-CG | -6.74 | 99.79 | 115.30 |
| 1 | A | 470 | LEU | CB-CA-C | -6.74 | 97.39 | 110.20 |
| 1 | A | 705 | LYS | N-CA-CB | 6.74 | 122.73 | 110.60 |
| 10 | L | 55 | ILE | CB-CA-C | -6.74 | 98.12 | 111.60 |
| 9 | K | 105 | PHE | CZ-CE2-CD2 | -6.74 | 112.01 | 120.10 |
| 6 | H | 80 | ARG | NE-CZ-NH2 | 6.74 | 123.67 | 120.30 |
| 1 | A | 386 | ASP | CB-CG-OD2 | -6.74 | 112.24 | 118.30 |
| 5 | F | 92 | ARG | NE-CZ-NH2 | -6.74 | 116.93 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 683 | ILE | CG1-CB-CG2 | -6.73 | 96.60 | 111.40 |
| 1 | A | 532 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | A | 1318 | THR | N-CA-CB | -6.72 | 97.53 | 110.30 |
| 7 | I | 111 | THR | OG1-CB-CG2 | -6.71 | 94.56 | 110.00 |
| 1 | A | 1433 | MET | CG-SD-CE | 6.71 | 110.94 | 100.20 |
| 2 | B | 894 | ASP | CB-CG-OD1 | 6.71 | 124.34 | 118.30 |
| 2 | B | 1223 | ASP | CB-CG-OD1 | -6.71 | 112.26 | 118.30 |
| 4 | E | 11 | ARG | NH1-CZ-NH2 | 6.71 | 126.78 | 119.40 |
| 1 | A | 239 | LEU | CA-CB-CG | 6.71 | 130.72 | 115.30 |
| 7 | I | 98 | VAL | CA-CB-CG2 | -6.71 | 100.84 | 110.90 |
| 1 | A | 351 | THR | CB-CA-C | -6.70 | 93.50 | 111.60 |
| 5 | F | 94 | LEU | C-N-CA | -6.70 | 108.22 | 122.30 |
| 1 | A | 1004 | ASN | N-CA-C | 6.68 | 129.05 | 111.00 |
| 2 | B | 501 | PRO | O-C-N | 6.68 | 133.40 | 122.70 |
| 2 | B | 813 | LYS | CD-CE-NZ | -6.68 | 96.33 | 111.70 |
| 10 | L | 58 | LYS | CA-C-N | 6.68 | 131.90 | 117.20 |
| 10 | L | 25 | ALA | C-N-CA | 6.68 | 138.40 | 121.70 |
| 6 | H | 63 | LEU | CA-CB-CG | 6.67 | 130.64 | 115.30 |
| 2 | B | 543 | SER | CB-CA-C | -6.67 | 97.44 | 110.10 |
| 4 | E | 121 | MET | CB-CG-SD | 6.67 | 132.40 | 112.40 |
| 2 | B | 1099 | VAL | CG1-CB-CG2 | 6.66 | 121.56 | 110.90 |
| 3 | C | 38 | ILE | CG1-CB-CG2 | -6.66 | 96.75 | 111.40 |
| 2 | B | 655 | LYS | CD-CE-NZ | 6.65 | 127.00 | 111.70 |
| 2 | B | 131 | ASP | CB-CG-OD2 | 6.65 | 124.28 | 118.30 |
| 1 | A | 1284 | MET | CG-SD-CE | -6.65 | 89.57 | 100.20 |
| 2 | B | 1201 | LYS | CD-CE-NZ | -6.65 | 96.42 | 111.70 |
| 2 | B | 1135 | ARG | CG-CD-NE | -6.64 | 97.85 | 111.80 |
| 4 | E | 161 | LYS | CA-CB-CG | 6.64 | 128.01 | 113.40 |
| 6 | H | 94 | ASP | CB-CG-OD2 | 6.64 | 124.28 | 118.30 |
| 7 | I | 5 | ARG | NE-CZ-NH1 | 6.63 | 123.62 | 120.30 |
| 2 | B | 993 | THR | OG1-CB-CG2 | -6.63 | 94.75 | 110.00 |
| 3 | C | 204 | SER | N-CA-CB | -6.62 | 100.57 | 110.50 |
| 1 | A | 755 | PHE | CB-CG-CD2 | 6.61 | 125.43 | 120.80 |
| 5 | F | 115 | THR | OG1-CB-CG2 | -6.61 | 94.79 | 110.00 |
| 2 | B | 1017 | ILE | CA-CB-CG1 | -6.61 | 98.44 | 111.00 |
| 2 | B | 699 | GLU | CB-CA-C | -6.61 | 97.18 | 110.40 |
| 7 | I | 55 | THR | CA-CB-CG2 | 6.61 | 121.65 | 112.40 |
| 1 | A | 655 | PHE | CB-CG-CD1 | 6.60 | 125.42 | 120.80 |
| 2 | B | 642 | ASP | N-CA-CB | 6.59 | 122.47 | 110.60 |
| 2 | B | 1083 | ALA | N-CA-CB | -6.59 | 100.87 | 110.10 |
| 1 | A | 726 | ARG | CG-CD-NE | -6.59 | 97.97 | 111.80 |
| 3 | C | 263 | THR | CA-CB-CG2 | 6.59 | 121.62 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1085 | ILE | CG1-CB-CG2 | -6.58 | 96.91 | 111.40 |
| 1 | A | 414 | ASP | CB-CG-OD1 | 6.58 | 124.22 | 118.30 |
| 1 | A | 1025 | ARG | NE-CZ-NH2 | 6.58 | 123.59 | 120.30 |
| 7 | I | 17 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | A | 781 | ASP | CB-CG-OD1 | 6.57 | 124.22 | 118.30 |
| 1 | A | 1375 | MET | CG-SD-CE | 6.57 | 110.72 | 100.20 |
| 1 | A | 279 | LEU | CB-CG-CD1 | 6.57 | 122.17 | 111.00 |
| 8 | J | 47 | ARG | NE-CZ-NH2 | -6.57 | 117.02 | 120.30 |
| 4 | E | 78 | LEU | CB-CG-CD2 | 6.56 | 122.16 | 111.00 |
| 1 | A | 597 | LEU | CB-CG-CD2 | -6.56 | 99.84 | 111.00 |
| 3 | C | 34 | ARG | CD-NE-CZ | 6.56 | 132.79 | 123.60 |
| 1 | A | 1349 | TYR | CG-CD1-CE1 | 6.56 | 126.55 | 121.30 |
| 2 | B | 884 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | A | 1203 | ASN | CB-CA-C | 6.56 | 123.52 | 110.40 |
| 2 | B | 576 | ASP | CB-CG-OD2 | 6.55 | 124.20 | 118.30 |
| 3 | C | 253 | LYS | CD-CE-NZ | -6.55 | 96.63 | 111.70 |
| 4 | E | 4 | GLU | OE1-CD-OE2 | -6.55 | 115.44 | 123.30 |
| 5 | F | 135 | ARG | NE-CZ-NH2 | 6.54 | 123.57 | 120.30 |
| 2 | B | 1183 | LYS | CA-CB-CG | 6.54 | 127.78 | 113.40 |
| 2 | B | 959 | ASP | OD1-CG-OD2 | -6.53 | 110.89 | 123.30 |
| 2 | B | 452 | THR | OG1-CB-CG2 | -6.53 | 94.98 | 110.00 |
| 2 | B | 1156 | ASP | CB-CG-OD1 | 6.53 | 124.18 | 118.30 |
| 2 | B | 650 | GLU | CG-CD-OE1 | -6.53 | 105.25 | 118.30 |
| 1 | A | 1172 | LEU | CB-CA-C | -6.52 | 97.81 | 110.20 |
| 10 | L | 58 | LYS | N-CA-C | 6.52 | 128.61 | 111.00 |
| 1 | A | 519 | PRO | N-CD-CG | 6.52 | 112.98 | 103.20 |
| 4 | E | 17 | ARG | CG-CD-NE | -6.51 | 98.13 | 111.80 |
| 3 | C | 23 | SER | N-CA-C | -6.50 | 93.46 | 111.00 |
| 1 | A | 1170 | ILE | CG1-CB-CG2 | -6.49 | 97.12 | 111.40 |
| 1 | A | 62 | ASP | CB-CG-OD2 | 6.49 | 124.14 | 118.30 |
| 2 | B | 895 | ASP | CB-CG-OD2 | 6.49 | 124.14 | 118.30 |
| 2 | B | 1219 | ASP | OD1-CG-OD2 | -6.49 | 110.97 | 123.30 |
| 1 | A | 1357 | ALA | CB-CA-C | -6.49 | 100.37 | 110.10 |
| 7 | I | 84 | VAL | N-CA-CB | -6.49 | 97.23 | 111.50 |
| 9 | K | 73 | LEU | CA-CB-CG | 6.48 | 130.21 | 115.30 |
| 1 | A | 1006 | ILE | CA-CB-CG1 | 6.48 | 123.31 | 111.00 |
| 3 | C | 193 | TYR | CD1-CE1-CZ | 6.48 | 125.63 | 119.80 |
| 10 | L | 40 | LEU | CB-CA-C | 6.48 | 122.51 | 110.20 |
| 1 | A | 1326 | ARG | NH1-CZ-NH2 | -6.48 | 112.27 | 119.40 |
| 1 | A | 79 | GLY | N-CA-C | -6.47 | 96.91 | 113.10 |
| 2 | B | 273 | LEU | CB-CG-CD1 | 6.47 | 122.00 | 111.00 |
| 6 | H | 142 | LEU | CB-CG-CD1 | -6.47 | 100.01 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1001 | ARG | CG-CD-NE | -6.45 | 98.25 | 111.80 |
| 2 | B | 217 | ARG | CG-CD-NE | -6.45 | 98.26 | 111.80 |
| 1 | A | 634 | THR | CA-CB-CG2 | -6.45 | 103.38 | 112.40 |
| 9 | K | 19 | LEU | CB-CG-CD1 | -6.44 | 100.05 | 111.00 |
| 1 | A | 830 | LYS | N-CA-CB | 6.43 | 122.18 | 110.60 |
| 2 | B | 38 | PHE | CB-CG-CD1 | -6.43 | 116.30 | 120.80 |
| 1 | A | 923 | LEU | CB-CG-CD1 | -6.43 | 100.07 | 111.00 |
| 2 | B | 272 | THR | OG1-CB-CG2 | -6.43 | 95.22 | 110.00 |
| 2 | B | 401 | PHE | CB-CG-CD2 | -6.42 | 116.30 | 120.80 |
| 3 | C | 35 | ARG | CG-CD-NE | -6.42 | 98.31 | 111.80 |
| 2 | B | 854 | LEU | CB-CG-CD2 | -6.42 | 100.08 | 111.00 |
| 1 | A | 1405 | THR | OG1-CB-CG2 | -6.41 | 95.26 | 110.00 |
| 3 | C | 124 | LEU | N-CA-C | 6.41 | 128.31 | 111.00 |
| 6 | H | 102 | TYR | CD1-CE1-CZ | -6.41 | 114.03 | 119.80 |
| 6 | H | 103 | LYS | CB-CG-CD | 6.41 | 128.26 | 111.60 |
| 9 | K | 114 | LEU | CB-CG-CD1 | -6.41 | 100.11 | 111.00 |
| 1 | A | 1281 | ARG | CB-CA-C | -6.40 | 97.60 | 110.40 |
| 1 | A | 1241 | ARG | CD-NE-CZ | 6.39 | 132.55 | 123.60 |
| 1 | A | 1299 | VAL | CB-CA-C | 6.39 | 123.55 | 111.40 |
| 1 | A | 938 | LYS | CB-CA-C | -6.39 | 97.62 | 110.40 |
| 1 | A | 1154 | TYR | N-CA-C | -6.39 | 93.75 | 111.00 |
| 2 | B | 646 | LEU | CB-CG-CD1 | 6.39 | 121.86 | 111.00 |
| 1 | A | 407 | ARG | NH1-CZ-NH2 | 6.38 | 126.42 | 119.40 |
| 7 | I | 83 | ASN | CB-CA-C | -6.38 | 97.64 | 110.40 |
| 1 | A | 985 | ASP | OD1-CG-OD2 | 6.38 | 135.41 | 123.30 |
| 2 | B | 759 | PRO | N-CD-CG | -6.37 | 93.64 | 103.20 |
| 1 | A | 720 | ARG | CG-CD-NE | 6.37 | 125.17 | 111.80 |
| 1 | A | 934 | LYS | CD-CE-NZ | -6.37 | 97.06 | 111.70 |
| 3 | C | 239 | PRO | CA-C-O | 6.36 | 135.47 | 120.20 |
| 4 | E | 77 | SER | N-CA-C | -6.36 | 93.82 | 111.00 |
| 1 | A | 446 | ARG | CG-CD-NE | 6.36 | 125.16 | 111.80 |
| 2 | B | 336 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 1 | A | 475 | THR | N-CA-CB | -6.36 | 98.22 | 110.30 |
| 1 | A | 44 | THR | N-CA-CB | 6.36 | 122.37 | 110.30 |
| 1 | A | 857 | ARG | CB-CA-C | -6.36 | 97.69 | 110.40 |
| 10 | L | 68 | GLU | CB-CG-CD | 6.35 | 131.34 | 114.20 |
| 1 | A | 416 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 3 | C | 183 | TRP | CA-C-N | 6.34 | 131.16 | 117.20 |
| 1 | A | 672 | ASP | OD1-CG-OD2 | -6.34 | 111.25 | 123.30 |
| 2 | B | 709 | ASP | CB-CG-OD2 | 6.34 | 124.00 | 118.30 |
| 1 | A | 1171 | GLN | N-CA-CB | 6.33 | 122.00 | 110.60 |
| 2 | B | 914 | LYS | CD-CE-NZ | -6.33 | 97.14 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1155 | ASP | CB-CG-OD1 | 6.32 | 123.99 | 118.30 |
| 2 | B | 399 | ASP | CB-CG-OD2 | 6.32 | 123.99 | 118.30 |
| 2 | B | 1108 | ARG | N-CA-C | 6.32 | 128.07 | 111.00 |
| 2 | B | 270 | LYS | CD-CE-NZ | -6.32 | 97.16 | 111.70 |
| 1 | A | 939 | ASP | CB-CG-OD2 | 6.32 | 123.99 | 118.30 |
| 2 | B | 608 | ASP | CB-CG-OD2 | 6.32 | 123.99 | 118.30 |
| 2 | B | 1103 | ILE | CB-CA-C | -6.32 | 98.97 | 111.60 |
| 3 | C | 16 | ASP | OD1-CG-OD2 | -6.32 | 111.30 | 123.30 |
| 7 | I | 92 | ARG | NE-CZ-NH1 | -6.32 | 117.14 | 120.30 |
| 2 | B | 446 | LEU | CB-CA-C | 6.31 | 122.19 | 110.20 |
| 2 | B | 634 | TYR | CB-CG-CD1 | -6.30 | 117.22 | 121.00 |
| 5 | F | 97 | ARG | CG-CD-NE | -6.30 | 98.57 | 111.80 |
| 2 | B | 56 | ASP | O-C-N | -6.30 | 112.62 | 122.70 |
| 1 | A | 462 | VAL | CG1-CB-CG2 | -6.30 | 100.82 | 110.90 |
| 2 | B | 434 | ARG | CG-CD-NE | 6.29 | 125.01 | 111.80 |
| 1 | A | 761 | MET | CG-SD-CE | 6.29 | 110.26 | 100.20 |
| 2 | B | 312 | GLU | N-CA-CB | -6.29 | 99.28 | 110.60 |
| 2 | B | 324 | ILE | CG1-CB-CG2 | -6.29 | 97.57 | 111.40 |
| 2 | B | 1073 | TYR | CZ-CE2-CD2 | 6.28 | 125.45 | 119.80 |
| 9 | K | 79 | GLU | OE1-CD-OE2 | -6.28 | 115.76 | 123.30 |
| 3 | C | 193 | TYR | CZ-CE2-CD2 | -6.28 | 114.15 | 119.80 |
| 1 | A | 1062 | GLU | CA-CB-CG | 6.28 | 127.21 | 113.40 |
| 2 | B | 1060 | ARG | NE-CZ-NH2 | -6.28 | 117.16 | 120.30 |
| 1 | A | 659 | HIS | CB-CG-ND1 | -6.27 | 107.52 | 123.20 |
| 9 | K | 26 | LYS | CG-CD-CE | 6.27 | 130.71 | 111.90 |
| 2 | B | 961 | LEU | CB-CG-CD1 | 6.27 | 121.66 | 111.00 |
| 7 | I | 35 | VAL | CB-CA-C | -6.27 | 99.49 | 111.40 |
| 2 | B | 735 | ALA | O-C-N | 6.27 | 132.73 | 122.70 |
| 2 | B | 629 | ASP | CB-CG-OD1 | -6.26 | 112.66 | 118.30 |
| 1 | A | 843 | LYS | CB-CA-C | 6.25 | 122.91 | 110.40 |
| 1 | A | 544 | ASP | OD1-CG-OD2 | -6.25 | 111.42 | 123.30 |
| 1 | A | 1325 | THR | N-CA-CB | -6.25 | 98.42 | 110.30 |
| 1 | A | 731 | ARG | NH1-CZ-NH2 | 6.24 | 126.27 | 119.40 |
| 2 | B | 124 | TYR | CB-CG-CD2 | 6.24 | 124.74 | 121.00 |
| 1 | A | 375 | THR | CA-CB-CG2 | -6.24 | 103.67 | 112.40 |
| 1 | A | 804 | TYR | CB-CG-CD1 | 6.24 | 124.74 | 121.00 |
| 2 | B | 1127 | GLY | N-CA-C | 6.24 | 128.69 | 113.10 |
| 2 | B | 722 | ASP | CB-CG-OD2 | 6.23 | 123.91 | 118.30 |
| 9 | K | 75 | ILE | CA-CB-CG1 | 6.23 | 122.84 | 111.00 |
| 1 | A | 555 | ASP | CB-CG-OD2 | 6.23 | 123.91 | 118.30 |
| 1 | A | 1103 | GLU | CB-CA-C | 6.23 | 122.85 | 110.40 |
| 2 | B | 167 | ILE | CB-CA-C | -6.23 | 99.15 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 566 | ILE | CB-CA-C | -6.23 | 99.15 | 111.60 |
| 7 | I | 82 | GLU | OE1-CD-OE2 | -6.22 | 115.83 | 123.30 |
| 1 | A | 739 | ASP | CB-CG-OD2 | 6.22 | 123.90 | 118.30 |
| 2 | B | 653 | VAL | CA-CB-CG1 | 6.22 | 120.23 | 110.90 |
| 2 | B | 759 | PRO | CA-CB-CG | -6.22 | 92.18 | 104.00 |
| 5 | F | 154 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | A | 541 | ILE | CG1-CB-CG2 | -6.21 | 97.73 | 111.40 |
| 7 | I | 24 | ARG | CB-CA-C | -6.21 | 97.97 | 110.40 |
| 7 | I | 78 | CYS | CA-CB-SG | 6.21 | 125.18 | 114.00 |
| 1 | A | 461 | LYS | CB-CA-C | -6.21 | 97.98 | 110.40 |
| 6 | H | 142 | LEU | CA-CB-CG | -6.20 | 101.03 | 115.30 |
| 10 | L | 70 | ARG | N-CA-C | 6.20 | 127.75 | 111.00 |
| 7 | I | 24 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 2 | B | 68 | THR | OG1-CB-CG2 | -6.20 | 95.74 | 110.00 |
| 2 | B | 365 | THR | OG1-CB-CG2 | -6.20 | 95.75 | 110.00 |
| 2 | B | 419 | THR | OG1-CB-CG2 | -6.20 | 95.74 | 110.00 |
| 1 | A | 1373 | ASP | OD1-CG-OD2 | -6.20 | 111.53 | 123.30 |
| 1 | A | 1235 | LYS | CD-CE-NZ | 6.19 | 125.95 | 111.70 |
| 3 | C | 127 | ARG | NE-CZ-NH1 | 6.19 | 123.40 | 120.30 |
| 2 | B | 43 | LEU | CB-CG-CD2 | -6.19 | 100.47 | 111.00 |
| 1 | A | 728 | LYS | CB-CG-CD | 6.19 | 127.70 | 111.60 |
| 7 | I | 4 | PHE | CB-CG-CD1 | -6.19 | 116.47 | 120.80 |
| 1 | A | 376 | TYR | CZ-CE2-CD2 | -6.19 | 114.23 | 119.80 |
| 4 | E | 103 | LYS | N-CA-CB | 6.18 | 121.73 | 110.60 |
| 1 | A | 1192 | LEU | CB-CG-CD1 | -6.17 | 100.50 | 111.00 |
| 2 | B | 942 | ARG | CA-CB-CG | 6.17 | 126.98 | 113.40 |
| 2 | B | 477 | ALA | CB-CA-C | 6.17 | 119.36 | 110.10 |
| 1 | A | 486 | GLU | CG-CD-OE1 | 6.17 | 130.63 | 118.30 |
| 2 | B | 1216 | LEU | CB-CG-CD2 | -6.16 | 100.52 | 111.00 |
| 1 | A | 879 | GLU | OE1-CD-OE2 | 6.16 | 130.69 | 123.30 |
| 1 | A | 1155 | ASP | OD1-CG-OD2 | -6.16 | 111.59 | 123.30 |
| 1 | A | 1342 | GLU | OE1-CD-OE2 | 6.16 | 130.69 | 123.30 |
| 9 | K | 68 | PHE | CB-CG-CD1 | -6.16 | 116.49 | 120.80 |
| 1 | A | 325 | ILE | CG1-CB-CG2 | -6.16 | 97.86 | 111.40 |
| 1 | A | 1155 | ASP | CB-CG-OD2 | 6.15 | 123.84 | 118.30 |
| 3 | C | 252 | GLN | CB-CA-C | 6.15 | 122.71 | 110.40 |
| 10 | L | 57 | LEU | N-CA-C | 6.15 | 127.61 | 111.00 |
| 1 | A | 493 | GLN | CB-CG-CD | 6.15 | 127.59 | 111.60 |
| 4 | E | 87 | SER | CB-CA-C | 6.15 | 121.78 | 110.10 |
| 1 | A | 1348 | LEU | CB-CG-CD1 | -6.15 | 100.55 | 111.00 |
| 1 | A | 1445 | ILE | O-C-N | 6.15 | 132.54 | 122.70 |
| 2 | B | 909 | ASP | OD1-CG-OD2 | -6.14 | 111.64 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 596 | THR | CB-CA-C | -6.13 | 95.04 | 111.60 |
| 2 | B | 297 | ILE | CA-CB-CG2 | -6.13 | 98.63 | 110.90 |
| 4 | E | 180 | ARG | CD-NE-CZ | 6.13 | 132.19 | 123.60 |
| 1 | A | 416 | ARG | CG-CD-NE | -6.13 | 98.93 | 111.80 |
| 9 | K | 74 | ARG | CG-CD-NE | -6.13 | 98.93 | 111.80 |
| 2 | B | 138 | GLU | OE1-CD-OE2 | -6.13 | 115.95 | 123.30 |
| 1 | A | 923 | LEU | CB-CA-C | -6.12 | 98.57 | 110.20 |
| 1 | A | 1066 | VAL | CG1-CB-CG2 | -6.12 | 101.11 | 110.90 |
| 1 | A | 922 | ASP | CB-CG-OD1 | 6.12 | 123.80 | 118.30 |
| 1 | A | 885 | THR | OG1-CB-CG2 | -6.11 | 95.94 | 110.00 |
| 2 | B | 979 | LYS | CD-CE-NZ | -6.11 | 97.64 | 111.70 |
| 1 | A | 466 | SER | N-CA-C | 6.11 | 127.49 | 111.00 |
| 4 | E | 41 | ASP | OD1-CG-OD2 | -6.11 | 111.70 | 123.30 |
| 1 | A | 1377 | THR | CA-CB-CG2 | 6.10 | 120.94 | 112.40 |
| 2 | B | 212 | LEU | CB-CG-CD2 | 6.10 | 121.37 | 111.00 |
| 2 | B | 959 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | A | 1111 | MET | N-CA-CB | -6.10 | 99.63 | 110.60 |
| 2 | B | 304 | ASP | N-CA-CB | 6.10 | 121.57 | 110.60 |
| 2 | B | 690 | VAL | CG1-CB-CG2 | -6.10 | 101.14 | 110.90 |
| 3 | C | 249 | ASP | CB-CG-OD1 | -6.10 | 112.81 | 118.30 |
| 1 | A | 839 | ARG | NE-CZ-NH1 | 6.09 | 123.35 | 120.30 |
| 2 | B | 89 | GLU | OE1-CD-OE2 | -6.09 | 115.99 | 123.30 |
| 2 | B | 990 | ILE | CA-CB-CG1 | 6.09 | 122.57 | 111.00 |
| 3 | C | 210 | GLU | CG-CD-OE1 | 6.09 | 130.48 | 118.30 |
| 4 | E | 204 | THR | N-CA-CB | -6.09 | 98.73 | 110.30 |
| 3 | C | 183 | TRP | O-C-N | -6.09 | 112.96 | 122.70 |
| 4 | E | 16 | PHE | CB-CG-CD1 | 6.09 | 125.06 | 120.80 |
| 1 | A | 1013 | ASP | CB-CG-OD1 | 6.08 | 123.78 | 118.30 |
| 1 | A | 1234 | GLU | CA-CB-CG | 6.08 | 126.79 | 113.40 |
| 4 | E | 62 | ALA | N-CA-CB | -6.08 | 101.58 | 110.10 |
| 4 | E | 195 | VAL | CA-CB-CG2 | -6.08 | 101.78 | 110.90 |
| 7 | I | 30 | ARG | CG-CD-NE | -6.08 | 99.03 | 111.80 |
| 1 | A | 898 | ARG | CB-CA-C | -6.08 | 98.25 | 110.40 |
| 1 | A | 608 | ILE | CA-CB-CG1 | 6.08 | 122.54 | 111.00 |
| 1 | A | 664 | THR | CB-CA-C | -6.08 | 95.20 | 111.60 |
| 6 | H | 82 | PRO | N-CA-C | -6.08 | 96.30 | 112.10 |
| 3 | C | 85 | ASP | CB-CG-OD1 | -6.07 | 112.83 | 118.30 |
| 2 | B | 596 | LEU | CB-CG-CD1 | -6.07 | 100.68 | 111.00 |
| 1 | A | 512 | VAL | CA-CB-CG1 | 6.07 | 120.00 | 110.90 |
| 3 | C | 55 | THR | OG1-CB-CG2 | -6.06 | 96.06 | 110.00 |
| 2 | B | 97 | VAL | CG1-CB-CG2 | -6.06 | 101.20 | 110.90 |
| 1 | A | 386 | ASP | CB-CG-OD1 | 6.06 | 123.75 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 116 | TYR | N-CA-C | 6.06 | 127.35 | 111.00 |
| 8 | J | 64 | ASN | CB-CA-C | 6.06 | 122.51 | 110.40 |
| 1 | A | 895 | LYS | CD-CE-NZ | -6.05 | 97.78 | 111.70 |
| 1 | A | 1371 | LEU | CB-CG-CD1 | -6.05 | 100.71 | 111.00 |
| 7 | I | 118 | ARG | CA-CB-CG | 6.05 | 126.71 | 113.40 |
| 1 | A | 305 | ASP | OD1-CG-OD2 | -6.05 | 111.81 | 123.30 |
| 4 | E | 26 | ARG | NE-CZ-NH2 | 6.05 | 123.33 | 120.30 |
| 2 | B | 537 | LYS | CD-CE-NZ | -6.04 | 97.80 | 111.70 |
| 1 | A | 918 | GLU | CA-CB-CG | 6.04 | 126.69 | 113.40 |
| 4 | E | 55 | ARG | NE-CZ-NH2 | 6.04 | 123.32 | 120.30 |
| 2 | B | 212 | LEU | CB-CG-CD1 | -6.04 | 100.73 | 111.00 |
| 2 | B | 711 | GLU | CB-CA-C | -6.04 | 98.33 | 110.40 |
| 6 | H | 11 | GLN | CB-CA-C | -6.03 | 98.33 | 110.40 |
| 7 | I | 1 | MET | CB-CG-SD | 6.03 | 130.49 | 112.40 |
| 7 | I | 112 | SER | N-CA-CB | -6.03 | 101.46 | 110.50 |
| 8 | J | 48 | ARG | CD-NE-CZ | 6.03 | 132.04 | 123.60 |
| 2 | B | 1220 | ARG | NH1-CZ-NH2 | -6.03 | 112.77 | 119.40 |
| 2 | B | 884 | ARG | CG-CD-NE | -6.03 | 99.15 | 111.80 |
| 2 | B | 904 | ARG | NE-CZ-NH2 | 6.03 | 123.31 | 120.30 |
| 1 | A | 578 | LEU | CB-CG-CD1 | -6.02 | 100.76 | 111.00 |
| 1 | A | 96 | ILE | CA-CB-CG1 | 6.02 | 122.44 | 111.00 |
| 3 | C | 206 | ASN | O-C-N | -6.02 | 113.07 | 122.70 |
| 2 | B | 19 | GLU | OE1-CD-OE2 | -6.02 | 116.08 | 123.30 |
| 2 | B | 135 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 2 | B | 354 | ASP | CB-CG-OD2 | -6.01 | 112.89 | 118.30 |
| 4 | E | 17 | ARG | NE-CZ-NH1 | -6.01 | 117.29 | 120.30 |
| 9 | K | 41 | THR | CA-CB-CG2 | -6.01 | 103.98 | 112.40 |
| 2 | B | 807 | ARG | CG-CD-NE | -6.01 | 99.18 | 111.80 |
| 7 | I | 92 | ARG | CA-C-N | -6.00 | 103.99 | 117.20 |
| 3 | C | 63 | ILE | CG1-CB-CG2 | -6.00 | 98.19 | 111.40 |
| 1 | A | 1227 | ILE | CG1-CB-CG2 | -6.00 | 98.20 | 111.40 |
| 1 | A | 677 | ARG | NE-CZ-NH2 | 6.00 | 123.30 | 120.30 |
| 2 | B | 1033 | LYS | CD-CE-NZ | -5.99 | 97.92 | 111.70 |
| 5 | F | 116 | ASP | OD1-CG-OD2 | -5.99 | 111.92 | 123.30 |
| 1 | A | 56 | PRO | O-C-N | 5.98 | 132.27 | 122.70 |
| 6 | H | 7 | ASP | CB-CG-OD2 | 5.98 | 123.68 | 118.30 |
| 10 | L | 42 | ARG | NE-CZ-NH2 | 5.98 | 123.29 | 120.30 |
| 1 | A | 680 | THR | OG1-CB-CG2 | -5.97 | 96.27 | 110.00 |
| 1 | A | 720 | ARG | NE-CZ-NH1 | -5.97 | 117.31 | 120.30 |
| 2 | B | 579 | ARG | NH1-CZ-NH2 | 5.97 | 125.97 | 119.40 |
| 2 | B | 1181 | GLU | CA-CB-CG | 5.97 | 126.54 | 113.40 |
| 7 | I | 55 | THR | N-CA-CB | -5.97 | 98.96 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1359 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 2 | B | 942 | ARG | CG-CD-NE | -5.97 | 99.27 | 111.80 |
| 2 | B | 598 | GLU | CG-CD-OE2 | 5.97 | 130.23 | 118.30 |
| 2 | B | 381 | MET | CG-SD-CE | -5.96 | 90.66 | 100.20 |
| 2 | B | 836 | GLU | O-C-N | 5.96 | 132.24 | 122.70 |
| 1 | A | 1225 | PHE | CB-CG-CD2 | 5.96 | 124.97 | 120.80 |
| 7 | I | 5 | ARG | CB-CG-CD | 5.96 | 127.10 | 111.60 |
| 1 | A | 295 | LEU | CA-CB-CG | 5.96 | 129.00 | 115.30 |
| 1 | A | 666 | ILE | CG1-CB-CG2 | 5.96 | 124.51 | 111.40 |
| 2 | B | 249 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | A | 724 | GLU | N-CA-C | -5.96 | 94.92 | 111.00 |
| 2 | B | 889 | THR | CB-CA-C | -5.96 | 95.52 | 111.60 |
| 1 | A | 327 | ALA | CA-C-N | -5.95 | 104.11 | 117.20 |
| 2 | B | 276 | ILE | CG1-CB-CG2 | -5.95 | 98.31 | 111.40 |
| 2 | B | 852 | ARG | N-CA-CB | -5.95 | 99.89 | 110.60 |
| 6 | H | 107 | VAL | N-CA-C | -5.95 | 94.94 | 111.00 |
| 1 | A | 885 | THR | CA-CB-CG2 | 5.95 | 120.73 | 112.40 |
| 1 | A | 896 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 2 | B | 621 | GLU | CG-CD-OE2 | 5.94 | 130.18 | 118.30 |
| 1 | A | 790 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 |
| 2 | B | 895 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 6 | H | 87 | ARG | CA-CB-CG | 5.93 | 126.46 | 113.40 |
| 2 | B | 397 | ASP | CB-CG-OD2 | 5.93 | 123.64 | 118.30 |
| 5 | F | 149 | GLU | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 2 | B | 883 | LEU | CB-CG-CD2 | 5.93 | 121.08 | 111.00 |
| 2 | B | 1154 | ALA | CB-CA-C | 5.93 | 118.99 | 110.10 |
| 3 | C | 183 | TRP | N-CA-C | -5.93 | 94.99 | 111.00 |
| 7 | I | 88 | SER | CB-CA-C | -5.92 | 98.84 | 110.10 |
| 1 | A | 589 | GLN | CB-CA-C | -5.92 | 98.56 | 110.40 |
| 1 | A | 708 | MET | CG-SD-CE | 5.92 | 109.67 | 100.20 |
| 4 | E | 39 | LEU | CB-CG-CD1 | 5.92 | 121.06 | 111.00 |
| 10 | L | 63 | ARG | N-CA-CB | 5.90 | 121.23 | 110.60 |
| 1 | A | 858 | ASN | CB-CG-OD1 | -5.90 | 109.80 | 121.60 |
| 1 | A | 1377 | THR | N-CA-CB | 5.90 | 121.51 | 110.30 |
| 8 | J | 7 | CYS | CB-CA-C | -5.90 | 98.60 | 110.40 |
| 1 | A | 438 | ASP | OD1-CG-OD2 | -5.90 | 112.09 | 123.30 |
| 3 | C | 40 | GLU | N-CA-C | 5.90 | 126.93 | 111.00 |
| 2 | B | 511 | PRO | N-CD-CG | -5.90 | 94.35 | 103.20 |
| 2 | B | 954 | VAL | CB-CA-C | -5.90 | 100.19 | 111.40 |
| 2 | B | 1153 | GLU | CG-CD-OE1 | -5.90 | 106.50 | 118.30 |
| 7 | I | 24 | ARG | CG-CD-NE | -5.89 | 99.42 | 111.80 |
| 2 | B | 589 | VAL | CB-CA-C | 5.89 | 122.59 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1019 | SER | C-N-CA | -5.89 | 106.98 | 121.70 |
| 3 | C | 76 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 3 | C | 191 | TYR | CZ-CE2-CD2 | 5.89 | 125.10 | 119.80 |
| 1 | A | 728 | LYS | N-CA-CB | 5.89 | 121.19 | 110.60 |
| 1 | A | 1243 | VAL | CA-CB-CG2 | 5.89 | 119.73 | 110.90 |
| 1 | A | 897 | TYR | CB-CG-CD1 | 5.88 | 124.53 | 121.00 |
| 9 | K | 74 | ARG | NE-CZ-NH1 | -5.88 | 117.36 | 120.30 |
| 1 | A | 1204 | ASP | OD1-CG-OD2 | -5.88 | 112.14 | 123.30 |
| 2 | B | 378 | LEU | CB-CG-CD1 | -5.88 | 101.01 | 111.00 |
| 6 | H | 63 | LEU | CB-CA-C | 5.87 | 121.36 | 110.20 |
| 10 | L | 48 | CYS | N-CA-C | 5.87 | 126.85 | 111.00 |
| 1 | A | 16 | GLU | CG-CD-OE2 | -5.87 | 106.57 | 118.30 |
| 1 | A | 658 | LEU | CB-CG-CD2 | -5.86 | 101.03 | 111.00 |
| 4 | E | 200 | ARG | N-CA-CB | 5.86 | 121.15 | 110.60 |
| 7 | I | 8 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | A | 1193 | LEU | CB-CG-CD2 | -5.86 | 101.04 | 111.00 |
| 10 | L | 40 | LEU | CB-CG-CD2 | 5.86 | 120.96 | 111.00 |
| 3 | C | 238 | ILE | CA-CB-CG2 | 5.85 | 122.60 | 110.90 |
| 1 | A | 516 | SER | N-CA-CB | -5.85 | 101.72 | 110.50 |
| 3 | C | 165 | LYS | N-CA-CB | 5.85 | 121.13 | 110.60 |
| 6 | H | 128 | ASN | N-CA-C | 5.85 | 126.78 | 111.00 |
| 2 | B | 65 | GLU | OE1-CD-OE2 | -5.84 | 116.29 | 123.30 |
| 1 | A | 1370 | LEU | CD1-CG-CD2 | -5.84 | 92.98 | 110.50 |
| 1 | A | 1371 | LEU | CB-CG-CD2 | 5.84 | 120.93 | 111.00 |
| 3 | C | 18 | VAL | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | A | 41 | MET | CG-SD-CE | 5.84 | 109.54 | 100.20 |
| 2 | B | 1101 | ASP | OD1-CG-OD2 | -5.84 | 112.20 | 123.30 |
| 1 | A | 1035 | TYR | CD1-CE1-CZ | 5.84 | 125.05 | 119.80 |
| 4 | E | 162 | ARG | CB-CA-C | 5.84 | 122.07 | 110.40 |
| 6 | H | 127 | GLY | N-CA-C | 5.84 | 127.69 | 113.10 |
| 2 | B | 895 | ASP | OD1-CG-OD2 | -5.83 | 112.21 | 123.30 |
| 2 | B | 853 | SER | CB-CA-C | -5.83 | 99.02 | 110.10 |
| 5 | F | 150 | GLU | CG-CD-OE1 | -5.83 | 106.64 | 118.30 |
| 8 | J | 64 | ASN | N-CA-CB | -5.83 | 100.11 | 110.60 |
| 1 | A | 613 | ILE | CG1-CB-CG2 | -5.82 | 98.59 | 111.40 |
| 3 | C | 127 | ARG | NE-CZ-NH2 | 5.82 | 123.21 | 120.30 |
| 1 | A | 914 | GLU | CG-CD-OE1 | 5.82 | 129.94 | 118.30 |
| 2 | B | 260 | GLY | N-CA-C | -5.82 | 98.55 | 113.10 |
| 2 | B | 436 | VAL | CB-CA-C | 5.82 | 122.46 | 111.40 |
| 9 | K | 93 | SER | N-CA-CB | 5.82 | 119.22 | 110.50 |
| 1 | A | 416 | ARG | CA-CB-CG | 5.81 | 126.19 | 113.40 |
| 3 | C | 90 | ASP | N-CA-C | 5.81 | 126.68 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 110 | ASP | OD1-CG-OD2 | -5.81 | 112.27 | 123.30 |
| 1 | A | 436 | ILE | CG1-CB-CG2 | -5.80 | 98.63 | 111.40 |
| 3 | C | 89 | GLU | N-CA-C | -5.80 | 95.33 | 111.00 |
| 2 | B | 20 | ASP | CB-CG-OD1 | 5.80 | 123.52 | 118.30 |
| 2 | B | 644 | GLU | N-CA-CB | -5.80 | 100.16 | 110.60 |
| 2 | B | 788 | ARG | NE-CZ-NH2 | -5.79 | 117.40 | 120.30 |
| 2 | B | 957 | ASN | N-CA-CB | -5.79 | 100.17 | 110.60 |
| 4 | E | 149 | LEU | CB-CG-CD1 | 5.79 | 120.85 | 111.00 |
| 1 | A | 86 | LEU | CB-CG-CD2 | 5.79 | 120.85 | 111.00 |
| 1 | A | 1176 | LEU | CB-CG-CD2 | 5.79 | 120.84 | 111.00 |
| 1 | A | 1241 | ARG | CG-CD-NE | -5.79 | 99.65 | 111.80 |
| 2 | B | 795 | ILE | CB-CA-C | -5.79 | 100.03 | 111.60 |
| 9 | K | 47 | ARG | NH1-CZ-NH2 | 5.79 | 125.76 | 119.40 |
| 9 | K | 39 | ASP | OD1-CG-OD2 | -5.78 | 112.31 | 123.30 |
| 6 | H | 117 | SER | CB-CA-C | -5.78 | 99.12 | 110.10 |
| 1 | A | 1134 | ILE | CG1-CB-CG2 | -5.78 | 98.69 | 111.40 |
| 3 | C | 116 | LYS | CD-CE-NZ | -5.78 | 98.42 | 111.70 |
| 7 | I | 45 | ARG | NE-CZ-NH2 | 5.77 | 123.19 | 120.30 |
| 1 | A | 238 | CYS | CA-CB-SG | -5.77 | 103.61 | 114.00 |
| 2 | B | 381 | MET | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 2 | B | 336 | ARG | NE-CZ-NH1 | -5.77 | 117.42 | 120.30 |
| 1 | A | 731 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 1 | A | 1409 | LEU | CB-CG-CD1 | 5.75 | 120.78 | 111.00 |
| 1 | A | 1014 | ALA | CA-C-O | 5.75 | 132.17 | 120.10 |
| 1 | A | 1237 | ILE | CG1-CB-CG2 | -5.75 | 98.75 | 111.40 |
| 2 | B | 589 | VAL | O-C-N | -5.75 | 113.50 | 122.70 |
| 1 | A | 1120 | LEU | CB-CG-CD1 | 5.74 | 120.77 | 111.00 |
| 1 | A | 1129 | GLU | OE1-CD-OE2 | -5.74 | 116.41 | 123.30 |
| 1 | A | 1135 | ARG | CD-NE-CZ | 5.74 | 131.64 | 123.60 |
| 1 | A | 1198 | ASP | CB-CG-OD2 | 5.74 | 123.47 | 118.30 |
| 1 | A | 980 | ASP | CB-CA-C | -5.74 | 98.92 | 110.40 |
| 2 | B | 1212 | ILE | CA-CB-CG1 | -5.74 | 100.09 | 111.00 |
| 4 | E | 53 | PRO | N-CD-CG | -5.74 | 94.59 | 103.20 |
| 4 | E | 112 | TYR | OH-CZ-CE2 | 5.74 | 135.60 | 120.10 |
| 7 | I | 17 | ARG | N-CA-CB | 5.74 | 120.93 | 110.60 |
| 1 | A | 836 | TYR | CB-CG-CD1 | -5.74 | 117.56 | 121.00 |
| 2 | B | 319 | GLU | OE1-CD-OE2 | -5.74 | 116.42 | 123.30 |
| 4 | E | 154 | ILE | CG1-CB-CG2 | -5.74 | 98.78 | 111.40 |
| 3 | C | 94 | LYS | CA-CB-CG | 5.73 | 126.02 | 113.40 |
| 3 | C | 34 | ARG | CG-CD-NE | -5.73 | 99.76 | 111.80 |
| 1 | A | 434 | ARG | CD-NE-CZ | 5.73 | 131.62 | 123.60 |
| 2 | B | 245 | GLU | CG-CD-OE2 | 5.73 | 129.76 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 684 | LEU | CB-CG-CD1 | -5.73 | 101.26 | 111.00 |
| 6 | H | 116 | TYR | CB-CA-C | -5.73 | 98.95 | 110.40 |
| 4 | E | 30 | ILE | CG1-CB-CG2 | -5.73 | 98.80 | 111.40 |
| 7 | I | 18 | GLU | N-CA-C | -5.73 | 95.54 | 111.00 |
| 9 | K | 32 | VAL | CG1-CB-CG2 | -5.73 | 101.74 | 110.90 |
| 1 | A | 1208 | THR | CB-CA-C | -5.72 | 96.14 | 111.60 |
| 1 | A | 1425 | SER | CA-CB-OG | -5.72 | 95.75 | 111.20 |
| 2 | B | 289 | LEU | O-C-N | -5.72 | 113.47 | 123.20 |
| 1 | A | 945 | GLU | OE1-CD-OE2 | 5.72 | 130.17 | 123.30 |
| 2 | B | 589 | VAL | N-CA-CB | -5.72 | 98.91 | 111.50 |
| 3 | C | 47 | ASP | CB-CG-OD1 | -5.72 | 113.16 | 118.30 |
| 1 | A | 739 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 6 | H | 52 | GLN | CA-C-N | 5.71 | 129.77 | 117.20 |
| 1 | A | 1280 | GLU | CG-CD-OE1 | -5.71 | 106.88 | 118.30 |
| 1 | A | 243 | PRO | N-CD-CG | -5.71 | 94.64 | 103.20 |
| 3 | C | 263 | THR | N-CA-CB | -5.71 | 99.45 | 110.30 |
| 1 | A | 235 | ILE | CB-CG1-CD1 | 5.71 | 129.88 | 113.90 |
| 4 | E | 194 | GLU | OE1-CD-OE2 | -5.71 | 116.45 | 123.30 |
| 8 | J | 31 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 9 | K | 47 | ARG | CG-CD-NE | 5.71 | 123.79 | 111.80 |
| 2 | B | 773 | MET | CA-CB-CG | -5.70 | 103.61 | 113.30 |
| 1 | A | 1212 | VAL | CG1-CB-CG2 | -5.70 | 101.78 | 110.90 |
| 2 | B | 239 | GLU | CB-CA-C | 5.70 | 121.80 | 110.40 |
| 8 | J | 58 | GLU | OE1-CD-OE2 | -5.70 | 116.46 | 123.30 |
| 1 | A | 968 | GLN | CA-CB-CG | -5.70 | 100.87 | 113.40 |
| 2 | B | 268 | THR | N-CA-CB | -5.70 | 99.47 | 110.30 |
| 8 | J | 28 | ASP | N-CA-CB | 5.70 | 120.85 | 110.60 |
| 2 | B | 911 | ILE | CG1-CB-CG2 | -5.69 | 98.87 | 111.40 |
| 8 | J | 51 | LEU | CB-CG-CD2 | -5.69 | 101.32 | 111.00 |
| 3 | C | 35 | ARG | CD-NE-CZ | 5.69 | 131.57 | 123.60 |
| 9 | K | 6 | ARG | N-CA-CB | -5.69 | 100.36 | 110.60 |
| 1 | A | 1287 | TYR | CD1-CE1-CZ | -5.69 | 114.68 | 119.80 |
| 2 | B | 1018 | PRO | CA-C-O | -5.69 | 106.55 | 120.20 |
| 4 | E | 57 | MET | CG-SD-CE | 5.69 | 109.30 | 100.20 |
| 6 | H | 16 | ASP | CB-CA-C | -5.69 | 99.03 | 110.40 |
| 9 | K | 93 | SER | CB-CA-C | -5.68 | 99.30 | 110.10 |
| 1 | A | 896 | ARG | NH1-CZ-NH2 | 5.68 | 125.65 | 119.40 |
| 1 | A | 1080 | THR | CA-CB-CG2 | 5.68 | 120.35 | 112.40 |
| 2 | B | 479 | VAL | CG1-CB-CG2 | -5.68 | 101.81 | 110.90 |
| 2 | B | 1026 | LEU | CB-CG-CD2 | 5.68 | 120.65 | 111.00 |
| 2 | B | 341 | LEU | CB-CG-CD1 | 5.67 | 120.65 | 111.00 |
| 2 | B | 131 | ASP | N-CA-C | -5.67 | 95.69 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 331 | LEU | CB-CG-CD1 | 5.67 | 120.64 | 111.00 |
| 1 | A | 701 | LEU | CB-CG-CD2 | -5.67 | 101.36 | 111.00 |
| 1 | A | 1025 | ARG | NE-CZ-NH1 | -5.67 | 117.47 | 120.30 |
| 2 | B | 289 | LEU | C-N-CA | -5.67 | 110.40 | 122.30 |
| 1 | A | 1135 | ARG | CA-CB-CG | 5.67 | 125.87 | 113.40 |
| 9 | K | 17 | SER | CB-CA-C | -5.67 | 99.33 | 110.10 |
| 4 | E | 72 | PHE | CG-CD2-CE2 | -5.67 | 114.57 | 120.80 |
| 1 | A | 266 | LEU | CB-CA-C | -5.66 | 99.44 | 110.20 |
| 8 | J | 24 | LEU | CB-CA-C | -5.66 | 99.44 | 110.20 |
| 3 | C | 58 | LEU | CB-CG-CD1 | -5.66 | 101.38 | 111.00 |
| 1 | A | 720 | ARG | CB-CG-CD | 5.66 | 126.31 | 111.60 |
| 4 | E | 169 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | A | 1116 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 9 | K | 111 | LEU | CD1-CG-CD2 | 5.66 | 127.47 | 110.50 |
| 5 | F | 133 | VAL | CA-CB-CG2 | -5.65 | 102.42 | 110.90 |
| 6 | H | 112 | ILE | CG1-CB-CG2 | -5.65 | 98.96 | 111.40 |
| 2 | B | 239 | GLU | N-CA-CB | -5.65 | 100.43 | 110.60 |
| 2 | B | 797 | TYR | CB-CG-CD2 | 5.65 | 124.39 | 121.00 |
| 3 | C | 254 | LYS | N-CA-CB | 5.65 | 120.77 | 110.60 |
| 10 | L | 26 | THR | CA-CB-CG2 | 5.65 | 120.31 | 112.40 |
| 7 | I | 54 | GLU | CG-CD-OE2 | -5.65 | 107.01 | 118.30 |
| 1 | A | 871 | ASP | CB-CG-OD2 | 5.64 | 123.38 | 118.30 |
| 2 | B | 857 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 4 | E | 80 | VAL | CB-CA-C | -5.64 | 100.67 | 111.40 |
| 1 | A | 764 | CYS | N-CA-CB | -5.64 | 100.44 | 110.60 |
| 1 | A | 1192 | LEU | CB-CG-CD2 | 5.64 | 120.59 | 111.00 |
| 2 | B | 595 | ARG | N-CA-CB | 5.64 | 120.75 | 110.60 |
| 2 | B | 642 | ASP | C-N-CA | -5.64 | 107.60 | 121.70 |
| 2 | B | 1064 | TYR | C-N-CA | -5.64 | 107.60 | 121.70 |
| 5 | F | 97 | ARG | CB-CG-CD | 5.64 | 126.26 | 111.60 |
| 1 | A | 962 | ARG | CG-CD-NE | -5.64 | 99.96 | 111.80 |
| 2 | B | 643 | ASP | CB-CG-OD1 | 5.64 | 123.37 | 118.30 |
| 7 | I | 10 | CYS | N-CA-C | 5.63 | 126.21 | 111.00 |
| 1 | A | 290 | GLU | OE1-CD-OE2 | 5.63 | 130.06 | 123.30 |
| 1 | A | 635 | ARG | CG-CD-NE | -5.63 | 99.97 | 111.80 |
| 6 | H | 52 | GLN | O-C-N | -5.63 | 113.69 | 122.70 |
| 2 | B | 315 | LYS | CB-CA-C | -5.63 | 99.14 | 110.40 |
| 1 | A | 886 | ILE | CG1-CB-CG2 | -5.63 | 99.02 | 111.40 |
| 1 | A | 1231 | ASP | CB-CG-OD2 | 5.63 | 123.36 | 118.30 |
| 2 | B | 1183 | LYS | CB-CA-C | 5.62 | 121.65 | 110.40 |
| 7 | I | 9 | ASP | CB-CG-OD1 | -5.62 | 113.24 | 118.30 |
| 2 | B | 646 | LEU | N-CA-C | 5.62 | 126.18 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 136 | LYS | CD-CE-NZ | 5.62 | 124.63 | 111.70 |
| 1 | A | 571 | LEU | CB-CG-CD2 | 5.62 | 120.55 | 111.00 |
| 2 | B | 1089 | PRO | N-CD-CG | 5.62 | 111.63 | 103.20 |
| 7 | I | 4 | PHE | N-CA-C | 5.62 | 126.17 | 111.00 |
| 1 | A | 1418 | LEU | CB-CG-CD2 | -5.62 | 101.45 | 111.00 |
| 1 | A | 1012 | ARG | CD-NE-CZ | 5.62 | 131.46 | 123.60 |
| 1 | A | 1440 | ALA | N-CA-CB | -5.62 | 102.24 | 110.10 |
| 1 | A | 913 | LEU | CB-CG-CD2 | 5.61 | 120.54 | 111.00 |
| 3 | C | 215 | GLU | OE1-CD-OE2 | -5.61 | 116.57 | 123.30 |
| 7 | I | 31 | THR | C-N-CA | 5.61 | 135.72 | 121.70 |
| 2 | B | 245 | GLU | CA-CB-CG | 5.61 | 125.73 | 113.40 |
| 1 | A | 1116 | LEU | N-CA-C | -5.60 | 95.87 | 111.00 |
| 1 | A | 74 | MET | CB-CG-SD | 5.60 | 129.21 | 112.40 |
| 1 | A | 739 | ASP | OD1-CG-OD2 | -5.60 | 112.66 | 123.30 |
| 3 | C | 152 | GLU | OE1-CD-OE2 | 5.60 | 130.02 | 123.30 |
| 3 | C | 191 | TYR | CB-CG-CD1 | 5.60 | 124.36 | 121.00 |
| 1 | A | 1284 | MET | O-C-N | 5.60 | 131.66 | 122.70 |
| 6 | H | 56 | THR | N-CA-C | -5.60 | 95.88 | 111.00 |
| 8 | J | 34 | THR | OG1-CB-CG2 | -5.60 | 97.12 | 110.00 |
| 1 | A | 1003 | LYS | CA-CB-CG | -5.60 | 101.08 | 113.40 |
| 3 | C | 260 | LEU | CB-CG-CD2 | 5.60 | 120.51 | 111.00 |
| 4 | E | 81 | GLU | N-CA-CB | -5.60 | 100.53 | 110.60 |
| 1 | A | 586 | ILE | CG1-CB-CG2 | -5.59 | 99.09 | 111.40 |
| 4 | E | 63 | ASN | N-CA-C | 5.59 | 126.10 | 111.00 |
| 7 | I | 24 | ARG | N-CA-CB | 5.59 | 120.67 | 110.60 |
| 1 | A | 1263 | ILE | CG1-CB-CG2 | -5.59 | 99.09 | 111.40 |
| 2 | B | 452 | THR | C-N-CA | 5.59 | 135.68 | 121.70 |
| 2 | B | 370 | PHE | CB-CA-C | 5.59 | 121.58 | 110.40 |
| 2 | B | 234 | ILE | CG1-CB-CG2 | 5.59 | 123.69 | 111.40 |
| 2 | B | 346 | GLU | CG-CD-OE1 | 5.59 | 129.48 | 118.30 |
| 1 | A | 244 | PRO | CA-C-O | -5.59 | 106.79 | 120.20 |
| 2 | B | 522 | VAL | N-CA-CB | -5.59 | 99.21 | 111.50 |
| 3 | C | 127 | ARG | NH1-CZ-NH2 | -5.59 | 113.25 | 119.40 |
| 1 | A | 466 | SER | N-CA-CB | 5.58 | 118.88 | 110.50 |
| 4 | E | 52 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 1 | A | 1450 | LEU | CA-CB-CG | 5.58 | 128.14 | 115.30 |
| 2 | B | 57 | TYR | CD1-CE1-CZ | 5.58 | 124.83 | 119.80 |
| 2 | B | 483 | LEU | CB-CG-CD2 | 5.58 | 120.49 | 111.00 |
| 3 | C | 163 | ILE | CB-CA-C | 5.58 | 122.77 | 111.60 |
| 2 | B | 1019 | SER | CA-CB-OG | -5.58 | 96.13 | 111.20 |
| 9 | K | 14 | GLU | CB-CA-C | 5.58 | 121.56 | 110.40 |
| 7 | I | 1 | MET | CG-SD-CE | 5.58 | 109.12 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 452 | LYS | CB-CG-CD | -5.58 | 97.10 | 111.60 |
| 1 | A | 465 | TYR | O-C-N | -5.58 | 113.78 | 122.70 |
| 2 | B | 459 | TYR | CB-CG-CD1 | -5.58 | 117.66 | 121.00 |
| 2 | B | 705 | MET | CB-CG-SD | -5.57 | 95.69 | 112.40 |
| 9 | K | 4 | PRO | N-CA-C | -5.57 | 97.62 | 112.10 |
| 2 | B | 903 | VAL | CG1-CB-CG2 | -5.57 | 101.99 | 110.90 |
| 2 | B | 1106 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 1 | A | 1307 | GLU | OE1-CD-OE2 | -5.57 | 116.62 | 123.30 |
| 2 | B | 353 | LYS | CD-CE-NZ | 5.57 | 124.51 | 111.70 |
| 2 | B | 133 | LYS | CD-CE-NZ | -5.56 | 98.90 | 111.70 |
| 1 | A | 173 | THR | N-CA-C | -5.56 | 95.98 | 111.00 |
| 1 | A | 495 | GLU | OE1-CD-OE2 | -5.56 | 116.63 | 123.30 |
| 1 | A | 1442 | ASP | O-C-N | 5.56 | 131.59 | 122.70 |
| 2 | B | 940 | PRO | N-CD-CG | -5.56 | 94.86 | 103.20 |
| 1 | A | 58 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 1 | A | 908 | LEU | CB-CG-CD2 | -5.55 | 101.56 | 111.00 |
| 2 | B | 273 | LEU | CB-CA-C | -5.55 | 99.65 | 110.20 |
| 1 | A | 441 | PRO | N-CD-CG | -5.55 | 94.87 | 103.20 |
| 2 | B | 852 | ARG | NE-CZ-NH2 | 5.55 | 123.07 | 120.30 |
| 2 | B | 56 | ASP | N-CA-C | 5.54 | 125.97 | 111.00 |
| 2 | B | 817 | LEU | CB-CG-CD2 | -5.54 | 101.57 | 111.00 |
| 8 | J | 14 | VAL | O-C-N | -5.54 | 113.77 | 123.20 |
| 1 | A | 1231 | ASP | CB-CG-OD1 | -5.54 | 113.31 | 118.30 |
| 1 | A | 1192 | LEU | CB-CA-C | -5.54 | 99.67 | 110.20 |
| 4 | E | 38 | PRO | O-C-N | 5.54 | 131.56 | 122.70 |
| 5 | F | 81 | THR | CA-CB-CG2 | 5.54 | 120.16 | 112.40 |
| 2 | B | 1010 | LEU | CB-CA-C | -5.54 | 99.68 | 110.20 |
| 4 | E | 166 | LYS | CD-CE-NZ | 5.54 | 124.43 | 111.70 |
| 1 | A | 992 | ASP | N-CA-CB | -5.53 | 100.64 | 110.60 |
| 1 | A | 1017 | LEU | CB-CG-CD2 | -5.53 | 101.59 | 111.00 |
| 2 | B | 1099 | VAL | CB-CA-C | -5.53 | 100.89 | 111.40 |
| 7 | I | 9 | ASP | CB-CG-OD2 | 5.53 | 123.28 | 118.30 |
| 9 | K | 111 | LEU | CB-CG-CD1 | -5.53 | 101.60 | 111.00 |
| 1 | A | 933 | TYR | CB-CG-CD2 | 5.53 | 124.32 | 121.00 |
| 2 | B | 134 | LYS | CD-CE-NZ | 5.53 | 124.41 | 111.70 |
| 1 | A | 1257 | ASP | CB-CG-OD1 | -5.53 | 113.33 | 118.30 |
| 5 | F | 144 | GLU | OE1-CD-OE2 | 5.52 | 129.93 | 123.30 |
| 6 | H | 117 | SER | O-C-N | 5.52 | 131.54 | 122.70 |
| 1 | A | 1146 | VAL | N-CA-CB | -5.52 | 99.36 | 111.50 |
| 2 | B | 665 | GLU | CA-CB-CG | 5.52 | 125.54 | 113.40 |
| 1 | A | 433 | GLU | OE1-CD-OE2 | 5.51 | 129.92 | 123.30 |
| 2 | B | 336 | ARG | NH1-CZ-NH2 | 5.51 | 125.47 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 119 | VAL | CA-CB-CG1 | -5.51 | 102.63 | 110.90 |
| 9 | K | 61 | TYR | CZ-CE2-CD2 | 5.51 | 124.76 | 119.80 |
| 1 | A | 434 | ARG | CG-CD-NE | -5.51 | 100.24 | 111.80 |
| 1 | A | 52 | GLY | CA-C-O | -5.50 | 110.69 | 120.60 |
| 2 | B | 841 | MET | CG-SD-CE | 5.50 | 109.00 | 100.20 |
| 1 | A | 1113 | THR | OG1-CB-CG2 | -5.50 | 97.35 | 110.00 |
| 1 | A | 934 | LYS | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | A | 1109 | LYS | CB-CA-C | 5.50 | 121.40 | 110.40 |
| 2 | B | 737 | THR | CA-CB-CG2 | -5.49 | 104.71 | 112.40 |
| 9 | K | 54 | ARG | CD-NE-CZ | 5.49 | 131.29 | 123.60 |
| 7 | I | 16 | PRO | N-CD-CG | -5.49 | 94.97 | 103.20 |
| 7 | I | 92 | ARG | O-C-N | 5.49 | 131.48 | 122.70 |
| 7 | I | 93 | LYS | CA-CB-CG | 5.49 | 125.48 | 113.40 |
| 3 | C | 180 | TYR | CD1-CE1-CZ | 5.49 | 124.74 | 119.80 |
| 8 | J | 18 | TRP | CD1-NE1-CE2 | -5.48 | 104.06 | 109.00 |
| 10 | L | 58 | LYS | O-C-N | -5.48 | 113.94 | 122.70 |
| 2 | B | 166 | PHE | N-CA-CB | -5.48 | 100.74 | 110.60 |
| 1 | A | 672 | ASP | CB-CA-C | -5.47 | 99.45 | 110.40 |
| 2 | B | 302 | CYS | CA-CB-SG | -5.47 | 104.15 | 114.00 |
| 2 | B | 387 | LEU | CA-CB-CG | 5.47 | 127.89 | 115.30 |
| 1 | A | 948 | VAL | N-CA-CB | -5.47 | 99.46 | 111.50 |
| 2 | B | 108 | VAL | CB-CA-C | 5.47 | 121.80 | 111.40 |
| 3 | C | 14 | SER | N-CA-C | -5.47 | 96.23 | 111.00 |
| 9 | K | 1 | MET | CB-CG-SD | -5.47 | 96.00 | 112.40 |
| 1 | A | 66 | LYS | CA-CB-CG | 5.46 | 125.42 | 113.40 |
| 6 | H | 87 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | A | 1274 | ARG | CB-CA-C | -5.46 | 99.49 | 110.40 |
| 2 | B | 973 | ILE | CG1-CB-CG2 | -5.46 | 99.40 | 111.40 |
| 1 | A | 836 | TYR | CB-CG-CD2 | 5.45 | 124.27 | 121.00 |
| 1 | A | 1290 | LYS | CD-CE-NZ | 5.45 | 124.24 | 111.70 |
| 2 | B | 710 | LEU | CB-CG-CD1 | -5.45 | 101.73 | 111.00 |
| 1 | A | 85 | ASP | N-CA-CB | 5.45 | 120.41 | 110.60 |
| 1 | A | 1228 | TRP | CA-CB-CG | 5.45 | 124.05 | 113.70 |
| 1 | A | 437 | MET | CB-CA-C | -5.45 | 99.51 | 110.40 |
| 2 | B | 277 | LYS | N-CA-CB | -5.45 | 100.80 | 110.60 |
| 2 | B | 1166 | CYS | N-CA-CB | -5.44 | 100.80 | 110.60 |
| 4 | E | 182 | ASP | OD1-CG-OD2 | -5.44 | 112.97 | 123.30 |
| 1 | A | 567 | LYS | CA-C-O | -5.44 | 108.69 | 120.10 |
| 6 | H | 9 | ILE | N-CA-CB | 5.44 | 123.30 | 110.80 |
| 1 | A | 607 | ILE | N-CA-C | -5.43 | 96.34 | 111.00 |
| 2 | B | 106 | ASP | N-CA-CB | -5.43 | 100.83 | 110.60 |
| 2 | B | 497 | ARG | NH1-CZ-NH2 | 5.43 | 125.37 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 118 | PHE | CG-CD2-CE2 | -5.43 | 114.83 | 120.80 |
| 2 | B | 198 | ASP | CB-CG-OD1 | 5.42 | 123.18 | 118.30 |
| 2 | B | 638 | PHE | CD1-CE1-CZ | -5.42 | 113.59 | 120.10 |
| 1 | A | 743 | VAL | CG1-CB-CG2 | -5.42 | 102.23 | 110.90 |
| 1 | A | 1233 | ASP | N-CA-CB | 5.42 | 120.36 | 110.60 |
| 4 | E | 192 | ARG | CD-NE-CZ | 5.42 | 131.19 | 123.60 |
| 1 | A | 1259 | MET | N-CA-C | -5.41 | 96.38 | 111.00 |
| 2 | B | 961 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 2 | B | 903 | VAL | CB-CA-C | -5.41 | 101.12 | 111.40 |
| 2 | B | 164 | LYS | CA-C-N | 5.41 | 129.10 | 117.20 |
| 9 | K | 70 | ARG | CB-CA-C | 5.41 | 121.22 | 110.40 |
| 3 | C | 180 | TYR | CG-CD2-CE2 | 5.41 | 125.63 | 121.30 |
| 1 | A | 764 | CYS | CA-CB-SG | 5.41 | 123.73 | 114.00 |
| 1 | A | 938 | LYS | CG-CD-CE | -5.40 | 95.69 | 111.90 |
| 2 | B | 501 | PRO | CA-C-O | -5.40 | 107.24 | 120.20 |
| 2 | B | 773 | MET | CG-SD-CE | 5.40 | 108.84 | 100.20 |
| 2 | B | 1028 | GLU | OE1-CD-OE2 | -5.40 | 116.82 | 123.30 |
| 1 | A | 352 | VAL | CA-CB-CG1 | 5.40 | 119.00 | 110.90 |
| 10 | L | 57 | LEU | CB-CA-C | -5.40 | 99.95 | 110.20 |
| 2 | B | 990 | ILE | CB-CA-C | -5.40 | 100.81 | 111.60 |
| 2 | B | 1073 | TYR | CB-CG-CD2 | 5.40 | 124.24 | 121.00 |
| 1 | A | 1081 | LEU | CB-CG-CD1 | -5.39 | 101.83 | 111.00 |
| 1 | A | 739 | ASP | N-CA-C | 5.39 | 125.56 | 111.00 |
| 2 | B | 303 | TYR | CB-CG-CD2 | -5.39 | 117.77 | 121.00 |
| 5 | F | 109 | VAL | CG1-CB-CG2 | -5.39 | 102.28 | 110.90 |
| 2 | B | 224 | GLN | CA-CB-CG | -5.38 | 101.55 | 113.40 |
| 6 | H | 60 | ALA | C-N-CA | -5.38 | 108.24 | 121.70 |
| 2 | B | 743 | ILE | CG1-CB-CG2 | -5.38 | 99.56 | 111.40 |
| 2 | B | 217 | ARG | CB-CG-CD | 5.38 | 125.59 | 111.60 |
| 9 | K | 73 | LEU | CB-CG-CD2 | 5.38 | 120.15 | 111.00 |
| 1 | A | 894 | GLU | CA-C-O | -5.38 | 108.80 | 120.10 |
| 2 | B | 633 | VAL | CB-CA-C | -5.38 | 101.18 | 111.40 |
| 2 | B | 731 | VAL | N-CA-C | -5.38 | 96.48 | 111.00 |
| 4 | E | 118 | PRO | N-CD-CG | 5.38 | 111.27 | 103.20 |
| 2 | B | 775 | LYS | CB-CG-CD | -5.38 | 97.62 | 111.60 |
| 3 | C | 240 | VAL | N-CA-C | 5.38 | 125.51 | 111.00 |
| 1 | A | 469 | ARG | CA-CB-CG | 5.37 | 125.21 | 113.40 |
| 1 | A | 1289 | ARG | NE-CZ-NH2 | 5.37 | 122.98 | 120.30 |
| 1 | A | 443 | LEU | CB-CG-CD1 | -5.37 | 101.88 | 111.00 |
| 2 | B | 1020 | ARG | CA-CB-CG | 5.36 | 125.20 | 113.40 |
| 1 | A | 1239 | ARG | CG-CD-NE | -5.36 | 100.54 | 111.80 |
| 2 | B | 635 | ARG | NH1-CZ-NH2 | -5.36 | 113.50 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 607 | GLY | O-C-N | -5.36 | 114.12 | 122.70 |
| 1 | A | 1311 | VAL | CG1-CB-CG2 | -5.36 | 102.33 | 110.90 |
| 1 | A | 840 | ARG | CD-NE-CZ | 5.36 | 131.10 | 123.60 |
| 1 | A | 72 | GLU | N-CA-C | 5.35 | 125.46 | 111.00 |
| 1 | A | 913 | LEU | N-CA-CB | -5.35 | 99.69 | 110.40 |
| 7 | I | 23 | ASN | CB-CA-C | 5.35 | 121.11 | 110.40 |
| 2 | B | 463 | THR | N-CA-C | 5.35 | 125.45 | 111.00 |
| 2 | B | 604 | ARG | CD-NE-CZ | 5.35 | 131.09 | 123.60 |
| 6 | H | 8 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 7 | I | 17 | ARG | CB-CG-CD | 5.35 | 125.50 | 111.60 |
| 1 | A | 1264 | GLU | OE1-CD-OE2 | -5.35 | 116.89 | 123.30 |
| 2 | B | 396 | ASP | O-C-N | 5.34 | 131.25 | 122.70 |
| 2 | B | 434 | ARG | CA-CB-CG | 5.34 | 125.16 | 113.40 |
| 1 | A | 678 | GLU | OE1-CD-OE2 | -5.34 | 116.89 | 123.30 |
| 2 | B | 707 | PRO | N-CD-CG | -5.34 | 95.19 | 103.20 |
| 2 | B | 889 | THR | N-CA-CB | 5.34 | 120.44 | 110.30 |
| 2 | B | 95 | ILE | CB-CA-C | -5.34 | 100.93 | 111.60 |
| 2 | B | 406 | LEU | CB-CG-CD2 | -5.34 | 101.93 | 111.00 |
| 8 | J | 21 | TYR | CG-CD1-CE1 | 5.34 | 125.57 | 121.30 |
| 9 | K | 110 | ASN | CB-CA-C | 5.34 | 121.07 | 110.40 |
| 1 | A | 576 | GLN | CB-CA-C | -5.33 | 99.73 | 110.40 |
| 1 | A | 883 | LEU | N-CA-C | -5.33 | 96.59 | 111.00 |
| 4 | E | 18 | THR | OG1-CB-CG2 | -5.33 | 97.73 | 110.00 |
| 1 | A | 385 | ILE | CG1-CB-CG2 | 5.33 | 123.12 | 111.40 |
| 1 | A | 917 | SER | CB-CA-C | -5.33 | 99.98 | 110.10 |
| 3 | C | 109 | SER | CB-CA-C | 5.33 | 120.22 | 110.10 |
| 2 | B | 995 | ARG | CD-NE-CZ | 5.32 | 131.05 | 123.60 |
| 1 | A | 995 | GLU | CG-CD-OE1 | -5.32 | 107.66 | 118.30 |
| 2 | B | 781 | PHE | CB-CG-CD1 | -5.32 | 117.08 | 120.80 |
| 2 | B | 35 | SER | CB-CA-C | -5.32 | 99.99 | 110.10 |
| 2 | B | 950 | ASP | N-CA-CB | -5.32 | 101.03 | 110.60 |
| 1 | A | 602 | ASP | C-N-CA | 5.31 | 134.98 | 121.70 |
| 2 | B | 1030 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 4 | E | 74 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | A | 1039 | LYS | CD-CE-NZ | -5.31 | 99.50 | 111.70 |
| 2 | B | 895 | ASP | N-CA-CB | 5.31 | 120.16 | 110.60 |
| 7 | I | 118 | ARG | N-CA-C | 5.31 | 125.33 | 111.00 |
| 4 | E | 31 | THR | CA-CB-CG2 | 5.31 | 119.83 | 112.40 |
| 2 | B | 568 | ASP | OD1-CG-OD2 | -5.30 | 113.22 | 123.30 |
| 5 | F | 103 | MET | CG-SD-CE | 5.30 | 108.69 | 100.20 |
| 1 | A | 366 | VAL | N-CA-C | -5.30 | 96.69 | 111.00 |
| 1 | A | 739 | ASP | N-CA-CB | -5.30 | 101.06 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 359 | GLU | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 4 | E | 181 | ALA | N-CA-CB | -5.30 | 102.68 | 110.10 |
| 1 | A | 577 | ILE | CG1-CB-CG2 | -5.30 | 99.74 | 111.40 |
| 9 | K | 11 | LEU | CB-CA-C | -5.30 | 100.14 | 110.20 |
| 2 | B | 122 | LEU | CA-CB-CG | -5.29 | 103.13 | 115.30 |
| 2 | B | 1110 | PRO | CA-C-O | 5.29 | 132.90 | 120.20 |
| 10 | L | 41 | SER | N-CA-C | 5.29 | 125.29 | 111.00 |
| 2 | B | 96 | TYR | CB-CG-CD2 | -5.29 | 117.83 | 121.00 |
| 4 | E | 66 | GLU | N-CA-CB | 5.29 | 120.12 | 110.60 |
| 1 | A | 1377 | THR | CB-CA-C | -5.29 | 97.32 | 111.60 |
| 3 | C | 207 | CYS | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 2 | B | 639 | ILE | CA-CB-CG1 | 5.29 | 121.04 | 111.00 |
| 4 | E | 204 | THR | CA-CB-OG1 | 5.28 | 120.09 | 109.00 |
| 1 | A | 710 | LEU | CB-CG-CD2 | 5.28 | 119.98 | 111.00 |
| 1 | A | 596 | THR | CA-C-O | -5.28 | 109.02 | 120.10 |
| 1 | A | 481 | ASP | N-CA-CB | -5.28 | 101.10 | 110.60 |
| 9 | K | 78 | THR | N-CA-CB | 5.28 | 120.33 | 110.30 |
| 1 | A | 1154 | TYR | OH-CZ-CE2 | 5.27 | 134.34 | 120.10 |
| 1 | A | 1003 | LYS | CB-CG-CD | 5.27 | 125.30 | 111.60 |
| 3 | C | 202 | PRO | N-CD-CG | -5.27 | 95.30 | 103.20 |
| 1 | A | 54 | ASN | CA-C-N | 5.27 | 128.79 | 117.20 |
| 1 | A | 1301 | GLU | CG-CD-OE2 | -5.27 | 107.76 | 118.30 |
| 1 | A | 426 | LEU | CB-CG-CD1 | 5.26 | 119.95 | 111.00 |
| 2 | B | 331 | LEU | CB-CG-CD2 | -5.26 | 102.05 | 111.00 |
| 9 | K | 101 | LEU | CA-CB-CG | 5.26 | 127.40 | 115.30 |
| 2 | B | 310 | MET | CG-SD-CE | 5.26 | 108.61 | 100.20 |
| 2 | B | 299 | GLU | CA-CB-CG | 5.26 | 124.96 | 113.40 |
| 5 | F | 93 | ILE | CG1-CB-CG2 | -5.25 | 99.85 | 111.40 |
| 2 | B | 254 | LEU | N-CA-C | -5.25 | 96.83 | 111.00 |
| 2 | B | 957 | ASN | N-CA-C | 5.25 | 125.17 | 111.00 |
| 4 | E | 28 | TYR | CD1-CE1-CZ | 5.25 | 124.53 | 119.80 |
| 8 | J | 42 | LYS | CD-CE-NZ | 5.25 | 123.78 | 111.70 |
| 7 | I | 91 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | A | 1012 | ARG | CA-CB-CG | 5.24 | 124.93 | 113.40 |
| 2 | B | 567 | GLU | CA-CB-CG | 5.24 | 124.94 | 113.40 |
| 3 | C | 119 | VAL | CA-CB-CG2 | 5.24 | 118.77 | 110.90 |
| 2 | B | 114 | PRO | N-CD-CG | 5.24 | 111.06 | 103.20 |
| 1 | A | 399 | HIS | C-N-CA | 5.24 | 144.01 | 122.00 |
| 1 | A | 834 | THR | CA-CB-CG2 | -5.24 | 105.07 | 112.40 |
| 1 | A | 1102 | LYS | N-CA-CB | -5.24 | 101.17 | 110.60 |
| 1 | A | 1147 | THR | OG1-CB-CG2 | -5.24 | 97.95 | 110.00 |
| 1 | A | 686 | ALA | N-CA-CB | 5.24 | 117.43 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 848 | ARG | NE-CZ-NH1 | -5.24 | 117.68 | 120.30 |
| 1 | A | 795 | GLU | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 3 | C | 232 | VAL | CG1-CB-CG2 | 5.23 | 119.27 | 110.90 |
| 6 | H | 6 | PHE | N-CA-C | -5.23 | 96.88 | 111.00 |
| 4 | E | 76 | GLY | N-CA-C | -5.23 | 100.03 | 113.10 |
| 1 | A | 15 | LYS | CA-CB-CG | 5.23 | 124.90 | 113.40 |
| 1 | A | 1022 | LEU | CB-CG-CD1 | -5.23 | 102.11 | 111.00 |
| 2 | B | 705 | MET | CG-SD-CE | -5.23 | 91.84 | 100.20 |
| 1 | A | 812 | GLU | OE1-CD-OE2 | -5.23 | 117.03 | 123.30 |
| 1 | A | 912 | LEU | CA-CB-CG | -5.22 | 103.29 | 115.30 |
| 2 | B | 539 | LEU | CB-CG-CD1 | -5.22 | 102.12 | 111.00 |
| 5 | F | 116 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | A | 1307 | GLU | CG-CD-OE1 | 5.22 | 128.75 | 118.30 |
| 4 | E | 108 | GLY | CA-C-O | 5.22 | 130.00 | 120.60 |
| 2 | B | 1082 | MET | CB-CG-SD | 5.22 | 128.06 | 112.40 |
| 1 | A | 918 | GLU | CG-CD-OE2 | 5.22 | 128.74 | 118.30 |
| 1 | A | 941 | LYS | N-CA-CB | 5.22 | 120.00 | 110.60 |
| 1 | A | 1027 | ALA | N-CA-CB | -5.21 | 102.80 | 110.10 |
| 3 | C | 57 | VAL | N-CA-CB | -5.21 | 100.03 | 111.50 |
| 1 | A | 63 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 2 | B | 648 | HIS | N-CA-C | 5.21 | 125.07 | 111.00 |
| 7 | I | 70 | ARG | NH1-CZ-NH2 | 5.21 | 125.13 | 119.40 |
| 2 | B | 20 | ASP | N-CA-CB | 5.21 | 119.98 | 110.60 |
| 1 | A | 901 | LEU | CB-CA-C | -5.21 | 100.30 | 110.20 |
| 2 | B | 969 | ARG | CD-NE-CZ | -5.21 | 116.31 | 123.60 |
| 3 | C | 220 | ASP | OD1-CG-OD2 | -5.21 | 113.41 | 123.30 |
| 3 | C | 37 | MET | CG-SD-CE | 5.21 | 108.53 | 100.20 |
| 10 | L | 70 | ARG | N-CA-CB | -5.21 | 101.23 | 110.60 |
| 6 | H | 32 | THR | N-CA-CB | 5.20 | 120.19 | 110.30 |
| 2 | B | 916 | THR | N-CA-C | 5.20 | 125.04 | 111.00 |
| 3 | C | 195 | GLN | N-CA-CB | 5.20 | 119.96 | 110.60 |
| 3 | C | 262 | LEU | CB-CG-CD1 | 5.20 | 119.84 | 111.00 |
| 1 | A | 369 | SER | CB-CA-C | -5.20 | 100.22 | 110.10 |
| 1 | A | 896 | ARG | CD-NE-CZ | -5.20 | 116.32 | 123.60 |
| 4 | E | 46 | TYR | CD1-CE1-CZ | 5.20 | 124.48 | 119.80 |
| 2 | B | 702 | LEU | CB-CG-CD2 | 5.20 | 119.83 | 111.00 |
| 1 | A | 26 | GLU | OE1-CD-OE2 | -5.19 | 117.07 | 123.30 |
| 2 | B | 890 | TYR | CB-CG-CD1 | 5.19 | 124.11 | 121.00 |
| 1 | A | 446 | ARG | NE-CZ-NH1 | -5.19 | 117.71 | 120.30 |
| 2 | B | 310 | MET | CA-CB-CG | -5.19 | 104.48 | 113.30 |
| 1 | A | 11 | LEU | CB-CG-CD2 | 5.18 | 119.81 | 111.00 |
| 1 | A | 476 | SER | CA-CB-OG | -5.18 | 97.20 | 111.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 857 | ARG | CG-CD-NE | -5.18 | 100.91 | 111.80 |
| 10 | L | 57 | LEU | CB-CG-CD2 | -5.18 | 102.19 | 111.00 |
| 2 | B | 898 | LEU | CB-CG-CD2 | 5.18 | 119.81 | 111.00 |
| 6 | H | 39 | THR | CA-CB-CG2 | -5.18 | 105.15 | 112.40 |
| 2 | B | 392 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 2 | B | 514 | LEU | CB-CG-CD2 | -5.18 | 102.20 | 111.00 |
| 2 | B | 1007 | VAL | N-CA-CB | -5.18 | 100.11 | 111.50 |
| 1 | A | 984 | LYS | CA-CB-CG | 5.17 | 124.78 | 113.40 |
| 1 | A | 651 | LYS | CB-CA-C | 5.17 | 120.75 | 110.40 |
| 7 | I | 1 | MET | CA-CB-CG | 5.17 | 122.09 | 113.30 |
| 1 | A | 900 | ASP | CB-CG-OD2 | -5.17 | 113.64 | 118.30 |
| 4 | E | 144 | ILE | CG1-CB-CG2 | 5.17 | 122.78 | 111.40 |
| 2 | B | 646 | LEU | CB-CG-CD2 | 5.17 | 119.79 | 111.00 |
| 2 | B | 165 | VAL | N-CA-CB | 5.17 | 122.87 | 111.50 |
| 8 | J | 63 | TYR | CB-CG-CD1 | 5.17 | 124.10 | 121.00 |
| 1 | A | 497 | THR | N-CA-CB | -5.17 | 100.48 | 110.30 |
| 1 | A | 1299 | VAL | N-CA-CB | -5.17 | 100.14 | 111.50 |
| 2 | B | 284 | ILE | CG1-CB-CG2 | -5.17 | 100.04 | 111.40 |
| 6 | H | 106 | GLU | CB-CA-C | 5.17 | 120.73 | 110.40 |
| 1 | A | 78 | PRO | N-CD-CG | 5.16 | 110.94 | 103.20 |
| 1 | A | 524 | VAL | CG1-CB-CG2 | -5.16 | 102.64 | 110.90 |
| 3 | C | 10 | ILE | CB-CA-C | -5.16 | 101.27 | 111.60 |
| 1 | A | 705 | LYS | CA-C-N | -5.16 | 105.84 | 117.20 |
| 10 | L | 59 | ALA | CB-CA-C | -5.16 | 102.36 | 110.10 |
| 8 | J | 56 | LEU | CD1-CG-CD2 | -5.16 | 95.03 | 110.50 |
| 7 | I | 13 | MET | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | A | 1028 | THR | OG1-CB-CG2 | -5.15 | 98.15 | 110.00 |
| 2 | B | 787 | VAL | N-CA-CB | -5.15 | 100.16 | 111.50 |
| 6 | H | 41 | ASP | OD1-CG-OD2 | -5.15 | 113.52 | 123.30 |
| 7 | I | 109 | ILE | CA-CB-CG1 | 5.15 | 120.79 | 111.00 |
| 1 | A | 897 | TYR | CG-CD2-CE2 | -5.15 | 117.18 | 121.30 |
| 4 | E | 207 | ARG | NH1-CZ-NH2 | -5.15 | 113.74 | 119.40 |
| 1 | A | 461 | LYS | CD-CE-NZ | -5.14 | 99.87 | 111.70 |
| 1 | A | 898 | ARG | NH1-CZ-NH2 | -5.14 | 113.74 | 119.40 |
| 2 | B | 1060 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | A | 1077 | THR | O-C-N | -5.14 | 114.47 | 122.70 |
| 2 | B | 621 | GLU | CG-CD-OE1 | -5.14 | 108.02 | 118.30 |
| 1 | A | 927 | VAL | CA-CB-CG2 | -5.14 | 103.19 | 110.90 |
| 2 | B | 1005 | GLY | N-CA-C | 5.14 | 125.95 | 113.10 |
| 1 | A | 351 | THR | CA-CB-CG2 | -5.14 | 105.21 | 112.40 |
| 1 | A | 814 | PHE | CB-CG-CD2 | 5.14 | 124.40 | 120.80 |
| 1 | A | 1275 | GLY | CA-C-N | -5.13 | 105.90 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1417 | GLU | N-CA-C | -5.13 | 97.14 | 111.00 |
| 1 | A | 831 | THR | CA-CB-CG2 | -5.13 | 105.21 | 112.40 |
| 2 | B | 1131 | GLY | N-CA-C | 5.13 | 125.93 | 113.10 |
| 2 | B | 935 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 4 | E | 200 | ARG | CG-CD-NE | -5.13 | 101.03 | 111.80 |
| 4 | E | 28 | TYR | CB-CG-CD2 | 5.13 | 124.08 | 121.00 |
| 4 | E | 28 | TYR | N-CA-C | -5.13 | 97.15 | 111.00 |
| 1 | A | 49 | LYS | CD-CE-NZ | 5.13 | 123.50 | 111.70 |
| 1 | A | 1148 | ILE | CG1-CB-CG2 | -5.13 | 100.12 | 111.40 |
| 1 | A | 400 | PRO | N-CD-CG | 5.13 | 110.89 | 103.20 |
| 2 | B | 1020 | ARG | NH1-CZ-NH2 | -5.13 | 113.76 | 119.40 |
| 1 | A | 968 | GLN | CB-CA-C | -5.12 | 100.15 | 110.40 |
| 2 | B | 412 | LEU | N-CA-CB | 5.12 | 120.65 | 110.40 |
| 1 | A | 4 | GLN | CB-CA-C | 5.12 | 120.64 | 110.40 |
| 2 | B | 522 | VAL | CA-CB-CG2 | -5.12 | 103.22 | 110.90 |
| 3 | C | 132 | PRO | CA-C-O | -5.12 | 107.91 | 120.20 |
| 6 | H | 91 | ASP | CA-C-O | 5.12 | 130.85 | 120.10 |
| 2 | B | 806 | THR | N-CA-CB | -5.12 | 100.58 | 110.30 |
| 2 | B | 90 | ILE | N-CA-C | 5.12 | 124.81 | 111.00 |
| 6 | H | 77 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 2 | B | 362 | PRO | CA-C-O | -5.11 | 107.93 | 120.20 |
| 2 | B | 945 | GLU | CG-CD-OE2 | -5.11 | 108.07 | 118.30 |
| 3 | C | 105 | GLY | N-CA-C | -5.11 | 100.32 | 113.10 |
| 9 | K | 42 | LEU | CB-CA-C | -5.11 | 100.48 | 110.20 |
| 3 | C | 72 | LEU | CB-CG-CD1 | -5.11 | 102.31 | 111.00 |
| 6 | H | 45 | GLU | CG-CD-OE2 | -5.11 | 108.08 | 118.30 |
| 10 | L | 54 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | A | 980 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | A | 1158 | PRO | CA-C-O | -5.11 | 107.94 | 120.20 |
| 2 | B | 1168 | LEU | CB-CG-CD2 | -5.11 | 102.32 | 111.00 |
| 2 | B | 586 | TRP | CB-CA-C | 5.10 | 120.60 | 110.40 |
| 1 | A | 804 | TYR | CG-CD2-CE2 | 5.10 | 125.38 | 121.30 |
| 2 | B | 395 | GLN | N-CA-CB | 5.10 | 119.77 | 110.60 |
| 3 | C | 125 | MET | CB-CG-SD | 5.10 | 127.69 | 112.40 |
| 10 | L | 50 | ASP | N-CA-CB | 5.10 | 119.77 | 110.60 |
| 1 | A | 1101 | LEU | CB-CA-C | 5.10 | 119.88 | 110.20 |
| 7 | I | 45 | ARG | CA-CB-CG | 5.10 | 124.61 | 113.40 |
| 1 | A | 795 | GLU | CB-CG-CD | 5.09 | 127.96 | 114.20 |
| 1 | A | 1326 | ARG | NE-CZ-NH2 | 5.09 | 122.85 | 120.30 |
| 1 | A | 1365 | TYR | CG-CD1-CE1 | -5.09 | 117.23 | 121.30 |
| 8 | J | 28 | ASP | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 7 | I | 28 | GLU | CA-CB-CG | 5.09 | 124.59 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 975 | HIS | N-CA-CB | -5.09 | 101.44 | 110.60 |
| 7 | I | 45 | ARG | CG-CD-NE | 5.08 | 122.47 | 111.80 |
| 1 | A | 65 | LEU | CB-CG-CD2 | 5.08 | 119.63 | 111.00 |
| 9 | K | 64 | GLU | CG-CD-OE1 | 5.08 | 128.46 | 118.30 |
| 1 | A | 32 | VAL | N-CA-CB | -5.08 | 100.33 | 111.50 |
| 3 | C | 89 | GLU | OE1-CD-OE2 | -5.08 | 117.21 | 123.30 |
| 2 | B | 567 | GLU | CB-CA-C | 5.07 | 120.55 | 110.40 |
| 1 | A | 793 | SER | N-CA-CB | -5.07 | 102.89 | 110.50 |
| 2 | B | 1220 | ARG | CG-CD-NE | 5.07 | 122.44 | 111.80 |
| 2 | B | 279 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 4 | E | 103 | LYS | CD-CE-NZ | 5.07 | 123.35 | 111.70 |
| 9 | K | 39 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 2 | B | 684 | LEU | CB-CG-CD2 | 5.06 | 119.61 | 111.00 |
| 3 | C | 240 | VAL | CB-CA-C | -5.06 | 101.78 | 111.40 |
| 6 | H | 89 | LEU | CA-C-N | 5.06 | 128.34 | 117.20 |
| 1 | A | 840 | ARG | CG-CD-NE | -5.06 | 101.18 | 111.80 |
| 2 | B | 1053 | GLU | N-CA-CB | 5.06 | 119.71 | 110.60 |
| 3 | C | 193 | TYR | CB-CG-CD2 | 5.06 | 124.04 | 121.00 |
| 8 | J | 29 | GLU | OE1-CD-OE2 | 5.05 | 129.36 | 123.30 |
| 2 | B | 1161 | HIS | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 4 | E | 177 | ARG | NE-CZ-NH2 | 5.05 | 122.83 | 120.30 |
| 7 | I | 75 | CYS | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 1 | A | 644 | LYS | CB-CA-C | -5.05 | 100.30 | 110.40 |
| 2 | B | 100 | PRO | CA-N-CD | -5.05 | 104.43 | 111.50 |
| 3 | C | 267 | GLN | N-CA-C | 5.05 | 124.63 | 111.00 |
| 6 | H | 7 | ASP | OD1-CG-OD2 | -5.04 | 113.72 | 123.30 |
| 8 | J | 39 | LEU | CB-CG-CD1 | 5.04 | 119.58 | 111.00 |
| 3 | C | 155 | LEU | CB-CG-CD2 | -5.04 | 102.42 | 111.00 |
| 1 | A | 932 | GLU | CB-CG-CD | 5.04 | 127.81 | 114.20 |
| 6 | H | 139 | ASN | N-CA-C | -5.04 | 97.39 | 111.00 |
| 1 | A | 912 | LEU | N-CA-CB | 5.04 | 120.48 | 110.40 |
| 2 | B | 446 | LEU | CB-CG-CD1 | 5.04 | 119.57 | 111.00 |
| 1 | A | 1374 | VAL | CA-CB-CG2 | -5.04 | 103.34 | 110.90 |
| 3 | C | 182 | PRO | N-CD-CG | -5.04 | 95.65 | 103.20 |
| 10 | L | 61 | THR | CA-CB-CG2 | 5.03 | 119.45 | 112.40 |
| 1 | A | 1233 | ASP | CB-CG-OD2 | 5.03 | 122.83 | 118.30 |
| 4 | E | 152 | LYS | CD-CE-NZ | -5.03 | 100.13 | 111.70 |
| 1 | A | 806 | ARG | CB-CA-C | -5.03 | 100.34 | 110.40 |
| 2 | B | 486 | TYR | CB-CG-CD2 | -5.03 | 117.98 | 121.00 |
| 5 | F | 132 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 2 | B | 1052 | VAL | CG1-CB-CG2 | -5.03 | 102.86 | 110.90 |
| 10 | L | 31 | CYS | CB-CA-C | -5.03 | 100.35 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1004 | ASN | N-CA-CB | -5.02 | 101.56 | 110.60 |
| 1 | A | 1221 | LYS | N-CA-CB | 5.02 | 119.64 | 110.60 |
| 2 | B | 1202 | LEU | CA-CB-CG | -5.02 | 103.75 | 115.30 |
| 10 | L | 38 | LEU | CB-CG-CD2 | 5.02 | 119.53 | 111.00 |
| 1 | A | 1135 | ARG | CG-CD-NE | -5.02 | 101.26 | 111.80 |
| 4 | E | 12 | LEU | CB-CG-CD2 | 5.02 | 119.53 | 111.00 |
| 10 | L | 40 | LEU | CB-CG-CD1 | 5.02 | 119.53 | 111.00 |
| 1 | A | 350 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 4 | E | 207 | ARG | CB-CG-CD | 5.01 | 124.64 | 111.60 |
| 1 | A | 656 | TRP | CD1-NE1-CE2 | -5.01 | 104.49 | 109.00 |
| 6 | H | 111 | LEU | CB-CG-CD1 | 5.01 | 119.52 | 111.00 |
| 1 | A | 788 | SER | CA-CB-OG | -5.01 | 97.67 | 111.20 |
| 1 | A | 1170 | ILE | N-CA-C | -5.01 | 97.47 | 111.00 |
| 1 | A | 1376 | THR | CA-CB-CG2 | 5.01 | 119.42 | 112.40 |
| 2 | B | 485 | ARG | CD-NE-CZ | 5.01 | 130.62 | 123.60 |
| 2 | B | 978 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 4 | E | 140 | LEU | CB-CG-CD2 | -5.01 | 102.48 | 111.00 |
| 1 | A | 887 | GLY | C-N-CA | -5.01 | 111.78 | 122.30 |
| 2 | B | 624 | LEU | CB-CG-CD1 | 5.01 | 119.52 | 111.00 |
| 1 | A | 962 | ARG | O-C-N | -5.01 | 114.69 | 122.70 |
| 2 | B | 1222 | ARG | NE-CZ-NH2 | -5.01 | 117.80 | 120.30 |
| 1 | A | 1043 | ASP | OD1-CG-OD2 | -5.00 | 113.79 | 123.30 |
| 1 | A | 495 | GLU | CB-CA-C | 5.00 | 120.40 | 110.40 |
| 1 | A | 917 | SER | CA-CB-OG | -5.00 | 97.70 | 111.20 |
| 3 | C | 4 | GLU | N-CA-C | 5.00 | 124.50 | 111.00 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 4 | E | 204 | THR | CB |

All (102) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1046 | LEU | Mainchain |
| 1 | A | 1093 | LYS | Peptide |
| 1 | A | 1111 | MET | Mainchain |
| 1 | A | 1119 | TYR | Sidechain |
| 1 | A | 1155 | ASP | Mainchain,Peptide |
| 1 | A | 1220 | PHE | Peptide |
| 1 | A | 1232 | ASN | Peptide |
| 1 | A | 1301 | GLU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1366 | ARG | Sidechain |
| 1 | A | 1384 | VAL | Peptide |
| 1 | A | 1434 | ALA | Mainchain |
| 1 | A | 31 | SER | Peptide |
| 1 | A | 399 | HIS | Peptide |
| 1 | A | 434 | ARG | Sidechain |
| 1 | A | 44 | THR | Peptide |
| 1 | A | 464 | PRO | Peptide |
| 1 | A | 465 | TYR | Sidechain |
| 1 | A | 555 | ASP | Peptide |
| 1 | A | 60 | SER | Peptide |
| 1 | A | 659 | HIS | Sidechain |
| 1 | A | 70 | CYS | Peptide |
| 1 | A | 705 | LYS | Peptide |
| 1 | A | 706 | HIS | Peptide |
| 1 | A | 74 | MET | Peptide |
| 1 | A | 741 | ASN | Mainchain |
| 1 | A | 821 | ARG | Sidechain |
| 1 | A | 936 | LEU | Mainchain |
| 2 | B | 1025 | HIS | Sidechain |
| 2 | B | 104 | GLU | Peptide |
| 2 | B | 107 | GLY | Peptide |
| 2 | B | 1097 | HIS | Sidechain |
| 2 | B | 1101 | ASP | Peptide |
| 2 | B | 1102 | LYS | Peptide |
| 2 | B | 1109 | GLY | Peptide |
| 2 | B | 1141 | HIS | Sidechain |
| 2 | B | 1152 | MET | Peptide |
| 2 | B | 1153 | GLU | Peptide |
| 2 | B | 1155 | SER | Peptide |
| 2 | B | 1221 | SER | Peptide |
| 2 | B | 1222 | ARG | Peptide |
| 2 | B | 238 | ALA | Mainchain |
| 2 | B | 244 | LEU | Peptide |
| 2 | B | 248 | SER | Peptide |
| 2 | B | 369 | GLY | Peptide |
| 2 | B | 431 | TYR | Peptide |
| 2 | B | 518 | HIS | Sidechain |
| 2 | B | 642 | ASP | Peptide |
| 2 | B | 643 | ASP | Peptide |
| 2 | B | 644 | GLU | Peptide |
| 2 | B | 667 | GLN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 732 | SER | Peptide |
| 2 | B | 868 | MET | Peptide |
| 2 | B | 882 | THR | Peptide |
| 2 | B | 884 | ARG | Peptide |
| 2 | B | 905 | VAL | Peptide |
| 2 | B | 956 | THR | Peptide |
| 2 | B | 963 | PHE | Mainchain |
| 2 | B | 968 | VAL | Mainchain |
| 2 | B | 98 | THR | Peptide |
| 3 | C | 103 | ALA | Mainchain |
| 3 | C | 155 | LEU | Mainchain,Peptide |
| 3 | C | 156 | THR | Mainchain |
| 3 | C | 184 | ASN | Peptide |
| 3 | C | 190 | ASP | Peptide |
| 3 | C | 238 | ILE | Mainchain |
| 3 | C | 240 | VAL | Mainchain |
| 3 | C | 261 | ALA | Peptide |
| 3 | C | 267 | GLN | Peptide |
| 3 | C | 34 | ARG | Sidechain |
| 3 | C | 35 | ARG | Sidechain |
| 3 | C | 4 | GLU | Peptide |
| 4 | E | 119 | SER | Peptide |
| 4 | E | 125 | PRO | Peptide |
| 4 | E | 128 | PRO | Peptide |
| 4 | E | 153 | HIS | Sidechain |
| 4 | E | 207 | ARG | Mainchain |
| 4 | E | 212 | ARG | Sidechain |
| 4 | E | 77 | SER | Peptide |
| 6 | H | 102 | TYR | Peptide |
| 6 | H | 103 | LYS | Peptide |
| 6 | H | 127 | GLY | Peptide |
| 6 | H | 131 | ASN | Peptide |
| 6 | H | 135 | LEU | Peptide |
| 6 | H | 136 | LYS | Peptide |
| 6 | H | 17 | PRO | Peptide |
| 6 | H | 26 | ILE | Peptide |
| 6 | H | 61 | SER | Peptide |
| 6 | H | 62 | SER | Peptide |
| 6 | H | 86 | ASP | Peptide |
| 6 | H | 87 | ARG | Peptide |
| 6 | H | 94 | ASP | Peptide |
| 7 | I | 3 | THR | Mainchain,Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | I | 43 | VAL | Mainchain |
| 9 | K | 6 | ARG | Sidechain |
| 9 | K | 70 | ARG | Mainchain |
| 10 | L | 27 | LEU | Peptide |
| 10 | L | 34 | CYS | Peptide |
| 10 | L | 35 | SER | Peptide |
| 10 | L | 59 | ALA | 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 | 10625 | 0 | 10693 | 807 | 0 |
| 2 | B | 8690 | 0 | 8713 | 507 | 0 |
| 3 | C | 2095 | 0 | 2051 | 140 | 0 |
| 4 | E | 1760 | 0 | 1788 | 125 | 0 |
| 5 | F | 670 | 0 | 690 | 48 | 0 |
| 6 | H | 1068 | 0 | 1040 | 155 | 0 |
| 7 | I | 990 | 0 | 949 | 70 | 0 |
| 8 | J | 525 | 0 | 535 | 39 | 0 |
| 9 | K | 919 | 0 | 929 | 64 | 0 |
| 10 | L | 364 | 0 | 386 | 51 | 0 |
| 11 | A | 2 | 0 | 0 | 0 | 0 |
| 11 | B | 1 | 0 | 0 | 0 | 0 |
| 11 | C | 1 | 0 | 0 | 0 | 0 |
| 11 | I | 2 | 0 | 0 | 0 | 0 |
| 11 | J | 1 | 0 | 0 | 0 | 0 |
| 11 | L | 1 | 0 | 0 | 0 | 0 |
| 12 | A | 2 | 0 | 0 | 0 | 0 |
| 13 | B | 32 | 0 | 11 | 8 | 0 |
| 14 | A | 11 | 0 | 0 | 3 | 0 |
| 14 | B | 11 | 0 | 0 | 4 | 0 |
| 14 | F | 1 | 0 | 0 | 0 | 0 |
| 14 | L | 1 | 0 | 0 | 1 | 0 |
| All | All | 27772 | 0 | 27785 | 1880 | 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 34.

All (1880) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:61:ILE:CA | 1:A:61:ILE:CB | 1.75 | 1.64 |
| 1:A:941:LYS:CD | 1:A:941:LYS:CG | 1.74 | 1.64 |
| 10:L:61:THR:CB | 10:L:61:THR:CG2 | 1.75 | 1.64 |
| 5:F:72:LYS:CD | 5:F:72:LYS:CE | 1.76 | 1.64 |
| 1:A:1405:THR:CB | 1:A:1405:THR:CA | 1.77 | 1.62 |
| 1:A:1132:LYS:CB | 1:A:1132:LYS:CG | 1.75 | 1.62 |
| 1:A:1055:ARG:CG | 1:A:1055:ARG:CD | 1.76 | 1.61 |
| 4:E:161:LYS:CD | 4:E:161:LYS:CE | 1.76 | 1.61 |
| 1:A:46:THR:CA | 1:A:46:THR:CB | 1.77 | 1.61 |
| 1:A:571:LEU:CD2 | 1:A:571:LEU:CG | 1.78 | 1.61 |
| 2:B:227:LYS:CG | 2:B:227:LYS:CD | 1.74 | 1.61 |
| 1:A:1081:LEU:CD2 | 1:A:1081:LEU:CG | 1.76 | 1.60 |
| 1:A:1215:ARG:CB | 1:A:1215:ARG:CG | 1.75 | 1.60 |
| 2:B:531:GLN:CB | 2:B:531:GLN:CG | 1.77 | 1.60 |
| 3:C:7:GLN:CB | 3:C:7:GLN:CG | 1.77 | 1.60 |
| 1:A:518:LYS:CE | 1:A:518:LYS:CD | 1.77 | 1.60 |
| 4:E:54:GLN:CG | 4:E:54:GLN:CB | 1.78 | 1.60 |
| 7:I:3:THR:CB | 7:I:3:THR:CG2 | 1.75 | 1.60 |
| 1:A:973:ILE:CB | 1:A:973:ILE:CG2 | 1.75 | 1.60 |
| 2:B:115:GLN:CB | 2:B:115:GLN:CG | 1.76 | 1.60 |
| 1:A:368:LYS:CG | 1:A:368:LYS:CD | 1.75 | 1.59 |
| 1:A:1102:LYS:CD | 1:A:1102:LYS:CE | 1.77 | 1.59 |
| 1:A:1261:LYS:CD | 1:A:1261:LYS:CE | 1.76 | 1.59 |
| 1:A:1385:THR:CB | 1:A:1385:THR:CG2 | 1.75 | 1.59 |
| 7:I:120:GLN:CG | 7:I:120:GLN:CB | 1.74 | 1.59 |
| 2:B:434:ARG:CG | 2:B:434:ARG:CD | 1.78 | 1.59 |
| 1:A:274:ILE:CA | 1:A:274:ILE:CB | 1.78 | 1.59 |
| 1:A:1262:LYS:CG | 1:A:1262:LYS:CD | 1.75 | 1.59 |
| 4:E:131:THR:CA | 4:E:131:THR:CB | 1.74 | 1.59 |
| 1:A:1080:THR:CA | 1:A:1080:THR:CB | 1.75 | 1.59 |
| 2:B:436:VAL:CA | 2:B:436:VAL:CB | 1.78 | 1.59 |
| 10:L:26:THR:CB | 10:L:26:THR:CG2 | 1.75 | 1.59 |
| 1:A:566:ILE:CB | 1:A:566:ILE:CG2 | 1.75 | 1.58 |
| 4:E:98:ILE:CA | 4:E:98:ILE:CB | 1.79 | 1.58 |
| 8:J:42:LYS:CD | 8:J:42:LYS:CE | 1.79 | 1.58 |
| 9:K:20:LYS:CG | 9:K:20:LYS:CD | 1.77 | 1.58 |
| 1:A:843:LYS:CD | 1:A:843:LYS:CE | 1.76 | 1.58 |
| 6:H:77:ARG:CB | 6:H:77:ARG:CG | 1.81 | 1.58 |
| 1:A:1286:LYS:CB | 1:A:1286:LYS:CG | 1.77 | 1.58 |
| 4:E:37:LEU:CD1 | 4:E:37:LEU:CG | 1.81 | 1.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:L:54:ARG:CG | 10:L:54:ARG:CD | 1.76 | 1.58 |
| 1:A:1112:LYS:CG | 1:A:1112:LYS:CB | 1.82 | 1.58 |
| 2:B:305:VAL:CG1 | 2:B:305:VAL:CB | 1.79 | 1.58 |
| 2:B:775:LYS:CB | 2:B:775:LYS:CG | 1.81 | 1.57 |
| 2:B:1057:LYS:CD | 2:B:1057:LYS:CG | 1.74 | 1.57 |
| 1:A:1132:LYS:CG | 1:A:1132:LYS:CD | 1.80 | 1.57 |
| 2:B:958:GLN:CB | 2:B:958:GLN:CG | 1.76 | 1.57 |
| 3:C:9:LYS:CG | 3:C:9:LYS:CD | 1.82 | 1.57 |
| 1:A:977:LYS:CB | 1:A:977:LYS:CG | 1.75 | 1.57 |
| 1:A:1093:LYS:CG | 1:A:1093:LYS:CB | 1.76 | 1.57 |
| 1:A:1162:VAL:CG1 | 1:A:1162:VAL:CB | 1.80 | 1.57 |
| 2:B:620:ARG:CG | 2:B:620:ARG:CD | 1.77 | 1.57 |
| 3:C:199:LYS:CD | 3:C:199:LYS:CE | 1.76 | 1.57 |
| 1:A:1109:LYS:CD | 1:A:1109:LYS:CG | 1.79 | 1.57 |
| 1:A:1272:THR:CG2 | 1:A:1272:THR:CB | 1.76 | 1.57 |
| 1:A:44:THR:CA | 1:A:44:THR:CB | 1.77 | 1.56 |
| 1:A:74:MET:CB | 1:A:74:MET:CG | 1.78 | 1.56 |
| 1:A:237:THR:CB | 1:A:237:THR:CG2 | 1.82 | 1.56 |
| 2:B:164:LYS:CE | 2:B:164:LYS:CD | 1.82 | 1.56 |
| 6:H:9:ILE:CB | 6:H:9:ILE:CA | 1.76 | 1.56 |
| 2:B:1097:HIS:CB | 2:B:1097:HIS:CA | 1.79 | 1.56 |
| 3:C:252:GLN:CG | 3:C:252:GLN:CB | 1.74 | 1.56 |
| 7:I:45:ARG:CG | 7:I:45:ARG:CD | 1.82 | 1.56 |
| 1:A:295:LEU:CD2 | 1:A:295:LEU:CG | 1.77 | 1.56 |
| 1:A:1130:GLN:CG | 1:A:1130:GLN:CD | 1.74 | 1.56 |
| 2:B:191:LYS:CG | 2:B:191:LYS:CB | 1.81 | 1.56 |
| 2:B:230:ALA:CA | 2:B:230:ALA:CB | 1.77 | 1.56 |
| 2:B:415:GLN:CG | 2:B:415:GLN:CB | 1.82 | 1.56 |
| 4:E:152:LYS:CG | 4:E:152:LYS:CD | 1.82 | 1.56 |
| 1:A:840:ARG:CG | 1:A:840:ARG:CD | 1.75 | 1.55 |
| 1:A:1135:ARG:CG | 1:A:1135:ARG:CD | 1.78 | 1.55 |
| 4:E:129:PRO:CG | 4:E:129:PRO:CD | 1.75 | 1.55 |
| 1:A:66:LYS:CB | 1:A:66:LYS:CG | 1.78 | 1.55 |
| 1:A:1003:LYS:CG | 1:A:1003:LYS:CB | 1.78 | 1.55 |
| 1:A:1187:GLN:CB | 1:A:1187:GLN:CG | 1.84 | 1.55 |
| 3:C:102:GLN:CB | 3:C:102:GLN:CG | 1.78 | 1.55 |
| 3:C:116:LYS:CD | 3:C:116:LYS:CE | 1.79 | 1.55 |
| 2:B:434:ARG:CG | 2:B:434:ARG:CB | 1.78 | 1.55 |
| 2:B:646:LEU:CD1 | 2:B:646:LEU:CG | 1.81 | 1.55 |
| 1:A:1445:ILE:CB | 1:A:1445:ILE:CG2 | 1.83 | 1.55 |
| 9:K:26:LYS:CG | 9:K:26:LYS:CD | 1.77 | 1.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:509:ALA:CA | 2:B:509:ALA:CB | 1.84 | 1.55 |
| 2:B:959:ASP:CB | 2:B:959:ASP:CG | 1.74 | 1.55 |
| 2:B:246:LYS:CA | 2:B:246:LYS:C | 1.76 | 1.54 |
| 5:F:123:LYS:NZ | 5:F:123:LYS:CE | 1.67 | 1.54 |
| 1:A:1171:GLN:CG | 1:A:1171:GLN:CD | 1.76 | 1.54 |
| 2:B:233:PRO:CB | 2:B:233:PRO:CG | 1.76 | 1.54 |
| 2:B:1102:LYS:CB | 2:B:1102:LYS:CG | 1.78 | 1.54 |
| 1:A:601:LYS:CD | 1:A:601:LYS:CE | 1.82 | 1.54 |
| 1:A:1350:LYS:CG | 1:A:1350:LYS:CD | 1.78 | 1.54 |
| 2:B:227:LYS:NZ | 2:B:227:LYS:CE | 1.70 | 1.54 |
| 1:A:1109:LYS:CG | 1:A:1109:LYS:CB | 1.79 | 1.54 |
| 2:B:646:LEU:CG | 2:B:646:LEU:CD2 | 1.81 | 1.54 |
| 6:H:52:GLN:CG | 6:H:52:GLN:CD | 1.74 | 1.54 |
| 2:B:962:LYS:CD | 2:B:962:LYS:CE | 1.82 | 1.53 |
| 1:A:720:ARG:CG | 1:A:720:ARG:CD | 1.79 | 1.53 |
| 1:A:1222:ASN:CG | 1:A:1222:ASN:CB | 1.76 | 1.53 |
| 2:B:477:ALA:CA | 2:B:477:ALA:CB | 1.85 | 1.53 |
| 2:B:598:GLU:CG | 2:B:598:GLU:CD | 1.76 | 1.53 |
| 2:B:723:VAL:CA | 2:B:723:VAL:CB | 1.84 | 1.53 |
| 1:A:830:LYS:CE | 1:A:830:LYS:CD | 1.81 | 1.53 |
| 1:A:1419:ASP:CG | 1:A:1419:ASP:CB | 1.75 | 1.53 |
| 2:B:723:VAL:CB | 2:B:723:VAL:CG1 | 1.82 | 1.53 |
| 10:L:43:THR:CB | 10:L:43:THR:CG2 | 1.76 | 1.53 |
| 1:A:5:GLN:CG | 1:A:5:GLN:CB | 1.80 | 1.53 |
| 2:B:346:GLU:CG | 2:B:346:GLU:CD | 1.77 | 1.53 |
| 3:C:154:LYS:CG | 3:C:154:LYS:CD | 1.82 | 1.53 |
| 1:A:941:LYS:NZ | 1:A:941:LYS:CE | 1.70 | 1.53 |
| 1:A:1235:LYS:NZ | 1:A:1235:LYS:CE | 1.69 | 1.53 |
| 1:A:544:ASP:CB | 1:A:544:ASP:CG | 1.77 | 1.52 |
| 1:A:1110:ASN:CG | 1:A:1110:ASN:CB | 1.78 | 1.52 |
| 2:B:962:LYS:CD | 2:B:962:LYS:CG | 1.87 | 1.52 |
| 4:E:162:ARG:CB | 4:E:162:ARG:CG | 1.86 | 1.52 |
| 9:K:111:LEU:CD1 | 9:K:111:LEU:CG | 1.86 | 1.52 |
| 1:A:934:LYS:CD | 1:A:934:LYS:CE | 1.87 | 1.52 |
| 3:C:94:LYS:NZ | 3:C:94:LYS:CE | 1.67 | 1.52 |
| 1:A:423:ASP:CB | 1:A:423:ASP:CG | 1.76 | 1.52 |
| 2:B:347:LYS:CD | 2:B:347:LYS:CE | 1.76 | 1.52 |
| 10:L:28:LYS:CA | 10:L:28:LYS:C | 1.77 | 1.52 |
| 2:B:706:GLN:CB | 2:B:706:GLN:CG | 1.84 | 1.51 |
| 2:B:986:GLN:CG | 2:B:986:GLN:CD | 1.75 | 1.51 |
| 2:B:1154:ALA:CA | 2:B:1154:ALA:CB | 1.87 | 1.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:41:ASP:CB | 4:E:41:ASP:CG | 1.77 | 1.51 |
| 3:C:50:GLU:CG | 3:C:50:GLU:CD | 1.77 | 1.51 |
| 10:L:48:CYS:C | 10:L:48:CYS:CA | 1.77 | 1.51 |
| 1:A:795:GLU:CG | 1:A:795:GLU:CD | 1.76 | 1.51 |
| 2:B:622:LYS:NZ | 2:B:622:LYS:CE | 1.70 | 1.51 |
| 2:B:1101:ASP:CB | 2:B:1101:ASP:CG | 1.77 | 1.51 |
| 4:E:191:LYS:NZ | 4:E:191:LYS:CE | 1.72 | 1.51 |
| 1:A:695:LYS:CE | 1:A:695:LYS:CD | 1.88 | 1.51 |
| 1:A:728:LYS:CE | 1:A:728:LYS:NZ | 1.70 | 1.51 |
| 2:B:115:GLN:CG | 2:B:115:GLN:CD | 1.78 | 1.51 |
| 1:A:597:LEU:CD1 | 1:A:597:LEU:CG | 1.87 | 1.50 |
| 1:A:620:LYS:CD | 1:A:620:LYS:CE | 1.86 | 1.50 |
| 4:E:180:ARG:CG | 4:E:180:ARG:CD | 1.87 | 1.50 |
| 1:A:830:LYS:CD | 1:A:830:LYS:CG | 1.87 | 1.50 |
| 1:A:481:ASP:CG | 1:A:481:ASP:CB | 1.76 | 1.50 |
| 2:B:951:GLN:CG | 2:B:951:GLN:CD | 1.74 | 1.50 |
| 1:A:895:LYS:CD | 1:A:895:LYS:CE | 1.85 | 1.50 |
| 2:B:870:ILE:CA | 2:B:870:ILE:CB | 1.87 | 1.50 |
| 4:E:152:LYS:CD | 4:E:152:LYS:CE | 1.86 | 1.50 |
| 1:A:555:ASP:CB | 1:A:555:ASP:CG | 1.78 | 1.49 |
| 1:A:843:LYS:CD | 1:A:843:LYS:CG | 1.87 | 1.49 |
| 10:L:26:THR:CB | 10:L:26:THR:CA | 1.89 | 1.49 |
| 1:A:69:THR:C | 1:A:69:THR:CA | 1.74 | 1.49 |
| 2:B:315:LYS:NZ | 2:B:315:LYS:CE | 1.72 | 1.49 |
| 1:A:1132:LYS:NZ | 1:A:1132:LYS:CE | 1.74 | 1.49 |
| 2:B:41:LYS:NZ | 2:B:41:LYS:CE | 1.72 | 1.49 |
| 3:C:15:LYS:CG | 3:C:15:LYS:CD | 1.90 | 1.49 |
| 1:A:1204:ASP:CB | 1:A:1204:ASP:CG | 1.79 | 1.48 |
| 1:A:978:PRO:CB | 1:A:978:PRO:CG | 1.78 | 1.48 |
| 2:B:641:GLU:CG | 2:B:641:GLU:CD | 1.79 | 1.48 |
| 1:A:941:LYS:CD | 1:A:941:LYS:CE | 1.88 | 1.48 |
| 2:B:199:MET:CE | 2:B:199:MET:SD | 2.02 | 1.48 |
| 2:B:231:PRO:CB | 2:B:231:PRO:CG | 1.85 | 1.47 |
| 4:E:53:PRO:CG | 4:E:53:PRO:CB | 1.74 | 1.47 |
| 5:F:129:LYS:NZ | 5:F:129:LYS:CE | 1.72 | 1.47 |
| 6:H:104:PHE:C | 6:H:104:PHE:CA | 1.82 | 1.47 |
| 4:E:50:MET:SD | 4:E:50:MET:CG | 2.02 | 1.47 |
| 2:B:432:MET:CE | 2:B:432:MET:SD | 2.03 | 1.46 |
| 4:E:106:GLN:CG | 4:E:106:GLN:CD | 1.79 | 1.46 |
| 7:I:17:ARG:CG | 7:I:17:ARG:CD | 1.91 | 1.46 |
| 4:E:93:MET:CG | 4:E:93:MET:SD | 2.02 | 1.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:201:LYS:CG | 4:E:201:LYS:CD | 1.93 | 1.45 |
| 1:A:705:LYS:CB | 1:A:705:LYS:CG | 1.90 | 1.45 |
| 1:A:41:MET:CE | 1:A:41:MET:SD | 2.05 | 1.45 |
| 1:A:676:MET:CE | 1:A:676:MET:SD | 2.05 | 1.45 |
| 2:B:789:MET:CE | 2:B:789:MET:SD | 2.05 | 1.45 |
| 1:A:676:MET:SD | 1:A:676:MET:CG | 2.04 | 1.44 |
| 2:B:999:MET:CG | 2:B:999:MET:SD | 2.05 | 1.44 |
| 6:H:139:ASN:CB | 6:H:139:ASN:CG | 1.86 | 1.44 |
| 1:A:346:ASP:CB | 1:A:346:ASP:CG | 1.86 | 1.44 |
| 1:A:56:PRO:O | 1:A:57:ARG:CD | 1.66 | 1.44 |
| 1:A:938:LYS:CD | 1:A:938:LYS:CE | 1.95 | 1.44 |
| 2:B:1169:MET:CE | 2:B:1169:MET:SD | 2.05 | 1.44 |
| 3:C:265:MET:CE | 3:C:265:MET:SD | 2.05 | 1.44 |
| 1:A:248:PRO:CB | 1:A:248:PRO:CG | 1.78 | 1.43 |
| 1:A:1111:MET:SD | 1:A:1111:MET:CG | 2.05 | 1.43 |
| 1:A:1350:LYS:NZ | 1:A:1350:LYS:CE | 1.75 | 1.43 |
| 1:A:728:LYS:CG | 1:A:728:LYS:CD | 1.92 | 1.43 |
| 2:B:987:LYS:NZ | 2:B:987:LYS:CE | 1.81 | 1.43 |
| 1:A:1290:LYS:NZ | 1:A:1290:LYS:CE | 1.80 | 1.43 |
| 2:B:593:PRO:CG | 2:B:593:PRO:CB | 1.86 | 1.43 |
| 2:B:531:GLN:CG | 2:B:531:GLN:CD | 1.88 | 1.42 |
| 7:I:1:MET:CE | 7:I:1:MET:SD | 2.07 | 1.42 |
| 2:B:736:THR:CB | 2:B:736:THR:CG2 | 1.96 | 1.42 |
| 13:B:3008:GTP:N9 | 13:B:3008:GTP:C1' | 1.81 | 1.42 |
| 10:L:68:GLU:CG | 10:L:68:GLU:CD | 1.85 | 1.41 |
| 2:B:382:ILE:CG1 | 2:B:382:ILE:CD1 | 1.95 | 1.41 |
| 3:C:154:LYS:CD | 3:C:154:LYS:CE | 1.98 | 1.41 |
| 1:A:1259:MET:SD | 1:A:1259:MET:CG | 2.09 | 1.41 |
| 2:B:347:LYS:CD | 2:B:347:LYS:CG | 1.98 | 1.41 |
| 4:E:93:MET:SD | 4:E:93:MET:CE | 2.08 | 1.40 |
| 8:J:1:MET:CE | 8:J:1:MET:SD | 2.07 | 1.40 |
| 1:A:1232:ASN:CG | 1:A:1232:ASN:CB | 1.89 | 1.40 |
| 6:H:19:ARG:CG | 6:H:19:ARG:CD | 1.98 | 1.40 |
| 4:E:121:MET:CE | 4:E:121:MET:SD | 2.08 | 1.40 |
| 1:A:620:LYS:CE | 1:A:620:LYS:NZ | 1.85 | 1.40 |
| 3:C:29:MET:CE | 3:C:29:MET:SD | 2.10 | 1.40 |
| 1:A:1302:PRO:CG | 1:A:1302:PRO:CB | 1.95 | 1.39 |
| 4:E:131:THR:CB | 4:E:131:THR:CG2 | 1.99 | 1.39 |
| 4:E:20:LYS:NZ | 4:E:20:LYS:CE | 1.84 | 1.38 |
| 1:A:74:MET:CE | 1:A:74:MET:SD | 2.09 | 1.38 |
| 4:E:162:ARG:CG | 4:E:162:ARG:CD | 2.01 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:I:1:MET:SD | 7:I:1:MET:CG | 2.13 | 1.35 |
| 1:A:1444:MET:CE | 1:A:1444:MET:SD | 2.14 | 1.35 |
| 2:B:1097:HIS:ND1 | 2:B:1097:HIS:HA | 1.37 | 1.35 |
| 7:I:55:THR:CB | 7:I:55:THR:CG2 | 2.05 | 1.35 |
| 4:E:121:MET:SD | 4:E:121:MET:CG | 2.13 | 1.34 |
| 6:H:104:PHE:O | 6:H:106:GLU:N | 1.63 | 1.32 |
| 1:A:172:PRO:CG | 1:A:185:TRP:CE2 | 2.11 | 1.31 |
| 1:A:728:LYS:CE | 1:A:728:LYS:CD | 2.09 | 1.31 |
| 1:A:1259:MET:SD | 1:A:1259:MET:CE | 2.18 | 1.30 |
| 1:A:437:MET:CE | 1:A:437:MET:SD | 2.18 | 1.30 |
| 2:B:999:MET:SD | 2:B:999:MET:CE | 1.20 | 1.30 |
| 4:E:1:MET:CE | 4:E:1:MET:SD | 2.21 | 1.29 |
| 1:A:156:ASP:O | 1:A:158:PRO:CD | 1.80 | 1.28 |
| 2:B:705:MET:CE | 2:B:705:MET:SD | 1.18 | 1.28 |
| 1:A:172:PRO:CD | 1:A:185:TRP:CE2 | 2.18 | 1.26 |
| 1:A:304:MET:CE | 1:A:304:MET:SD | 2.25 | 1.24 |
| 3:C:75:MET:CE | 3:C:75:MET:SD | 2.25 | 1.24 |
| 1:A:172:PRO:CG | 1:A:185:TRP:CZ2 | 2.18 | 1.24 |
| 1:A:186:LYS:HE2 | 1:A:197:PRO:CD | 1.66 | 1.24 |
| 1:A:172:PRO:CD | 1:A:185:TRP:NE1 | 2.01 | 1.24 |
| 3:C:165:LYS:NZ | 3:C:165:LYS:CE | 2.01 | 1.24 |
| 1:A:56:PRO:O | 1:A:57:ARG:HD2 | 1.11 | 1.23 |
| 3:C:125:MET:CE | 3:C:125:MET:SD | 2.27 | 1.23 |
| 1:A:172:PRO:HG2 | 1:A:185:TRP:CZ2 | 1.71 | 1.22 |
| 1:A:156:ASP:O | 1:A:158:PRO:HD2 | 1.07 | 1.21 |
| 1:A:369:SER:OG | 9:K:2:ASN:ND2 | 1.73 | 1.20 |
| 1:A:153:PRO:HD3 | 1:A:161:LEU:CD2 | 1.71 | 1.20 |
| 1:A:605:MET:CE | 1:A:607:ILE:HD11 | 1.71 | 1.19 |
| 2:B:999:MET:SD | 2:B:999:MET:HE3 | 1.77 | 1.19 |
| 1:A:487:MET:CE | 1:A:487:MET:SD | 1.09 | 1.19 |
| 2:B:662:MET:CE | 2:B:662:MET:SD | 2.31 | 1.18 |
| 1:A:535:THR:HG21 | 1:A:617:VAL:H | 1.07 | 1.16 |
| 10:L:68:GLU:OE1 | 14:L:3006:HOH:O | 1.63 | 1.16 |
| 9:K:1:MET:SD | 9:K:1:MET:CE | 2.35 | 1.15 |
| 5:F:103:MET:CE | 5:F:103:MET:SD | 2.33 | 1.15 |
| 2:B:999:MET:SD | 2:B:999:MET:HE1 | 1.77 | 1.14 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:CD1 | 1.82 | 1.14 |
| 1:A:172:PRO:HD2 | 1:A:185:TRP:NE1 | 1.60 | 1.14 |
| 2:B:999:MET:SD | 2:B:999:MET:HE2 | 1.77 | 1.14 |
| 1:A:42:ASP:OD2 | 1:A:47:ARG:N | 1.81 | 1.14 |
| 2:B:101:MET:SD | 2:B:101:MET:CE | 2.35 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:885:THR:HG21 | 14:A:3013:HOH:O | 1.45 | 1.13 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CE2 | 1.80 | 1.13 |
| 2:B:705:MET:SD | 2:B:705:MET:HE3 | 1.76 | 1.13 |
| 1:A:487:MET:CE | 1:A:487:MET:CG | 2.25 | 1.12 |
| 2:B:846:ILE:HD11 | 2:B:974:PRO:HB2 | 1.13 | 1.12 |
| 1:A:708:MET:CE | 1:A:708:MET:SD | 2.37 | 1.12 |
| 1:A:518:LYS:CD | 1:A:518:LYS:NZ | 2.11 | 1.11 |
| 2:B:705:MET:SD | 2:B:705:MET:HE1 | 1.76 | 1.11 |
| 7:I:45:ARG:HG2 | 7:I:45:ARG:HH11 | 1.10 | 1.11 |
| 2:B:705:MET:CE | 2:B:705:MET:CG | 2.28 | 1.10 |
| 1:A:186:LYS:HE2 | 1:A:197:PRO:HD3 | 1.22 | 1.10 |
| 1:A:605:MET:HE2 | 1:A:607:ILE:CD1 | 1.80 | 1.10 |
| 6:H:128:ASN:O | 6:H:131:ASN:ND2 | 1.85 | 1.09 |
| 2:B:130:VAL:HG22 | 2:B:167:ILE:HD11 | 1.30 | 1.09 |
| 3:C:54:ASN:OD1 | 3:C:56:THR:HB | 1.53 | 1.09 |
| 1:A:487:MET:SD | 1:A:487:MET:HE2 | 1.68 | 1.09 |
| 1:A:107:CYS:HB2 | 1:A:148:CYS:SG | 1.93 | 1.08 |
| 1:A:487:MET:SD | 1:A:487:MET:HE3 | 1.68 | 1.08 |
| 1:A:567:LYS:HB3 | 6:H:96:VAL:H | 1.16 | 1.08 |
| 2:B:792:MET:SD | 2:B:792:MET:CE | 2.42 | 1.08 |
| 6:H:138:GLU:O | 6:H:139:ASN:C | 1.92 | 1.07 |
| 1:A:487:MET:SD | 1:A:487:MET:HE1 | 1.68 | 1.07 |
| 7:I:16:PRO:O | 7:I:17:ARG:HD3 | 1.53 | 1.06 |
| 2:B:1097:HIS:CA | 2:B:1097:HIS:ND1 | 2.12 | 1.06 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CD2 | 1.88 | 1.05 |
| 2:B:705:MET:SD | 2:B:705:MET:HE2 | 1.76 | 1.05 |
| 7:I:45:ARG:CG | 7:I:45:ARG:HH11 | 1.69 | 1.05 |
| 7:I:4:PHE:HE1 | 7:I:13:MET:HE2 | 1.19 | 1.05 |
| 2:B:999:MET:CG | 2:B:999:MET:CE | 2.35 | 1.04 |
| 1:A:1233:ASP:O | 1:A:1234:GLU:HB3 | 1.55 | 1.03 |
| 1:A:1285:MET:CE | 1:A:1285:MET:SD | 2.46 | 1.03 |
| 5:F:93:ILE:HD11 | 5:F:134:ILE:HD11 | 1.40 | 1.03 |
| 8:J:14:VAL:HG13 | 8:J:50:ILE:HD11 | 1.41 | 1.03 |
| 9:K:110:ASN:O | 9:K:112:GLN:N | 1.92 | 1.03 |
| 2:B:955:THR:HG22 | 10:L:54:ARG:O | 1.57 | 1.03 |
| 4:E:12:LEU:HD21 | 4:E:58:MET:SD | 1.99 | 1.03 |
| 6:H:63:LEU:C | 6:H:90:ALA:HB3 | 1.77 | 1.03 |
| 4:E:57:MET:CE | 4:E:57:MET:SD | 2.47 | 1.02 |
| 2:B:552:MET:CG | 2:B:552:MET:SD | 2.48 | 1.02 |
| 6:H:106:GLU:O | 6:H:107:VAL:C | 1.98 | 1.02 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:HG13 | 1.58 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:679:ILE:HD11 | 1:A:732:LEU:HB2 | 1.42 | 1.01 |
| 1:A:1079:MET:SD | 1:A:1359:ASP:OD2 | 2.19 | 1.01 |
| 1:A:187:LYS:HB2 | 1:A:194:ALA:HB3 | 1.44 | 1.00 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:CG | 1.95 | 0.99 |
| 1:A:89:PRO:HB2 | 1:A:204:THR:HG21 | 1.39 | 0.99 |
| 1:A:567:LYS:HB3 | 6:H:96:VAL:N | 1.78 | 0.99 |
| 1:A:72:GLU:OE2 | 2:B:1175:LEU:HD11 | 1.63 | 0.98 |
| 1:A:153:PRO:HD3 | 1:A:161:LEU:HD22 | 1.43 | 0.97 |
| 1:A:119:ASN:O | 1:A:120:GLU:HB2 | 1.63 | 0.97 |
| 2:B:643:ASP:O | 2:B:644:GLU:HB2 | 1.63 | 0.96 |
| 1:A:107:CYS:CB | 1:A:148:CYS:SG | 2.53 | 0.96 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:NE1 | 1.77 | 0.96 |
| 1:A:186:LYS:CE | 1:A:197:PRO:HD3 | 1.95 | 0.96 |
| 1:A:153:PRO:HD3 | 1:A:161:LEU:HD23 | 1.48 | 0.95 |
| 2:B:885:MET:CE | 2:B:885:MET:SD | 2.54 | 0.95 |
| 1:A:186:LYS:HE2 | 1:A:197:PRO:HD2 | 1.45 | 0.95 |
| 7:I:78:CYS:SG | 7:I:103:CYS:SG | 2.64 | 0.95 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:H | 1.29 | 0.95 |
| 8:J:2:ILE:HD13 | 8:J:2:ILE:N | 1.80 | 0.95 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:HD3 | 1.48 | 0.95 |
| 1:A:1081:LEU:CD2 | 1:A:1081:LEU:HG | 1.97 | 0.94 |
| 2:B:552:MET:SD | 2:B:552:MET:CE | 2.55 | 0.94 |
| 1:A:186:LYS:NZ | 1:A:195:ASP:HA | 1.82 | 0.94 |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:H | 1.33 | 0.94 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HD2 | 1.83 | 0.94 |
| 4:E:63:ASN:O | 4:E:64:PRO:O | 1.86 | 0.93 |
| 1:A:325:ILE:C | 1:A:327:ALA:H | 1.68 | 0.93 |
| 1:A:605:MET:HE2 | 1:A:607:ILE:HD11 | 0.95 | 0.93 |
| 2:B:555:ILE:CD1 | 2:B:587:HIS:CE1 | 2.51 | 0.93 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:CE1 | 2.03 | 0.92 |
| 1:A:487:MET:CG | 1:A:487:MET:HE2 | 1.92 | 0.92 |
| 1:A:176:LYS:NZ | 1:A:178:GLY:O | 2.01 | 0.92 |
| 1:A:775:ILE:CG1 | 1:A:775:ILE:CD1 | 2.48 | 0.92 |
| 2:B:1190:ASP:O | 2:B:1191:ILE:HG13 | 1.68 | 0.92 |
| 5:F:77:ASP:O | 5:F:78:GLN:HB2 | 1.66 | 0.92 |
| 7:I:116:ASN:HD21 | 7:I:118:ARG:HB2 | 1.35 | 0.92 |
| 2:B:846:ILE:CD1 | 2:B:974:PRO:HB2 | 2.00 | 0.92 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:CD2 | 2.00 | 0.91 |
| 1:A:1055:ARG:CG | 1:A:1055:ARG:NE | 2.33 | 0.91 |
| 1:A:1079:MET:HG2 | 1:A:1359:ASP:OD2 | 1.71 | 0.91 |
| 2:B:130:VAL:H | 2:B:167:ILE:HD11 | 1.32 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:F:81:THR:CG2 | 5:F:136:ARG:HH11 | 1.83 | 0.91 |
| 1:A:1236:LEU:O | 1:A:1237:ILE:HD12 | 1.71 | 0.91 |
| 2:B:846:ILE:HD11 | 2:B:974:PRO:CB | 1.98 | 0.91 |
| 1:A:535:THR:CG2 | 1:A:617:VAL:H | 1.84 | 0.90 |
| 6:H:55:LEU:HD22 | 6:H:144:ILE:HD12 | 1.53 | 0.90 |
| 7:I:4:PHE:HE1 | 7:I:13:MET:CE | 1.83 | 0.90 |
| 1:A:605:MET:CE | 1:A:607:ILE:CD1 | 2.43 | 0.90 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:CG1 | 2.19 | 0.89 |
| 2:B:58:THR:O | 2:B:62:ILE:HG12 | 1.71 | 0.89 |
| 2:B:1097:HIS:CA | 2:B:1097:HIS:CG | 2.55 | 0.89 |
| 2:B:620:ARG:CG | 2:B:620:ARG:NE | 2.36 | 0.89 |
| 4:E:117:THR:O | 4:E:119:SER:N | 2.06 | 0.89 |
| 1:A:369:SER:H | 9:K:2:ASN:HD21 | 1.21 | 0.89 |
| 8:J:1:MET:CE | 8:J:1:MET:CG | 2.51 | 0.89 |
| 2:B:846:ILE:HD11 | 2:B:974:PRO:O | 1.73 | 0.88 |
| 2:B:775:LYS:CB | 2:B:775:LYS:CD | 2.51 | 0.88 |
| 6:H:89:LEU:O | 6:H:91:ASP:N | 2.06 | 0.88 |
| 7:I:45:ARG:HG2 | 7:I:45:ARG:NH1 | 1.88 | 0.88 |
| 1:A:795:GLU:HG2 | 2:B:731:VAL:HG21 | 1.54 | 0.88 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:HA2 | 1.54 | 0.88 |
| 3:C:167:HIS:HD2 | 3:C:169:LYS:H | 1.22 | 0.88 |
| 1:A:1286:LYS:CB | 1:A:1286:LYS:CD | 2.51 | 0.88 |
| 1:A:89:PRO:HB2 | 1:A:204:THR:CG2 | 2.02 | 0.88 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:HA | 1.54 | 0.88 |
| 1:A:1166:ASP:HB3 | 1:A:1169:ILE:CG2 | 2.05 | 0.88 |
| 4:E:147:HIS:HD2 | 4:E:149:LEU:H | 1.17 | 0.87 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CZ2 | 2.02 | 0.87 |
| 1:A:56:PRO:O | 1:A:57:ARG:HD3 | 1.69 | 0.87 |
| 2:B:555:ILE:HD12 | 2:B:587:HIS:CE1 | 2.09 | 0.87 |
| 1:A:567:LYS:CB | 6:H:96:VAL:H | 1.87 | 0.87 |
| 5:F:93:ILE:CD1 | 5:F:134:ILE:HD11 | 2.04 | 0.87 |
| 1:A:1079:MET:CG | 1:A:1359:ASP:OD2 | 2.22 | 0.87 |
| 2:B:1025:HIS:HE1 | 2:B:1090:THR:HG21 | 1.41 | 0.86 |
| 3:C:167:HIS:HE1 | 10:L:70:ARG:O | 1.58 | 0.86 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:CE2 | 2.10 | 0.86 |
| 2:B:846:ILE:CD1 | 2:B:974:PRO:O | 2.24 | 0.86 |
| 6:H:57:VAL:HG22 | 6:H:144:ILE:HD11 | 1.57 | 0.86 |
| 6:H:104:PHE:O | 6:H:105:GLU:C | 2.10 | 0.86 |
| 4:E:79:TRP:HB2 | 4:E:105:PHE:CE1 | 2.10 | 0.86 |
| 1:A:1134:ILE:CG2 | 1:A:1138:ILE:HD11 | 2.06 | 0.86 |
| 1:A:567:LYS:CD | 6:H:95:TYR:HA | 2.06 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:J:2:ILE:N | 8:J:2:ILE:CD1 | 2.37 | 0.85 |
| 1:A:567:LYS:CG | 1:A:568:PRO:CD | 2.54 | 0.85 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:CA | 2.05 | 0.85 |
| 7:I:4:PHE:CE1 | 7:I:13:MET:HE2 | 2.10 | 0.85 |
| 5:F:123:LYS:NZ | 5:F:123:LYS:CD | 2.39 | 0.85 |
| 1:A:64:ASN:OD1 | 1:A:64:ASN:O | 1.93 | 0.85 |
| 1:A:1166:ASP:HB3 | 1:A:1169:ILE:HG21 | 1.59 | 0.85 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CE3 | 2.10 | 0.85 |
| 1:A:164:ARG:O | 1:A:166:GLY:N | 2.08 | 0.85 |
| 1:A:679:ILE:HD12 | 1:A:729:ALA:HA | 1.58 | 0.85 |
| 2:B:104:GLU:OE1 | 10:L:54:ARG:NE | 2.10 | 0.85 |
| 6:H:106:GLU:O | 6:H:107:VAL:O | 1.94 | 0.84 |
| 1:A:55:ASP:OD1 | 1:A:55:ASP:O | 1.94 | 0.84 |
| 3:C:46:ILE:HD12 | 3:C:72:LEU:HD11 | 1.59 | 0.84 |
| 7:I:32:CYS:HB2 | 7:I:34:TYR:H | 1.43 | 0.83 |
| 10:L:48:CYS:C | 10:L:48:CYS:HA | 1.98 | 0.83 |
| 1:A:61:ILE:CB | 1:A:61:ILE:HA | 2.04 | 0.83 |
| 2:B:1220:ARG:O | 2:B:1222:ARG:HD3 | 1.77 | 0.83 |
| 2:B:542:MET:HG3 | 2:B:747:MET:CE | 2.07 | 0.83 |
| 2:B:477:ALA:CB | 2:B:477:ALA:HA | 2.08 | 0.83 |
| 4:E:98:ILE:CB | 4:E:98:ILE:HA | 2.03 | 0.83 |
| 1:A:679:ILE:HD13 | 1:A:732:LEU:HD12 | 1.59 | 0.83 |
| 1:A:31:SER:CB | 1:A:83:HIS:HD2 | 1.91 | 0.83 |
| 2:B:286:PHE:HB3 | 2:B:297:ILE:HD12 | 1.58 | 0.83 |
| 2:B:431:TYR:CD2 | 2:B:431:TYR:O | 2.31 | 0.83 |
| 1:A:108:MET:H | 1:A:171:GLN:HE22 | 1.23 | 0.82 |
| 13:B:3008:GTP:C1' | 13:B:3008:GTP:C8 | 2.61 | 0.82 |
| 4:E:2:ASP:HB3 | 4:E:6:GLU:HB2 | 1.61 | 0.82 |
| 1:A:1233:ASP:O | 1:A:1234:GLU:CB | 2.26 | 0.82 |
| 2:B:561:TRP:O | 2:B:590:HIS:HE1 | 1.61 | 0.82 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:N | 1.93 | 0.82 |
| 1:A:1003:LYS:CG | 1:A:1003:LYS:CA | 2.56 | 0.82 |
| 1:A:407:ARG:HD2 | 1:A:413:ILE:HD11 | 1.59 | 0.82 |
| 7:I:4:PHE:CE1 | 7:I:13:MET:CE | 2.62 | 0.82 |
| 1:A:325:ILE:O | 1:A:327:ALA:N | 2.12 | 0.82 |
| 10:L:28:LYS:C | 10:L:28:LYS:HA | 1.98 | 0.82 |
| 2:B:25:ILE:HD11 | 2:B:651:LEU:HD12 | 1.62 | 0.81 |
| 6:H:63:LEU:C | 6:H:90:ALA:CB | 2.49 | 0.81 |
| 2:B:644:GLU:OE1 | 2:B:646:LEU:HB2 | 1.79 | 0.81 |
| 1:A:55:ASP:N | 1:A:56:PRO:CD | 2.44 | 0.81 |
| 1:A:531:ILE:HD12 | 1:A:617:VAL:HB | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:169:ARG:HB2 | 2:B:454:THR:HG23 | 1.63 | 0.81 |
| 2:B:515:HIS:H | 2:B:518:HIS:CD2 | 1.99 | 0.81 |
| 1:A:347:PHE:H | 2:B:1107:ALA:HA | 1.46 | 0.81 |
| 1:A:901:LEU:H | 1:A:926:GLN:NE2 | 1.77 | 0.81 |
| 1:A:1111:MET:CG | 1:A:1111:MET:CE | 2.58 | 0.81 |
| 1:A:265:LYS:CD | 1:A:302:THR:HG22 | 2.11 | 0.81 |
| 6:H:138:GLU:O | 6:H:140:ALA:N | 2.14 | 0.80 |
| 1:A:535:THR:HG21 | 1:A:617:VAL:N | 1.93 | 0.80 |
| 7:I:45:ARG:CG | 7:I:45:ARG:NH1 | 2.45 | 0.80 |
| 2:B:542:MET:HG3 | 2:B:747:MET:HE3 | 1.63 | 0.80 |
| 1:A:567:LYS:HG3 | 1:A:568:PRO:CD | 2.10 | 0.80 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:CG | 2.15 | 0.80 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD3 | 2.11 | 0.80 |
| 1:A:982:THR:HG22 | 1:A:985:ASP:H | 1.47 | 0.80 |
| 2:B:515:HIS:H | 2:B:518:HIS:HD2 | 1.25 | 0.80 |
| 6:H:103:LYS:HB3 | 6:H:105:GLU:OE1 | 1.82 | 0.80 |
| 2:B:417:PHE:CD2 | 2:B:417:PHE:O | 2.36 | 0.79 |
| 2:B:90:ILE:HA | 2:B:133:LYS:O | 1.83 | 0.79 |
| 5:F:77:ASP:O | 5:F:78:GLN:CB | 2.28 | 0.79 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CE2 | 2.17 | 0.79 |
| 1:A:265:LYS:NZ | 1:A:302:THR:HG21 | 1.98 | 0.79 |
| 2:B:114:PRO:HD3 | 2:B:124:TYR:CE1 | 2.17 | 0.79 |
| 2:B:643:ASP:O | 2:B:644:GLU:CB | 2.31 | 0.79 |
| 1:A:55:ASP:O | 1:A:57:ARG:N | 2.15 | 0.79 |
| 2:B:130:VAL:HG22 | 2:B:167:ILE:CD1 | 2.10 | 0.79 |
| 4:E:50:MET:SD | 4:E:50:MET:CE | 2.70 | 0.79 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:H | 1.47 | 0.78 |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:H | 1.29 | 0.78 |
| 3:C:260:LEU:HD12 | 3:C:260:LEU:O | 1.82 | 0.78 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:CD | 2.13 | 0.78 |
| 1:A:869:GLY:O | 4:E:204:THR:HG21 | 1.84 | 0.78 |
| 1:A:571:LEU:CD2 | 1:A:571:LEU:HG | 2.08 | 0.78 |
| 1:A:711:ARG:HE | 7:I:95:THR:HG22 | 1.48 | 0.78 |
| 1:A:69:THR:C | 1:A:69:THR:HA | 2.03 | 0.78 |
| 1:A:134:ARG:O | 1:A:138:ILE:HG23 | 1.84 | 0.78 |
| 1:A:941:LYS:CD | 1:A:941:LYS:NZ | 2.47 | 0.78 |
| 2:B:754:SER:O | 2:B:806:THR:HG21 | 1.84 | 0.78 |
| 1:A:46:THR:CA | 1:A:46:THR:HB | 2.10 | 0.77 |
| 2:B:281:PRO:HB2 | 2:B:284:ILE:HD13 | 1.63 | 0.77 |
| 1:A:481:ASP:CG | 1:A:481:ASP:CA | 2.50 | 0.77 |
| 2:B:1128:LEU:HD12 | 2:B:1128:LEU:C | 2.03 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1055:ARG:CD | 1:A:1055:ARG:CB | 2.62 | 0.77 |
| 1:A:1151:GLU:CG | 7:I:45:ARG:HD2 | 2.14 | 0.77 |
| 1:A:636:GLU:OE1 | 1:A:966:ASN:ND2 | 2.16 | 0.77 |
| 2:B:431:TYR:CE1 | 2:B:447:ALA:HB1 | 2.19 | 0.77 |
| 2:B:1084:GLN:NE2 | 3:C:192:TRP:H | 1.82 | 0.77 |
| 2:B:431:TYR:O | 2:B:431:TYR:HD2 | 1.66 | 0.77 |
| 6:H:104:PHE:O | 6:H:106:GLU:CA | 2.32 | 0.77 |
| 1:A:567:LYS:HG3 | 1:A:568:PRO:HD2 | 1.65 | 0.77 |
| 1:A:909:ASP:OD1 | 1:A:911:SER:N | 2.17 | 0.77 |
| 4:E:98:ILE:CA | 4:E:98:ILE:HB | 2.12 | 0.77 |
| 6:H:77:ARG:O | 6:H:78:SER:O | 2.03 | 0.77 |
| 1:A:325:ILE:C | 1:A:327:ALA:N | 2.37 | 0.76 |
| 1:A:587:HIS:HD2 | 1:A:966:ASN:OD1 | 1.69 | 0.76 |
| 6:H:84:ALA:O | 6:H:88:SER:OG | 2.02 | 0.76 |
| 6:H:91:ASP:OD1 | 6:H:91:ASP:O | 2.01 | 0.76 |
| 2:B:305:VAL:CG1 | 2:B:305:VAL:CA | 2.62 | 0.76 |
| 9:K:111:LEU:CD1 | 9:K:111:LEU:CB | 2.62 | 0.76 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:HD12 | 1.68 | 0.76 |
| 1:A:327:ALA:O | 2:B:1206:GLU:OE1 | 2.03 | 0.76 |
| 1:A:156:ASP:C | 1:A:158:PRO:CD | 2.53 | 0.76 |
| 1:A:1118:VAL:HB | 1:A:1327:ILE:HD12 | 1.66 | 0.76 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:H | 1.33 | 0.76 |
| 1:A:567:LYS:CD | 6:H:95:TYR:CG | 2.69 | 0.75 |
| 2:B:680:THR:HG22 | 2:B:682:SER:H | 1.50 | 0.75 |
| 1:A:172:PRO:HD2 | 1:A:185:TRP:HE1 | 1.48 | 0.75 |
| 1:A:941:LYS:CD | 1:A:941:LYS:CB | 2.62 | 0.75 |
| 1:A:871:ASP:HB3 | 4:E:204:THR:HG23 | 1.68 | 0.75 |
| 2:B:549:THR:HG22 | 2:B:628:THR:HB | 1.69 | 0.75 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CH2 | 2.21 | 0.75 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:HD22 | 1.68 | 0.75 |
| 3:C:40:GLU:HA | 3:C:163:ILE:HD12 | 1.69 | 0.75 |
| 1:A:73:GLY:O | 1:A:75:ASN:N | 2.19 | 0.75 |
| 1:A:172:PRO:CG | 1:A:185:TRP:CH2 | 2.70 | 0.75 |
| 1:A:1350:LYS:CD | 1:A:1350:LYS:CB | 2.65 | 0.75 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:CD2 | 2.21 | 0.75 |
| 6:H:89:LEU:C | 6:H:91:ASP:H | 1.90 | 0.75 |
| 6:H:9:ILE:CB | 6:H:9:ILE:HA | 2.14 | 0.74 |
| 6:H:130:ARG:HD2 | 6:H:130:ARG:C | 2.06 | 0.74 |
| 1:A:61:ILE:O | 1:A:62:ASP:HB2 | 1.86 | 0.74 |
| 10:L:47:ARG:HG2 | 10:L:48:CYS:H | 1.53 | 0.74 |
| 1:A:186:LYS:HZ1 | 1:A:195:ASP:HA | 1.50 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:H:101:ALA:HB2 | 6:H:116:TYR:CE2 | 2.23 | 0.74 |
| 1:A:1259:MET:SD | 1:A:1259:MET:CB | 2.75 | 0.74 |
| 1:A:1445:ILE:CG2 | 1:A:1445:ILE:CA | 2.65 | 0.74 |
| 8:J:1:MET:C | 8:J:2:ILE:HD13 | 2.07 | 0.74 |
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:H | 1.32 | 0.74 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:CD1 | 2.18 | 0.74 |
| 5:F:75:PRO:O | 5:F:77:ASP:O | 2.06 | 0.74 |
| 7:I:116:ASN:ND2 | 7:I:118:ARG:HB2 | 2.03 | 0.73 |
| 4:E:147:HIS:CD2 | 4:E:149:LEU:H | 2.05 | 0.73 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:HD21 | 1.68 | 0.73 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:H | 1.86 | 0.73 |
| 1:A:14:VAL:H | 1:A:1432:GLN:HE22 | 1.36 | 0.73 |
| 1:A:1151:GLU:OE2 | 7:I:45:ARG:HD3 | 1.88 | 0.73 |
| 1:A:1236:LEU:O | 1:A:1237:ILE:CD1 | 2.36 | 0.73 |
| 2:B:723:VAL:CB | 2:B:723:VAL:HA | 2.16 | 0.73 |
| 3:C:33:LEU:HD13 | 3:C:248:ILE:HD13 | 1.70 | 0.73 |
| 4:E:29:PHE:O | 4:E:30:ILE:HD13 | 1.87 | 0.73 |
| 10:L:34:CYS:O | 10:L:34:CYS:SG | 2.41 | 0.73 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:HD11 | 1.71 | 0.73 |
| 5:F:111:LEU:O | 5:F:113:GLY:N | 2.20 | 0.73 |
| 1:A:938:LYS:CE | 1:A:938:LYS:CG | 2.67 | 0.73 |
| 1:A:328:ARG:HG3 | 1:A:329:LEU:H | 1.53 | 0.73 |
| 1:A:368:LYS:CD | 1:A:368:LYS:CB | 2.66 | 0.73 |
| 1:A:1134:ILE:HG22 | 1:A:1138:ILE:HD11 | 1.69 | 0.73 |
| 1:A:1341:ILE:HD11 | 1:A:1376:THR:O | 1.88 | 0.73 |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HB2 | 1.53 | 0.73 |
| 1:A:156:ASP:OD2 | 1:A:156:ASP:N | 2.21 | 0.73 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CZ3 | 2.24 | 0.73 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:NH2 | 2.03 | 0.73 |
| 1:A:156:ASP:O | 1:A:158:PRO:HD3 | 1.84 | 0.72 |
| 2:B:357:GLN:NE2 | 2:B:368:GLU:HG2 | 2.03 | 0.72 |
| 2:B:999:MET:CG | 2:B:999:MET:HE3 | 2.17 | 0.72 |
| 6:H:27:GLU:OE1 | 6:H:39:THR:OG1 | 2.05 | 0.72 |
| 1:A:26:GLU:O | 1:A:30:ILE:HD13 | 1.90 | 0.72 |
| 2:B:251:ILE:O | 2:B:251:ILE:HG22 | 1.89 | 0.72 |
| 2:B:313:MET:HE3 | 2:B:386:LEU:HD22 | 1.69 | 0.72 |
| 1:A:503:GLN:NE2 | 5:F:90:ARG:NH2 | 2.38 | 0.72 |
| 1:A:903:ASN:ND2 | 1:A:905:ASP:H | 1.88 | 0.72 |
| 1:A:977:LYS:CG | 1:A:977:LYS:CA | 2.67 | 0.72 |
| 2:B:515:HIS:N | 2:B:518:HIS:HD2 | 1.88 | 0.72 |
| 2:B:1162:ILE:CD1 | 2:B:1194:ILE:HG12 | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:566:ILE:CG2 | 1:A:566:ILE:CA | 2.66 | 0.72 |
| 9:K:35:PHE:HE1 | 9:K:73:LEU:HD12 | 1.54 | 0.72 |
| 2:B:315:LYS:NZ | 2:B:315:LYS:CD | 2.50 | 0.72 |
| 5:F:93:ILE:HD11 | 5:F:134:ILE:CD1 | 2.19 | 0.72 |
| 1:A:172:PRO:CG | 1:A:185:TRP:CD2 | 2.62 | 0.72 |
| 1:A:1134:ILE:HG23 | 1:A:1138:ILE:HD11 | 1.70 | 0.72 |
| 2:B:663:ALA:O | 2:B:667:GLN:HG3 | 1.89 | 0.72 |
| 3:C:102:GLN:CG | 3:C:102:GLN:CA | 2.66 | 0.72 |
| 2:B:294:ASP:H | 7:I:12:ASN:HD22 | 1.36 | 0.71 |
| 6:H:105:GLU:HG2 | 6:H:136:LYS:NZ | 2.04 | 0.71 |
| 2:B:357:GLN:HE21 | 2:B:368:GLU:HG2 | 1.56 | 0.71 |
| 2:B:996:ARG:NH1 | 14:B:3012:HOH:O | 2.22 | 0.71 |
| 1:A:154:SER:O | 1:A:155:GLU:O | 2.08 | 0.71 |
| 3:C:77:ILE:HD12 | 3:C:80:LEU:HB3 | 1.73 | 0.71 |
| 1:A:247:ARG:NH1 | 1:A:263:THR:HG23 | 2.05 | 0.71 |
| 4:E:112:TYR:CG | 4:E:116:ILE:HD11 | 2.25 | 0.71 |
| 1:A:23:SER:O | 1:A:27:VAL:HG23 | 1.89 | 0.71 |
| 1:A:518:LYS:CD | 1:A:518:LYS:HZ2 | 2.03 | 0.71 |
| 1:A:187:LYS:CB | 1:A:194:ALA:HB3 | 2.19 | 0.71 |
| 3:C:241:ASP:HB3 | 9:K:109:TRP:CE2 | 2.25 | 0.71 |
| 6:H:6:PHE:CD2 | 6:H:7:ASP:N | 2.59 | 0.71 |
| 1:A:531:ILE:O | 1:A:535:THR:HB | 1.90 | 0.71 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:H | 1.88 | 0.71 |
| 1:A:265:LYS:HD3 | 1:A:302:THR:HG22 | 1.71 | 0.71 |
| 2:B:294:ASP:H | 7:I:12:ASN:ND2 | 1.87 | 0.71 |
| 1:A:1385:THR:CG2 | 1:A:1385:THR:CA | 2.68 | 0.71 |
| 8:J:1:MET:HB3 | 8:J:2:ILE:HD13 | 1.71 | 0.71 |
| 1:A:186:LYS:CE | 1:A:197:PRO:CD | 2.56 | 0.71 |
| 1:A:560:ILE:HD12 | 1:A:560:ILE:H | 1.56 | 0.70 |
| 1:A:1080:THR:CA | 1:A:1080:THR:HB | 2.13 | 0.70 |
| 1:A:53:LEU:HD23 | 1:A:54:ASN:N | 2.06 | 0.70 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:HE1 | 1.55 | 0.70 |
| 4:E:47:CYS:SG | 4:E:52:ARG:O | 2.50 | 0.70 |
| 1:A:261:ASP:N | 1:A:261:ASP:OD1 | 2.24 | 0.70 |
| 2:B:242:SER:HG | 2:B:363:HIS:HD1 | 1.35 | 0.70 |
| 2:B:877:PRO:O | 2:B:878:GLN:HG2 | 1.92 | 0.70 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:H | 1.56 | 0.70 |
| 1:A:107:CYS:SG | 1:A:171:GLN:OE1 | 2.49 | 0.70 |
| 1:A:547:LEU:HB3 | 9:K:58:PHE:CE1 | 2.27 | 0.70 |
| 2:B:227:LYS:CG | 2:B:227:LYS:CE | 2.70 | 0.70 |
| 1:A:42:ASP:OD2 | 1:A:47:ARG:CA | 2.40 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1162:VAL:CG1 | 1:A:1162:VAL:CA | 2.69 | 0.70 |
| 2:B:484:ASN:OD1 | 2:B:486:TYR:CE1 | 2.45 | 0.70 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:HG11 | 1.74 | 0.70 |
| 3:C:172:PRO:O | 3:C:235:VAL:HG12 | 1.90 | 0.70 |
| 9:K:65:HIS:HD2 | 9:K:67:PHE:H | 1.36 | 0.70 |
| 1:A:369:SER:CB | 9:K:2:ASN:ND2 | 2.54 | 0.70 |
| 1:A:1135:ARG:CG | 1:A:1135:ARG:NE | 2.53 | 0.70 |
| 1:A:1405:THR:CA | 1:A:1405:THR:HB | 2.14 | 0.70 |
| 8:J:1:MET:C | 8:J:2:ILE:CD1 | 2.60 | 0.70 |
| 1:A:150:THR:HA | 1:A:166:GLY:HA2 | 1.73 | 0.70 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:CA | 2.21 | 0.70 |
| 3:C:181:ASP:OD2 | 3:C:186:LEU:HB2 | 1.92 | 0.70 |
| 1:A:679:ILE:HD12 | 1:A:729:ALA:CA | 2.21 | 0.69 |
| 1:A:32:VAL:HG23 | 1:A:33:ALA:H | 1.57 | 0.69 |
| 1:A:567:LYS:CD | 1:A:568:PRO:CD | 2.70 | 0.69 |
| 2:B:119:LEU:O | 2:B:965:LYS:NZ | 2.24 | 0.69 |
| 2:B:463:THR:HG21 | 2:B:465:ASN:OD1 | 1.91 | 0.69 |
| 2:B:645:SER:OG | 2:B:646:LEU:N | 2.23 | 0.69 |
| 2:B:1025:HIS:CE1 | 2:B:1090:THR:HG21 | 2.25 | 0.69 |
| 2:B:1166:CYS:O | 2:B:1168:LEU:N | 2.25 | 0.69 |
| 2:B:1031:LEU:HB2 | 2:B:1055:ILE:CD1 | 2.22 | 0.69 |
| 2:B:1077:THR:CG2 | 2:B:1079:LYS:H | 2.05 | 0.69 |
| 1:A:608:ILE:HD12 | 1:A:613:ILE:HG13 | 1.74 | 0.69 |
| 2:B:1222:ARG:HH11 | 2:B:1222:ARG:HB2 | 1.57 | 0.69 |
| 3:C:209:TYR:HD1 | 3:C:209:TYR:H | 1.41 | 0.69 |
| 1:A:46:THR:O | 1:A:48:ALA:N | 2.26 | 0.69 |
| 1:A:885:THR:CG2 | 14:A:3013:HOH:O | 2.19 | 0.69 |
| 2:B:217:ARG:HD3 | 2:B:407:ASP:OD2 | 1.93 | 0.69 |
| 3:C:50:GLU:HB3 | 10:L:64:LEU:HD13 | 1.73 | 0.69 |
| 3:C:199:LYS:CD | 3:C:199:LYS:NZ | 2.56 | 0.69 |
| 7:I:120:GLN:O | 7:I:121:PHE:HB2 | 1.91 | 0.69 |
| 8:J:2:ILE:HG22 | 8:J:3:VAL:N | 2.07 | 0.69 |
| 1:A:328:ARG:CG | 1:A:329:LEU:H | 2.03 | 0.69 |
| 1:A:523:ILE:HB | 1:A:622:VAL:HG13 | 1.75 | 0.69 |
| 1:A:282:ASN:C | 1:A:283:GLY:O | 2.28 | 0.69 |
| 1:A:679:ILE:CD1 | 1:A:729:ALA:HA | 2.21 | 0.69 |
| 1:A:840:ARG:CG | 1:A:840:ARG:NE | 2.54 | 0.69 |
| 1:A:849:MET:HE2 | 1:A:1061:GLY:HA2 | 1.75 | 0.69 |
| 2:B:744:HIS:HD2 | 2:B:746:SER:H | 1.41 | 0.69 |
| 1:A:243:PRO:HB2 | 1:A:245:PRO:HD2 | 1.74 | 0.69 |
| 4:E:100:ILE:HG22 | 4:E:101:GLN:N | 2.07 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:839:MET:CE | 2:B:1010:LEU:HD11 | 2.23 | 0.68 |
| 2:B:955:THR:CG2 | 10:L:54:ARG:O | 2.39 | 0.68 |
| 1:A:166:GLY:O | 1:A:167:CYS:HB3 | 1.92 | 0.68 |
| 2:B:1161:HIS:C | 2:B:1162:ILE:HD12 | 2.13 | 0.68 |
| 1:A:351:THR:HG21 | 2:B:1103:ILE:HG12 | 1.75 | 0.68 |
| 6:H:103:LYS:O | 6:H:115:TYR:HD1 | 1.76 | 0.68 |
| 5:F:76:LYS:O | 5:F:79:ARG:HD2 | 1.93 | 0.68 |
| 1:A:567:LYS:HE2 | 6:H:95:TYR:CE2 | 2.26 | 0.68 |
| 1:A:587:HIS:CE1 | 1:A:969:GLN:HG2 | 2.28 | 0.68 |
| 6:H:105:GLU:HG2 | 6:H:136:LYS:HZ2 | 1.58 | 0.68 |
| 1:A:265:LYS:CE | 1:A:302:THR:HG22 | 2.23 | 0.68 |
| 1:A:69:THR:HG22 | 2:B:1174:LYS:HE2 | 1.75 | 0.68 |
| 4:E:112:TYR:CD2 | 4:E:116:ILE:HD11 | 2.28 | 0.68 |
| 5:F:81:THR:CG2 | 5:F:136:ARG:NH1 | 2.56 | 0.68 |
| 6:H:105:GLU:HB3 | 6:H:107:VAL:HG23 | 1.76 | 0.68 |
| 1:A:1161:THR:CG2 | 1:A:1163:ILE:H | 2.06 | 0.68 |
| 4:E:98:ILE:O | 4:E:101:GLN:HB3 | 1.93 | 0.68 |
| 9:K:55:LYS:HB2 | 9:K:81:TYR:CE1 | 2.28 | 0.68 |
| 1:A:679:ILE:HD13 | 1:A:732:LEU:CD1 | 2.24 | 0.68 |
| 2:B:531:GLN:CD | 2:B:531:GLN:H | 1.97 | 0.68 |
| 1:A:1385:THR:O | 1:A:1385:THR:HG22 | 1.94 | 0.67 |
| 4:E:79:TRP:HB2 | 4:E:105:PHE:CD1 | 2.28 | 0.67 |
| 2:B:417:PHE:CD2 | 2:B:417:PHE:C | 2.67 | 0.67 |
| 1:A:46:THR:CB | 1:A:46:THR:C | 2.63 | 0.67 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:OG1 | 1.94 | 0.67 |
| 3:C:116:LYS:CD | 3:C:116:LYS:NZ | 2.56 | 0.67 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HG12 | 2.24 | 0.67 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD3 | 2.25 | 0.67 |
| 1:A:184:SER:HB2 | 1:A:199:LEU:HD23 | 1.75 | 0.67 |
| 1:A:912:LEU:HD23 | 1:A:912:LEU:N | 2.10 | 0.67 |
| 2:B:435:THR:O | 2:B:435:THR:HG22 | 1.95 | 0.67 |
| 2:B:654:ARG:H | 2:B:657:HIS:HD2 | 1.42 | 0.67 |
| 2:B:1222:ARG:HG2 | 2:B:1222:ARG:NH1 | 2.09 | 0.67 |
| 1:A:567:LYS:CB | 6:H:95:TYR:HA | 2.25 | 0.67 |
| 2:B:51:PHE:CZ | 2:B:172:ILE:HD13 | 2.30 | 0.67 |
| 2:B:227:LYS:CD | 2:B:227:LYS:CB | 2.70 | 0.67 |
| 2:B:487:THR:HG22 | 2:B:490:SER:H | 1.58 | 0.67 |
| 2:B:1162:ILE:HD13 | 2:B:1194:ILE:HG12 | 1.77 | 0.67 |
| 1:A:503:GLN:NE2 | 5:F:90:ARG:HH21 | 1.93 | 0.67 |
| 1:A:63:ARG:HA | 1:A:74:MET:HG2 | 1.77 | 0.67 |
| 2:B:90:ILE:HD13 | 2:B:134:LYS:HA | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:180:TYR:OH | 3:C:188:HIS:ND1 | 2.26 | 0.67 |
| 9:K:55:LYS:HB3 | 9:K:81:TYR:HD1 | 1.60 | 0.67 |
| 1:A:46:THR:HB | 1:A:46:THR:O | 1.95 | 0.67 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:CD2 | 2.30 | 0.67 |
| 7:I:3:THR:CG2 | 7:I:3:THR:CA | 2.70 | 0.67 |
| 1:A:1195:LEU:HD11 | 1:A:1267:MET:CE | 2.25 | 0.66 |
| 1:A:328:ARG:HA | 2:B:1206:GLU:OE1 | 1.95 | 0.66 |
| 1:A:492:PRO:HB2 | 1:A:497:THR:HG22 | 1.75 | 0.66 |
| 9:K:20:LYS:CG | 9:K:20:LYS:CE | 2.73 | 0.66 |
| 2:B:899:ILE:CD1 | 2:B:911:ILE:HA | 2.25 | 0.66 |
| 1:A:567:LYS:CG | 6:H:96:VAL:H | 2.09 | 0.66 |
| 1:A:849:MET:CE | 1:A:1061:GLY:HA2 | 2.26 | 0.66 |
| 6:H:123:MET:HE3 | 6:H:142:LEU:HD22 | 1.76 | 0.66 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:CG1 | 2.74 | 0.66 |
| 1:A:369:SER:N | 9:K:2:ASN:HD21 | 1.90 | 0.66 |
| 1:A:1350:LYS:CG | 1:A:1350:LYS:CE | 2.74 | 0.66 |
| 2:B:206:ASN:OD1 | 2:B:458:LYS:CE | 2.44 | 0.66 |
| 2:B:243:ALA:C | 2:B:244:LEU:HG | 2.14 | 0.66 |
| 2:B:291:ILE:HG22 | 2:B:297:ILE:HD13 | 1.76 | 0.66 |
| 6:H:115:TYR:O | 6:H:123:MET:O | 2.13 | 0.66 |
| 1:A:265:LYS:NZ | 1:A:302:THR:CG2 | 2.59 | 0.66 |
| 1:A:534:LEU:O | 1:A:574:GLY:HA3 | 1.96 | 0.66 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:HD3 | 1.78 | 0.66 |
| 9:K:93:SER:O | 9:K:97:LYS:HG3 | 1.95 | 0.66 |
| 1:A:172:PRO:CD | 1:A:185:TRP:CD2 | 2.79 | 0.66 |
| 4:E:117:THR:O | 4:E:118:PRO:C | 2.34 | 0.66 |
| 1:A:99:ILE:HD13 | 1:A:235:ILE:HD13 | 1.77 | 0.66 |
| 4:E:36:GLU:O | 4:E:37:LEU:C | 2.30 | 0.66 |
| 6:H:131:ASN:H | 6:H:131:ASN:HD22 | 1.42 | 0.66 |
| 1:A:57:ARG:HB3 | 1:A:68:GLN:HG2 | 1.75 | 0.65 |
| 1:A:135:PHE:CD1 | 1:A:222:LEU:HD22 | 2.31 | 0.65 |
| 1:A:172:PRO:HD2 | 1:A:185:TRP:CE2 | 2.11 | 0.65 |
| 1:A:537:ARG:NH2 | 1:A:600:PRO:O | 2.29 | 0.65 |
| 2:B:1019:SER:CB | 13:B:3008:GTP:O6 | 2.43 | 0.65 |
| 1:A:224:PHE:CG | 1:A:231:PRO:HD3 | 2.31 | 0.65 |
| 8:J:53:HIS:HE1 | 8:J:55:ASP:HA | 1.62 | 0.65 |
| 1:A:156:ASP:C | 1:A:158:PRO:HD3 | 2.17 | 0.65 |
| 1:A:187:LYS:HB2 | 1:A:194:ALA:CB | 2.21 | 0.65 |
| 1:A:919:ILE:HD13 | 1:A:983:ILE:HD13 | 1.79 | 0.65 |
| 3:C:7:GLN:CB | 3:C:7:GLN:CD | 2.63 | 0.65 |
| 2:B:228:LYS:O | 2:B:261:ARG:NH2 | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:38:ILE:HG13 | 3:C:176:ILE:HD12 | 1.78 | 0.65 |
| 3:C:167:HIS:CE1 | 10:L:70:ARG:O | 2.47 | 0.65 |
| 9:K:24:ASP:OD1 | 9:K:74:ARG:NH1 | 2.29 | 0.65 |
| 2:B:191:LYS:CG | 2:B:191:LYS:CA | 2.74 | 0.65 |
| 2:B:341:LEU:HD12 | 2:B:342:GLY:H | 1.60 | 0.65 |
| 1:A:960:ILE:O | 1:A:964:ILE:HD13 | 1.97 | 0.65 |
| 1:A:562:THR:CG2 | 6:H:98:TYR:CD2 | 2.80 | 0.65 |
| 2:B:246:LYS:C | 2:B:246:LYS:HA | 2.07 | 0.65 |
| 1:A:741:ASN:HD21 | 1:A:743:VAL:HB | 1.61 | 0.64 |
| 1:A:1151:GLU:HG2 | 7:I:45:ARG:HD2 | 1.79 | 0.64 |
| 1:A:1298:TYR:O | 1:A:1299:VAL:HG23 | 1.97 | 0.64 |
| 4:E:152:LYS:CD | 4:E:152:LYS:CB | 2.75 | 0.64 |
| 7:I:120:GLN:O | 7:I:121:PHE:CB | 2.45 | 0.64 |
| 1:A:934:LYS:CD | 1:A:934:LYS:NZ | 2.60 | 0.64 |
| 2:B:115:GLN:CG | 2:B:115:GLN:CA | 2.74 | 0.64 |
| 2:B:1222:ARG:HH11 | 2:B:1222:ARG:CG | 2.10 | 0.64 |
| 5:F:109:VAL:CG1 | 5:F:110:ASP:N | 2.60 | 0.64 |
| 6:H:89:LEU:HB3 | 6:H:91:ASP:OD1 | 1.98 | 0.64 |
| 7:I:4:PHE:CE1 | 7:I:13:MET:HE1 | 2.31 | 0.64 |
| 1:A:1272:THR:CG2 | 1:A:1272:THR:CA | 2.72 | 0.64 |
| 2:B:1163:CYS:SG | 2:B:1165:ILE:HG13 | 2.38 | 0.64 |
| 1:A:407:ARG:CD | 1:A:413:ILE:HD11 | 2.27 | 0.64 |
| 2:B:291:ILE:O | 2:B:297:ILE:HD11 | 1.97 | 0.64 |
| 3:C:41:ILE:N | 3:C:163:ILE:HD11 | 2.13 | 0.64 |
| 4:E:115:ASN:O | 4:E:116:ILE:HD13 | 1.96 | 0.64 |
| 5:F:105:ALA:HB1 | 5:F:106:PRO:HD2 | 1.77 | 0.64 |
| 3:C:77:ILE:CD1 | 3:C:80:LEU:HB3 | 2.28 | 0.64 |
| 6:H:47:PHE:CG | 6:H:95:TYR:HD1 | 2.16 | 0.64 |
| 1:A:265:LYS:HZ2 | 1:A:302:THR:HG21 | 1.62 | 0.64 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H | 1.62 | 0.64 |
| 1:A:1172:LEU:O | 1:A:1173:HIS:CD2 | 2.49 | 0.64 |
| 1:A:1155:ASP:O | 1:A:1241:ARG:NH2 | 2.31 | 0.64 |
| 2:B:841:MET:HB2 | 2:B:990:ILE:HD12 | 1.78 | 0.64 |
| 3:C:77:ILE:HD12 | 3:C:77:ILE:O | 1.98 | 0.64 |
| 6:H:105:GLU:H | 6:H:105:GLU:CD | 2.01 | 0.64 |
| 1:A:894:GLU:HB2 | 1:A:933:TYR:OH | 1.98 | 0.64 |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CD | 2.01 | 0.64 |
| 8:J:1:MET:CE | 8:J:1:MET:CB | 2.76 | 0.64 |
| 1:A:84:ILE:HD12 | 1:A:270:LEU:HD13 | 1.80 | 0.63 |
| 1:A:446:ARG:HG2 | 1:A:446:ARG:HH11 | 1.62 | 0.63 |
| 2:B:94:LYS:HG2 | 2:B:96:TYR:CE1 | 2.34 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:40:GLU:HA | 3:C:163:ILE:CD1 | 2.28 | 0.63 |
| 1:A:709:THR:HG22 | 1:A:712:GLU:H | 1.63 | 0.63 |
| 2:B:120:ARG:NH2 | 2:B:956:THR:O | 2.29 | 0.63 |
| 2:B:393:LYS:NZ | 2:B:621:GLU:OE2 | 2.23 | 0.63 |
| 4:E:117:THR:OG1 | 4:E:120:ALA:CB | 2.47 | 0.63 |
| 10:L:26:THR:CA | 10:L:26:THR:HB | 2.19 | 0.63 |
| 2:B:127:GLY:HA2 | 2:B:168:GLY:O | 1.98 | 0.63 |
| 4:E:152:LYS:CD | 4:E:152:LYS:NZ | 2.62 | 0.63 |
| 8:J:53:HIS:HE1 | 8:J:55:ASP:CA | 2.10 | 0.63 |
| 9:K:55:LYS:HB2 | 9:K:81:TYR:CD1 | 2.34 | 0.63 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:CG1 | 2.29 | 0.63 |
| 3:C:99:LEU:HD12 | 3:C:99:LEU:N | 2.14 | 0.63 |
| 1:A:11:LEU:HD11 | 2:B:1195:HIS:CD2 | 2.34 | 0.63 |
| 1:A:579:SER:HA | 1:A:582:ILE:HD12 | 1.80 | 0.63 |
| 1:A:589:GLN:HB2 | 1:A:961:ARG:HH22 | 1.63 | 0.63 |
| 1:A:1265:ASN:O | 1:A:1266:THR:C | 2.35 | 0.63 |
| 6:H:76:THR:O | 6:H:76:THR:HG22 | 1.99 | 0.63 |
| 1:A:531:ILE:CD1 | 1:A:578:LEU:HD22 | 2.29 | 0.63 |
| 2:B:1222:ARG:NH1 | 2:B:1222:ARG:CG | 2.59 | 0.63 |
| 6:H:32:THR:CG2 | 6:H:33:GLN:OE1 | 2.47 | 0.63 |
| 6:H:93:TYR:HB3 | 6:H:144:ILE:O | 1.98 | 0.63 |
| 1:A:31:SER:HB3 | 1:A:83:HIS:HD2 | 1.62 | 0.63 |
| 4:E:161:LYS:CE | 4:E:161:LYS:CG | 2.69 | 0.63 |
| 1:A:224:PHE:CD2 | 1:A:231:PRO:HD3 | 2.34 | 0.62 |
| 1:A:1162:VAL:O | 1:A:1162:VAL:HG12 | 1.98 | 0.62 |
| 2:B:531:GLN:CG | 2:B:531:GLN:CA | 2.71 | 0.62 |
| 9:K:55:LYS:CB | 9:K:81:TYR:CD1 | 2.82 | 0.62 |
| 1:A:164:ARG:C | 1:A:166:GLY:H | 2.02 | 0.62 |
| 2:B:955:THR:HG23 | 10:L:55:ILE:HA | 1.80 | 0.62 |
| 5:F:81:THR:HG23 | 5:F:136:ARG:HH11 | 1.62 | 0.62 |
| 6:H:96:VAL:HG22 | 6:H:143:LEU:HD23 | 1.80 | 0.62 |
| 1:A:237:THR:CG2 | 1:A:237:THR:CA | 2.73 | 0.62 |
| 2:B:436:VAL:CA | 2:B:436:VAL:HB | 2.16 | 0.62 |
| 1:A:901:LEU:H | 1:A:926:GLN:HE22 | 1.47 | 0.62 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:CZ | 2.35 | 0.62 |
| 10:L:58:LYS:O | 10:L:59:ALA:HB3 | 2.00 | 0.62 |
| 2:B:899:ILE:HD12 | 2:B:911:ILE:HG13 | 1.80 | 0.62 |
| 6:H:47:PHE:CB | 6:H:95:TYR:HD1 | 2.12 | 0.62 |
| 6:H:63:LEU:HB2 | 6:H:90:ALA:HB2 | 1.81 | 0.62 |
| 1:A:1111:MET:CG | 1:A:1111:MET:HE2 | 2.29 | 0.62 |
| 2:B:884:ARG:NH1 | 2:B:884:ARG:HG2 | 2.13 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:N | 1.98 | 0.62 |
| 1:A:186:LYS:CD | 1:A:197:PRO:HD3 | 2.29 | 0.62 |
| 1:A:518:LYS:CE | 1:A:518:LYS:CG | 2.75 | 0.62 |
| 2:B:531:GLN:NE2 | 2:B:532:ALA:H | 1.97 | 0.62 |
| 2:B:787:VAL:O | 2:B:787:VAL:CG1 | 2.47 | 0.62 |
| 6:H:57:VAL:HG22 | 6:H:144:ILE:CD1 | 2.30 | 0.62 |
| 1:A:55:ASP:N | 1:A:56:PRO:HD3 | 2.12 | 0.62 |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:N | 2.12 | 0.62 |
| 3:C:255:VAL:O | 3:C:255:VAL:HG12 | 1.99 | 0.62 |
| 1:A:84:ILE:HD12 | 1:A:270:LEU:CD1 | 2.30 | 0.62 |
| 1:A:751:SER:O | 1:A:752:LYS:HB2 | 1.99 | 0.62 |
| 1:A:328:ARG:HH11 | 1:A:1405:THR:HG22 | 1.65 | 0.61 |
| 1:A:837:ILE:HD11 | 1:A:1102:LYS:HG2 | 1.81 | 0.61 |
| 3:C:46:ILE:CD1 | 3:C:72:LEU:HD11 | 2.29 | 0.61 |
| 2:B:843:GLN:NE2 | 2:B:846:ILE:CG2 | 2.62 | 0.61 |
| 1:A:14:VAL:H | 1:A:1432:GLN:NE2 | 1.98 | 0.61 |
| 1:A:1259:MET:SD | 1:A:1259:MET:HB2 | 2.40 | 0.61 |
| 2:B:130:VAL:CG2 | 2:B:167:ILE:HD11 | 2.20 | 0.61 |
| 2:B:498:THR:CG2 | 2:B:537:LYS:HB2 | 2.30 | 0.61 |
| 9:K:110:ASN:C | 9:K:112:GLN:H | 2.00 | 0.61 |
| 1:A:636:GLU:OE2 | 1:A:962:ARG:HD2 | 2.01 | 0.61 |
| 1:A:1436:ILE:HD12 | 1:A:1436:ILE:O | 2.00 | 0.61 |
| 2:B:251:ILE:O | 2:B:251:ILE:CG2 | 2.48 | 0.61 |
| 1:A:44:THR:CB | 1:A:44:THR:C | 2.67 | 0.61 |
| 1:A:567:LYS:CE | 6:H:95:TYR:CE2 | 2.83 | 0.61 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:N | 2.11 | 0.61 |
| 1:A:1118:VAL:HB | 1:A:1327:ILE:CD1 | 2.30 | 0.61 |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CG | 2.12 | 0.61 |
| 7:I:4:PHE:CZ | 7:I:13:MET:HE1 | 2.34 | 0.61 |
| 1:A:1323:ASP:OD1 | 1:A:1325:THR:HB | 1.99 | 0.61 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HB | 1.83 | 0.61 |
| 6:H:47:PHE:CZ | 6:H:146:ARG:HD2 | 2.36 | 0.61 |
| 5:F:81:THR:HG23 | 5:F:136:ARG:NH1 | 2.16 | 0.61 |
| 8:J:2:ILE:HG22 | 8:J:3:VAL:H | 1.65 | 0.61 |
| 9:K:12:LEU:N | 9:K:12:LEU:HD12 | 2.15 | 0.61 |
| 1:A:107:CYS:SG | 1:A:148:CYS:HB2 | 2.40 | 0.61 |
| 2:B:128:LEU:O | 2:B:167:ILE:HD12 | 2.00 | 0.61 |
| 4:E:129:PRO:CD | 4:E:130:ALA:H | 2.13 | 0.61 |
| 5:F:73:ALA:HB2 | 5:F:143:PHE:CZ | 2.35 | 0.61 |
| 6:H:26:ILE:HD12 | 6:H:42:ILE:HD12 | 1.81 | 0.61 |
| 1:A:1318:THR:HG23 | 4:E:11:ARG:HH12 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:191:LYS:NZ | 4:E:191:LYS:CD | 2.64 | 0.61 |
| 6:H:8:ASP:OD2 | 6:H:9:ILE:N | 2.27 | 0.61 |
| 6:H:114:VAL:HG11 | 6:H:134:ASN:HD22 | 1.66 | 0.61 |
| 1:A:567:LYS:CB | 1:A:568:PRO:CD | 2.79 | 0.60 |
| 4:E:65:THR:O | 4:E:69:ILE:HG13 | 2.01 | 0.60 |
| 8:J:53:HIS:CE1 | 8:J:54:VAL:C | 2.74 | 0.60 |
| 1:A:72:GLU:OE2 | 2:B:1175:LEU:CD1 | 2.45 | 0.60 |
| 1:A:1266:THR:O | 1:A:1267:MET:C | 2.39 | 0.60 |
| 2:B:550:ASP:OD1 | 2:B:551:PRO:HD2 | 2.01 | 0.60 |
| 2:B:995:ARG:HD2 | 2:B:997:GLU:OE2 | 2.01 | 0.60 |
| 3:C:242:GLN:NE2 | 3:C:246:ARG:HE | 1.98 | 0.60 |
| 1:A:858:ASN:HD21 | 1:A:860:LEU:HB2 | 1.65 | 0.60 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:CD2 | 2.31 | 0.60 |
| 7:I:16:PRO:HG3 | 7:I:27:PHE:CE2 | 2.37 | 0.60 |
| 1:A:595:THR:HG22 | 1:A:596:THR:N | 2.16 | 0.60 |
| 2:B:879:ARG:NH2 | 2:B:885:MET:CE | 2.65 | 0.60 |
| 1:A:369:SER:CB | 9:K:2:ASN:HD21 | 2.12 | 0.60 |
| 1:A:571:LEU:CD2 | 1:A:571:LEU:CD1 | 2.73 | 0.60 |
| 1:A:715:GLU:OE1 | 1:A:774:ARG:HD3 | 2.01 | 0.60 |
| 1:A:1236:LEU:C | 1:A:1237:ILE:CD1 | 2.70 | 0.60 |
| 6:H:130:ARG:HD2 | 6:H:130:ARG:O | 2.01 | 0.60 |
| 8:J:14:VAL:CG1 | 8:J:50:ILE:HD11 | 2.23 | 0.60 |
| 1:A:658:LEU:HD12 | 1:A:658:LEU:O | 2.01 | 0.60 |
| 1:A:895:LYS:CD | 1:A:895:LYS:NZ | 2.62 | 0.60 |
| 2:B:249:ARG:CZ | 2:B:415:GLN:HG3 | 2.32 | 0.60 |
| 2:B:775:LYS:CB | 2:B:775:LYS:HD2 | 2.31 | 0.60 |
| 1:A:562:THR:HG22 | 6:H:98:TYR:CD2 | 2.36 | 0.60 |
| 2:B:121:ASN:HA | 2:B:207:GLY:HA3 | 1.84 | 0.60 |
| 4:E:153:HIS:CE1 | 4:E:184:VAL:HG11 | 2.36 | 0.60 |
| 1:A:172:PRO:CD | 1:A:185:TRP:CD1 | 2.59 | 0.60 |
| 1:A:378:GLU:OE1 | 1:A:434:ARG:HD3 | 2.02 | 0.60 |
| 1:A:1146:VAL:O | 1:A:1146:VAL:CG1 | 2.50 | 0.60 |
| 1:A:1172:LEU:O | 1:A:1173:HIS:CG | 2.55 | 0.60 |
| 2:B:885:MET:CE | 2:B:885:MET:HB3 | 2.31 | 0.60 |
| 2:B:1166:CYS:O | 2:B:1167:GLY:C | 2.40 | 0.60 |
| 3:C:252:GLN:HE22 | 9:K:99:GLY:N | 2.00 | 0.60 |
| 1:A:500:GLU:OE2 | 1:A:1438:THR:HG21 | 2.01 | 0.59 |
| 2:B:787:VAL:O | 2:B:787:VAL:HG12 | 2.02 | 0.59 |
| 3:C:55:THR:O | 3:C:55:THR:HG22 | 2.01 | 0.59 |
| 3:C:162:GLY:HA3 | 3:C:170:TRP:CE2 | 2.38 | 0.59 |
| 6:H:11:GLN:NE2 | 6:H:52:GLN:HG2 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:680:THR:HG22 | 2:B:682:SER:N | 2.14 | 0.59 |
| 2:B:879:ARG:NH2 | 2:B:885:MET:HE2 | 2.17 | 0.59 |
| 2:B:916:THR:N | 2:B:935:ARG:O | 2.34 | 0.59 |
| 4:E:37:LEU:HD23 | 4:E:42:PHE:HB2 | 1.84 | 0.59 |
| 1:A:42:ASP:OD2 | 1:A:46:THR:C | 2.39 | 0.59 |
| 1:A:353:ILE:HD12 | 1:A:482:PHE:CE2 | 2.38 | 0.59 |
| 1:A:265:LYS:CE | 1:A:302:THR:CG2 | 2.80 | 0.59 |
| 2:B:118:ARG:HG3 | 2:B:204:ILE:HD13 | 1.83 | 0.59 |
| 4:E:78:LEU:HD11 | 4:E:109:ILE:HD12 | 1.84 | 0.59 |
| 9:K:55:LYS:CB | 9:K:81:TYR:HD1 | 2.15 | 0.59 |
| 1:A:804:TYR:O | 2:B:761:HIS:ND1 | 2.35 | 0.59 |
| 2:B:862:GLN:HE22 | 2:B:961:LEU:HD13 | 1.67 | 0.59 |
| 1:A:189:ARG:HG2 | 1:A:189:ARG:O | 2.03 | 0.59 |
| 1:A:679:ILE:CD1 | 1:A:732:LEU:HD12 | 2.32 | 0.59 |
| 1:A:1198:ASP:OD1 | 1:A:1200:ALA:HB3 | 2.02 | 0.59 |
| 2:B:899:ILE:HD11 | 2:B:911:ILE:HA | 1.84 | 0.59 |
| 3:C:40:GLU:C | 3:C:163:ILE:HD11 | 2.22 | 0.59 |
| 1:A:567:LYS:HB2 | 6:H:95:TYR:HA | 1.83 | 0.59 |
| 1:A:744:LYS:HD3 | 1:A:748:MET:SD | 2.43 | 0.59 |
| 1:A:1263:ILE:O | 1:A:1267:MET:HG3 | 2.03 | 0.59 |
| 1:A:1424:VAL:O | 1:A:1428:VAL:HG23 | 2.02 | 0.59 |
| 2:B:843:GLN:NE2 | 2:B:846:ILE:HG22 | 2.16 | 0.59 |
| 2:B:998:ASP:OD1 | 3:C:35:ARG:NH2 | 2.35 | 0.59 |
| 6:H:9:ILE:CB | 6:H:9:ILE:C | 2.68 | 0.59 |
| 1:A:3:GLY:CA | 1:A:76:GLU:HG2 | 2.33 | 0.59 |
| 1:A:679:ILE:HD11 | 1:A:729:ALA:O | 2.02 | 0.59 |
| 1:A:903:ASN:ND2 | 1:A:905:ASP:N | 2.50 | 0.59 |
| 2:B:282:ILE:HD11 | 2:B:317:CYS:HB3 | 1.85 | 0.59 |
| 2:B:1222:ARG:HH11 | 2:B:1222:ARG:CB | 2.15 | 0.59 |
| 3:C:94:LYS:NZ | 3:C:94:LYS:CD | 2.59 | 0.59 |
| 4:E:131:THR:CB | 4:E:131:THR:HA | 2.17 | 0.59 |
| 8:J:53:HIS:ND1 | 8:J:54:VAL:N | 2.50 | 0.59 |
| 1:A:122:MET:HG3 | 1:A:122:MET:O | 2.02 | 0.59 |
| 1:A:1077:THR:HG22 | 1:A:1078:GLN:NE2 | 2.17 | 0.59 |
| 6:H:103:LYS:HE3 | 6:H:135:LEU:O | 2.03 | 0.59 |
| 9:K:65:HIS:CD2 | 9:K:67:PHE:H | 2.19 | 0.59 |
| 2:B:1097:HIS:CE1 | 2:B:1102:LYS:HG3 | 2.38 | 0.58 |
| 3:C:120:ILE:H | 3:C:120:ILE:HD12 | 1.68 | 0.58 |
| 6:H:32:THR:HB | 6:H:33:GLN:OE1 | 2.03 | 0.58 |
| 1:A:535:THR:O | 1:A:575:LYS:HE2 | 2.03 | 0.58 |
| 2:B:531:GLN:HE21 | 2:B:532:ALA:H | 1.49 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1221:SER:OG | 5:F:72:LYS:HD2 | 2.02 | 0.58 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD2 | 2.27 | 0.58 |
| 1:A:683:ILE:HD13 | 1:A:725:ALA:HB1 | 1.85 | 0.58 |
| 3:C:239:PRO:O | 3:C:242:GLN:HB2 | 2.03 | 0.58 |
| 1:A:770:VAL:HG23 | 1:A:775:ILE:HD13 | 1.85 | 0.58 |
| 1:A:1325:THR:O | 4:E:148:GLU:HG2 | 2.02 | 0.58 |
| 2:B:705:MET:HB3 | 2:B:706:GLN:HE21 | 1.67 | 0.58 |
| 2:B:870:ILE:CB | 2:B:870:ILE:HA | 2.17 | 0.58 |
| 4:E:131:THR:CB | 4:E:131:THR:C | 2.65 | 0.58 |
| 7:I:7:CYS:SG | 7:I:32:CYS:SG | 3.00 | 0.58 |
| 1:A:40:THR:HG23 | 1:A:54:ASN:ND2 | 2.18 | 0.58 |
| 2:B:1097:HIS:HA | 2:B:1097:HIS:CG | 2.22 | 0.58 |
| 2:B:1154:ALA:CB | 2:B:1154:ALA:HA | 2.19 | 0.58 |
| 4:E:83:CYS:O | 4:E:113:GLN:NE2 | 2.35 | 0.58 |
| 1:A:280:GLU:HG3 | 1:A:289:ILE:HD12 | 1.86 | 0.58 |
| 1:A:464:PRO:O | 1:A:465:TYR:O | 2.22 | 0.58 |
| 2:B:134:LYS:O | 2:B:135:ARG:HG3 | 2.03 | 0.58 |
| 6:H:89:LEU:C | 6:H:91:ASP:N | 2.49 | 0.58 |
| 6:H:123:MET:CE | 6:H:142:LEU:HD22 | 2.33 | 0.58 |
| 1:A:107:CYS:SG | 1:A:148:CYS:CB | 2.92 | 0.58 |
| 1:A:247:ARG:HH11 | 1:A:263:THR:HG23 | 1.69 | 0.58 |
| 1:A:533:LYS:NZ | 1:A:745:GLN:HE22 | 2.01 | 0.58 |
| 1:A:56:PRO:O | 1:A:57:ARG:CG | 2.50 | 0.58 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:HH22 | 1.69 | 0.58 |
| 2:B:555:ILE:CD1 | 2:B:587:HIS:NE2 | 2.67 | 0.58 |
| 5:F:123:LYS:NZ | 5:F:123:LYS:HD2 | 2.16 | 0.58 |
| 6:H:113:ALA:CB | 6:H:124:ARG:HH21 | 2.17 | 0.58 |
| 7:I:111:THR:HG21 | 7:I:113:ASP:HB2 | 1.86 | 0.58 |
| 1:A:555:ASP:OD1 | 9:K:26:LYS:NZ | 2.37 | 0.58 |
| 2:B:51:PHE:HZ | 2:B:172:ILE:HD13 | 1.68 | 0.58 |
| 2:B:561:TRP:O | 2:B:590:HIS:CE1 | 2.51 | 0.58 |
| 10:L:38:LEU:HG | 10:L:39:SER:H | 1.67 | 0.58 |
| 2:B:1152:MET:HA | 2:B:1152:MET:CE | 2.34 | 0.58 |
| 10:L:47:ARG:HG2 | 10:L:48:CYS:N | 2.18 | 0.58 |
| 1:A:1166:ASP:CB | 1:A:1169:ILE:CG2 | 2.82 | 0.57 |
| 6:H:130:ARG:HB2 | 6:H:133:ASN:CB | 2.33 | 0.57 |
| 7:I:3:THR:CG2 | 7:I:3:THR:OG1 | 2.47 | 0.57 |
| 8:J:3:VAL:HA | 8:J:53:HIS:CD2 | 2.39 | 0.57 |
| 9:K:26:LYS:CD | 9:K:26:LYS:CB | 2.81 | 0.57 |
| 2:B:914:LYS:H | 2:B:938:SER:HB2 | 1.69 | 0.57 |
| 9:K:35:PHE:CE1 | 9:K:73:LEU:HD12 | 2.36 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:362:ASP:OD1 | 1:A:459:ARG:HD3 | 2.04 | 0.57 |
| 2:B:1084:GLN:C | 2:B:1085:ILE:HD12 | 2.25 | 0.57 |
| 3:C:80:LEU:HD22 | 3:C:129:ILE:CD1 | 2.34 | 0.57 |
| 3:C:252:GLN:HE22 | 9:K:99:GLY:CA | 2.18 | 0.57 |
| 5:F:74:ILE:HD12 | 5:F:144:GLU:HG2 | 1.86 | 0.57 |
| 3:C:10:ILE:HD12 | 9:K:108:GLU:O | 2.04 | 0.57 |
| 3:C:55:THR:HB | 3:C:152:GLU:H | 1.69 | 0.57 |
| 1:A:231:PRO:O | 1:A:234:MET:HG3 | 2.05 | 0.57 |
| 1:A:1080:THR:CB | 1:A:1080:THR:N | 2.64 | 0.57 |
| 5:F:89:GLU:HG2 | 5:F:134:ILE:HD13 | 1.85 | 0.57 |
| 6:H:32:THR:HG22 | 6:H:33:GLN:CD | 2.25 | 0.57 |
| 10:L:34:CYS:SG | 10:L:36:SER:OG | 2.63 | 0.57 |
| 1:A:61:ILE:CA | 1:A:61:ILE:CG1 | 2.78 | 0.57 |
| 1:A:587:HIS:NE2 | 1:A:969:GLN:HG2 | 2.19 | 0.57 |
| 2:B:890:TYR:OH | 2:B:936:ASP:OD1 | 2.19 | 0.57 |
| 6:H:47:PHE:CB | 6:H:95:TYR:CD1 | 2.88 | 0.57 |
| 6:H:114:VAL:HG11 | 6:H:134:ASN:ND2 | 2.18 | 0.57 |
| 7:I:16:PRO:O | 7:I:17:ARG:CD | 2.42 | 0.57 |
| 1:A:351:THR:HG21 | 2:B:1103:ILE:CG1 | 2.35 | 0.57 |
| 9:K:18:LYS:HE3 | 9:K:38:GLU:HG2 | 1.85 | 0.57 |
| 2:B:167:ILE:HG22 | 2:B:167:ILE:O | 2.05 | 0.57 |
| 2:B:516:ASN:HD22 | 2:B:516:ASN:H | 1.51 | 0.57 |
| 4:E:169:ARG:HD3 | 5:F:140:ASP:OD2 | 2.05 | 0.57 |
| 8:J:14:VAL:HG13 | 8:J:50:ILE:CD1 | 2.27 | 0.57 |
| 2:B:117:ALA:HA | 2:B:122:LEU:HB2 | 1.86 | 0.56 |
| 2:B:95:ILE:HG22 | 2:B:96:TYR:N | 2.20 | 0.56 |
| 2:B:555:ILE:HD13 | 2:B:587:HIS:CE1 | 2.37 | 0.56 |
| 1:A:903:ASN:HD21 | 1:A:905:ASP:HB2 | 1.70 | 0.56 |
| 1:A:982:THR:HB | 1:A:985:ASP:OD2 | 2.05 | 0.56 |
| 6:H:6:PHE:CG | 6:H:7:ASP:N | 2.73 | 0.56 |
| 6:H:118:PHE:O | 6:H:119:GLY:C | 2.44 | 0.56 |
| 3:C:102:GLN:CG | 3:C:102:GLN:N | 2.68 | 0.56 |
| 3:C:133:ILE:O | 3:C:134:ILE:HD13 | 2.05 | 0.56 |
| 1:A:155:GLU:HB2 | 1:A:156:ASP:OD2 | 2.06 | 0.56 |
| 3:C:114:TYR:CD2 | 3:C:140:ASN:HB3 | 2.40 | 0.56 |
| 5:F:114:GLU:HB2 | 5:F:120:ILE:HD13 | 1.88 | 0.56 |
| 1:A:1385:THR:CG2 | 1:A:1385:THR:C | 2.74 | 0.56 |
| 2:B:705:MET:HE3 | 2:B:705:MET:CG | 2.24 | 0.56 |
| 1:A:843:LYS:CD | 1:A:843:LYS:NZ | 2.67 | 0.56 |
| 3:C:209:TYR:N | 3:C:209:TYR:CD1 | 2.73 | 0.56 |
| 1:A:120:GLU:HG2 | 1:A:123:ARG:HH22 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:385:ILE:O | 1:A:385:ILE:HD13 | 2.06 | 0.56 |
| 1:A:846:GLU:HA | 1:A:1066:VAL:HG23 | 1.86 | 0.56 |
| 2:B:566:LEU:HD13 | 2:B:588:GLY:HA2 | 1.87 | 0.56 |
| 3:C:33:LEU:CD1 | 3:C:248:ILE:HD13 | 2.36 | 0.56 |
| 4:E:117:THR:OG1 | 4:E:120:ALA:HB3 | 2.06 | 0.56 |
| 4:E:129:PRO:HD2 | 4:E:130:ALA:H | 1.70 | 0.56 |
| 6:H:55:LEU:HD22 | 6:H:144:ILE:CD1 | 2.33 | 0.56 |
| 1:A:844:ALA:CB | 1:A:1384:VAL:HG12 | 2.35 | 0.56 |
| 2:B:864:LYS:HD2 | 2:B:871:THR:OG1 | 2.05 | 0.56 |
| 1:A:44:THR:CA | 1:A:44:THR:HB | 2.18 | 0.56 |
| 1:A:567:LYS:CB | 1:A:568:PRO:HD3 | 2.35 | 0.56 |
| 1:A:1410:PHE:HD2 | 2:B:1212:ILE:HD11 | 1.71 | 0.56 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:N | 2.21 | 0.56 |
| 6:H:104:PHE:C | 6:H:104:PHE:HA | 2.10 | 0.56 |
| 6:H:127:GLY:O | 6:H:128:ASN:HB2 | 2.05 | 0.56 |
| 1:A:84:ILE:CG2 | 1:A:241:VAL:CG2 | 2.84 | 0.55 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:CB | 2.34 | 0.55 |
| 1:A:1127:ASP:HB3 | 1:A:1130:GLN:H | 1.70 | 0.55 |
| 2:B:605:ARG:NE | 2:B:639:ILE:HD11 | 2.21 | 0.55 |
| 1:A:679:ILE:HD12 | 1:A:729:ALA:CB | 2.36 | 0.55 |
| 1:A:50:ILE:HG22 | 1:A:52:GLY:N | 2.20 | 0.55 |
| 1:A:1215:ARG:CG | 1:A:1215:ARG:CA | 2.79 | 0.55 |
| 2:B:436:VAL:CB | 2:B:436:VAL:HA | 2.20 | 0.55 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HG12 | 1.87 | 0.55 |
| 1:A:784:LEU:HB3 | 1:A:786:HIS:HD2 | 1.71 | 0.55 |
| 2:B:280:ILE:HD12 | 2:B:280:ILE:N | 2.21 | 0.55 |
| 3:C:265:MET:CE | 3:C:265:MET:CG | 2.84 | 0.55 |
| 7:I:64:SER:O | 7:I:66:PRO:HD3 | 2.07 | 0.55 |
| 10:L:61:THR:CG2 | 10:L:61:THR:OG1 | 2.48 | 0.55 |
| 10:L:51:CYS:SG | 10:L:53:HIS:HB2 | 2.47 | 0.55 |
| 9:K:18:LYS:CE | 9:K:38:GLU:OE2 | 2.55 | 0.55 |
| 1:A:135:PHE:CE1 | 1:A:222:LEU:HD22 | 2.42 | 0.55 |
| 1:A:897:TYR:CD2 | 1:A:936:LEU:HD13 | 2.42 | 0.55 |
| 2:B:68:THR:HG23 | 2:B:91:SER:HB3 | 1.89 | 0.55 |
| 2:B:620:ARG:CG | 2:B:620:ARG:HE | 2.18 | 0.55 |
| 1:A:41:MET:O | 1:A:50:ILE:HD11 | 2.06 | 0.55 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:CA | 2.37 | 0.55 |
| 1:A:1105:LEU:O | 1:A:1383:SER:OG | 2.23 | 0.55 |
| 1:A:903:ASN:C | 1:A:903:ASN:HD22 | 2.09 | 0.55 |
| 1:A:1146:VAL:O | 1:A:1146:VAL:HG13 | 2.07 | 0.55 |
| 1:A:1445:ILE:CG2 | 1:A:1445:ILE:HA | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:840:ARG:CD | 1:A:840:ARG:CB | 2.79 | 0.55 |
| 2:B:984:HIS:CD2 | 2:B:1025:HIS:HA | 2.42 | 0.55 |
| 3:C:15:LYS:CD | 3:C:15:LYS:CB | 2.84 | 0.55 |
| 3:C:29:MET:CE | 3:C:29:MET:HB2 | 2.37 | 0.55 |
| 6:H:47:PHE:CG | 6:H:95:TYR:CD1 | 2.95 | 0.55 |
| 6:H:106:GLU:O | 6:H:108:SER:N | 2.40 | 0.55 |
| 1:A:3:GLY:HA3 | 1:A:76:GLU:HG2 | 1.90 | 0.54 |
| 2:B:98:THR:HB | 2:B:99:LYS:O | 2.08 | 0.54 |
| 4:E:147:HIS:CD2 | 4:E:149:LEU:HB2 | 2.43 | 0.54 |
| 6:H:32:THR:CB | 6:H:33:GLN:OE1 | 2.55 | 0.54 |
| 1:A:567:LYS:CD | 6:H:95:TYR:CD1 | 2.91 | 0.54 |
| 1:A:597:LEU:CD1 | 1:A:597:LEU:HG | 2.21 | 0.54 |
| 1:A:1261:LYS:CD | 1:A:1261:LYS:NZ | 2.67 | 0.54 |
| 2:B:1198:TYR:CE1 | 2:B:1201:LYS:HD2 | 2.42 | 0.54 |
| 3:C:102:GLN:N | 3:C:102:GLN:HG2 | 2.21 | 0.54 |
| 3:C:116:LYS:CE | 3:C:116:LYS:CG | 2.81 | 0.54 |
| 6:H:138:GLU:O | 6:H:139:ASN:O | 2.25 | 0.54 |
| 7:I:98:VAL:HG22 | 7:I:99:LEU:N | 2.20 | 0.54 |
| 1:A:540:PHE:O | 1:A:541:ILE:HD13 | 2.07 | 0.54 |
| 1:A:1169:ILE:HD11 | 1:A:1227:ILE:HD12 | 1.89 | 0.54 |
| 2:B:526:GLU:HG2 | 2:B:538:ASN:ND2 | 2.23 | 0.54 |
| 6:H:4:THR:O | 6:H:5:LEU:HD23 | 2.08 | 0.54 |
| 10:L:28:LYS:O | 10:L:59:ALA:HB3 | 2.07 | 0.54 |
| 1:A:295:LEU:CD2 | 1:A:295:LEU:CD1 | 2.79 | 0.54 |
| 1:A:679:ILE:CD1 | 1:A:732:LEU:HB2 | 2.25 | 0.54 |
| 2:B:203:PHE:HB3 | 2:B:205:ILE:CD1 | 2.36 | 0.54 |
| 3:C:252:GLN:CB | 3:C:252:GLN:CD | 2.72 | 0.54 |
| 6:H:103:LYS:CB | 6:H:105:GLU:OE1 | 2.54 | 0.54 |
| 1:A:53:LEU:HD23 | 1:A:54:ASN:H | 1.70 | 0.54 |
| 1:A:237:THR:CG2 | 1:A:237:THR:HB | 2.19 | 0.54 |
| 1:A:1151:GLU:CG | 7:I:45:ARG:CD | 2.85 | 0.54 |
| 2:B:1006:ILE:HD11 | 8:J:43:ARG:HB2 | 1.90 | 0.54 |
| 8:J:42:LYS:CE | 8:J:42:LYS:CG | 2.83 | 0.54 |
| 4:E:154:ILE:HD13 | 4:E:199:ILE:HD12 | 1.90 | 0.54 |
| 1:A:1172:LEU:C | 1:A:1173:HIS:CD2 | 2.81 | 0.54 |
| 1:A:1226:VAL:HG12 | 1:A:1227:ILE:N | 2.20 | 0.54 |
| 2:B:98:THR:OG1 | 2:B:127:GLY:O | 2.25 | 0.54 |
| 2:B:864:LYS:HG3 | 2:B:865:LYS:N | 2.21 | 0.54 |
| 7:I:35:VAL:O | 7:I:35:VAL:HG23 | 2.06 | 0.54 |
| 1:A:605:MET:HE3 | 1:A:607:ILE:CD1 | 2.32 | 0.54 |
| 1:A:31:SER:CB | 1:A:83:HIS:CD2 | 2.83 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:369:SER:H | 9:K:2:ASN:ND2 | 2.00 | 0.54 |
| 1:A:903:ASN:HD22 | 1:A:905:ASP:N | 2.05 | 0.54 |
| 1:A:1166:ASP:CA | 1:A:1169:ILE:HG22 | 2.37 | 0.54 |
| 2:B:26:THR:O | 2:B:27:ALA:C | 2.45 | 0.54 |
| 2:B:899:ILE:HG22 | 2:B:900:ALA:H | 1.72 | 0.54 |
| 2:B:983:ARG:HD3 | 14:B:3009:HOH:O | 2.08 | 0.54 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:N | 2.71 | 0.54 |
| 1:A:446:ARG:HH11 | 1:A:446:ARG:CG | 2.19 | 0.53 |
| 2:B:841:MET:CE | 2:B:990:ILE:HD11 | 2.37 | 0.53 |
| 6:H:59:ILE:HG22 | 6:H:60:ALA:N | 2.23 | 0.53 |
| 4:E:117:THR:OG1 | 4:E:120:ALA:HB2 | 2.09 | 0.53 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:CD2 | 2.44 | 0.53 |
| 2:B:102:VAL:O | 2:B:109:THR:HA | 2.09 | 0.53 |
| 2:B:906:SER:O | 2:B:907:GLY:C | 2.46 | 0.53 |
| 3:C:80:LEU:HD12 | 3:C:94:LYS:O | 2.08 | 0.53 |
| 1:A:84:ILE:HG22 | 1:A:241:VAL:CG2 | 2.38 | 0.53 |
| 1:A:134:ARG:O | 1:A:138:ILE:CG2 | 2.55 | 0.53 |
| 1:A:189:ARG:O | 1:A:190:ALA:CB | 2.55 | 0.53 |
| 1:A:518:LYS:NZ | 1:A:518:LYS:HD3 | 2.14 | 0.53 |
| 1:A:601:LYS:CD | 1:A:601:LYS:NZ | 2.70 | 0.53 |
| 1:A:913:LEU:HD11 | 1:A:981:LEU:O | 2.08 | 0.53 |
| 3:C:40:GLU:OE1 | 3:C:254:LYS:NZ | 2.42 | 0.53 |
| 3:C:80:LEU:HD22 | 3:C:129:ILE:HD13 | 1.91 | 0.53 |
| 5:F:109:VAL:HG22 | 5:F:127:GLU:OE1 | 2.09 | 0.53 |
| 6:H:91:ASP:OD1 | 6:H:91:ASP:C | 2.45 | 0.53 |
| 9:K:88:LYS:O | 9:K:89:ASN:C | 2.45 | 0.53 |
| 1:A:172:PRO:HG2 | 1:A:185:TRP:CH2 | 2.31 | 0.53 |
| 1:A:636:GLU:OE2 | 1:A:962:ARG:CD | 2.56 | 0.53 |
| 2:B:999:MET:HB3 | 2:B:1000:PRO:HD2 | 1.89 | 0.53 |
| 3:C:8:VAL:CG1 | 3:C:9:LYS:H | 2.22 | 0.53 |
| 3:C:70:ILE:HD11 | 3:C:144:ILE:HD12 | 1.90 | 0.53 |
| 6:H:95:TYR:CD2 | 6:H:95:TYR:C | 2.82 | 0.53 |
| 2:B:620:ARG:HG2 | 7:I:62:ILE:CD1 | 2.38 | 0.53 |
| 3:C:242:GLN:HE21 | 3:C:246:ARG:HH21 | 1.56 | 0.53 |
| 1:A:93:VAL:HA | 1:A:96:ILE:CD1 | 2.39 | 0.53 |
| 1:A:154:SER:O | 1:A:155:GLU:C | 2.47 | 0.53 |
| 1:A:1130:GLN:CG | 1:A:1130:GLN:NE2 | 2.65 | 0.53 |
| 2:B:249:ARG:NH1 | 2:B:418:LYS:NZ | 2.57 | 0.53 |
| 6:H:81:PRO:HB2 | 6:H:82:PRO:CD | 2.37 | 0.53 |
| 6:H:62:SER:O | 6:H:63:LEU:O | 2.26 | 0.53 |
| 1:A:704:ALA:HB1 | 1:A:708:MET:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:N | 2.24 | 0.53 |
| 2:B:1152:MET:HA | 2:B:1152:MET:HE2 | 1.90 | 0.53 |
| 5:F:72:LYS:CE | 5:F:72:LYS:CG | 2.85 | 0.53 |
| 10:L:58:LYS:O | 10:L:59:ALA:CB | 2.54 | 0.53 |
| 1:A:106:VAL:HG21 | 1:A:214:ILE:HG12 | 1.90 | 0.53 |
| 1:A:458:HIS:CE1 | 1:A:507:VAL:HG21 | 2.43 | 0.53 |
| 1:A:1151:GLU:HG2 | 7:I:45:ARG:CD | 2.39 | 0.53 |
| 3:C:169:LYS:NZ | 10:L:69:ALA:O | 2.41 | 0.53 |
| 4:E:93:MET:HE3 | 4:E:116:ILE:HG21 | 1.91 | 0.53 |
| 6:H:37:LYS:O | 6:H:125:LEU:HA | 2.09 | 0.53 |
| 7:I:49:ILE:HG22 | 7:I:49:ILE:O | 2.09 | 0.53 |
| 1:A:63:ARG:HA | 1:A:74:MET:SD | 2.49 | 0.52 |
| 1:A:535:THR:HG23 | 1:A:616:VAL:HA | 1.91 | 0.52 |
| 1:A:741:ASN:HD22 | 1:A:741:ASN:C | 2.12 | 0.52 |
| 2:B:313:MET:CE | 2:B:386:LEU:HD22 | 2.39 | 0.52 |
| 4:E:37:LEU:CD1 | 4:E:37:LEU:HG | 2.20 | 0.52 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:CE1 | 2.42 | 0.52 |
| 1:A:752:LYS:HD2 | 2:B:1015:HIS:O | 2.09 | 0.52 |
| 2:B:431:TYR:CE1 | 2:B:447:ALA:CB | 2.91 | 0.52 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:N | 2.56 | 0.52 |
| 1:A:541:ILE:HD11 | 1:A:656:TRP:HE1 | 1.73 | 0.52 |
| 6:H:9:ILE:CA | 6:H:9:ILE:CG2 | 2.81 | 0.52 |
| 1:A:407:ARG:O | 1:A:408:ASP:C | 2.48 | 0.52 |
| 1:A:588:LEU:HD23 | 1:A:588:LEU:C | 2.29 | 0.52 |
| 1:A:964:ILE:CD1 | 1:A:964:ILE:N | 2.72 | 0.52 |
| 1:A:1262:LYS:CG | 1:A:1262:LYS:CE | 2.82 | 0.52 |
| 4:E:127:ILE:N | 4:E:128:PRO:CD | 2.72 | 0.52 |
| 1:A:351:THR:HG23 | 2:B:1103:ILE:CG1 | 2.40 | 0.52 |
| 1:A:1318:THR:CG2 | 4:E:11:ARG:HH12 | 2.22 | 0.52 |
| 2:B:424:LEU:O | 2:B:428:ILE:HG13 | 2.08 | 0.52 |
| 6:H:55:LEU:CD2 | 6:H:144:ILE:HD12 | 2.33 | 0.52 |
| 1:A:98:LYS:HB3 | 1:A:234:MET:CE | 2.39 | 0.52 |
| 1:A:120:GLU:HG2 | 1:A:123:ARG:NH2 | 2.25 | 0.52 |
| 1:A:186:LYS:HZ3 | 1:A:195:ASP:HA | 1.69 | 0.52 |
| 1:A:1341:ILE:HD13 | 4:E:212:ARG:NH2 | 2.24 | 0.52 |
| 3:C:114:TYR:HB3 | 3:C:140:ASN:O | 2.10 | 0.52 |
| 3:C:148:ARG:O | 3:C:149:LYS:C | 2.48 | 0.52 |
| 5:F:83:PRO:HA | 5:F:146:TRP:CZ3 | 2.44 | 0.52 |
| 1:A:42:ASP:OD2 | 1:A:47:ARG:CG | 2.58 | 0.52 |
| 2:B:789:MET:CE | 2:B:789:MET:CG | 2.88 | 0.52 |
| 13:B:3008:GTP:N9 | 13:B:3008:GTP:C2' | 2.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:973:ILE:CG2 | 1:A:973:ILE:CA | 2.82 | 0.52 |
| 1:A:973:ILE:CG2 | 1:A:973:ILE:CG1 | 2.81 | 0.52 |
| 1:A:1035:TYR:O | 1:A:1036:ARG:HB2 | 2.10 | 0.52 |
| 1:A:1256:GLU:HB3 | 1:A:1259:MET:HE2 | 1.92 | 0.52 |
| 2:B:59:LEU:HG | 2:B:95:ILE:HD13 | 1.92 | 0.52 |
| 2:B:775:LYS:CG | 2:B:775:LYS:CA | 2.82 | 0.52 |
| 3:C:94:LYS:NZ | 3:C:94:LYS:CG | 2.72 | 0.52 |
| 7:I:43:VAL:O | 7:I:43:VAL:HG12 | 2.09 | 0.52 |
| 1:A:186:LYS:HG3 | 1:A:197:PRO:HD3 | 1.92 | 0.51 |
| 1:A:1236:LEU:C | 1:A:1237:ILE:HD13 | 2.31 | 0.51 |
| 2:B:757:PRO:HG2 | 2:B:984:HIS:HE1 | 1.75 | 0.51 |
| 3:C:178:PHE:C | 3:C:178:PHE:CD2 | 2.84 | 0.51 |
| 4:E:52:ARG:HG3 | 4:E:53:PRO:HD3 | 1.91 | 0.51 |
| 10:L:68:GLU:O | 10:L:69:ALA:HB3 | 2.10 | 0.51 |
| 1:A:186:LYS:NZ | 1:A:195:ASP:CA | 2.67 | 0.51 |
| 1:A:1287:TYR:O | 1:A:1302:PRO:HA | 2.10 | 0.51 |
| 1:A:1341:ILE:CD1 | 1:A:1379:GLY:HA2 | 2.36 | 0.51 |
| 2:B:864:LYS:HB2 | 2:B:871:THR:HA | 1.92 | 0.51 |
| 3:C:73:GLN:HA | 3:C:133:ILE:HD11 | 1.91 | 0.51 |
| 7:I:45:ARG:CD | 7:I:45:ARG:CB | 2.80 | 0.51 |
| 1:A:34:LYS:O | 1:A:35:ILE:C | 2.48 | 0.51 |
| 1:A:73:GLY:C | 1:A:75:ASN:N | 2.61 | 0.51 |
| 1:A:598:LEU:HD21 | 6:H:124:ARG:HB2 | 1.92 | 0.51 |
| 2:B:612:GLU:O | 2:B:612:GLU:HG3 | 2.11 | 0.51 |
| 2:B:43:LEU:HD11 | 2:B:811:TYR:O | 2.11 | 0.51 |
| 2:B:705:MET:CE | 2:B:705:MET:HG3 | 2.36 | 0.51 |
| 2:B:843:GLN:HE22 | 2:B:846:ILE:HG21 | 1.75 | 0.51 |
| 3:C:209:TYR:HD1 | 3:C:209:TYR:N | 2.08 | 0.51 |
| 7:I:10:CYS:SG | 7:I:32:CYS:SG | 3.09 | 0.51 |
| 1:A:274:ILE:CB | 1:A:274:ILE:C | 2.70 | 0.51 |
| 1:A:689:LYS:O | 1:A:693:VAL:HG23 | 2.10 | 0.51 |
| 6:H:113:ALA:HB2 | 6:H:124:ARG:NH2 | 2.25 | 0.51 |
| 1:A:551:TYR:CD2 | 9:K:62:LYS:HD3 | 2.46 | 0.51 |
| 2:B:744:HIS:CD2 | 2:B:746:SER:H | 2.24 | 0.51 |
| 2:B:792:MET:SD | 2:B:857:ARG:NH2 | 2.84 | 0.51 |
| 2:B:1019:SER:HB2 | 13:B:3008:GTP:N7 | 2.26 | 0.51 |
| 4:E:162:ARG:CG | 4:E:162:ARG:CA | 2.86 | 0.51 |
| 7:I:14:LEU:HB3 | 7:I:27:PHE:HB3 | 1.92 | 0.51 |
| 1:A:110:CYS:SG | 1:A:167:CYS:SG | 3.09 | 0.51 |
| 1:A:229:SER:O | 1:A:229:SER:OG | 2.25 | 0.51 |
| 9:K:18:LYS:HE2 | 9:K:38:GLU:OE2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:F:81:THR:HG22 | 5:F:136:ARG:HH11 | 1.71 | 0.51 |
| 6:H:44:VAL:O | 6:H:44:VAL:HG13 | 2.11 | 0.51 |
| 1:A:55:ASP:C | 1:A:57:ARG:H | 2.09 | 0.51 |
| 1:A:135:PHE:HD1 | 1:A:222:LEU:HD22 | 1.75 | 0.51 |
| 1:A:189:ARG:O | 1:A:190:ALA:HB3 | 2.11 | 0.51 |
| 2:B:884:ARG:HG2 | 2:B:884:ARG:HH11 | 1.76 | 0.51 |
| 4:E:176:PRO:O | 4:E:212:ARG:HA | 2.11 | 0.51 |
| 6:H:6:PHE:CD2 | 6:H:6:PHE:C | 2.84 | 0.51 |
| 6:H:130:ARG:HB2 | 6:H:133:ASN:HB3 | 1.92 | 0.51 |
| 6:H:135:LEU:HD13 | 6:H:139:ASN:O | 2.11 | 0.51 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HG13 | 2.40 | 0.51 |
| 2:B:900:ALA:O | 2:B:901:PRO:C | 2.48 | 0.51 |
| 3:C:196:ASP:HB3 | 3:C:199:LYS:HG3 | 1.91 | 0.51 |
| 3:C:214:ASN:O | 3:C:217:ASP:HB2 | 2.11 | 0.51 |
| 6:H:142:LEU:HG | 6:H:143:LEU:N | 2.26 | 0.51 |
| 1:A:328:ARG:NH1 | 1:A:1405:THR:HG22 | 2.24 | 0.50 |
| 2:B:1051:THR:CG2 | 2:B:1053:GLU:H | 2.14 | 0.50 |
| 2:B:486:TYR:CZ | 2:B:1096:ARG:NH2 | 2.79 | 0.50 |
| 1:A:35:ILE:HD13 | 1:A:241:VAL:HG11 | 1.93 | 0.50 |
| 1:A:279:LEU:H | 1:A:281:HIS:H | 1.59 | 0.50 |
| 2:B:435:THR:O | 2:B:435:THR:CG2 | 2.59 | 0.50 |
| 2:B:436:VAL:CA | 2:B:436:VAL:CG2 | 2.79 | 0.50 |
| 2:B:662:MET:CE | 2:B:662:MET:CG | 2.90 | 0.50 |
| 3:C:41:ILE:C | 3:C:163:ILE:HD11 | 2.32 | 0.50 |
| 3:C:252:GLN:NE2 | 9:K:99:GLY:H | 2.09 | 0.50 |
| 9:K:111:LEU:N | 9:K:111:LEU:HD23 | 2.27 | 0.50 |
| 1:A:1348:LEU:HG | 1:A:1372:VAL:HG22 | 1.94 | 0.50 |
| 2:B:435:THR:HG23 | 2:B:437:GLU:HB2 | 1.93 | 0.50 |
| 3:C:29:MET:HB2 | 3:C:29:MET:HE2 | 1.92 | 0.50 |
| 3:C:162:GLY:HA3 | 3:C:170:TRP:CD2 | 2.46 | 0.50 |
| 6:H:77:ARG:HB2 | 6:H:77:ARG:HH11 | 1.76 | 0.50 |
| 1:A:121:LEU:HB3 | 1:A:141:LEU:HD21 | 1.94 | 0.50 |
| 1:A:365:GLY:HA2 | 1:A:461:LYS:O | 2.11 | 0.50 |
| 1:A:679:ILE:HD12 | 1:A:729:ALA:HB1 | 1.94 | 0.50 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:CD1 | 2.59 | 0.50 |
| 1:A:1449:SER:HB2 | 5:F:149:GLU:OE2 | 2.11 | 0.50 |
| 2:B:167:ILE:HD12 | 2:B:167:ILE:N | 2.26 | 0.50 |
| 2:B:846:ILE:HD11 | 2:B:974:PRO:C | 2.31 | 0.50 |
| 5:F:109:VAL:HG12 | 5:F:110:ASP:N | 2.24 | 0.50 |
| 9:K:46:ILE:O | 9:K:47:ARG:C | 2.40 | 0.50 |
| 1:A:93:VAL:HA | 1:A:96:ILE:HD13 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:466:SER:CB | 2:B:1103:ILE:HD11 | 2.41 | 0.50 |
| 1:A:587:HIS:CD2 | 1:A:966:ASN:OD1 | 2.58 | 0.50 |
| 1:A:664:THR:HG22 | 1:A:742:ASN:HB3 | 1.93 | 0.50 |
| 2:B:458:LYS:NZ | 2:B:958:GLN:NE2 | 2.59 | 0.50 |
| 2:B:757:PRO:HG2 | 2:B:984:HIS:CE1 | 2.47 | 0.50 |
| 2:B:436:VAL:CB | 2:B:436:VAL:N | 2.69 | 0.50 |
| 2:B:1097:HIS:CB | 2:B:1097:HIS:N | 2.66 | 0.50 |
| 1:A:1112:LYS:CG | 1:A:1112:LYS:CA | 2.81 | 0.50 |
| 8:J:4:PRO:HD3 | 8:J:53:HIS:HD2 | 1.77 | 0.50 |
| 1:A:63:ARG:HA | 1:A:74:MET:CG | 2.40 | 0.50 |
| 1:A:89:PRO:CB | 1:A:204:THR:HG21 | 2.28 | 0.50 |
| 2:B:512:ARG:HB2 | 14:B:3017:HOH:O | 2.12 | 0.50 |
| 2:B:843:GLN:NE2 | 2:B:846:ILE:HG21 | 2.27 | 0.50 |
| 1:A:55:ASP:N | 1:A:56:PRO:HD2 | 2.25 | 0.49 |
| 1:A:328:ARG:NH1 | 1:A:1405:THR:CG2 | 2.75 | 0.49 |
| 1:A:1081:LEU:CD2 | 1:A:1081:LEU:CD1 | 2.81 | 0.49 |
| 2:B:516:ASN:H | 2:B:516:ASN:ND2 | 2.10 | 0.49 |
| 2:B:956:THR:HA | 2:B:961:LEU:O | 2.12 | 0.49 |
| 7:I:16:PRO:HG3 | 7:I:27:PHE:HE2 | 1.76 | 0.49 |
| 1:A:69:THR:CG2 | 2:B:1174:LYS:HE2 | 2.42 | 0.49 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:N | 2.27 | 0.49 |
| 1:A:1224:LEU:HG | 1:A:1225:PHE:N | 2.27 | 0.49 |
| 3:C:252:GLN:NE2 | 9:K:99:GLY:N | 2.60 | 0.49 |
| 6:H:77:ARG:C | 6:H:78:SER:O | 2.49 | 0.49 |
| 10:L:48:CYS:HB3 | 10:L:51:CYS:O | 2.13 | 0.49 |
| 1:A:853:ASP:O | 1:A:854:ASN:HB2 | 2.12 | 0.49 |
| 1:A:867:ILE:HD12 | 1:A:1000:LEU:HD21 | 1.95 | 0.49 |
| 1:A:1195:LEU:HD11 | 1:A:1267:MET:HE1 | 1.93 | 0.49 |
| 2:B:235:SER:OG | 2:B:236:HIS:HD2 | 1.96 | 0.49 |
| 3:C:19:ASP:C | 3:C:19:ASP:OD1 | 2.50 | 0.49 |
| 6:H:103:LYS:HG2 | 6:H:105:GLU:OE2 | 2.12 | 0.49 |
| 10:L:26:THR:CG2 | 10:L:27:LEU:H | 2.26 | 0.49 |
| 2:B:393:LYS:HZ1 | 2:B:621:GLU:CD | 2.15 | 0.49 |
| 2:B:1014:PRO:HA | 2:B:1017:ILE:HD12 | 1.94 | 0.49 |
| 2:B:365:THR:HG22 | 2:B:367:LEU:H | 1.76 | 0.49 |
| 7:I:55:THR:CG2 | 7:I:55:THR:HB | 2.29 | 0.49 |
| 10:L:30:ILE:HG22 | 10:L:31:CYS:N | 2.27 | 0.49 |
| 10:L:32:ALA:HB2 | 10:L:55:ILE:HG22 | 1.93 | 0.49 |
| 1:A:1162:VAL:CG1 | 1:A:1162:VAL:O | 2.61 | 0.49 |
| 2:B:237:VAL:HG12 | 2:B:238:ALA:N | 2.28 | 0.49 |
| 2:B:360:PHE:O | 2:B:361:LEU:C | 2.51 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:252:GLN:HE22 | 9:K:99:GLY:HA2 | 1.75 | 0.49 |
| 6:H:19:ARG:CD | 6:H:19:ARG:HA | 2.43 | 0.49 |
| 7:I:65:ASP:C | 7:I:65:ASP:OD1 | 2.50 | 0.49 |
| 8:J:1:MET:C | 8:J:2:ILE:HD12 | 2.32 | 0.49 |
| 1:A:387:ARG:O | 1:A:388:LEU:C | 2.51 | 0.49 |
| 1:A:507:VAL:N | 1:A:508:PRO:CD | 2.75 | 0.49 |
| 1:A:560:ILE:HD12 | 1:A:560:ILE:N | 2.26 | 0.49 |
| 1:A:983:ILE:N | 1:A:983:ILE:HD12 | 2.28 | 0.49 |
| 2:B:284:ILE:HD11 | 2:B:321:GLY:HA2 | 1.94 | 0.49 |
| 2:B:453:ILE:HG22 | 2:B:454:THR:N | 2.28 | 0.49 |
| 3:C:177:GLU:HB2 | 3:C:231:ASN:HB3 | 1.95 | 0.49 |
| 1:A:156:ASP:C | 1:A:158:PRO:HD2 | 2.10 | 0.49 |
| 1:A:706:HIS:CE1 | 1:A:1135:ARG:HD3 | 2.48 | 0.49 |
| 1:A:1151:GLU:OE2 | 7:I:45:ARG:CD | 2.59 | 0.49 |
| 2:B:531:GLN:HE21 | 2:B:532:ALA:N | 2.10 | 0.49 |
| 6:H:103:LYS:CE | 6:H:135:LEU:O | 2.60 | 0.49 |
| 1:A:741:ASN:C | 1:A:741:ASN:ND2 | 2.67 | 0.49 |
| 1:A:1166:ASP:CA | 1:A:1169:ILE:CG2 | 2.91 | 0.49 |
| 1:A:1436:ILE:CD1 | 2:B:1144:ALA:HB2 | 2.42 | 0.49 |
| 2:B:121:ASN:HD21 | 2:B:965:LYS:NZ | 2.10 | 0.49 |
| 2:B:821:GLN:OE1 | 2:B:850:LEU:HD12 | 2.12 | 0.49 |
| 7:I:71:SER:OG | 7:I:83:ASN:ND2 | 2.45 | 0.49 |
| 1:A:1162:VAL:CG1 | 1:A:1162:VAL:CG2 | 2.81 | 0.48 |
| 4:E:124:VAL:HB | 4:E:125:PRO:HD3 | 1.95 | 0.48 |
| 10:L:38:LEU:O | 10:L:39:SER:HB2 | 2.13 | 0.48 |
| 1:A:44:THR:CB | 1:A:44:THR:HA | 2.21 | 0.48 |
| 1:A:531:ILE:O | 1:A:531:ILE:HD13 | 2.13 | 0.48 |
| 1:A:768:GLN:NE2 | 1:A:816:HIS:HA | 2.28 | 0.48 |
| 1:A:1111:MET:SD | 1:A:1111:MET:CB | 2.92 | 0.48 |
| 1:A:1161:THR:HG23 | 1:A:1163:ILE:H | 1.77 | 0.48 |
| 6:H:103:LYS:O | 6:H:115:TYR:CD1 | 2.63 | 0.48 |
| 1:A:144:THR:HG22 | 1:A:145:LYS:N | 2.28 | 0.48 |
| 1:A:278:THR:O | 1:A:278:THR:HG22 | 2.13 | 0.48 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:HD12 | 1.94 | 0.48 |
| 1:A:1318:THR:HG23 | 4:E:11:ARG:NH1 | 2.28 | 0.48 |
| 2:B:498:THR:HG21 | 2:B:537:LYS:HB2 | 1.95 | 0.48 |
| 2:B:1006:ILE:HD11 | 8:J:43:ARG:CB | 2.43 | 0.48 |
| 2:B:1153:GLU:OE1 | 2:B:1153:GLU:HA | 2.13 | 0.48 |
| 4:E:65:THR:O | 4:E:69:ILE:CG1 | 2.60 | 0.48 |
| 7:I:29:CYS:SG | 7:I:31:THR:HB | 2.54 | 0.48 |
| 1:A:786:HIS:N | 1:A:786:HIS:CD2 | 2.81 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:C | 2.33 | 0.48 |
| 8:J:1:MET:CE | 8:J:1:MET:HG3 | 2.43 | 0.48 |
| 10:L:47:ARG:CG | 10:L:48:CYS:N | 2.75 | 0.48 |
| 1:A:66:LYS:CB | 1:A:66:LYS:CD | 2.84 | 0.48 |
| 1:A:187:LYS:HD2 | 1:A:194:ALA:HB2 | 1.94 | 0.48 |
| 1:A:295:LEU:CD2 | 1:A:295:LEU:HG | 2.19 | 0.48 |
| 1:A:503:GLN:HE21 | 5:F:90:ARG:HH21 | 1.61 | 0.48 |
| 3:C:183:TRP:NE1 | 3:C:207:CYS:HB3 | 2.28 | 0.48 |
| 6:H:4:THR:C | 6:H:5:LEU:HD23 | 2.33 | 0.48 |
| 6:H:9:ILE:CA | 6:H:9:ILE:CG1 | 2.83 | 0.48 |
| 1:A:901:LEU:CD2 | 1:A:919:ILE:HD12 | 2.43 | 0.48 |
| 2:B:65:GLU:HG2 | 2:B:66:ASP:N | 2.27 | 0.48 |
| 2:B:213:ILE:HD13 | 2:B:481:GLN:HG3 | 1.95 | 0.48 |
| 2:B:350:GLN:HG3 | 2:B:350:GLN:O | 2.13 | 0.48 |
| 2:B:640:VAL:HG22 | 2:B:651:LEU:HD23 | 1.96 | 0.48 |
| 2:B:999:MET:HE3 | 2:B:999:MET:HG2 | 1.93 | 0.48 |
| 4:E:5:ASN:O | 4:E:9:ILE:HG13 | 2.13 | 0.48 |
| 6:H:5:LEU:O | 6:H:133:ASN:ND2 | 2.46 | 0.48 |
| 6:H:100:THR:O | 6:H:116:TYR:HA | 2.13 | 0.48 |
| 1:A:373:THR:O | 1:A:373:THR:HG22 | 2.12 | 0.48 |
| 2:B:758:PHE:N | 2:B:759:PRO:CD | 2.76 | 0.48 |
| 4:E:93:MET:CE | 4:E:116:ILE:HG21 | 2.43 | 0.48 |
| 7:I:58:VAL:HG11 | 7:I:109:ILE:HD11 | 1.96 | 0.48 |
| 9:K:10:PHE:HD1 | 9:K:11:LEU:HD13 | 1.78 | 0.48 |
| 1:A:153:PRO:CD | 1:A:161:LEU:CD2 | 2.66 | 0.48 |
| 1:A:466:SER:HB3 | 2:B:1103:ILE:HD11 | 1.94 | 0.48 |
| 1:A:476:SER:N | 1:A:477:PRO:HD2 | 2.29 | 0.48 |
| 1:A:518:LYS:CD | 1:A:518:LYS:HZ3 | 2.20 | 0.48 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:CD | 2.40 | 0.48 |
| 1:A:901:LEU:HD21 | 1:A:919:ILE:HD12 | 1.95 | 0.48 |
| 1:A:1102:LYS:CD | 1:A:1102:LYS:NZ | 2.69 | 0.48 |
| 2:B:1128:LEU:HG | 2:B:1128:LEU:O | 2.14 | 0.48 |
| 1:A:92:HIS:HD2 | 1:A:94:GLY:N | 2.12 | 0.48 |
| 2:B:1220:ARG:O | 2:B:1222:ARG:CD | 2.57 | 0.48 |
| 4:E:63:ASN:O | 4:E:64:PRO:C | 2.44 | 0.48 |
| 6:H:40:LEU:HD12 | 6:H:41:ASP:H | 1.78 | 0.48 |
| 1:A:55:ASP:H | 1:A:56:PRO:HD3 | 1.77 | 0.48 |
| 1:A:472:LEU:O | 1:A:475:THR:HB | 2.14 | 0.48 |
| 1:A:664:THR:HG21 | 1:A:746:MET:CE | 2.44 | 0.48 |
| 2:B:121:ASN:N | 2:B:121:ASN:HD22 | 2.11 | 0.48 |
| 2:B:185:THR:HG23 | 2:B:188:ASP:OD2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:203:PHE:HB3 | 2:B:205:ILE:HD11 | 1.96 | 0.48 |
| 2:B:498:THR:HG22 | 2:B:537:LYS:HB2 | 1.95 | 0.48 |
| 3:C:94:LYS:NZ | 3:C:94:LYS:HG2 | 2.28 | 0.48 |
| 9:K:18:LYS:HE3 | 9:K:38:GLU:CG | 2.44 | 0.48 |
| 9:K:82:ASP:OD1 | 9:K:83:PRO:HG2 | 2.14 | 0.48 |
| 5:F:109:VAL:HG13 | 5:F:110:ASP:N | 2.29 | 0.47 |
| 1:A:670:ILE:HD13 | 2:B:1067:ARG:CZ | 2.43 | 0.47 |
| 1:A:1232:ASN:CB | 1:A:1232:ASN:ND2 | 2.73 | 0.47 |
| 2:B:117:ALA:O | 2:B:207:GLY:HA2 | 2.14 | 0.47 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:N | 2.08 | 0.47 |
| 4:E:37:LEU:C | 4:E:38:PRO:O | 2.50 | 0.47 |
| 1:A:274:ILE:CA | 1:A:274:ILE:CG1 | 2.84 | 0.47 |
| 1:A:1291:VAL:O | 1:A:1291:VAL:HG12 | 2.10 | 0.47 |
| 2:B:864:LYS:O | 2:B:961:LEU:CD2 | 2.62 | 0.47 |
| 2:B:899:ILE:HD12 | 2:B:911:ILE:HA | 1.97 | 0.47 |
| 4:E:61:GLN:HG3 | 4:E:62:ALA:N | 2.29 | 0.47 |
| 9:K:65:HIS:CD2 | 9:K:66:PRO:HD2 | 2.49 | 0.47 |
| 1:A:64:ASN:O | 1:A:66:LYS:N | 2.46 | 0.47 |
| 1:A:399:HIS:HE1 | 1:A:436:ILE:O | 1.97 | 0.47 |
| 1:A:720:ARG:O | 1:A:724:GLU:HB3 | 2.14 | 0.47 |
| 1:A:1155:ASP:OD1 | 1:A:1162:VAL:HG23 | 2.14 | 0.47 |
| 1:A:1436:ILE:HD12 | 2:B:1144:ALA:HB2 | 1.97 | 0.47 |
| 4:E:117:THR:C | 4:E:119:SER:N | 2.67 | 0.47 |
| 6:H:105:GLU:C | 6:H:107:VAL:N | 2.63 | 0.47 |
| 1:A:84:ILE:HG22 | 1:A:241:VAL:HG21 | 1.96 | 0.47 |
| 1:A:138:ILE:HD12 | 1:A:142:CYS:SG | 2.54 | 0.47 |
| 1:A:913:LEU:HD12 | 1:A:913:LEU:C | 2.30 | 0.47 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N | 2.28 | 0.47 |
| 2:B:1177:HIS:HB2 | 2:B:1179:GLN:NE2 | 2.29 | 0.47 |
| 10:L:47:ARG:CG | 10:L:48:CYS:H | 2.18 | 0.47 |
| 2:B:101:MET:HA | 2:B:110:HIS:O | 2.14 | 0.47 |
| 2:B:616:ILE:HG12 | 2:B:697:GLU:HA | 1.96 | 0.47 |
| 2:B:724:ASP:O | 2:B:725:PRO:C | 2.51 | 0.47 |
| 2:B:727:LYS:HE2 | 2:B:1049:ASP:CG | 2.35 | 0.47 |
| 1:A:34:LYS:HG2 | 1:A:83:HIS:HE1 | 1.80 | 0.47 |
| 1:A:752:LYS:CD | 2:B:1015:HIS:O | 2.62 | 0.47 |
| 1:A:875:ALA:HB2 | 1:A:1366:ARG:HD3 | 1.96 | 0.47 |
| 1:A:1134:ILE:HG22 | 1:A:1306:LEU:HD11 | 1.97 | 0.47 |
| 1:A:1150:SER:OG | 7:I:46:HIS:HB3 | 2.15 | 0.47 |
| 1:A:1287:TYR:CD1 | 1:A:1305:VAL:HG21 | 2.49 | 0.47 |
| 2:B:169:ARG:O | 2:B:457:LEU:HD12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:259:TYR:HB2 | 2:B:268:THR:HG22 | 1.97 | 0.47 |
| 2:B:864:LYS:O | 2:B:961:LEU:HD23 | 2.13 | 0.47 |
| 2:B:1212:ILE:O | 2:B:1214:PRO:HD3 | 2.15 | 0.47 |
| 6:H:37:LYS:O | 6:H:125:LEU:HD23 | 2.14 | 0.47 |
| 6:H:76:THR:O | 6:H:76:THR:CG2 | 2.61 | 0.47 |
| 1:A:605:MET:HG3 | 1:A:607:ILE:HD12 | 1.97 | 0.47 |
| 2:B:97:VAL:HG12 | 2:B:178:ASN:HD21 | 1.80 | 0.47 |
| 2:B:616:ILE:HD13 | 2:B:696:GLU:HG3 | 1.97 | 0.47 |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:HB | 2.44 | 0.47 |
| 6:H:113:ALA:HA | 6:H:125:LEU:O | 2.15 | 0.47 |
| 1:A:269:ILE:HD11 | 1:A:300:VAL:HA | 1.97 | 0.47 |
| 1:A:1143:LEU:O | 1:A:1144:LYS:C | 2.53 | 0.47 |
| 2:B:955:THR:CG2 | 10:L:55:ILE:HA | 2.45 | 0.47 |
| 3:C:120:ILE:HD12 | 3:C:120:ILE:N | 2.29 | 0.47 |
| 1:A:237:THR:CG2 | 1:A:237:THR:C | 2.82 | 0.47 |
| 1:A:555:ASP:OD1 | 9:K:26:LYS:CE | 2.63 | 0.47 |
| 2:B:755:ILE:O | 2:B:755:ILE:HG22 | 2.14 | 0.47 |
| 1:A:413:ILE:N | 1:A:413:ILE:HD12 | 2.30 | 0.46 |
| 1:A:1445:ILE:HD13 | 1:A:1445:ILE:N | 2.30 | 0.46 |
| 2:B:916:THR:O | 2:B:916:THR:HG22 | 2.14 | 0.46 |
| 3:C:52:GLU:HA | 10:L:64:LEU:HD21 | 1.97 | 0.46 |
| 6:H:9:ILE:CA | 6:H:9:ILE:HB | 2.20 | 0.46 |
| 2:B:755:ILE:HD12 | 2:B:814:PHE:CD1 | 2.51 | 0.46 |
| 2:B:827:ILE:HG12 | 2:B:1012:ILE:HD11 | 1.96 | 0.46 |
| 2:B:1027:ILE:HG21 | 2:B:1027:ILE:HD13 | 1.56 | 0.46 |
| 1:A:110:CYS:SG | 1:A:167:CYS:CB | 3.04 | 0.46 |
| 1:A:119:ASN:O | 1:A:120:GLU:CB | 2.45 | 0.46 |
| 1:A:1154:TYR:CZ | 1:A:1156:PRO:HB3 | 2.51 | 0.46 |
| 2:B:566:LEU:HD12 | 2:B:566:LEU:HA | 1.78 | 0.46 |
| 2:B:844:SER:O | 2:B:847:ASP:HB2 | 2.15 | 0.46 |
| 3:C:66:ARG:O | 3:C:67:LEU:C | 2.53 | 0.46 |
| 1:A:26:GLU:HA | 1:A:29:ALA:HB3 | 1.96 | 0.46 |
| 1:A:1127:ASP:OD2 | 1:A:1130:GLN:HB2 | 2.15 | 0.46 |
| 2:B:134:LYS:HE3 | 2:B:134:LYS:HB2 | 1.74 | 0.46 |
| 2:B:820:GLY:HA3 | 2:B:1091:TYR:CZ | 2.51 | 0.46 |
| 6:H:101:ALA:HA | 6:H:116:TYR:H | 1.81 | 0.46 |
| 2:B:65:GLU:O | 2:B:67:SER:N | 2.49 | 0.46 |
| 2:B:1058:LEU:O | 2:B:1062:HIS:HD2 | 1.98 | 0.46 |
| 1:A:64:ASN:OD1 | 1:A:64:ASN:C | 2.53 | 0.46 |
| 1:A:153:PRO:CD | 1:A:161:LEU:HD22 | 2.30 | 0.46 |
| 1:A:523:ILE:HB | 1:A:622:VAL:CG1 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:567:LYS:HG2 | 6:H:96:VAL:O | 2.14 | 0.46 |
| 1:A:901:LEU:HD11 | 1:A:919:ILE:HD12 | 1.98 | 0.46 |
| 2:B:952:VAL:HG22 | 2:B:966:VAL:HG22 | 1.97 | 0.46 |
| 1:A:80:HIS:O | 1:A:243:PRO:HD3 | 2.16 | 0.46 |
| 1:A:551:TYR:CE2 | 9:K:62:LYS:HD3 | 2.50 | 0.46 |
| 1:A:595:THR:CG2 | 1:A:596:THR:N | 2.77 | 0.46 |
| 1:A:956:LEU:HB3 | 1:A:957:PRO:HD2 | 1.97 | 0.46 |
| 1:A:1055:ARG:NE | 1:A:1055:ARG:HG3 | 2.25 | 0.46 |
| 2:B:515:HIS:CB | 2:B:518:HIS:CD2 | 2.98 | 0.46 |
| 4:E:41:ASP:O | 4:E:42:PHE:C | 2.53 | 0.46 |
| 6:H:106:GLU:HB2 | 6:H:113:ALA:HB3 | 1.96 | 0.46 |
| 1:A:328:ARG:HH11 | 1:A:1405:THR:CG2 | 2.28 | 0.46 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD2 | 2.43 | 0.46 |
| 2:B:261:ARG:O | 2:B:264:SER:N | 2.48 | 0.46 |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:H | 1.80 | 0.46 |
| 4:E:44:ALA:O | 4:E:46:TYR:N | 2.49 | 0.46 |
| 4:E:61:GLN:HB2 | 4:E:79:TRP:HE3 | 1.81 | 0.46 |
| 9:K:78:THR:HG22 | 9:K:79:GLU:H | 1.81 | 0.46 |
| 10:L:26:THR:CG2 | 10:L:26:THR:OG1 | 2.57 | 0.46 |
| 1:A:34:LYS:HG2 | 1:A:83:HIS:CE1 | 2.51 | 0.46 |
| 2:B:622:LYS:NZ | 2:B:622:LYS:CD | 2.70 | 0.46 |
| 4:E:55:ARG:O | 4:E:58:MET:HB2 | 2.16 | 0.46 |
| 8:J:53:HIS:HD1 | 8:J:54:VAL:N | 2.13 | 0.46 |
| 1:A:919:ILE:HD13 | 1:A:983:ILE:CD1 | 2.45 | 0.46 |
| 1:A:920:LEU:HD22 | 1:A:921:GLY:N | 2.31 | 0.46 |
| 2:B:227:LYS:NZ | 2:B:236:HIS:HE1 | 2.13 | 0.46 |
| 4:E:161:LYS:CE | 4:E:172:GLU:OE2 | 2.64 | 0.46 |
| 5:F:89:GLU:CG | 5:F:134:ILE:HD13 | 2.45 | 0.46 |
| 6:H:113:ALA:CB | 6:H:124:ARG:NH2 | 2.79 | 0.46 |
| 6:H:113:ALA:HB2 | 6:H:124:ARG:HH21 | 1.81 | 0.46 |
| 1:A:535:THR:CG2 | 1:A:617:VAL:N | 2.66 | 0.45 |
| 1:A:1293:SER:HB2 | 1:A:1294:PRO:HD2 | 1.98 | 0.45 |
| 4:E:117:THR:C | 4:E:119:SER:H | 2.19 | 0.45 |
| 1:A:195:ASP:O | 1:A:196:GLU:CB | 2.64 | 0.45 |
| 1:A:265:LYS:HZ3 | 1:A:302:THR:HG21 | 1.77 | 0.45 |
| 1:A:1345:ARG:HG3 | 1:A:1376:THR:HG21 | 1.98 | 0.45 |
| 1:A:1410:PHE:HD2 | 2:B:1212:ILE:CD1 | 2.29 | 0.45 |
| 2:B:723:VAL:CA | 2:B:723:VAL:HB | 2.23 | 0.45 |
| 3:C:41:ILE:HA | 3:C:42:PRO:HD3 | 1.76 | 0.45 |
| 4:E:12:LEU:CD2 | 4:E:58:MET:SD | 2.88 | 0.45 |
| 5:F:128:LYS:NZ | 5:F:151:LEU:O | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:H:48:PRO:C | 6:H:49:VAL:HG23 | 2.36 | 0.45 |
| 6:H:123:MET:HE3 | 6:H:142:LEU:HD13 | 1.97 | 0.45 |
| 1:A:92:HIS:HD2 | 1:A:94:GLY:H | 1.64 | 0.45 |
| 1:A:436:ILE:HD13 | 1:A:436:ILE:HG21 | 1.63 | 0.45 |
| 3:C:15:LYS:O | 3:C:240:VAL:CG2 | 2.64 | 0.45 |
| 8:J:42:LYS:HG3 | 8:J:43:ARG:N | 2.32 | 0.45 |
| 1:A:98:LYS:O | 1:A:102:VAL:HG23 | 2.15 | 0.45 |
| 1:A:216:VAL:HA | 1:A:219:PHE:CE2 | 2.52 | 0.45 |
| 1:A:264:PHE:O | 1:A:267:ALA:HB3 | 2.17 | 0.45 |
| 1:A:1055:ARG:CG | 1:A:1055:ARG:HE | 2.27 | 0.45 |
| 1:A:1256:GLU:CB | 1:A:1259:MET:HE2 | 2.46 | 0.45 |
| 2:B:102:VAL:HG22 | 2:B:112:LEU:HD22 | 1.98 | 0.45 |
| 1:A:605:MET:CE | 1:A:607:ILE:CG1 | 2.95 | 0.45 |
| 1:A:1109:LYS:CG | 1:A:1109:LYS:CA | 2.80 | 0.45 |
| 2:B:121:ASN:HD22 | 2:B:121:ASN:H | 1.63 | 0.45 |
| 2:B:282:ILE:HD11 | 2:B:317:CYS:SG | 2.57 | 0.45 |
| 2:B:417:PHE:C | 2:B:417:PHE:HD2 | 2.16 | 0.45 |
| 2:B:642:ASP:HA | 2:B:643:ASP:HA | 1.29 | 0.45 |
| 7:I:43:VAL:O | 7:I:43:VAL:CG1 | 2.64 | 0.45 |
| 9:K:102:LYS:O | 9:K:106:GLU:HB2 | 2.17 | 0.45 |
| 1:A:98:LYS:HB3 | 1:A:234:MET:HE1 | 1.99 | 0.45 |
| 1:A:523:ILE:CB | 1:A:622:VAL:HG13 | 2.45 | 0.45 |
| 1:A:925:LEU:HD23 | 1:A:925:LEU:HA | 1.82 | 0.45 |
| 1:A:1166:ASP:O | 1:A:1169:ILE:HG23 | 2.16 | 0.45 |
| 1:A:1385:THR:CG2 | 1:A:1385:THR:HB | 2.19 | 0.45 |
| 2:B:206:ASN:OD1 | 2:B:458:LYS:HE3 | 2.15 | 0.45 |
| 2:B:215:GLN:HE22 | 2:B:499:ASN:HD22 | 1.65 | 0.45 |
| 2:B:916:THR:HB | 2:B:935:ARG:HB2 | 1.98 | 0.45 |
| 4:E:39:LEU:O | 4:E:42:PHE:HB3 | 2.17 | 0.45 |
| 1:A:511:ILE:HD13 | 1:A:646:PHE:HE1 | 1.81 | 0.45 |
| 1:A:597:LEU:H | 1:A:597:LEU:HD12 | 1.81 | 0.45 |
| 1:A:908:LEU:HA | 1:A:908:LEU:HD23 | 1.77 | 0.45 |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:HB2 | 1.99 | 0.45 |
| 2:B:246:LYS:CA | 2:B:247:GLY:N | 2.66 | 0.45 |
| 2:B:841:MET:HE1 | 2:B:990:ILE:HD11 | 1.97 | 0.45 |
| 3:C:56:THR:CG2 | 3:C:58:LEU:H | 2.29 | 0.45 |
| 5:F:128:LYS:HD3 | 5:F:128:LYS:HA | 1.76 | 0.45 |
| 8:J:53:HIS:CE1 | 8:J:55:ASP:N | 2.85 | 0.45 |
| 8:J:62:ARG:HE | 8:J:62:ARG:HB3 | 1.29 | 0.45 |
| 1:A:61:ILE:CA | 1:A:61:ILE:CG2 | 2.86 | 0.45 |
| 2:B:345:LYS:O | 2:B:346:GLU:C | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:455:SER:O | 2:B:459:TYR:HB3 | 2.16 | 0.45 |
| 3:C:218:PRO:O | 3:C:219:PHE:C | 2.55 | 0.45 |
| 1:A:858:ASN:C | 1:A:858:ASN:HD22 | 2.20 | 0.45 |
| 1:A:1111:MET:HE1 | 1:A:1331:SER:HA | 1.99 | 0.45 |
| 2:B:859:TYR:N | 2:B:859:TYR:CD1 | 2.85 | 0.45 |
| 4:E:63:ASN:C | 4:E:64:PRO:O | 2.55 | 0.45 |
| 1:A:910:PRO:HA | 1:A:916:GLY:HA3 | 1.99 | 0.45 |
| 3:C:80:LEU:HD12 | 3:C:80:LEU:HA | 1.58 | 0.45 |
| 4:E:129:PRO:CD | 4:E:130:ALA:N | 2.78 | 0.45 |
| 7:I:51:ASN:HB2 | 7:I:118:ARG:CZ | 2.46 | 0.45 |
| 1:A:566:ILE:CG2 | 1:A:566:ILE:HB | 2.20 | 0.44 |
| 2:B:210:LYS:HE3 | 2:B:461:LEU:O | 2.17 | 0.44 |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21 | 1.99 | 0.44 |
| 2:B:1019:SER:OG | 13:B:3008:GTP:C6 | 2.57 | 0.44 |
| 4:E:31:THR:O | 4:E:32:GLN:C | 2.55 | 0.44 |
| 4:E:80:VAL:HG12 | 4:E:81:GLU:N | 2.32 | 0.44 |
| 4:E:131:THR:CB | 4:E:131:THR:N | 2.67 | 0.44 |
| 5:F:107:VAL:HG12 | 5:F:109:VAL:H | 1.81 | 0.44 |
| 7:I:75:CYS:HB3 | 7:I:110:PHE:CE2 | 2.52 | 0.44 |
| 1:A:515:GLN:OE1 | 14:A:3018:HOH:O | 2.21 | 0.44 |
| 1:A:941:LYS:NZ | 1:A:941:LYS:HD3 | 2.30 | 0.44 |
| 2:B:806:THR:HG23 | 2:B:808:ALA:H | 1.82 | 0.44 |
| 3:C:196:ASP:CG | 3:C:199:LYS:HG3 | 2.38 | 0.44 |
| 1:A:481:ASP:CG | 1:A:481:ASP:N | 2.70 | 0.44 |
| 1:A:543:LEU:O | 1:A:543:LEU:HG | 2.15 | 0.44 |
| 1:A:1157:ASP:O | 1:A:1160:SER:O | 2.36 | 0.44 |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:N | 2.31 | 0.44 |
| 4:E:116:ILE:HG22 | 4:E:120:ALA:HB3 | 2.00 | 0.44 |
| 6:H:40:LEU:HD12 | 6:H:41:ASP:N | 2.31 | 0.44 |
| 7:I:120:GLN:O | 7:I:121:PHE:CD1 | 2.71 | 0.44 |
| 1:A:58:LEU:O | 1:A:59:GLY:O | 2.34 | 0.44 |
| 1:A:328:ARG:NH1 | 1:A:1405:THR:HB | 2.32 | 0.44 |
| 1:A:356:ASP:OD2 | 1:A:469:ARG:HD3 | 2.17 | 0.44 |
| 1:A:809:THR:HB | 1:A:810:PRO:CD | 2.47 | 0.44 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:CZ | 2.52 | 0.44 |
| 2:B:249:ARG:NH1 | 2:B:418:LYS:HZ2 | 2.15 | 0.44 |
| 6:H:93:TYR:CD1 | 6:H:93:TYR:N | 2.86 | 0.44 |
| 8:J:53:HIS:ND1 | 8:J:53:HIS:C | 2.70 | 0.44 |
| 1:A:503:GLN:HE21 | 5:F:90:ARG:NH2 | 2.12 | 0.44 |
| 1:A:531:ILE:CD1 | 1:A:617:VAL:HB | 2.39 | 0.44 |
| 1:A:596:THR:CG2 | 1:A:597:LEU:N | 2.77 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:843:LYS:CE | 1:A:843:LYS:CG | 2.93 | 0.44 |
| 1:A:901:LEU:CD1 | 1:A:919:ILE:HD12 | 2.48 | 0.44 |
| 1:A:982:THR:O | 1:A:985:ASP:HB2 | 2.18 | 0.44 |
| 2:B:983:ARG:CD | 14:B:3009:HOH:O | 2.66 | 0.44 |
| 2:B:1019:SER:CB | 13:B:3008:GTP:N7 | 2.81 | 0.44 |
| 2:B:1190:ASP:C | 2:B:1191:ILE:HG13 | 2.36 | 0.44 |
| 4:E:36:GLU:O | 4:E:38:PRO:N | 2.50 | 0.44 |
| 4:E:213:ILE:HG23 | 4:E:213:ILE:O | 2.17 | 0.44 |
| 2:B:56:ASP:OD1 | 2:B:56:ASP:N | 2.45 | 0.44 |
| 2:B:755:ILE:O | 2:B:755:ILE:CG2 | 2.66 | 0.44 |
| 3:C:54:ASN:OD1 | 3:C:56:THR:CB | 2.44 | 0.44 |
| 3:C:255:VAL:O | 3:C:255:VAL:CG1 | 2.65 | 0.44 |
| 3:C:260:LEU:O | 3:C:260:LEU:CD1 | 2.59 | 0.44 |
| 7:I:91:ARG:HD3 | 7:I:91:ARG:HA | 1.77 | 0.44 |
| 10:L:48:CYS:CA | 10:L:49:LYS:N | 2.66 | 0.44 |
| 1:A:555:ASP:OD1 | 9:K:26:LYS:HE3 | 2.17 | 0.44 |
| 1:A:599:SER:O | 1:A:600:PRO:C | 2.56 | 0.44 |
| 1:A:1111:MET:CE | 1:A:1111:MET:CB | 2.96 | 0.44 |
| 2:B:284:ILE:CD1 | 2:B:321:GLY:HA2 | 2.48 | 0.44 |
| 6:H:10:PHE:HA | 6:H:29:ALA:O | 2.18 | 0.44 |
| 6:H:82:PRO:O | 6:H:83:GLN:HB2 | 2.18 | 0.44 |
| 10:L:38:LEU:HG | 10:L:39:SER:N | 2.32 | 0.44 |
| 10:L:38:LEU:HD13 | 10:L:48:CYS:HA | 1.99 | 0.44 |
| 1:A:1333:ILE:HD12 | 1:A:1333:ILE:N | 2.33 | 0.44 |
| 2:B:114:PRO:HD3 | 2:B:124:TYR:HE1 | 1.78 | 0.44 |
| 2:B:130:VAL:H | 2:B:167:ILE:CD1 | 2.17 | 0.44 |
| 4:E:36:GLU:O | 4:E:38:PRO:HD3 | 2.18 | 0.44 |
| 1:A:1151:GLU:HG3 | 7:I:45:ARG:HD2 | 1.95 | 0.44 |
| 1:A:1166:ASP:HA | 1:A:1169:ILE:HG22 | 1.98 | 0.44 |
| 2:B:969:ARG:HH11 | 2:B:969:ARG:HD3 | 1.43 | 0.44 |
| 3:C:252:GLN:CG | 3:C:252:GLN:HB3 | 2.20 | 0.44 |
| 3:C:262:LEU:HA | 3:C:262:LEU:HD23 | 1.78 | 0.44 |
| 4:E:116:ILE:HG22 | 4:E:120:ALA:CB | 2.48 | 0.44 |
| 6:H:89:LEU:O | 6:H:90:ALA:C | 2.50 | 0.44 |
| 6:H:95:TYR:CE2 | 6:H:97:MET:HG3 | 2.53 | 0.44 |
| 1:A:145:LYS:HE2 | 1:A:149:GLU:OE1 | 2.18 | 0.43 |
| 2:B:555:ILE:HD12 | 2:B:587:HIS:HE1 | 1.75 | 0.43 |
| 1:A:587:HIS:CE1 | 1:A:609:ASP:H | 2.36 | 0.43 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:N | 2.33 | 0.43 |
| 1:A:882:SER:CB | 1:A:953:ASN:OD1 | 2.66 | 0.43 |
| 1:A:979:SER:OG | 1:A:981:LEU:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:118:ARG:NH2 | 2:B:194:GLU:CG | 2.80 | 0.43 |
| 2:B:276:ILE:HD12 | 2:B:276:ILE:HG23 | 1.71 | 0.43 |
| 2:B:323:VAL:O | 2:B:323:VAL:CG1 | 2.65 | 0.43 |
| 2:B:654:ARG:N | 2:B:657:HIS:HD2 | 2.14 | 0.43 |
| 2:B:789:MET:CE | 2:B:965:LYS:HB3 | 2.48 | 0.43 |
| 2:B:999:MET:CE | 2:B:1011:ILE:HD11 | 2.48 | 0.43 |
| 2:B:1202:LEU:HD23 | 2:B:1202:LEU:HA | 1.88 | 0.43 |
| 3:C:47:ASP:CG | 3:C:47:ASP:O | 2.56 | 0.43 |
| 1:A:605:MET:HE3 | 1:A:607:ILE:HG13 | 2.00 | 0.43 |
| 2:B:620:ARG:CD | 2:B:620:ARG:CB | 2.82 | 0.43 |
| 4:E:78:LEU:HG | 4:E:79:TRP:N | 2.33 | 0.43 |
| 6:H:27:GLU:OE1 | 6:H:39:THR:CG2 | 2.66 | 0.43 |
| 6:H:96:VAL:HA | 6:H:142:LEU:O | 2.18 | 0.43 |
| 1:A:11:LEU:O | 1:A:12:ARG:HG2 | 2.18 | 0.43 |
| 1:A:353:ILE:HD12 | 1:A:482:PHE:CD2 | 2.54 | 0.43 |
| 1:A:666:ILE:O | 1:A:666:ILE:HD13 | 2.19 | 0.43 |
| 1:A:676:MET:SD | 1:A:676:MET:CB | 2.98 | 0.43 |
| 1:A:977:LYS:CG | 1:A:977:LYS:HA | 2.49 | 0.43 |
| 1:A:1242:VAL:HG11 | 1:A:1259:MET:CE | 2.48 | 0.43 |
| 1:A:1438:THR:HB | 2:B:1142:GLY:O | 2.18 | 0.43 |
| 2:B:25:ILE:CD1 | 2:B:651:LEU:HD12 | 2.41 | 0.43 |
| 2:B:293:PRO:HA | 7:I:12:ASN:HD21 | 1.83 | 0.43 |
| 2:B:387:LEU:HD12 | 2:B:387:LEU:HA | 1.55 | 0.43 |
| 2:B:1166:CYS:O | 2:B:1166:CYS:SG | 2.76 | 0.43 |
| 3:C:74:SER:HB2 | 3:C:238:ILE:HD12 | 2.01 | 0.43 |
| 3:C:179:GLU:CG | 3:C:180:TYR:N | 2.81 | 0.43 |
| 3:C:196:ASP:CB | 3:C:199:LYS:HG3 | 2.49 | 0.43 |
| 6:H:98:TYR:C | 6:H:118:PHE:HD2 | 2.21 | 0.43 |
| 1:A:243:PRO:CB | 1:A:245:PRO:HD2 | 2.46 | 0.43 |
| 1:A:567:LYS:CD | 6:H:95:TYR:CD2 | 2.97 | 0.43 |
| 1:A:901:LEU:HB2 | 1:A:926:GLN:HE21 | 1.83 | 0.43 |
| 1:A:1339:LEU:HA | 1:A:1339:LEU:HD23 | 1.77 | 0.43 |
| 2:B:870:ILE:CA | 2:B:870:ILE:HB | 2.24 | 0.43 |
| 2:B:1150:ARG:HH11 | 2:B:1150:ARG:HD2 | 1.45 | 0.43 |
| 4:E:115:ASN:C | 4:E:116:ILE:HD13 | 2.38 | 0.43 |
| 5:F:81:THR:HG22 | 5:F:136:ARG:NH1 | 2.32 | 0.43 |
| 1:A:483:ASP:O | 2:B:987:LYS:NZ | 2.37 | 0.43 |
| 1:A:503:GLN:HE22 | 5:F:90:ARG:NH2 | 2.14 | 0.43 |
| 2:B:705:MET:CG | 2:B:705:MET:HE2 | 2.31 | 0.43 |
| 3:C:131:HIS:O | 3:C:132:PRO:C | 2.57 | 0.43 |
| 2:B:896:ASP:OD2 | 10:L:29:TYR:OH | 2.24 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:4:GLU:HG2 | 3:C:5:GLY:H | 1.84 | 0.43 |
| 4:E:96:PHE:CZ | 4:E:100:ILE:HD11 | 2.54 | 0.43 |
| 5:F:114:GLU:CB | 5:F:120:ILE:HD13 | 2.49 | 0.43 |
| 7:I:10:CYS:SG | 7:I:31:THR:HG22 | 2.58 | 0.43 |
| 7:I:55:THR:HG21 | 7:I:121:PHE:O | 2.19 | 0.43 |
| 8:J:43:ARG:O | 8:J:47:ARG:HG3 | 2.19 | 0.43 |
| 1:A:34:LYS:CG | 1:A:83:HIS:CE1 | 3.02 | 0.43 |
| 1:A:359:LEU:HA | 1:A:359:LEU:HD23 | 1.75 | 0.43 |
| 1:A:886:ILE:HD12 | 1:A:943:LEU:HB3 | 2.01 | 0.43 |
| 1:A:1383:SER:OG | 1:A:1384:VAL:N | 2.51 | 0.43 |
| 2:B:169:ARG:HB2 | 2:B:454:THR:CG2 | 2.41 | 0.43 |
| 2:B:451:LYS:HA | 2:B:454:THR:HB | 2.00 | 0.43 |
| 2:B:529:GLU:O | 2:B:531:GLN:NE2 | 2.52 | 0.43 |
| 2:B:863:GLU:OE1 | 2:B:962:LYS:HD3 | 2.18 | 0.43 |
| 2:B:986:GLN:CG | 2:B:986:GLN:OE1 | 2.53 | 0.43 |
| 3:C:163:ILE:HA | 3:C:163:ILE:HD13 | 1.43 | 0.43 |
| 4:E:78:LEU:HD11 | 4:E:109:ILE:CD1 | 2.49 | 0.43 |
| 6:H:13:SER:O | 6:H:14:GLU:HG3 | 2.19 | 0.43 |
| 6:H:81:PRO:C | 6:H:82:PRO:O | 2.55 | 0.43 |
| 1:A:562:THR:HG21 | 6:H:98:TYR:CD2 | 2.53 | 0.43 |
| 1:A:593:GLU:O | 1:A:593:GLU:HG2 | 2.18 | 0.43 |
| 1:A:597:LEU:CD1 | 1:A:597:LEU:CB | 2.86 | 0.43 |
| 1:A:700:ASN:O | 7:I:115:LYS:HE3 | 2.19 | 0.43 |
| 2:B:274:PRO:CG | 2:B:359:GLU:HB3 | 2.48 | 0.43 |
| 2:B:542:MET:CE | 2:B:747:MET:HG3 | 2.49 | 0.43 |
| 1:A:295:LEU:CD2 | 1:A:295:LEU:CB | 2.82 | 0.43 |
| 1:A:853:ASP:OD2 | 1:A:857:ARG:NH2 | 2.50 | 0.43 |
| 1:A:1169:ILE:HD11 | 1:A:1227:ILE:CD1 | 2.48 | 0.43 |
| 2:B:118:ARG:HG3 | 2:B:204:ILE:CD1 | 2.47 | 0.43 |
| 2:B:542:MET:HE2 | 2:B:747:MET:HG3 | 1.99 | 0.43 |
| 3:C:77:ILE:HD11 | 3:C:80:LEU:HD23 | 2.00 | 0.43 |
| 3:C:180:TYR:CD1 | 3:C:180:TYR:C | 2.93 | 0.43 |
| 6:H:33:GLN:C | 6:H:35:GLN:H | 2.22 | 0.43 |
| 9:K:18:LYS:HE3 | 9:K:38:GLU:OE2 | 2.19 | 0.43 |
| 1:A:14:VAL:N | 1:A:1432:GLN:HE22 | 2.11 | 0.42 |
| 1:A:186:LYS:CG | 1:A:197:PRO:HD3 | 2.48 | 0.42 |
| 1:A:563:PRO:HB3 | 1:A:572:TRP:CD2 | 2.53 | 0.42 |
| 2:B:132:VAL:HG12 | 2:B:133:LYS:N | 2.34 | 0.42 |
| 2:B:461:LEU:N | 2:B:461:LEU:HD12 | 2.34 | 0.42 |
| 2:B:885:MET:HB3 | 2:B:885:MET:HE3 | 1.99 | 0.42 |
| 2:B:914:LYS:N | 2:B:938:SER:HB2 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:43:THR:HG23 | 3:C:44:LEU:N | 2.33 | 0.42 |
| 6:H:95:TYR:C | 6:H:95:TYR:HD2 | 2.22 | 0.42 |
| 1:A:391:LEU:CD2 | 1:A:400:PRO:HB2 | 2.50 | 0.42 |
| 1:A:560:ILE:H | 1:A:560:ILE:CD1 | 2.30 | 0.42 |
| 1:A:1165:GLU:H | 1:A:1165:GLU:HG2 | 1.56 | 0.42 |
| 2:B:51:PHE:CE2 | 2:B:172:ILE:HD13 | 2.54 | 0.42 |
| 2:B:213:ILE:CD1 | 2:B:481:GLN:CD | 2.88 | 0.42 |
| 2:B:1194:ILE:O | 2:B:1194:ILE:HG13 | 2.19 | 0.42 |
| 6:H:32:THR:CG2 | 6:H:33:GLN:CD | 2.87 | 0.42 |
| 8:J:6:ARG:HD2 | 8:J:11:GLY:O | 2.18 | 0.42 |
| 1:A:157:ASP:O | 1:A:160:GLN:HG3 | 2.19 | 0.42 |
| 1:A:868:TYR:CE1 | 1:A:1064:VAL:HG13 | 2.54 | 0.42 |
| 2:B:1169:MET:CE | 2:B:1204:PHE:HB2 | 2.49 | 0.42 |
| 4:E:147:HIS:HD2 | 4:E:149:LEU:HB2 | 1.84 | 0.42 |
| 6:H:32:THR:HG22 | 6:H:33:GLN:OE1 | 2.17 | 0.42 |
| 7:I:17:ARG:HG3 | 7:I:28:GLU:OE1 | 2.19 | 0.42 |
| 1:A:664:THR:HG21 | 1:A:746:MET:HE1 | 2.00 | 0.42 |
| 1:A:744:LYS:HD3 | 1:A:748:MET:CE | 2.49 | 0.42 |
| 1:A:1435:PRO:HA | 1:A:1439:GLY:O | 2.20 | 0.42 |
| 2:B:554:ILE:HD12 | 2:B:554:ILE:H | 1.84 | 0.42 |
| 3:C:240:VAL:C | 3:C:242:GLN:N | 2.70 | 0.42 |
| 4:E:37:LEU:CD1 | 4:E:37:LEU:CB | 2.84 | 0.42 |
| 4:E:59:SER:O | 4:E:60:PHE:HB3 | 2.20 | 0.42 |
| 5:F:74:ILE:CD1 | 5:F:144:GLU:HG2 | 2.49 | 0.42 |
| 6:H:95:TYR:HE2 | 6:H:97:MET:HG3 | 1.85 | 0.42 |
| 6:H:105:GLU:CD | 6:H:105:GLU:N | 2.69 | 0.42 |
| 9:K:12:LEU:HD12 | 9:K:12:LEU:H | 1.85 | 0.42 |
| 1:A:599:SER:HB2 | 1:A:602:ASP:H | 1.85 | 0.42 |
| 1:A:722:LEU:HD23 | 1:A:722:LEU:HA | 1.90 | 0.42 |
| 1:A:913:LEU:HD12 | 1:A:913:LEU:HA | 1.61 | 0.42 |
| 2:B:509:ALA:C | 2:B:511:PRO:HD3 | 2.39 | 0.42 |
| 2:B:554:ILE:HD12 | 2:B:554:ILE:N | 2.34 | 0.42 |
| 2:B:996:ARG:HH11 | 2:B:996:ARG:HD3 | 1.53 | 0.42 |
| 3:C:7:GLN:CG | 3:C:7:GLN:CA | 2.87 | 0.42 |
| 6:H:44:VAL:O | 6:H:44:VAL:CG1 | 2.67 | 0.42 |
| 9:K:111:LEU:HD23 | 9:K:111:LEU:H | 1.85 | 0.42 |
| 10:L:34:CYS:HB3 | 10:L:51:CYS:HB3 | 2.02 | 0.42 |
| 1:A:195:ASP:O | 1:A:196:GLU:HB3 | 2.20 | 0.42 |
| 1:A:922:ASP:OD1 | 1:A:922:ASP:C | 2.58 | 0.42 |
| 2:B:70:ILE:HD12 | 2:B:70:ILE:N | 2.34 | 0.42 |
| 2:B:121:ASN:ND2 | 2:B:965:LYS:NZ | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:646:LEU:CD1 | 2:B:646:LEU:CD2 | 2.95 | 0.42 |
| 2:B:976:ILE:O | 2:B:1099:VAL:HG21 | 2.19 | 0.42 |
| 1:A:1336:MET:HE2 | 1:A:1381:LEU:H | 1.85 | 0.42 |
| 2:B:286:PHE:CB | 2:B:297:ILE:HD12 | 2.40 | 0.42 |
| 2:B:773:MET:O | 2:B:774:GLY:C | 2.55 | 0.42 |
| 2:B:834:ASN:O | 2:B:1013:ASN:HB2 | 2.20 | 0.42 |
| 2:B:1002:THR:O | 2:B:1005:GLY:N | 2.42 | 0.42 |
| 4:E:43:LYS:O | 4:E:47:CYS:CB | 2.68 | 0.42 |
| 1:A:709:THR:HG22 | 1:A:711:ARG:N | 2.35 | 0.42 |
| 1:A:786:HIS:CD2 | 1:A:786:HIS:H | 2.36 | 0.42 |
| 2:B:199:MET:HE1 | 2:B:488:TYR:CE1 | 2.55 | 0.42 |
| 4:E:79:TRP:HE1 | 4:E:81:GLU:HB2 | 1.84 | 0.42 |
| 6:H:138:GLU:C | 6:H:140:ALA:N | 2.67 | 0.42 |
| 10:L:49:LYS:O | 10:L:50:ASP:HB2 | 2.20 | 0.42 |
| 1:A:809:THR:OG1 | 1:A:812:GLU:HG3 | 2.20 | 0.42 |
| 1:A:830:LYS:CD | 1:A:830:LYS:CB | 2.84 | 0.42 |
| 1:A:1102:LYS:CE | 1:A:1102:LYS:CG | 2.87 | 0.42 |
| 1:A:1146:VAL:HG12 | 1:A:1197:LEU:HD22 | 2.02 | 0.42 |
| 1:A:1385:THR:CG2 | 1:A:1385:THR:O | 2.66 | 0.42 |
| 2:B:95:ILE:HG22 | 2:B:96:TYR:O | 2.20 | 0.42 |
| 2:B:104:GLU:HB2 | 2:B:108:VAL:HA | 2.02 | 0.42 |
| 2:B:757:PRO:HD2 | 2:B:984:HIS:HE1 | 1.85 | 0.42 |
| 2:B:902:GLY:O | 10:L:65:VAL:HG11 | 2.19 | 0.42 |
| 2:B:1006:ILE:CD1 | 8:J:43:ARG:HD2 | 2.50 | 0.42 |
| 8:J:16:ASP:OD1 | 8:J:17:LYS:HG3 | 2.19 | 0.42 |
| 1:A:93:VAL:HG13 | 1:A:301:ALA:HB1 | 2.01 | 0.41 |
| 1:A:230:ARG:NH1 | 1:A:232:GLU:OE2 | 2.52 | 0.41 |
| 2:B:274:PRO:HG3 | 2:B:359:GLU:O | 2.20 | 0.41 |
| 2:B:282:ILE:HD11 | 2:B:317:CYS:CB | 2.50 | 0.41 |
| 1:A:70:CYS:HB3 | 2:B:1172:ILE:HG23 | 2.02 | 0.41 |
| 1:A:492:PRO:HB2 | 1:A:497:THR:CG2 | 2.48 | 0.41 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:HD11 | 2.21 | 0.41 |
| 3:C:7:GLN:OE1 | 9:K:104:ASN:ND2 | 2.54 | 0.41 |
| 3:C:214:ASN:O | 3:C:217:ASP:N | 2.54 | 0.41 |
| 4:E:61:GLN:HB2 | 4:E:79:TRP:CE3 | 2.56 | 0.41 |
| 6:H:47:PHE:HB2 | 6:H:95:TYR:HD1 | 1.83 | 0.41 |
| 7:I:40:SER:CB | 7:I:41:PRO:CD | 2.97 | 0.41 |
| 1:A:145:LYS:HE2 | 1:A:149:GLU:CD | 2.40 | 0.41 |
| 1:A:807:GLY:CA | 2:B:761:HIS:CE1 | 3.04 | 0.41 |
| 1:A:1170:ILE:HD13 | 1:A:1170:ILE:HA | 1.96 | 0.41 |
| 2:B:879:ARG:HH21 | 2:B:885:MET:HE1 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:446:ARG:CG | 1:A:446:ARG:NH1 | 2.83 | 0.41 |
| 1:A:1322:ILE:HD12 | 1:A:1322:ILE:C | 2.41 | 0.41 |
| 2:B:1195:HIS:C | 2:B:1196:ILE:HG23 | 2.40 | 0.41 |
| 4:E:154:ILE:CD1 | 4:E:199:ILE:HD12 | 2.50 | 0.41 |
| 4:E:168:TYR:O | 4:E:169:ARG:HB2 | 2.20 | 0.41 |
| 7:I:71:SER:O | 7:I:83:ASN:ND2 | 2.53 | 0.41 |
| 1:A:95:PHE:O | 1:A:99:ILE:HG13 | 2.21 | 0.41 |
| 1:A:96:ILE:HG21 | 1:A:176:LYS:HE2 | 2.03 | 0.41 |
| 1:A:138:ILE:HG13 | 1:A:139:TRP:N | 2.35 | 0.41 |
| 1:A:557:ASP:O | 1:A:559:VAL:N | 2.53 | 0.41 |
| 1:A:666:ILE:HD12 | 2:B:1052:VAL:HG11 | 2.02 | 0.41 |
| 1:A:752:LYS:HE2 | 13:B:3008:GTP:N1 | 2.35 | 0.41 |
| 1:A:973:ILE:CD1 | 1:A:1038:THR:HG23 | 2.51 | 0.41 |
| 1:A:1166:ASP:CB | 1:A:1169:ILE:HG21 | 2.39 | 0.41 |
| 1:A:1237:ILE:HD12 | 1:A:1237:ILE:HA | 1.75 | 0.41 |
| 2:B:28:GLU:OE1 | 2:B:807:ARG:NH2 | 2.54 | 0.41 |
| 2:B:900:ALA:HA | 10:L:58:LYS:HD2 | 2.02 | 0.41 |
| 2:B:1189:ILE:N | 2:B:1189:ILE:HD12 | 2.35 | 0.41 |
| 4:E:98:ILE:CA | 4:E:98:ILE:CG2 | 2.88 | 0.41 |
| 7:I:103:CYS:SG | 7:I:106:CYS:SG | 3.18 | 0.41 |
| 1:A:846:GLU:HA | 1:A:1066:VAL:CG2 | 2.50 | 0.41 |
| 2:B:280:ILE:HD12 | 2:B:280:ILE:H | 1.86 | 0.41 |
| 4:E:79:TRP:NE1 | 4:E:81:GLU:HB2 | 2.36 | 0.41 |
| 5:F:128:LYS:NZ | 5:F:149:GLU:O | 2.48 | 0.41 |
| 6:H:138:GLU:HG2 | 6:H:139:ASN:N | 2.36 | 0.41 |
| 8:J:14:VAL:CG1 | 8:J:50:ILE:CD1 | 2.95 | 0.41 |
| 9:K:47:ARG:C | 9:K:47:ARG:HD2 | 2.41 | 0.41 |
| 1:A:9:ALA:O | 2:B:1193:GLN:OE1 | 2.39 | 0.41 |
| 1:A:351:THR:HG23 | 2:B:1103:ILE:HG12 | 1.98 | 0.41 |
| 1:A:571:LEU:HA | 1:A:571:LEU:HD12 | 1.70 | 0.41 |
| 1:A:741:ASN:ND2 | 1:A:743:VAL:H | 2.19 | 0.41 |
| 1:A:834:THR:CG2 | 1:A:1077:THR:OG1 | 2.66 | 0.41 |
| 2:B:780:VAL:HG21 | 8:J:56:LEU:HD11 | 2.03 | 0.41 |
| 2:B:914:LYS:HD2 | 2:B:937:ALA:HB3 | 2.02 | 0.41 |
| 2:B:939:THR:HA | 2:B:940:PRO:HD3 | 1.93 | 0.41 |
| 3:C:44:LEU:HD22 | 3:C:129:ILE:HD12 | 2.03 | 0.41 |
| 4:E:161:LYS:NZ | 4:E:172:GLU:OE2 | 2.51 | 0.41 |
| 6:H:145:ARG:HG2 | 6:H:145:ARG:NH1 | 2.36 | 0.41 |
| 1:A:516:SER:OG | 1:A:1362:TYR:O | 2.39 | 0.41 |
| 1:A:1023:ARG:HH21 | 1:A:1023:ARG:HD3 | 1.66 | 0.41 |
| 1:A:186:LYS:HD2 | 1:A:197:PRO:HG3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:269:ILE:CD1 | 1:A:300:VAL:HG22 | 2.50 | 0.41 |
| 1:A:541:ILE:HG22 | 1:A:546:VAL:HG23 | 2.03 | 0.41 |
| 1:A:582:ILE:HA | 1:A:583:PRO:HD3 | 1.92 | 0.41 |
| 1:A:1207:LEU:HD23 | 1:A:1211:GLN:OE1 | 2.21 | 0.41 |
| 1:A:1258:HIS:O | 1:A:1259:MET:C | 2.59 | 0.41 |
| 1:A:1267:MET:HA | 1:A:1271:ILE:HD13 | 2.03 | 0.41 |
| 1:A:1362:TYR:CD2 | 1:A:1362:TYR:C | 2.93 | 0.41 |
| 2:B:90:ILE:HD11 | 2:B:134:LYS:HE2 | 2.03 | 0.41 |
| 2:B:323:VAL:O | 2:B:323:VAL:HG12 | 2.20 | 0.41 |
| 2:B:1161:HIS:HA | 2:B:1192:TYR:O | 2.21 | 0.41 |
| 2:B:1179:GLN:HE21 | 2:B:1179:GLN:HB2 | 1.70 | 0.41 |
| 3:C:29:MET:CE | 3:C:29:MET:CB | 2.99 | 0.41 |
| 3:C:216:GLY:O | 3:C:217:ASP:C | 2.60 | 0.41 |
| 5:F:94:LEU:HD23 | 5:F:94:LEU:HA | 1.85 | 0.41 |
| 6:H:142:LEU:HA | 6:H:142:LEU:HD12 | 1.76 | 0.41 |
| 8:J:1:MET:HG3 | 8:J:60:PHE:HE2 | 1.86 | 0.41 |
| 9:K:98:LEU:O | 9:K:99:GLY:C | 2.58 | 0.41 |
| 10:L:54:ARG:CG | 10:L:54:ARG:NE | 2.66 | 0.41 |
| 1:A:93:VAL:HG22 | 1:A:301:ALA:HA | 2.02 | 0.41 |
| 1:A:1220:PHE:HB3 | 1:A:1224:LEU:HB3 | 2.03 | 0.41 |
| 2:B:643:ASP:HB3 | 2:B:644:GLU:C | 2.42 | 0.41 |
| 1:A:83:HIS:ND1 | 1:A:83:HIS:C | 2.74 | 0.40 |
| 1:A:210:ILE:HD13 | 1:A:210:ILE:HA | 1.91 | 0.40 |
| 1:A:274:ILE:CA | 1:A:274:ILE:HB | 2.21 | 0.40 |
| 1:A:547:LEU:HD22 | 9:K:58:PHE:CD1 | 2.56 | 0.40 |
| 1:A:679:ILE:CD1 | 1:A:729:ALA:O | 2.68 | 0.40 |
| 1:A:983:ILE:HD12 | 1:A:983:ILE:H | 1.86 | 0.40 |
| 1:A:1025:ARG:HD3 | 1:A:1025:ARG:HA | 1.88 | 0.40 |
| 1:A:1039:LYS:O | 1:A:1039:LYS:HG3 | 2.21 | 0.40 |
| 1:A:1166:ASP:HB3 | 1:A:1169:ILE:HG23 | 1.97 | 0.40 |
| 3:C:40:GLU:CD | 3:C:254:LYS:NZ | 2.75 | 0.40 |
| 3:C:102:GLN:CB | 3:C:102:GLN:CD | 2.78 | 0.40 |
| 4:E:55:ARG:O | 4:E:56:LYS:C | 2.59 | 0.40 |
| 5:F:93:ILE:HD12 | 5:F:134:ILE:HD11 | 1.98 | 0.40 |
| 6:H:101:ALA:HA | 6:H:116:TYR:HA | 2.01 | 0.40 |
| 9:K:27:ALA:HB1 | 9:K:28:PRO:CD | 2.51 | 0.40 |
| 9:K:59:ALA:HA | 9:K:74:ARG:O | 2.21 | 0.40 |
| 1:A:587:HIS:HE2 | 1:A:969:GLN:HG2 | 1.84 | 0.40 |
| 1:A:1004:ASN:OD1 | 4:E:167:ARG:HG3 | 2.21 | 0.40 |
| 2:B:113:TYR:CD2 | 2:B:192:LEU:HD22 | 2.57 | 0.40 |
| 2:B:724:ASP:O | 2:B:726:ALA:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:70:ILE:HD11 | 3:C:144:ILE:CD1 | 2.51 | 0.40 |
| 4:E:161:LYS:NZ | 4:E:193:GLY:O | 2.54 | 0.40 |
| 8:J:1:MET:HG3 | 8:J:1:MET:HE2 | 2.04 | 0.40 |
| 9:K:110:ASN:C | 9:K:112:GLN:N | 2.63 | 0.40 |
| 1:A:44:THR:CA | 1:A:44:THR:CG2 | 2.86 | 0.40 |
| 1:A:497:THR:HG21 | 2:B:1149:GLU:OE1 | 2.20 | 0.40 |
| 1:A:599:SER:HA | 1:A:600:PRO:HD2 | 1.82 | 0.40 |
| 1:A:1166:ASP:O | 1:A:1169:ILE:CG2 | 2.69 | 0.40 |
| 1:A:1209:MET:SD | 1:A:1236:LEU:HD22 | 2.62 | 0.40 |
| 2:B:361:LEU:N | 2:B:362:PRO:CD | 2.85 | 0.40 |
| 2:B:840:ILE:HB | 2:B:1011:ILE:HB | 2.03 | 0.40 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:HB2 | 2.28 | 0.40 |
| 3:C:11:ARG:NE | 3:C:209:TYR:CE2 | 2.89 | 0.40 |
| 4:E:43:LYS:O | 4:E:47:CYS:HB3 | 2.21 | 0.40 |
| 1:A:35:ILE:H | 1:A:35:ILE:HG13 | 1.65 | 0.40 |
| 1:A:127:ALA:O | 1:A:128:ILE:C | 2.59 | 0.40 |
| 1:A:1003:LYS:CG | 1:A:1003:LYS:HA | 2.43 | 0.40 |
| 2:B:121:ASN:HD21 | 2:B:965:LYS:CE | 2.35 | 0.40 |
| 2:B:165:VAL:O | 2:B:165:VAL:HG12 | 2.20 | 0.40 |
| 3:C:29:MET:HE2 | 3:C:29:MET:CB | 2.52 | 0.40 |
| 4:E:61:GLN:HE21 | 4:E:63:ASN:HD21 | 1.68 | 0.40 |
| 1:A:35:ILE:HA | 1:A:52:GLY:O | 2.22 | 0.40 |
| 1:A:771:GLU:CD | 2:B:510:LYS:HZ3 | 2.24 | 0.40 |
| 1:A:1098:VAL:N | 1:A:1099:PRO:CD | 2.84 | 0.40 |
| 1:A:1259:MET:O | 1:A:1260:LEU:C | 2.58 | 0.40 |
| 2:B:270:LYS:HB3 | 2:B:279:ASP:HB3 | 2.02 | 0.40 |
| 2:B:291:ILE:O | 2:B:297:ILE:CD1 | 2.67 | 0.40 |
| 2:B:458:LYS:HZ1 | 2:B:958:GLN:NE2 | 2.18 | 0.40 |
| 2:B:1160:VAL:HG12 | 2:B:1161:HIS:N | 2.35 | 0.40 |
| 3:C:248:ILE:HD12 | 9:K:101:LEU:HD12 | 2.03 | 0.40 |
| 4:E:28:TYR:CE1 | 4:E:75:MET:CE | 3.04 | 0.40 |
| 4:E:76:GLY:HA3 | 4:E:106:GLN:HB3 | 2.02 | 0.40 |
| 7:I:10:CYS:SG | 7:I:31:THR:CG2 | 3.10 | 0.40 |
| 8:J:53:HIS:HD1 | 8:J:53:HIS:C | 2.24 | 0.40 |
| 9:K:42:LEU:HA | 9:K:42:LEU:HD12 | 1.64 | 0.40 |
| 10:L:29:TYR:O | 10:L:30:ILE:HG13 | 2.21 | 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 | 1334/1733 (77%) | 1196 (90%) | 84 (6%) | 54 (4%) | 3 17 |
| 2 | B | 1071/1224 (88%) | 931 (87%) | 104 (10%) | 36 (3%) | 3 20 |
| 3 | C | 264/318 (83%) | 225 (85%) | 30 (11%) | 9 (3%) | 3 20 |
| 4 | E | 213/215 (99%) | 181 (85%) | 20 (9%) | 12 (6%) | 2 10 |
| 5 | F | 81/155 (52%) | 72 (89%) | 8 (10%) | 1 (1%) | 13 48 |
| 6 | H | 129/146 (88%) | 89 (69%) | 17 (13%) | 23 (18%) | 0 0 |
| 7 | I | 119/122 (98%) | 108 (91%) | 10 (8%) | 1 (1%) | 19 57 |
| 8 | J | 62/70 (89%) | 60 (97%) | 2 (3%) | 0 | 100 100 |
| 9 | K | 112/120 (93%) | 99 (88%) | 10 (9%) | 3 (3%) | 5 26 |
| 10 | L | 44/70 (63%) | 25 (57%) | 11 (25%) | 8 (18%) | 0 0 |
| All | All | 3429/4173 (82%) | 2986 (87%) | 296 (9%) | 147 (4%) | 2 15 |

All (147) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 35 | ILE |
| 1 | A | 45 | GLN |
| 1 | A | 47 | ARG |
| 1 | A | 59 | GLY |
| 1 | A | 62 | ASP |
| 1 | A | 65 | LEU |
| 1 | A | 69 | THR |
| 1 | A | 72 | GLU |
| 1 | A | 74 | MET |
| 1 | A | 120 | GLU |
| 1 | A | 155 | GLU |
| 1 | A | 156 | ASP |
| 1 | A | 157 | ASP |
| 1 | A | 165 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 190 | ALA |
| 1 | A | 286 | HIS |
| 1 | A | 418 | SER |
| 1 | A | 465 | TYR |
| 1 | A | 567 | LYS |
| 1 | A | 707 | GLY |
| 1 | A | 752 | LYS |
| 1 | A | 885 | THR |
| 1 | A | 1080 | THR |
| 1 | A | 1221 | LYS |
| 1 | A | 1448 | GLU |
| 2 | B | 66 | ASP |
| 2 | B | 105 | SER |
| 2 | B | 108 | VAL |
| 2 | B | 109 | THR |
| 2 | B | 165 | VAL |
| 2 | B | 230 | ALA |
| 2 | B | 436 | VAL |
| 2 | B | 645 | SER |
| 2 | B | 646 | LEU |
| 2 | B | 733 | HIS |
| 2 | B | 864 | LYS |
| 2 | B | 879 | ARG |
| 2 | B | 957 | ASN |
| 2 | B | 1108 | ARG |
| 2 | B | 1128 | LEU |
| 2 | B | 1167 | GLY |
| 3 | C | 4 | GLU |
| 3 | C | 9 | LYS |
| 3 | C | 206 | ASN |
| 4 | E | 48 | ASP |
| 4 | E | 64 | PRO |
| 4 | E | 118 | PRO |
| 5 | F | 73 | ALA |
| 6 | H | 32 | THR |
| 6 | H | 52 | GLN |
| 6 | H | 53 | ASP |
| 6 | H | 78 | SER |
| 6 | H | 90 | ALA |
| 6 | H | 104 | PHE |
| 6 | H | 105 | GLU |
| 6 | H | 116 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | H | 136 | LYS |
| 7 | I | 4 | PHE |
| 9 | K | 111 | LEU |
| 10 | L | 28 | LYS |
| 10 | L | 45 | ALA |
| 10 | L | 50 | ASP |
| 1 | A | 56 | PRO |
| 1 | A | 57 | ARG |
| 1 | A | 158 | PRO |
| 1 | A | 167 | CYS |
| 1 | A | 279 | LEU |
| 1 | A | 326 | ARG |
| 1 | A | 464 | PRO |
| 1 | A | 672 | ASP |
| 1 | A | 975 | HIS |
| 1 | A | 1223 | ASP |
| 1 | A | 1359 | ASP |
| 2 | B | 266 | ALA |
| 2 | B | 432 | MET |
| 2 | B | 451 | LYS |
| 2 | B | 466 | TRP |
| 2 | B | 887 | HIS |
| 2 | B | 1097 | HIS |
| 2 | B | 1105 | ALA |
| 3 | C | 209 | TYR |
| 3 | C | 231 | ASN |
| 4 | E | 44 | ALA |
| 4 | E | 45 | LYS |
| 4 | E | 50 | MET |
| 4 | E | 126 | SER |
| 6 | H | 77 | ARG |
| 6 | H | 81 | PRO |
| 6 | H | 86 | ASP |
| 6 | H | 89 | LEU |
| 6 | H | 107 | VAL |
| 6 | H | 135 | LEU |
| 6 | H | 139 | ASN |
| 9 | K | 99 | GLY |
| 10 | L | 39 | SER |
| 10 | L | 58 | LYS |
| 1 | A | 38 | PRO |
| 1 | A | 60 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 278 | THR |
| 1 | A | 1002 | GLY |
| 1 | A | 1255 | GLU |
| 2 | B | 865 | LYS |
| 2 | B | 1155 | SER |
| 2 | B | 1190 | ASP |
| 3 | C | 267 | GLN |
| 4 | E | 74 | ASP |
| 6 | H | 82 | PRO |
| 6 | H | 83 | GLN |
| 6 | H | 128 | ASN |
| 9 | K | 50 | LEU |
| 10 | L | 41 | SER |
| 1 | A | 32 | VAL |
| 1 | A | 75 | ASN |
| 1 | A | 706 | HIS |
| 2 | B | 90 | ILE |
| 2 | B | 447 | ALA |
| 2 | B | 643 | ASP |
| 3 | C | 137 | LYS |
| 4 | E | 2 | ASP |
| 4 | E | 56 | LYS |
| 6 | H | 19 | ARG |
| 10 | L | 46 | VAL |
| 1 | A | 42 | ASP |
| 1 | A | 196 | GLU |
| 1 | A | 599 | SER |
| 1 | A | 958 | VAL |
| 1 | A | 1204 | ASP |
| 1 | A | 1280 | GLU |
| 2 | B | 19 | GLU |
| 2 | B | 137 | TYR |
| 2 | B | 424 | LEU |
| 2 | B | 831 | SER |
| 2 | B | 1189 | ILE |
| 4 | E | 59 | SER |
| 6 | H | 119 | GLY |
| 10 | L | 59 | ALA |
| 1 | A | 400 | PRO |
| 2 | B | 940 | PRO |
| 2 | B | 1017 | ILE |
| 3 | C | 217 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | H | 5 | LEU |
| 6 | H | 103 | LYS |
| 1 | A | 52 | GLY |
| 1 | A | 55 | ASP |
| 3 | C | 126 | GLY |
| 4 | E | 38 | PRO |
| 1 | A | 1123 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 1183/1520 (78%) | 993 (84%) | 190 (16%) | 2 12 |
| 2 | B | 947/1061 (89%) | 801 (85%) | 146 (15%) | 2 13 |
| 3 | C | 234/274 (85%) | 194 (83%) | 40 (17%) | 2 10 |
| 4 | E | 197/197 (100%) | 153 (78%) | 44 (22%) | 1 4 |
| 5 | F | 73/137 (53%) | 62 (85%) | 11 (15%) | 3 14 |
| 6 | H | 117/128 (91%) | 74 (63%) | 43 (37%) | 0 0 |
| 7 | I | 115/116 (99%) | 93 (81%) | 22 (19%) | 1 8 |
| 8 | J | 59/65 (91%) | 49 (83%) | 10 (17%) | 2 11 |
| 9 | K | 99/102 (97%) | 83 (84%) | 16 (16%) | 2 12 |
| 10 | L | 40/57 (70%) | 20 (50%) | 20 (50%) | 0 0 |
| All | All | 3064/3657 (84%) | 2522 (82%) | 542 (18%) | 2 9 |

All (542) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | GLN |
| 1 | A | 11 | LEU |
| 1 | A | 15 | LYS |
| 1 | A | 22 | PHE |
| 1 | A | 30 | ILE |
| 1 | A | 34 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 36 | ARG |
| 1 | A | 39 | GLU |
| 1 | A | 44 | THR |
| 1 | A | 46 | THR |
| 1 | A | 49 | LYS |
| 1 | A | 58 | LEU |
| 1 | A | 60 | SER |
| 1 | A | 62 | ASP |
| 1 | A | 68 | GLN |
| 1 | A | 70 | CYS |
| 1 | A | 74 | MET |
| 1 | A | 81 | PHE |
| 1 | A | 84 | ILE |
| 1 | A | 90 | VAL |
| 1 | A | 93 | VAL |
| 1 | A | 98 | LYS |
| 1 | A | 106 | VAL |
| 1 | A | 110 | CYS |
| 1 | A | 112 | LYS |
| 1 | A | 114 | LEU |
| 1 | A | 120 | GLU |
| 1 | A | 121 | LEU |
| 1 | A | 122 | MET |
| 1 | A | 129 | LYS |
| 1 | A | 131 | SER |
| 1 | A | 138 | ILE |
| 1 | A | 144 | THR |
| 1 | A | 145 | LYS |
| 1 | A | 148 | CYS |
| 1 | A | 153 | PRO |
| 1 | A | 156 | ASP |
| 1 | A | 158 | PRO |
| 1 | A | 160 | GLN |
| 1 | A | 167 | CYS |
| 1 | A | 172 | PRO |
| 1 | A | 173 | THR |
| 1 | A | 176 | LYS |
| 1 | A | 191 | THR |
| 1 | A | 193 | ASP |
| 1 | A | 195 | ASP |
| 1 | A | 197 | PRO |
| 1 | A | 198 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 206 | GLU |
| 1 | A | 215 | SER |
| 1 | A | 230 | ARG |
| 1 | A | 231 | PRO |
| 1 | A | 235 | ILE |
| 1 | A | 239 | LEU |
| 1 | A | 247 | ARG |
| 1 | A | 261 | ASP |
| 1 | A | 263 | THR |
| 1 | A | 265 | LYS |
| 1 | A | 268 | ASP |
| 1 | A | 269 | ILE |
| 1 | A | 270 | LEU |
| 1 | A | 275 | SER |
| 1 | A | 286 | HIS |
| 1 | A | 294 | SER |
| 1 | A | 328 | ARG |
| 1 | A | 329 | LEU |
| 1 | A | 346 | ASP |
| 1 | A | 351 | THR |
| 1 | A | 354 | SER |
| 1 | A | 368 | LYS |
| 1 | A | 385 | ILE |
| 1 | A | 409 | SER |
| 1 | A | 416 | ARG |
| 1 | A | 419 | LYS |
| 1 | A | 434 | ARG |
| 1 | A | 451 | HIS |
| 1 | A | 461 | LYS |
| 1 | A | 466 | SER |
| 1 | A | 472 | LEU |
| 1 | A | 474 | VAL |
| 1 | A | 475 | THR |
| 1 | A | 493 | GLN |
| 1 | A | 495 | GLU |
| 1 | A | 498 | ARG |
| 1 | A | 504 | LEU |
| 1 | A | 508 | PRO |
| 1 | A | 513 | SER |
| 1 | A | 531 | ILE |
| 1 | A | 535 | THR |
| 1 | A | 537 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 543 | LEU |
| 1 | A | 571 | LEU |
| 1 | A | 588 | LEU |
| 1 | A | 590 | ARG |
| 1 | A | 597 | LEU |
| 1 | A | 599 | SER |
| 1 | A | 618 | GLU |
| 1 | A | 622 | VAL |
| 1 | A | 626 | ASN |
| 1 | A | 636 | GLU |
| 1 | A | 666 | ILE |
| 1 | A | 679 | ILE |
| 1 | A | 681 | GLU |
| 1 | A | 683 | ILE |
| 1 | A | 688 | LYS |
| 1 | A | 702 | LEU |
| 1 | A | 703 | THR |
| 1 | A | 705 | LYS |
| 1 | A | 708 | MET |
| 1 | A | 709 | THR |
| 1 | A | 710 | LEU |
| 1 | A | 720 | ARG |
| 1 | A | 724 | GLU |
| 1 | A | 728 | LYS |
| 1 | A | 741 | ASN |
| 1 | A | 794 | PRO |
| 1 | A | 810 | PRO |
| 1 | A | 821 | ARG |
| 1 | A | 830 | LYS |
| 1 | A | 843 | LYS |
| 1 | A | 858 | ASN |
| 1 | A | 882 | SER |
| 1 | A | 885 | THR |
| 1 | A | 895 | LYS |
| 1 | A | 903 | ASN |
| 1 | A | 907 | THR |
| 1 | A | 909 | ASP |
| 1 | A | 918 | GLU |
| 1 | A | 920 | LEU |
| 1 | A | 940 | ARG |
| 1 | A | 964 | ILE |
| 1 | A | 973 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 974 | ASP |
| 1 | A | 979 | SER |
| 1 | A | 982 | THR |
| 1 | A | 1003 | LYS |
| 1 | A | 1006 | ILE |
| 1 | A | 1015 | VAL |
| 1 | A | 1030 | ARG |
| 1 | A | 1064 | VAL |
| 1 | A | 1078 | GLN |
| 1 | A | 1081 | LEU |
| 1 | A | 1092 | LYS |
| 1 | A | 1093 | LYS |
| 1 | A | 1096 | SER |
| 1 | A | 1102 | LYS |
| 1 | A | 1109 | LYS |
| 1 | A | 1129 | GLU |
| 1 | A | 1138 | ILE |
| 1 | A | 1146 | VAL |
| 1 | A | 1161 | THR |
| 1 | A | 1165 | GLU |
| 1 | A | 1171 | GLN |
| 1 | A | 1172 | LEU |
| 1 | A | 1176 | LEU |
| 1 | A | 1187 | GLN |
| 1 | A | 1204 | ASP |
| 1 | A | 1208 | THR |
| 1 | A | 1217 | LYS |
| 1 | A | 1225 | PHE |
| 1 | A | 1230 | GLU |
| 1 | A | 1235 | LYS |
| 1 | A | 1236 | LEU |
| 1 | A | 1237 | ILE |
| 1 | A | 1239 | ARG |
| 1 | A | 1258 | HIS |
| 1 | A | 1259 | MET |
| 1 | A | 1267 | MET |
| 1 | A | 1269 | GLU |
| 1 | A | 1277 | GLU |
| 1 | A | 1281 | ARG |
| 1 | A | 1293 | SER |
| 1 | A | 1309 | ASP |
| 1 | A | 1317 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1318 | THR |
| 1 | A | 1325 | THR |
| 1 | A | 1327 | ILE |
| 1 | A | 1335 | ILE |
| 1 | A | 1359 | ASP |
| 1 | A | 1361 | SER |
| 1 | A | 1366 | ARG |
| 1 | A | 1376 | THR |
| 1 | A | 1377 | THR |
| 1 | A | 1384 | VAL |
| 1 | A | 1405 | THR |
| 1 | A | 1426 | GLU |
| 1 | A | 1438 | THR |
| 1 | A | 1445 | ILE |
| 1 | A | 1448 | GLU |
| 1 | A | 1449 | SER |
| 2 | B | 18 | PHE |
| 2 | B | 20 | ASP |
| 2 | B | 25 | ILE |
| 2 | B | 46 | GLN |
| 2 | B | 65 | GLU |
| 2 | B | 68 | THR |
| 2 | B | 69 | LEU |
| 2 | B | 70 | ILE |
| 2 | B | 89 | GLU |
| 2 | B | 92 | PHE |
| 2 | B | 98 | THR |
| 2 | B | 102 | VAL |
| 2 | B | 106 | ASP |
| 2 | B | 128 | LEU |
| 2 | B | 130 | VAL |
| 2 | B | 133 | LYS |
| 2 | B | 134 | LYS |
| 2 | B | 136 | THR |
| 2 | B | 138 | GLU |
| 2 | B | 164 | LYS |
| 2 | B | 167 | ILE |
| 2 | B | 178 | ASN |
| 2 | B | 179 | CYS |
| 2 | B | 183 | GLU |
| 2 | B | 194 | GLU |
| 2 | B | 199 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 204 | ILE |
| 2 | B | 217 | ARG |
| 2 | B | 228 | LYS |
| 2 | B | 239 | GLU |
| 2 | B | 242 | SER |
| 2 | B | 244 | LEU |
| 2 | B | 248 | SER |
| 2 | B | 252 | SER |
| 2 | B | 261 | ARG |
| 2 | B | 264 | SER |
| 2 | B | 277 | LYS |
| 2 | B | 282 | ILE |
| 2 | B | 358 | LYS |
| 2 | B | 367 | LEU |
| 2 | B | 373 | ARG |
| 2 | B | 384 | ARG |
| 2 | B | 387 | LEU |
| 2 | B | 417 | PHE |
| 2 | B | 422 | LYS |
| 2 | B | 423 | LYS |
| 2 | B | 425 | THR |
| 2 | B | 434 | ARG |
| 2 | B | 435 | THR |
| 2 | B | 463 | THR |
| 2 | B | 466 | TRP |
| 2 | B | 485 | ARG |
| 2 | B | 487 | THR |
| 2 | B | 498 | THR |
| 2 | B | 502 | ILE |
| 2 | B | 513 | GLN |
| 2 | B | 516 | ASN |
| 2 | B | 524 | PRO |
| 2 | B | 531 | GLN |
| 2 | B | 547 | VAL |
| 2 | B | 549 | THR |
| 2 | B | 550 | ASP |
| 2 | B | 566 | LEU |
| 2 | B | 567 | GLU |
| 2 | B | 589 | VAL |
| 2 | B | 591 | ARG |
| 2 | B | 595 | ARG |
| 2 | B | 598 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 606 | LYS |
| 2 | B | 614 | SER |
| 2 | B | 639 | ILE |
| 2 | B | 641 | GLU |
| 2 | B | 645 | SER |
| 2 | B | 648 | HIS |
| 2 | B | 650 | GLU |
| 2 | B | 653 | VAL |
| 2 | B | 666 | TYR |
| 2 | B | 680 | THR |
| 2 | B | 691 | GLU |
| 2 | B | 706 | GLN |
| 2 | B | 710 | LEU |
| 2 | B | 722 | ASP |
| 2 | B | 723 | VAL |
| 2 | B | 730 | ARG |
| 2 | B | 733 | HIS |
| 2 | B | 736 | THR |
| 2 | B | 775 | LYS |
| 2 | B | 788 | ARG |
| 2 | B | 806 | THR |
| 2 | B | 838 | SER |
| 2 | B | 846 | ILE |
| 2 | B | 857 | ARG |
| 2 | B | 863 | GLU |
| 2 | B | 864 | LYS |
| 2 | B | 868 | MET |
| 2 | B | 871 | THR |
| 2 | B | 878 | GLN |
| 2 | B | 879 | ARG |
| 2 | B | 881 | ASN |
| 2 | B | 882 | THR |
| 2 | B | 883 | LEU |
| 2 | B | 884 | ARG |
| 2 | B | 889 | THR |
| 2 | B | 895 | ASP |
| 2 | B | 896 | ASP |
| 2 | B | 908 | GLU |
| 2 | B | 914 | LYS |
| 2 | B | 933 | SER |
| 2 | B | 938 | SER |
| 2 | B | 955 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 956 | THR |
| 2 | B | 958 | GLN |
| 2 | B | 962 | LYS |
| 2 | B | 964 | VAL |
| 2 | B | 975 | GLN |
| 2 | B | 987 | LYS |
| 2 | B | 996 | ARG |
| 2 | B | 997 | GLU |
| 2 | B | 1007 | VAL |
| 2 | B | 1010 | LEU |
| 2 | B | 1055 | ILE |
| 2 | B | 1056 | SER |
| 2 | B | 1060 | ARG |
| 2 | B | 1065 | GLN |
| 2 | B | 1077 | THR |
| 2 | B | 1097 | HIS |
| 2 | B | 1099 | VAL |
| 2 | B | 1101 | ASP |
| 2 | B | 1106 | ARG |
| 2 | B | 1150 | ARG |
| 2 | B | 1152 | MET |
| 2 | B | 1155 | SER |
| 2 | B | 1156 | ASP |
| 2 | B | 1159 | ARG |
| 2 | B | 1165 | ILE |
| 2 | B | 1166 | CYS |
| 2 | B | 1174 | LYS |
| 2 | B | 1179 | GLN |
| 2 | B | 1182 | CYS |
| 2 | B | 1183 | LYS |
| 2 | B | 1185 | CYS |
| 2 | B | 1187 | ASN |
| 2 | B | 1211 | ASN |
| 2 | B | 1220 | ARG |
| 2 | B | 1222 | ARG |
| 2 | B | 1224 | PHE |
| 3 | C | 3 | GLU |
| 3 | C | 4 | GLU |
| 3 | C | 9 | LYS |
| 3 | C | 14 | SER |
| 3 | C | 23 | SER |
| 3 | C | 25 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 26 | ASP |
| 3 | C | 29 | MET |
| 3 | C | 33 | LEU |
| 3 | C | 43 | THR |
| 3 | C | 56 | THR |
| 3 | C | 57 | VAL |
| 3 | C | 77 | ILE |
| 3 | C | 86 | CYS |
| 3 | C | 93 | ASP |
| 3 | C | 102 | GLN |
| 3 | C | 119 | VAL |
| 3 | C | 125 | MET |
| 3 | C | 127 | ARG |
| 3 | C | 132 | PRO |
| 3 | C | 137 | LYS |
| 3 | C | 154 | LYS |
| 3 | C | 163 | ILE |
| 3 | C | 178 | PHE |
| 3 | C | 184 | ASN |
| 3 | C | 185 | LYS |
| 3 | C | 186 | LEU |
| 3 | C | 197 | SER |
| 3 | C | 205 | LYS |
| 3 | C | 209 | TYR |
| 3 | C | 214 | ASN |
| 3 | C | 238 | ILE |
| 3 | C | 240 | VAL |
| 3 | C | 245 | VAL |
| 3 | C | 251 | LEU |
| 3 | C | 264 | GLN |
| 3 | C | 265 | MET |
| 3 | C | 266 | ASP |
| 3 | C | 267 | GLN |
| 3 | C | 268 | ASP |
| 4 | E | 3 | GLN |
| 4 | E | 10 | SER |
| 4 | E | 14 | ARG |
| 4 | E | 33 | GLU |
| 4 | E | 34 | GLU |
| 4 | E | 36 | GLU |
| 4 | E | 37 | LEU |
| 4 | E | 47 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | E | 49 | SER |
| 4 | E | 50 | MET |
| 4 | E | 52 | ARG |
| 4 | E | 57 | MET |
| 4 | E | 60 | PHE |
| 4 | E | 61 | GLN |
| 4 | E | 69 | ILE |
| 4 | E | 70 | SER |
| 4 | E | 72 | PHE |
| 4 | E | 74 | ASP |
| 4 | E | 78 | LEU |
| 4 | E | 81 | GLU |
| 4 | E | 82 | PHE |
| 4 | E | 84 | ASP |
| 4 | E | 91 | LYS |
| 4 | E | 92 | THR |
| 4 | E | 95 | THR |
| 4 | E | 101 | GLN |
| 4 | E | 103 | LYS |
| 4 | E | 107 | THR |
| 4 | E | 116 | ILE |
| 4 | E | 119 | SER |
| 4 | E | 121 | MET |
| 4 | E | 123 | LEU |
| 4 | E | 129 | PRO |
| 4 | E | 137 | GLU |
| 4 | E | 149 | LEU |
| 4 | E | 158 | SER |
| 4 | E | 159 | ASP |
| 4 | E | 161 | LYS |
| 4 | E | 162 | ARG |
| 4 | E | 171 | LYS |
| 4 | E | 192 | ARG |
| 4 | E | 200 | ARG |
| 4 | E | 204 | THR |
| 4 | E | 212 | ARG |
| 5 | F | 72 | LYS |
| 5 | F | 77 | ASP |
| 5 | F | 79 | ARG |
| 5 | F | 81 | THR |
| 5 | F | 82 | THR |
| 5 | F | 87 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | F | 97 | ARG |
| 5 | F | 110 | ASP |
| 5 | F | 111 | LEU |
| 5 | F | 117 | PRO |
| 5 | F | 119 | ARG |
| 6 | H | 4 | THR |
| 6 | H | 5 | LEU |
| 6 | H | 6 | PHE |
| 6 | H | 7 | ASP |
| 6 | H | 9 | ILE |
| 6 | H | 13 | SER |
| 6 | H | 27 | GLU |
| 6 | H | 34 | ASP |
| 6 | H | 35 | GLN |
| 6 | H | 36 | CYS |
| 6 | H | 40 | LEU |
| 6 | H | 42 | ILE |
| 6 | H | 45 | GLU |
| 6 | H | 46 | LEU |
| 6 | H | 52 | GLN |
| 6 | H | 53 | ASP |
| 6 | H | 54 | SER |
| 6 | H | 56 | THR |
| 6 | H | 63 | LEU |
| 6 | H | 77 | ARG |
| 6 | H | 78 | SER |
| 6 | H | 80 | ARG |
| 6 | H | 86 | ASP |
| 6 | H | 87 | ARG |
| 6 | H | 88 | SER |
| 6 | H | 89 | LEU |
| 6 | H | 91 | ASP |
| 6 | H | 92 | ASP |
| 6 | H | 93 | TYR |
| 6 | H | 105 | GLU |
| 6 | H | 106 | GLU |
| 6 | H | 108 | SER |
| 6 | H | 109 | LYS |
| 6 | H | 111 | LEU |
| 6 | H | 112 | ILE |
| 6 | H | 121 | LEU |
| 6 | H | 126 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | H | 129 | TYR |
| 6 | H | 130 | ARG |
| 6 | H | 131 | ASN |
| 6 | H | 136 | LYS |
| 6 | H | 144 | ILE |
| 6 | H | 145 | ARG |
| 7 | I | 1 | MET |
| 7 | I | 2 | THR |
| 7 | I | 4 | PHE |
| 7 | I | 10 | CYS |
| 7 | I | 18 | GLU |
| 7 | I | 31 | THR |
| 7 | I | 40 | SER |
| 7 | I | 45 | ARG |
| 7 | I | 46 | HIS |
| 7 | I | 55 | THR |
| 7 | I | 61 | ASP |
| 7 | I | 76 | PRO |
| 7 | I | 77 | LYS |
| 7 | I | 78 | CYS |
| 7 | I | 82 | GLU |
| 7 | I | 84 | VAL |
| 7 | I | 95 | THR |
| 7 | I | 116 | ASN |
| 7 | I | 117 | LYS |
| 7 | I | 118 | ARG |
| 7 | I | 119 | THR |
| 7 | I | 120 | GLN |
| 8 | J | 1 | MET |
| 8 | J | 2 | ILE |
| 8 | J | 3 | VAL |
| 8 | J | 14 | VAL |
| 8 | J | 20 | SER |
| 8 | J | 28 | ASP |
| 8 | J | 38 | ARG |
| 8 | J | 48 | ARG |
| 8 | J | 62 | ARG |
| 8 | J | 64 | ASN |
| 9 | K | 1 | MET |
| 9 | K | 2 | ASN |
| 9 | K | 11 | LEU |
| 9 | K | 18 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | K | 20 | LYS |
| 9 | K | 31 | VAL |
| 9 | K | 42 | LEU |
| 9 | K | 47 | ARG |
| 9 | K | 63 | VAL |
| 9 | K | 73 | LEU |
| 9 | K | 75 | ILE |
| 9 | K | 78 | THR |
| 9 | K | 93 | SER |
| 9 | K | 112 | GLN |
| 9 | K | 113 | THR |
| 9 | K | 114 | LEU |
| 10 | L | 27 | LEU |
| 10 | L | 28 | LYS |
| 10 | L | 33 | GLU |
| 10 | L | 36 | SER |
| 10 | L | 42 | ARG |
| 10 | L | 44 | ASP |
| 10 | L | 46 | VAL |
| 10 | L | 47 | ARG |
| 10 | L | 48 | CYS |
| 10 | L | 49 | LYS |
| 10 | L | 50 | ASP |
| 10 | L | 51 | CYS |
| 10 | L | 54 | ARG |
| 10 | L | 58 | LYS |
| 10 | L | 60 | ARG |
| 10 | L | 61 | THR |
| 10 | L | 63 | ARG |
| 10 | L | 64 | LEU |
| 10 | L | 65 | VAL |
| 10 | L | 68 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 83 | HIS |
| 1 | A | 92 | HIS |
| 1 | A | 171 | GLN |
| 1 | A | 299 | HIS |
| 1 | A | 390 | GLN |
| 1 | A | 399 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 451 | HIS |
| 1 | A | 479 | ASN |
| 1 | A | 503 | GLN |
| 1 | A | 515 | GLN |
| 1 | A | 517 | ASN |
| 1 | A | 587 | HIS |
| 1 | A | 736 | ASN |
| 1 | A | 741 | ASN |
| 1 | A | 745 | GLN |
| 1 | A | 768 | GLN |
| 1 | A | 786 | HIS |
| 1 | A | 854 | ASN |
| 1 | A | 858 | ASN |
| 1 | A | 903 | ASN |
| 1 | A | 926 | GLN |
| 1 | A | 994 | GLN |
| 1 | A | 1078 | GLN |
| 1 | A | 1124 | HIS |
| 1 | A | 1173 | HIS |
| 1 | A | 1364 | ASN |
| 1 | A | 1432 | GLN |
| 2 | B | 121 | ASN |
| 2 | B | 178 | ASN |
| 2 | B | 215 | GLN |
| 2 | B | 236 | HIS |
| 2 | B | 325 | GLN |
| 2 | B | 357 | GLN |
| 2 | B | 366 | GLN |
| 2 | B | 383 | ASN |
| 2 | B | 433 | GLN |
| 2 | B | 516 | ASN |
| 2 | B | 518 | HIS |
| 2 | B | 531 | GLN |
| 2 | B | 538 | ASN |
| 2 | B | 587 | HIS |
| 2 | B | 590 | HIS |
| 2 | B | 657 | HIS |
| 2 | B | 706 | GLN |
| 2 | B | 744 | HIS |
| 2 | B | 843 | GLN |
| 2 | B | 862 | GLN |
| 2 | B | 878 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 958 | GLN |
| 2 | B | 984 | HIS |
| 2 | B | 1015 | HIS |
| 2 | B | 1025 | HIS |
| 2 | B | 1062 | HIS |
| 2 | B | 1065 | GLN |
| 2 | B | 1084 | GLN |
| 2 | B | 1093 | GLN |
| 2 | B | 1161 | HIS |
| 2 | B | 1179 | GLN |
| 2 | B | 1187 | ASN |
| 3 | C | 73 | GLN |
| 3 | C | 112 | ASN |
| 3 | C | 167 | HIS |
| 3 | C | 242 | GLN |
| 3 | C | 252 | GLN |
| 4 | E | 5 | ASN |
| 4 | E | 61 | GLN |
| 4 | E | 113 | GLN |
| 4 | E | 147 | HIS |
| 6 | H | 11 | GLN |
| 6 | H | 131 | ASN |
| 6 | H | 133 | ASN |
| 7 | I | 12 | ASN |
| 7 | I | 83 | ASN |
| 7 | I | 116 | ASN |
| 8 | J | 53 | HIS |
| 9 | K | 2 | ASN |
| 9 | K | 65 | HIS |
| 9 | K | 76 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 13 | GTP | B | 3008 | 2,12 | 26,34,34 | 1.38 | 2 (7%) | 32,54,54 | 1.53 | 4 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 13 | GTP | B | 3008 | 2,12 | 1/1/7/7 | 8/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 13 | B | 3008 | GTP | C8-N7 | -5.08 | 1.26 | 1.35 |
| 13 | B | 3008 | GTP | C2-N3 | 3.35 | 1.41 | 1.33 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | B | 3008 | GTP | O4'-C1'-C2' | 4.26 | 113.16 | 106.93 |
| 13 | B | 3008 | GTP | PA-O3A-PB | -3.55 | 120.63 | 132.83 |
| 13 | B | 3008 | GTP | PB-O3B-PG | -3.43 | 121.06 | 132.83 |
| 13 | B | 3008 | GTP | C2'-C3'-C4' | 2.37 | 107.25 | 102.64 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 13 | B | 3008 | GTP | C1' |

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 13 | B | 3008 | GTP | C5'-O5'-PA-O3A |
| 13 | B | 3008 | GTP | O4'-C4'-C5'-O5' |
| 13 | B | 3008 | GTP | C3'-C4'-C5'-O5' |
| 13 | B | 3008 | GTP | PB-O3B-PG-O2G |
| 13 | B | 3008 | GTP | C5'-O5'-PA-O2A |
| 13 | B | 3008 | GTP | C4'-C5'-O5'-PA |
| 13 | B | 3008 | GTP | PB-O3B-PG-O3G |
| 13 | B | 3008 | GTP | C5'-O5'-PA-O1A |

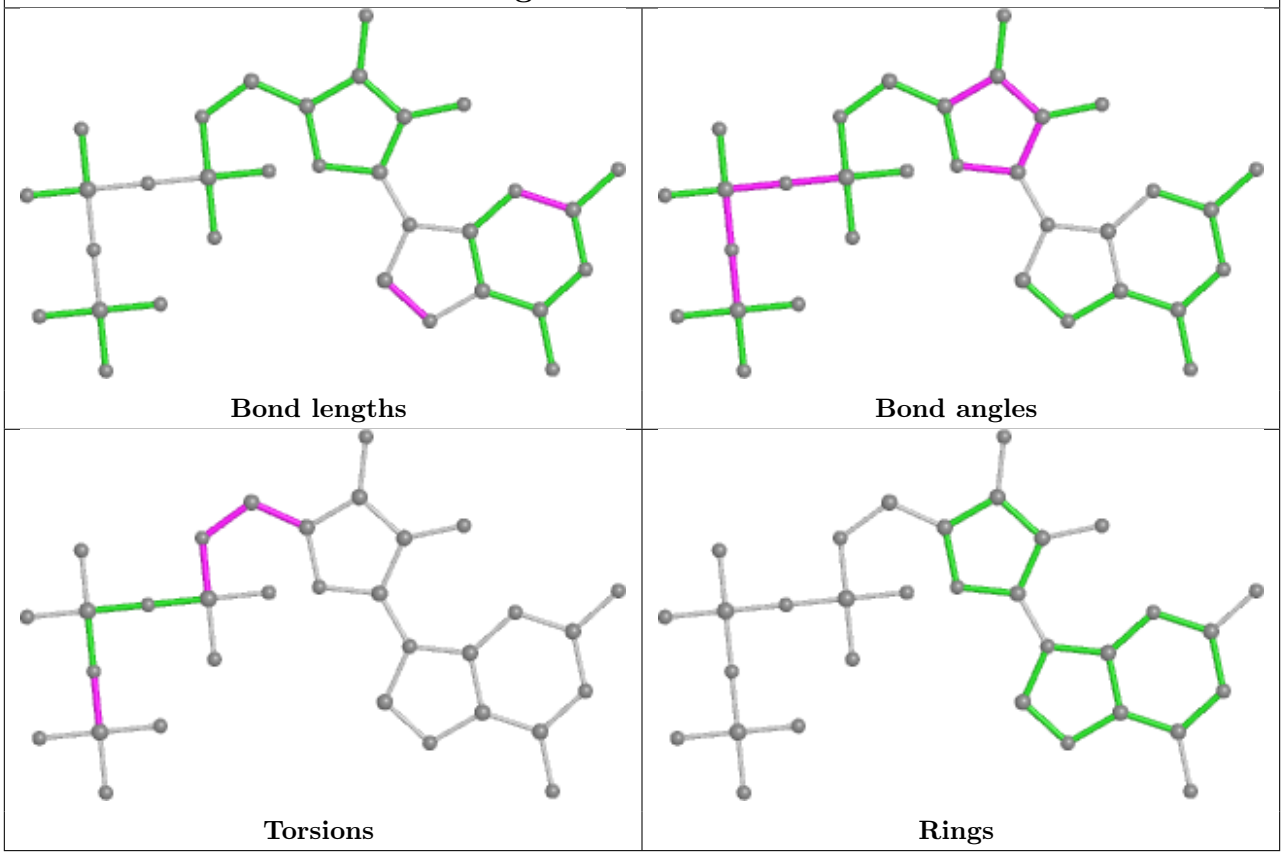
There are no ring outliers.

1 monomer is involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 13 | B | 3008 | GTP | 8 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand GTP B 3008**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 366:VAL | C | 367:PRO | N | 1.20 |

# 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 | 1351/1733 (77%) | -0.44 | 23 (1%) 70 41 | 20, 46, 110, 159 | 0 |
| 2 | B | 1091/1224 (89%) | -0.34 | 37 (3%) 45 19 | 21, 44, 116, 146 | 0 |
| 3 | C | 266/318 (83%) | -0.51 | 2 (0%) 86 65 | 29, 50, 79, 131 | 0 |
| 4 | E | 215/215 (100%) | -0.35 | 5 (2%) 60 31 | 23, 60, 108, 138 | 0 |
| 5 | F | 83/155 (53%) | -0.50 | 0 100 100 | 24, 45, 71, 80 | 0 |
| 6 | H | 133/146 (91%) | 0.06 | 4 (3%) 50 22 | 56, 88, 128, 135 | 0 |
| 7 | I | 121/122 (99%) | -0.44 | 1 (0%) 86 65 | 30, 50, 81, 111 | 0 |
| 8 | J | 64/70 (91%) | -0.59 | 0 100 100 | 31, 42, 71, 81 | 0 |
| 9 | K | 114/120 (95%) | -0.41 | 0 100 100 | 31, 58, 79, 86 | 0 |
| 10 | L | 46/70 (65%) | 0.15 | 4 (8%) 10 3 | 49, 95, 122, 125 | 0 |
| All | All | 3484/4173 (83%) | -0.38 | 76 (2%) 62 33 | 20, 49, 113, 159 | 0 |

All (76) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | B | 1109 | GLY | 7.4 |
| 2 | B | 246 | LYS | 7.4 |
| 2 | B | 882 | THR | 7.0 |
| 1 | A | 44 | THR | 6.8 |
| 1 | A | 188 | ASP | 6.4 |
| 1 | A | 69 | THR | 6.0 |
| 2 | B | 870 | ILE | 5.6 |
| 1 | A | 248 | PRO | 5.5 |
| 2 | B | 1223 | ASP | 5.4 |
| 2 | B | 1110 | PRO | 5.3 |
| 6 | H | 85 | GLY | 5.2 |
| 2 | B | 1106 | ARG | 5.1 |
| 2 | B | 247 | GLY | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 45 | GLN | 5.0 |
| 2 | B | 1105 | ALA | 4.9 |
| 1 | A | 1450 | LEU | 4.8 |
| 1 | A | 191 | THR | 4.8 |
| 3 | C | 268 | ASP | 4.5 |
| 6 | H | 132 | LEU | 4.1 |
| 2 | B | 734 | HIS | 3.9 |
| 10 | L | 25 | ALA | 3.7 |
| 1 | A | 190 | ALA | 3.6 |
| 2 | B | 1176 | ASN | 3.6 |
| 4 | E | 1 | MET | 3.6 |
| 2 | B | 1104 | HIS | 3.6 |
| 10 | L | 43 | THR | 3.5 |
| 2 | B | 245 | GLU | 3.4 |
| 2 | B | 869 | SER | 3.4 |
| 3 | C | 267 | GLN | 3.4 |
| 6 | H | 131 | ASN | 3.4 |
| 1 | A | 192 | GLY | 3.3 |
| 2 | B | 868 | MET | 3.2 |
| 2 | B | 883 | LEU | 3.2 |
| 1 | A | 43 | GLU | 3.2 |
| 2 | B | 137 | TYR | 3.1 |
| 2 | B | 888 | GLY | 3.1 |
| 2 | B | 89 | GLU | 3.1 |
| 2 | B | 733 | HIS | 3.0 |
| 1 | A | 189 | ARG | 3.0 |
| 1 | A | 1449 | SER | 2.9 |
| 4 | E | 2 | ASP | 2.9 |
| 2 | B | 135 | ARG | 2.8 |
| 2 | B | 1179 | GLN | 2.8 |
| 2 | B | 436 | VAL | 2.8 |
| 1 | A | 1092 | LYS | 2.8 |
| 2 | B | 136 | THR | 2.7 |
| 10 | L | 26 | THR | 2.7 |
| 2 | B | 1108 | ARG | 2.7 |
| 1 | A | 1222 | ASN | 2.7 |
| 2 | B | 1221 | SER | 2.6 |
| 2 | B | 1101 | ASP | 2.6 |
| 1 | A | 1448 | GLU | 2.6 |
| 4 | E | 50 | MET | 2.6 |
| 2 | B | 1102 | LYS | 2.6 |
| 2 | B | 887 | HIS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 3 | GLY | 2.5 |
| 1 | A | 833 | GLU | 2.5 |
| 2 | B | 871 | THR | 2.5 |
| 7 | I | 79 | HIS | 2.4 |
| 1 | A | 157 | ASP | 2.4 |
| 2 | B | 866 | TYR | 2.4 |
| 1 | A | 1080 | THR | 2.4 |
| 2 | B | 1224 | PHE | 2.4 |
| 1 | A | 193 | ASP | 2.3 |
| 2 | B | 432 | MET | 2.3 |
| 2 | B | 90 | ILE | 2.3 |
| 2 | B | 1155 | SER | 2.3 |
| 1 | A | 37 | PHE | 2.2 |
| 2 | B | 1189 | ILE | 2.1 |
| 1 | A | 1173 | HIS | 2.1 |
| 4 | E | 3 | GLN | 2.1 |
| 4 | E | 52 | ARG | 2.1 |
| 10 | L | 45 | ALA | 2.1 |
| 2 | B | 131 | ASP | 2.1 |
| 1 | A | 8 | SER | 2.1 |
| 6 | H | 35 | GLN | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 12 | MN | A | 3010 | 1/1 | 0.85 | 0.13 | 48,48,48,48 | 0 |
| 13 | GTP | B | 3008 | 32/32 | 0.90 | 0.23 | 96,112,119,119 | 0 |

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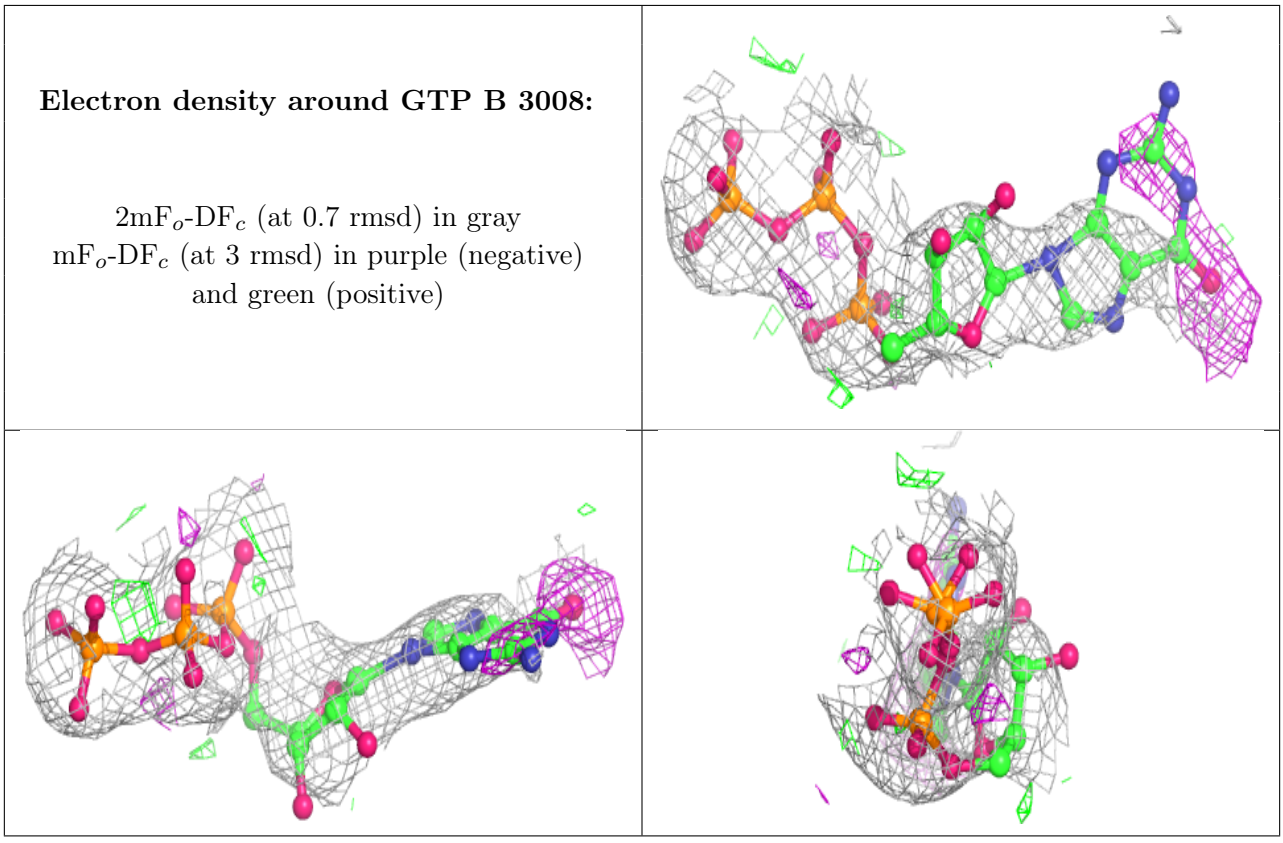
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 11 | ZN | A | 3006 | 1/1 | 0.93 | 0.12 | 67,67,67,67 | 0 |
| 11 | ZN | L | 3005 | 1/1 | 0.93 | 0.09 | 96,96,96,96 | 0 |
| 11 | ZN | B | 3007 | 1/1 | 0.96 | 0.11 | 64,64,64,64 | 0 |
| 12 | MN | A | 3009 | 1/1 | 0.97 | 0.13 | 36,36,36,36 | 0 |
| 11 | ZN | A | 3008 | 1/1 | 0.98 | 0.12 | 91,91,91,91 | 0 |
| 11 | ZN | C | 3002 | 1/1 | 0.99 | 0.09 | 53,53,53,53 | 0 |
| 11 | ZN | I | 3003 | 1/1 | 0.99 | 0.12 | 59,59,59,59 | 0 |
| 11 | ZN | I | 3004 | 1/1 | 0.99 | 0.05 | 80,80,80,80 | 0 |
| 11 | ZN | J | 3001 | 1/1 | 0.99 | 0.16 | 47,47,47,47 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GTP B 3008:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.