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

Jun 12, 2024 – 09:20 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1DLP |
| Title | : | STRUCTURAL CHARACTERIZATION OF THE NATIVE FETUIN-BINDING PROTEIN SCILLA CAMPANULATA AGGLUTININ (SCAFET): A NOVEL TWO-DOMAIN LECTIN |
| Authors | : | Wright, L.M.; Reynolds, C.D.; Rizkallah, P.J.; Allen, A.K.; VanDamme, E.J.M.; Donovan, M.J.; Peumans, W.J. |
| Deposited on | : | 1999-12-11 |
| Resolution | : | 3.30 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.

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

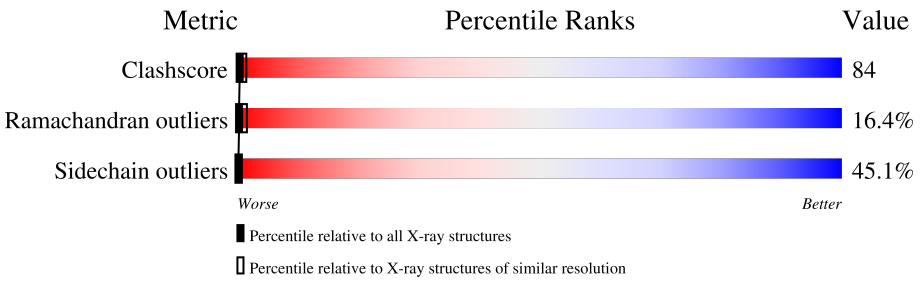
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 3.30 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 1205 (3.34-3.26) |
| Ramachandran outliers | 138981 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |

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%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 236 | 13% 35% 51% • |
| 1 | B | 236 | • 11% 34% 48% 6% |
| 1 | C | 236 | • 17% 32% 48% • |
| 1 | D | 236 | 11% 35% 49% 6% |
| 1 | E | 236 | • 14% 39% 43% • |
| 1 | F | 236 | • 14% 37% 40% 8% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10431 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 LECTIN SCAFET PRECURSOR.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 233 | 1778 | 1102 | 322 | 347 | 7 | 18 | 0 | 0 |
| 1 | B | 221 | 1694 | 1053 | 305 | 329 | 7 | 21 | 0 | 0 |
| 1 | C | 234 | 1772 | 1097 | 323 | 345 | 7 | 25 | 0 | 0 |
| 1 | D | 223 | 1702 | 1057 | 307 | 331 | 7 | 28 | 0 | 0 |
| 1 | E | 231 | 1759 | 1093 | 318 | 341 | 7 | 17 | 0 | 0 |
| 1 | F | 216 | 1659 | 1034 | 298 | 320 | 7 | 40 | 0 | 0 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | A | 19 | 19 | 19 | 0 | 0 |
| 2 | B | 15 | 15 | 15 | 0 | 0 |
| 2 | C | 6 | 6 | 6 | 0 | 0 |
| 2 | D | 8 | 8 | 8 | 0 | 0 |
| 2 | E | 8 | 8 | 8 | 0 | 0 |
| 2 | F | 11 | 11 | 11 | 0 | 0 |

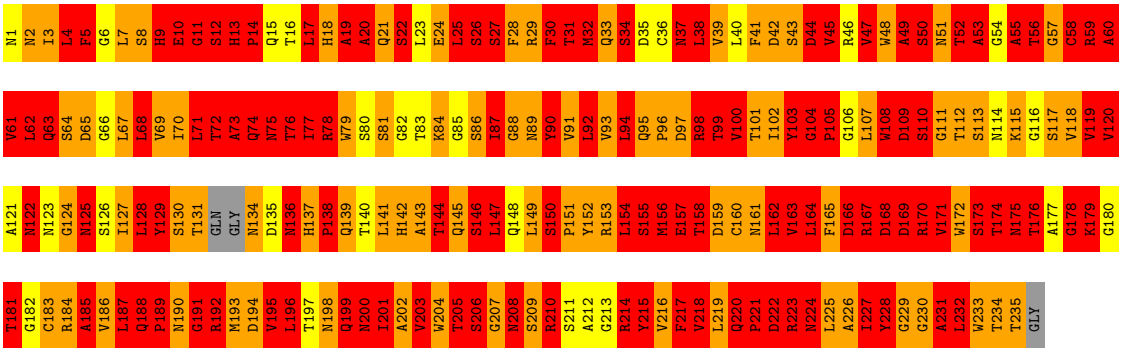
# 3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

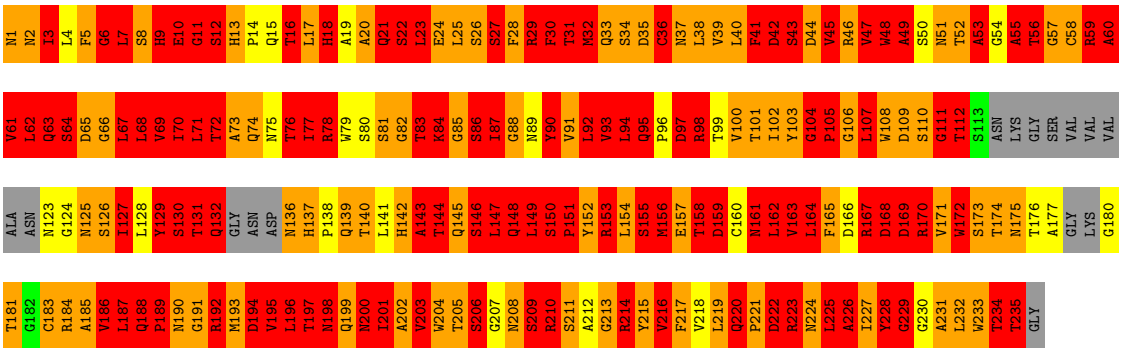
• Molecule 1: LECTIN SCAFET PRECURSOR

Chain A: 13% 35% 51%



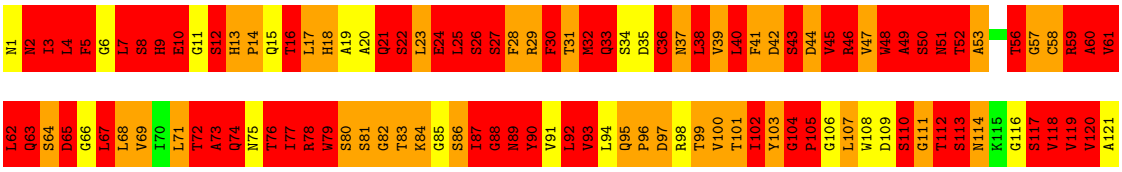

• Molecule 1: LECTIN SCAFET PRECURSOR

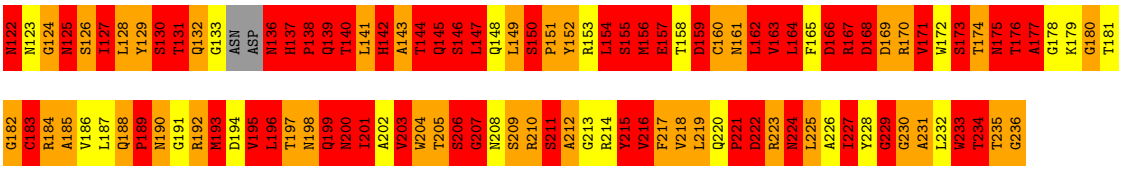
Chain B: 11% 34% 48% 6%




• Molecule 1: LECTIN SCAFET PRECURSOR

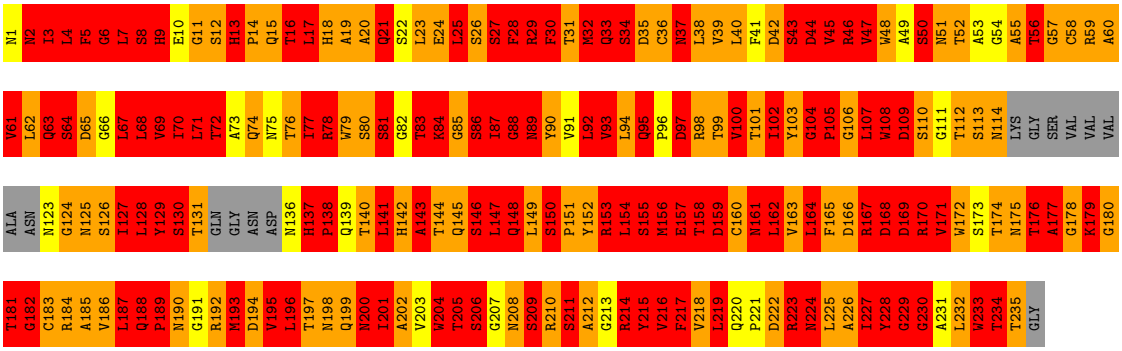
Chain C: 17% 32% 48%





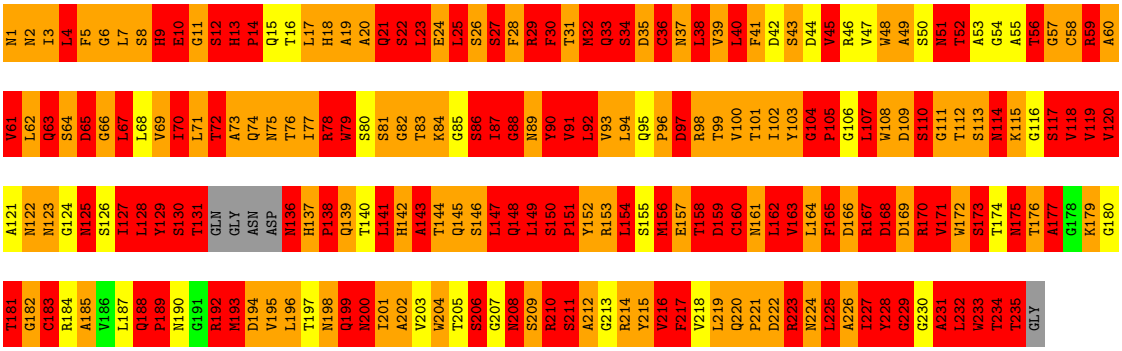

• Molecule 1: LECTIN SCAFET PRECURSOR

Chain D:



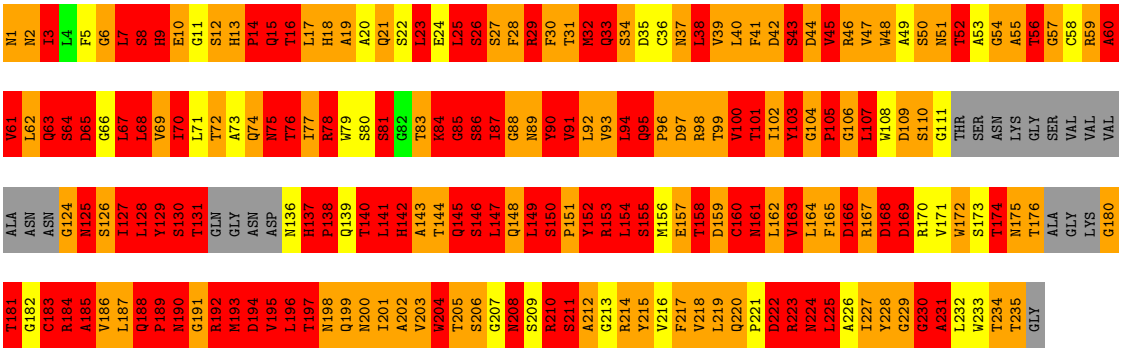

• Molecule 1: LECTIN SCAFET PRECURSOR

Chain E:




• Molecule 1: LECTIN SCAFET PRECURSOR

Chain F:



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 277.94Å 164.10Å 53.60Å<br>90.00° 95.38° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.30 | Depositor |
| % Data completeness<br>(in resolution range) | 95.3 (20.00-3.30) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | REFMAC | Depositor |
| R, $R_{free}$ | 0.189 , 0.293 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 10431 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 27.0 | wwPDB-VP |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 2.62 | 91/1812 (5.0%) | 6.89 | 912/2470 (36.9%) |
| 1 | B | 2.44 | 80/1726 (4.6%) | 6.84 | 897/2351 (38.2%) |
| 1 | C | 2.34 | 58/1805 (3.2%) | 6.48 | 838/2459 (34.1%) |
| 1 | D | 3.14 | 88/1735 (5.1%) | 7.13 | 928/2365 (39.2%) |
| 1 | E | 2.06 | 35/1793 (2.0%) | 5.99 | 765/2444 (31.3%) |
| 1 | F | 2.14 | 38/1691 (2.2%) | 6.60 | 810/2303 (35.2%) |
| All | All | 2.48 | 390/10562 (3.7%) | 6.66 | 5150/14392 (35.8%) |

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 | 2 | 60 |
| 1 | B | 2 | 73 |
| 1 | C | 0 | 66 |
| 1 | D | 0 | 51 |
| 1 | E | 0 | 39 |
| 1 | F | 2 | 53 |
| All | All | 6 | 342 |

All (390) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 1 | ASN | CG-ND2 | 50.13 | 2.58 | 1.32 |
| 1 | D | 78 | ARG | CG-CD | 46.82 | 2.69 | 1.51 |
| 1 | A | 44 | ASP | CB-CG | -34.10 | 0.80 | 1.51 |
| 1 | C | 168 | ASP | CG-OD1 | 30.06 | 1.94 | 1.25 |
| 1 | D | 167 | ARG | CD-NE | -29.28 | 0.96 | 1.46 |
| 1 | A | 136 | ASN | CB-CG | -23.90 | 0.96 | 1.51 |
| 1 | C | 9 | HIS | CB-CG | -20.03 | 1.14 | 1.50 |
| 1 | F | 224 | ASN | CA-CB | -19.84 | 1.01 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 12 | SER | CB-OG | -19.60 | 1.16 | 1.42 |
| 1 | D | 64 | SER | CB-OG | 19.02 | 1.67 | 1.42 |
| 1 | D | 230 | GLY | N-CA | -18.84 | 1.17 | 1.46 |
| 1 | F | 59 | ARG | CD-NE | -18.77 | 1.14 | 1.46 |
| 1 | E | 168 | ASP | CA-CB | -17.48 | 1.15 | 1.53 |
| 1 | D | 210 | ARG | CB-CG | -17.09 | 1.06 | 1.52 |
| 1 | D | 84 | LYS | CG-CD | -16.43 | 0.96 | 1.52 |
| 1 | A | 59 | ARG | CZ-NH1 | 16.11 | 1.53 | 1.33 |
| 1 | C | 44 | ASP | CA-CB | 16.02 | 1.89 | 1.53 |
| 1 | D | 233 | TRP | CG-CD1 | -14.94 | 1.15 | 1.36 |
| 1 | E | 136 | ASN | CA-CB | 13.41 | 1.88 | 1.53 |
| 1 | C | 130 | SER | CB-OG | -13.16 | 1.25 | 1.42 |
| 1 | D | 233 | TRP | CB-CG | -12.90 | 1.27 | 1.50 |
| 1 | D | 8 | SER | C-O | 12.59 | 1.47 | 1.23 |
| 1 | E | 46 | ARG | CA-CB | -12.06 | 1.27 | 1.53 |
| 1 | D | 12 | SER | C-O | -12.00 | 1.00 | 1.23 |
| 1 | D | 105 | PRO | N-CD | 11.92 | 1.64 | 1.47 |
| 1 | E | 131 | THR | C-O | 11.90 | 1.46 | 1.23 |
| 1 | B | 57 | GLY | N-CA | -11.78 | 1.28 | 1.46 |
| 1 | F | 81 | SER | CB-OG | -11.73 | 1.27 | 1.42 |
| 1 | F | 170 | ARG | CB-CG | -11.38 | 1.21 | 1.52 |
| 1 | A | 207 | GLY | N-CA | -11.34 | 1.29 | 1.46 |
| 1 | D | 229 | GLY | N-CA | -11.24 | 1.29 | 1.46 |
| 1 | B | 90 | TYR | CG-CD1 | -10.88 | 1.25 | 1.39 |
| 1 | A | 126 | SER | CB-OG | -10.88 | 1.28 | 1.42 |
| 1 | B | 138 | PRO | N-CD | -10.86 | 1.32 | 1.47 |
| 1 | D | 12 | SER | CB-OG | -10.82 | 1.28 | 1.42 |
| 1 | E | 130 | SER | CB-OG | 10.78 | 1.56 | 1.42 |
| 1 | A | 180 | GLY | N-CA | -10.74 | 1.29 | 1.46 |
| 1 | A | 131 | THR | CB-OG1 | 10.45 | 1.64 | 1.43 |
| 1 | C | 215 | TYR | CG-CD2 | -10.27 | 1.25 | 1.39 |
| 1 | F | 105 | PRO | N-CA | -10.23 | 1.29 | 1.47 |
| 1 | C | 59 | ARG | CZ-NH1 | 10.08 | 1.46 | 1.33 |
| 1 | C | 167 | ARG | CA-CB | -10.02 | 1.31 | 1.53 |
| 1 | C | 46 | ARG | CA-CB | -9.97 | 1.32 | 1.53 |
| 1 | A | 215 | TYR | CG-CD2 | -9.87 | 1.26 | 1.39 |
| 1 | E | 231 | ALA | CA-CB | -9.85 | 1.31 | 1.52 |
| 1 | C | 136 | ASN | N-CA | 9.79 | 1.66 | 1.46 |
| 1 | B | 150 | SER | CA-CB | -9.62 | 1.38 | 1.52 |
| 1 | A | 187 | LEU | N-CA | -9.58 | 1.27 | 1.46 |
| 1 | C | 168 | ASP | CG-OD2 | 9.42 | 1.47 | 1.25 |
| 1 | A | 157 | GLU | CD-OE1 | 9.41 | 1.36 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 126 | SER | CB-OG | -9.37 | 1.30 | 1.42 |
| 1 | B | 235 | THR | C-O | 9.31 | 1.41 | 1.23 |
| 1 | B | 61 | VAL | N-CA | 9.20 | 1.64 | 1.46 |
| 1 | D | 105 | PRO | N-CA | -9.17 | 1.31 | 1.47 |
| 1 | E | 160 | CYS | CB-SG | -9.14 | 1.66 | 1.82 |
| 1 | B | 66 | GLY | C-O | 9.10 | 1.38 | 1.23 |
| 1 | A | 59 | ARG | CZ-NH2 | 9.08 | 1.44 | 1.33 |
| 1 | B | 60 | ALA | C-O | 9.00 | 1.40 | 1.23 |
| 1 | B | 54 | GLY | C-O | 8.96 | 1.38 | 1.23 |
| 1 | E | 110 | SER | CB-OG | -8.88 | 1.30 | 1.42 |
| 1 | D | 98 | ARG | CZ-NH1 | 8.84 | 1.44 | 1.33 |
| 1 | E | 131 | THR | CA-C | 8.82 | 1.75 | 1.52 |
| 1 | A | 206 | SER | CB-OG | 8.79 | 1.53 | 1.42 |
| 1 | B | 61 | VAL | C-N | 8.79 | 1.54 | 1.34 |
| 1 | F | 34 | SER | CA-CB | 8.78 | 1.66 | 1.52 |
| 1 | A | 48 | TRP | CG-CD1 | -8.73 | 1.24 | 1.36 |
| 1 | D | 89 | ASN | CG-ND2 | 8.64 | 1.54 | 1.32 |
| 1 | A | 194 | ASP | CA-CB | -8.62 | 1.34 | 1.53 |
| 1 | B | 22 | SER | CA-CB | 8.61 | 1.65 | 1.52 |
| 1 | B | 61 | VAL | C-O | -8.60 | 1.07 | 1.23 |
| 1 | A | 215 | TYR | N-CA | -8.59 | 1.29 | 1.46 |
| 1 | D | 126 | SER | CA-CB | -8.52 | 1.40 | 1.52 |
| 1 | E | 232 | LEU | CA-C | -8.43 | 1.31 | 1.52 |
| 1 | B | 34 | SER | CB-OG | -8.43 | 1.31 | 1.42 |
| 1 | D | 217 | PHE | C-O | -8.40 | 1.07 | 1.23 |
| 1 | A | 101 | THR | CB-OG1 | -8.39 | 1.26 | 1.43 |
| 1 | A | 235 | THR | C-O | 8.39 | 1.39 | 1.23 |
| 1 | A | 26 | SER | CB-OG | -8.30 | 1.31 | 1.42 |
| 1 | B | 225 | LEU | C-N | -8.28 | 1.15 | 1.34 |
| 1 | F | 8 | SER | C-O | 8.28 | 1.39 | 1.23 |
| 1 | B | 64 | SER | N-CA | 8.27 | 1.62 | 1.46 |
| 1 | F | 131 | THR | C-O | 8.26 | 1.39 | 1.23 |
| 1 | D | 136 | ASN | N-CA | 8.24 | 1.62 | 1.46 |
| 1 | E | 167 | ARG | CB-CG | -8.19 | 1.30 | 1.52 |
| 1 | D | 106 | GLY | C-O | 8.17 | 1.36 | 1.23 |
| 1 | B | 98 | ARG | CZ-NH2 | 8.15 | 1.43 | 1.33 |
| 1 | C | 28 | PHE | CG-CD2 | -8.14 | 1.26 | 1.38 |
| 1 | A | 131 | THR | C-O | 8.09 | 1.38 | 1.23 |
| 1 | D | 130 | SER | CB-OG | 8.02 | 1.52 | 1.42 |
| 1 | F | 78 | ARG | CG-CD | -8.01 | 1.31 | 1.51 |
| 1 | C | 150 | SER | CB-OG | 7.99 | 1.52 | 1.42 |
| 1 | D | 221 | PRO | CA-CB | -7.99 | 1.37 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 61 | VAL | N-CA | 7.98 | 1.62 | 1.46 |
| 1 | F | 210 | ARG | CB-CG | 7.81 | 1.73 | 1.52 |
| 1 | A | 139 | GLN | C-N | 7.81 | 1.52 | 1.34 |
| 1 | B | 18 | HIS | N-CA | -7.79 | 1.30 | 1.46 |
| 1 | B | 191 | GLY | CA-C | -7.67 | 1.39 | 1.51 |
| 1 | F | 14 | PRO | N-CA | -7.65 | 1.34 | 1.47 |
| 1 | C | 215 | TYR | CE1-CZ | -7.61 | 1.28 | 1.38 |
| 1 | D | 157 | GLU | CD-OE1 | 7.61 | 1.34 | 1.25 |
| 1 | C | 88 | GLY | N-CA | 7.60 | 1.57 | 1.46 |
| 1 | A | 217 | PHE | CE1-CZ | -7.58 | 1.23 | 1.37 |
| 1 | A | 59 | ARG | NE-CZ | 7.57 | 1.42 | 1.33 |
| 1 | D | 209 | SER | CA-CB | 7.56 | 1.64 | 1.52 |
| 1 | B | 30 | PHE | C-N | -7.52 | 1.16 | 1.34 |
| 1 | C | 229 | GLY | C-N | -7.43 | 1.19 | 1.33 |
| 1 | C | 165 | PHE | CB-CG | -7.42 | 1.38 | 1.51 |
| 1 | F | 129 | TYR | CD2-CE2 | -7.41 | 1.28 | 1.39 |
| 1 | D | 168 | ASP | CA-CB | 7.40 | 1.70 | 1.53 |
| 1 | F | 98 | ARG | CZ-NH1 | 7.37 | 1.42 | 1.33 |
| 1 | A | 12 | SER | CA-CB | -7.35 | 1.42 | 1.52 |
| 1 | A | 6 | GLY | N-CA | 7.29 | 1.56 | 1.46 |
| 1 | A | 138 | PRO | N-CD | 7.28 | 1.58 | 1.47 |
| 1 | E | 15 | GLN | C-O | 7.26 | 1.37 | 1.23 |
| 1 | D | 217 | PHE | CD2-CE2 | -7.25 | 1.24 | 1.39 |
| 1 | A | 209 | SER | CB-OG | 7.23 | 1.51 | 1.42 |
| 1 | D | 21 | GLN | CA-CB | -7.21 | 1.38 | 1.53 |
| 1 | A | 86 | SER | CB-OG | -7.18 | 1.32 | 1.42 |
| 1 | F | 66 | GLY | C-O | 7.18 | 1.35 | 1.23 |
| 1 | B | 184 | ARG | CD-NE | -7.14 | 1.34 | 1.46 |
| 1 | B | 192 | ARG | CD-NE | -7.13 | 1.34 | 1.46 |
| 1 | B | 129 | TYR | N-CA | -7.12 | 1.32 | 1.46 |
| 1 | A | 30 | PHE | CG-CD1 | -7.11 | 1.28 | 1.38 |
| 1 | C | 5 | PHE | CB-CG | -7.07 | 1.39 | 1.51 |
| 1 | F | 129 | TYR | CZ-OH | 7.07 | 1.49 | 1.37 |
| 1 | B | 5 | PHE | C-O | 7.06 | 1.36 | 1.23 |
| 1 | D | 14 | PRO | N-CA | -7.04 | 1.35 | 1.47 |
| 1 | B | 152 | TYR | CE2-CZ | -7.04 | 1.29 | 1.38 |
| 1 | D | 198 | ASN | CA-CB | -6.95 | 1.35 | 1.53 |
| 1 | D | 230 | GLY | C-O | 6.89 | 1.34 | 1.23 |
| 1 | A | 92 | LEU | C-O | -6.88 | 1.10 | 1.23 |
| 1 | C | 59 | ARG | NE-CZ | 6.87 | 1.42 | 1.33 |
| 1 | C | 104 | GLY | N-CA | -6.86 | 1.35 | 1.46 |
| 1 | B | 105 | PRO | N-CA | -6.85 | 1.35 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 11 | GLY | CA-C | -6.84 | 1.41 | 1.51 |
| 1 | E | 104 | GLY | N-CA | -6.81 | 1.35 | 1.46 |
| 1 | D | 108 | TRP | CB-CG | -6.79 | 1.38 | 1.50 |
| 1 | A | 100 | VAL | CA-CB | 6.78 | 1.69 | 1.54 |
| 1 | B | 110 | SER | N-CA | -6.78 | 1.32 | 1.46 |
| 1 | D | 216 | VAL | CB-CG2 | -6.76 | 1.38 | 1.52 |
| 1 | A | 182 | GLY | CA-C | -6.75 | 1.41 | 1.51 |
| 1 | D | 233 | TRP | CA-CB | -6.73 | 1.39 | 1.53 |
| 1 | B | 60 | ALA | CA-C | -6.73 | 1.35 | 1.52 |
| 1 | D | 194 | ASP | N-CA | -6.72 | 1.32 | 1.46 |
| 1 | A | 229 | GLY | N-CA | -6.70 | 1.36 | 1.46 |
| 1 | D | 217 | PHE | CA-CB | -6.67 | 1.39 | 1.53 |
| 1 | A | 233 | TRP | CZ2-CH2 | -6.65 | 1.24 | 1.37 |
| 1 | C | 231 | ALA | N-CA | -6.65 | 1.33 | 1.46 |
| 1 | A | 124 | GLY | N-CA | -6.64 | 1.36 | 1.46 |
| 1 | D | 64 | SER | CA-CB | -6.64 | 1.43 | 1.52 |
| 1 | B | 29 | ARG | CZ-NH1 | 6.63 | 1.41 | 1.33 |
| 1 | B | 98 | ARG | CZ-NH1 | 6.63 | 1.41 | 1.33 |
| 1 | E | 6 | GLY | N-CA | 6.56 | 1.55 | 1.46 |
| 1 | C | 90 | TYR | CE1-CZ | -6.54 | 1.30 | 1.38 |
| 1 | C | 28 | PHE | CE1-CZ | 6.54 | 1.49 | 1.37 |
| 1 | B | 194 | ASP | N-CA | -6.53 | 1.33 | 1.46 |
| 1 | A | 155 | SER | CA-CB | -6.53 | 1.43 | 1.52 |
| 1 | A | 189 | PRO | CA-CB | -6.48 | 1.40 | 1.53 |
| 1 | D | 229 | GLY | CA-C | -6.47 | 1.41 | 1.51 |
| 1 | B | 87 | ILE | N-CA | -6.46 | 1.33 | 1.46 |
| 1 | E | 66 | GLY | N-CA | -6.45 | 1.36 | 1.46 |
| 1 | B | 84 | LYS | C-N | -6.44 | 1.21 | 1.33 |
| 1 | B | 55 | ALA | C-O | 6.42 | 1.35 | 1.23 |
| 1 | A | 48 | TRP | CB-CG | -6.41 | 1.38 | 1.50 |
| 1 | A | 146 | SER | CB-OG | 6.39 | 1.50 | 1.42 |
| 1 | D | 131 | THR | C-O | 6.37 | 1.35 | 1.23 |
| 1 | E | 136 | ASN | N-CA | 6.37 | 1.59 | 1.46 |
| 1 | B | 54 | GLY | C-N | 6.36 | 1.48 | 1.34 |
| 1 | C | 180 | GLY | N-CA | -6.33 | 1.36 | 1.46 |
| 1 | C | 110 | SER | CB-OG | -6.33 | 1.34 | 1.42 |
| 1 | B | 214 | ARG | NE-CZ | 6.33 | 1.41 | 1.33 |
| 1 | E | 215 | TYR | CG-CD2 | -6.32 | 1.30 | 1.39 |
| 1 | A | 204 | TRP | CD2-CE2 | -6.31 | 1.33 | 1.41 |
| 1 | C | 48 | TRP | CG-CD1 | -6.31 | 1.27 | 1.36 |
| 1 | E | 233 | TRP | N-CA | 6.31 | 1.58 | 1.46 |
| 1 | D | 146 | SER | C-O | 6.30 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 150 | SER | N-CA | 6.27 | 1.58 | 1.46 |
| 1 | F | 98 | ARG | NE-CZ | 6.26 | 1.41 | 1.33 |
| 1 | B | 223 | ARG | N-CA | -6.26 | 1.33 | 1.46 |
| 1 | B | 8 | SER | C-N | -6.24 | 1.19 | 1.34 |
| 1 | C | 126 | SER | CA-CB | 6.21 | 1.62 | 1.52 |
| 1 | F | 136 | ASN | N-CA | 6.21 | 1.58 | 1.46 |
| 1 | D | 191 | GLY | N-CA | -6.20 | 1.36 | 1.46 |
| 1 | A | 25 | LEU | C-N | -6.20 | 1.19 | 1.34 |
| 1 | D | 174 | THR | N-CA | -6.19 | 1.33 | 1.46 |
| 1 | E | 85 | GLY | C-N | -6.19 | 1.19 | 1.34 |
| 1 | D | 20 | ALA | N-CA | 6.18 | 1.58 | 1.46 |
| 1 | A | 48 | TRP | CA-CB | -6.18 | 1.40 | 1.53 |
| 1 | B | 231 | ALA | N-CA | -6.18 | 1.33 | 1.46 |
| 1 | B | 228 | TYR | C-N | -6.18 | 1.22 | 1.33 |
| 1 | A | 232 | LEU | N-CA | -6.17 | 1.34 | 1.46 |
| 1 | D | 105 | PRO | CA-CB | 6.16 | 1.65 | 1.53 |
| 1 | A | 233 | TRP | NE1-CE2 | -6.13 | 1.29 | 1.37 |
| 1 | A | 229 | GLY | C-N | -6.09 | 1.22 | 1.33 |
| 1 | B | 59 | ARG | CA-CB | -6.09 | 1.40 | 1.53 |
| 1 | B | 29 | ARG | CZ-NH2 | 6.09 | 1.41 | 1.33 |
| 1 | D | 142 | HIS | N-CA | -6.08 | 1.34 | 1.46 |
| 1 | B | 147 | LEU | CB-CG | -6.08 | 1.34 | 1.52 |
| 1 | A | 170 | ARG | CZ-NH2 | 6.08 | 1.41 | 1.33 |
| 1 | A | 214 | ARG | CB-CG | -6.07 | 1.36 | 1.52 |
| 1 | A | 12 | SER | C-O | -6.05 | 1.11 | 1.23 |
| 1 | F | 6 | GLY | CA-C | 6.04 | 1.61 | 1.51 |
| 1 | F | 194 | ASP | N-CA | -6.04 | 1.34 | 1.46 |
| 1 | C | 58 | CYS | CA-CB | -6.03 | 1.40 | 1.53 |
| 1 | A | 14 | PRO | N-CD | -6.03 | 1.39 | 1.47 |
| 1 | F | 105 | PRO | N-CD | 6.03 | 1.56 | 1.47 |
| 1 | C | 217 | PHE | CG-CD1 | -6.02 | 1.29 | 1.38 |
| 1 | A | 138 | PRO | N-CA | -6.00 | 1.37 | 1.47 |
| 1 | B | 191 | GLY | C-O | 6.00 | 1.33 | 1.23 |
| 1 | A | 48 | TRP | CE3-CZ3 | -5.98 | 1.28 | 1.38 |
| 1 | F | 34 | SER | CB-OG | 5.98 | 1.50 | 1.42 |
| 1 | E | 48 | TRP | CG-CD1 | -5.98 | 1.28 | 1.36 |
| 1 | B | 78 | ARG | NE-CZ | 5.96 | 1.40 | 1.33 |
| 1 | A | 188 | GLN | CB-CG | 5.93 | 1.68 | 1.52 |
| 1 | A | 9 | HIS | N-CA | -5.91 | 1.34 | 1.46 |
| 1 | A | 231 | ALA | N-CA | -5.91 | 1.34 | 1.46 |
| 1 | D | 66 | GLY | C-O | 5.90 | 1.33 | 1.23 |
| 1 | F | 129 | TYR | CD1-CE1 | -5.89 | 1.30 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 199 | GLN | N-CA | -5.89 | 1.34 | 1.46 |
| 1 | F | 184 | ARG | N-CA | -5.87 | 1.34 | 1.46 |
| 1 | D | 9 | HIS | N-CA | -5.87 | 1.34 | 1.46 |
| 1 | B | 146 | SER | CB-OG | -5.86 | 1.34 | 1.42 |
| 1 | F | 6 | GLY | C-O | 5.86 | 1.33 | 1.23 |
| 1 | C | 145 | GLN | CA-CB | -5.86 | 1.41 | 1.53 |
| 1 | E | 183 | CYS | N-CA | -5.85 | 1.34 | 1.46 |
| 1 | D | 235 | THR | C-O | 5.85 | 1.34 | 1.23 |
| 1 | D | 59 | ARG | CA-CB | -5.85 | 1.41 | 1.53 |
| 1 | C | 36 | CYS | CB-SG | -5.85 | 1.72 | 1.81 |
| 1 | C | 203 | VAL | CB-CG2 | -5.83 | 1.40 | 1.52 |
| 1 | C | 138 | PRO | C-N | 5.83 | 1.47 | 1.34 |
| 1 | F | 12 | SER | CB-OG | 5.83 | 1.49 | 1.42 |
| 1 | A | 129 | TYR | CZ-OH | -5.82 | 1.27 | 1.37 |
| 1 | D | 27 | SER | CA-CB | 5.82 | 1.61 | 1.52 |
| 1 | A | 90 | TYR | C-N | -5.81 | 1.20 | 1.34 |
| 1 | E | 66 | GLY | C-O | 5.79 | 1.32 | 1.23 |
| 1 | D | 203 | VAL | CB-CG2 | 5.79 | 1.65 | 1.52 |
| 1 | A | 57 | GLY | N-CA | -5.78 | 1.37 | 1.46 |
| 1 | C | 57 | GLY | N-CA | -5.78 | 1.37 | 1.46 |
| 1 | B | 184 | ARG | CZ-NH1 | 5.78 | 1.40 | 1.33 |
| 1 | E | 20 | ALA | CA-CB | -5.77 | 1.40 | 1.52 |
| 1 | B | 129 | TYR | CE2-CZ | -5.76 | 1.31 | 1.38 |
| 1 | B | 72 | THR | N-CA | -5.76 | 1.34 | 1.46 |
| 1 | D | 160 | CYS | CB-SG | -5.76 | 1.72 | 1.81 |
| 1 | D | 11 | GLY | N-CA | 5.75 | 1.54 | 1.46 |
| 1 | A | 85 | GLY | C-O | 5.73 | 1.32 | 1.23 |
| 1 | B | 138 | PRO | CA-CB | -5.72 | 1.42 | 1.53 |
| 1 | D | 13 | HIS | C-N | -5.72 | 1.23 | 1.34 |
| 1 | D | 148 | GLN | CA-CB | -5.72 | 1.41 | 1.53 |
| 1 | B | 1 | ASN | CG-OD1 | 5.71 | 1.36 | 1.24 |
| 1 | B | 14 | PRO | N-CA | -5.70 | 1.37 | 1.47 |
| 1 | E | 10 | GLU | N-CA | -5.70 | 1.34 | 1.46 |
| 1 | C | 141 | LEU | CA-CB | -5.70 | 1.40 | 1.53 |
| 1 | D | 183 | CYS | CB-SG | -5.69 | 1.72 | 1.81 |
| 1 | F | 7 | LEU | C-O | 5.68 | 1.34 | 1.23 |
| 1 | B | 222 | ASP | C-N | -5.68 | 1.21 | 1.34 |
| 1 | B | 10 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | D | 187 | LEU | C-O | -5.67 | 1.12 | 1.23 |
| 1 | A | 61 | VAL | CB-CG1 | -5.67 | 1.41 | 1.52 |
| 1 | B | 225 | LEU | CA-CB | -5.65 | 1.40 | 1.53 |
| 1 | A | 80 | SER | CB-OG | -5.65 | 1.34 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 34 | SER | CA-C | -5.65 | 1.38 | 1.52 |
| 1 | A | 83 | THR | C-N | -5.64 | 1.21 | 1.34 |
| 1 | D | 88 | GLY | N-CA | 5.64 | 1.54 | 1.46 |
| 1 | C | 83 | THR | C-N | -5.63 | 1.21 | 1.34 |
| 1 | B | 230 | GLY | N-CA | -5.63 | 1.37 | 1.46 |
| 1 | C | 124 | GLY | N-CA | -5.63 | 1.37 | 1.46 |
| 1 | A | 192 | ARG | CZ-NH2 | -5.63 | 1.25 | 1.33 |
| 1 | C | 196 | LEU | CB-CG | -5.63 | 1.36 | 1.52 |
| 1 | F | 98 | ARG | CZ-NH2 | 5.63 | 1.40 | 1.33 |
| 1 | F | 67 | LEU | CG-CD2 | 5.63 | 1.72 | 1.51 |
| 1 | A | 68 | LEU | C-O | -5.61 | 1.12 | 1.23 |
| 1 | D | 146 | SER | CA-CB | 5.61 | 1.61 | 1.52 |
| 1 | B | 74 | GLN | N-CA | -5.61 | 1.35 | 1.46 |
| 1 | A | 217 | PHE | CD1-CE1 | 5.57 | 1.50 | 1.39 |
| 1 | C | 192 | ARG | CA-CB | -5.57 | 1.41 | 1.53 |
| 1 | F | 130 | SER | C-N | 5.56 | 1.46 | 1.34 |
| 1 | A | 170 | ARG | CZ-NH1 | 5.54 | 1.40 | 1.33 |
| 1 | A | 221 | PRO | N-CA | 5.53 | 1.56 | 1.47 |
| 1 | E | 5 | PHE | C-O | 5.53 | 1.33 | 1.23 |
| 1 | B | 193 | MET | CA-CB | -5.52 | 1.41 | 1.53 |
| 1 | A | 218 | VAL | CB-CG2 | 5.52 | 1.64 | 1.52 |
| 1 | A | 114 | ASN | N-CA | -5.51 | 1.35 | 1.46 |
| 1 | A | 214 | ARG | CZ-NH2 | 5.51 | 1.40 | 1.33 |
| 1 | C | 27 | SER | CA-CB | -5.51 | 1.44 | 1.52 |
| 1 | C | 183 | CYS | CB-SG | -5.51 | 1.72 | 1.81 |
| 1 | A | 156 | MET | CG-SD | -5.50 | 1.66 | 1.81 |
| 1 | D | 15 | GLN | CA-CB | -5.50 | 1.41 | 1.53 |
| 1 | D | 196 | LEU | CA-CB | -5.49 | 1.41 | 1.53 |
| 1 | A | 60 | ALA | C-O | 5.49 | 1.33 | 1.23 |
| 1 | D | 52 | THR | N-CA | -5.47 | 1.35 | 1.46 |
| 1 | D | 183 | CYS | C-N | -5.46 | 1.21 | 1.34 |
| 1 | D | 48 | TRP | CA-CB | -5.45 | 1.42 | 1.53 |
| 1 | A | 186 | VAL | C-N | 5.44 | 1.46 | 1.34 |
| 1 | C | 139 | GLN | CA-CB | -5.44 | 1.42 | 1.53 |
| 1 | D | 61 | VAL | C-N | -5.44 | 1.21 | 1.34 |
| 1 | A | 104 | GLY | N-CA | -5.44 | 1.37 | 1.46 |
| 1 | B | 160 | CYS | N-CA | -5.43 | 1.35 | 1.46 |
| 1 | F | 139 | GLN | CB-CG | -5.42 | 1.38 | 1.52 |
| 1 | E | 129 | TYR | CE1-CZ | -5.41 | 1.31 | 1.38 |
| 1 | C | 207 | GLY | CA-C | -5.41 | 1.43 | 1.51 |
| 1 | F | 128 | LEU | C-N | -5.41 | 1.21 | 1.34 |
| 1 | B | 109 | ASP | N-CA | -5.40 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 8 | SER | CB-OG | 5.39 | 1.49 | 1.42 |
| 1 | F | 129 | TYR | CB-CG | 5.39 | 1.59 | 1.51 |
| 1 | B | 98 | ARG | NE-CZ | 5.39 | 1.40 | 1.33 |
| 1 | D | 227 | ILE | C-N | -5.38 | 1.21 | 1.34 |
| 1 | A | 125 | ASN | N-CA | -5.38 | 1.35 | 1.46 |
| 1 | D | 44 | ASP | C-N | -5.38 | 1.21 | 1.34 |
| 1 | E | 138 | PRO | N-CA | -5.37 | 1.38 | 1.47 |
| 1 | D | 139 | GLN | CB-CG | -5.36 | 1.38 | 1.52 |
| 1 | B | 89 | ASN | CG-ND2 | 5.35 | 1.46 | 1.32 |
| 1 | A | 230 | GLY | C-N | -5.34 | 1.21 | 1.34 |
| 1 | E | 11 | GLY | CA-C | -5.34 | 1.43 | 1.51 |
| 1 | C | 88 | GLY | C-O | -5.34 | 1.15 | 1.23 |
| 1 | A | 105 | PRO | N-CA | -5.34 | 1.38 | 1.47 |
| 1 | B | 60 | ALA | C-N | -5.33 | 1.21 | 1.34 |
| 1 | E | 146 | SER | CA-CB | 5.32 | 1.60 | 1.52 |
| 1 | B | 78 | ARG | CZ-NH2 | 5.31 | 1.40 | 1.33 |
| 1 | C | 205 | THR | C-O | 5.29 | 1.33 | 1.23 |
| 1 | A | 30 | PHE | CA-CB | -5.29 | 1.42 | 1.53 |
| 1 | D | 221 | PRO | N-CD | -5.29 | 1.40 | 1.47 |
| 1 | D | 28 | PHE | N-CA | -5.28 | 1.35 | 1.46 |
| 1 | D | 139 | GLN | CA-CB | -5.28 | 1.42 | 1.53 |
| 1 | C | 133 | GLY | CA-C | 5.26 | 1.60 | 1.51 |
| 1 | B | 149 | LEU | N-CA | -5.26 | 1.35 | 1.46 |
| 1 | B | 183 | CYS | CB-SG | -5.26 | 1.73 | 1.81 |
| 1 | A | 25 | LEU | CA-CB | -5.25 | 1.41 | 1.53 |
| 1 | B | 28 | PHE | CB-CG | -5.25 | 1.42 | 1.51 |
| 1 | D | 147 | LEU | N-CA | 5.25 | 1.56 | 1.46 |
| 1 | C | 172 | TRP | CD2-CE2 | -5.24 | 1.35 | 1.41 |
| 1 | C | 138 | PRO | C-O | 5.24 | 1.33 | 1.23 |
| 1 | B | 1 | ASN | N-CA | 5.23 | 1.56 | 1.46 |
| 1 | C | 143 | ALA | CA-CB | -5.22 | 1.41 | 1.52 |
| 1 | D | 69 | VAL | C-N | -5.22 | 1.22 | 1.34 |
| 1 | B | 190 | ASN | N-CA | -5.22 | 1.35 | 1.46 |
| 1 | A | 137 | HIS | ND1-CE1 | -5.22 | 1.21 | 1.34 |
| 1 | A | 125 | ASN | CG-OD1 | 5.21 | 1.35 | 1.24 |
| 1 | E | 13 | HIS | C-N | -5.21 | 1.24 | 1.34 |
| 1 | A | 50 | SER | CB-OG | 5.21 | 1.49 | 1.42 |
| 1 | A | 96 | PRO | N-CD | -5.20 | 1.40 | 1.47 |
| 1 | C | 199 | GLN | N-CA | -5.20 | 1.35 | 1.46 |
| 1 | A | 29 | ARG | CA-CB | -5.19 | 1.42 | 1.53 |
| 1 | A | 186 | VAL | CB-CG1 | -5.19 | 1.42 | 1.52 |
| 1 | D | 92 | LEU | C-O | 5.19 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 167 | ARG | CA-CB | 5.19 | 1.65 | 1.53 |
| 1 | B | 28 | PHE | CG-CD1 | -5.18 | 1.30 | 1.38 |
| 1 | F | 61 | VAL | N-CA | 5.18 | 1.56 | 1.46 |
| 1 | D | 21 | GLN | CB-CG | -5.17 | 1.38 | 1.52 |
| 1 | B | 211 | SER | CB-OG | 5.17 | 1.49 | 1.42 |
| 1 | D | 184 | ARG | NE-CZ | 5.16 | 1.39 | 1.33 |
| 1 | C | 130 | SER | C-O | -5.16 | 1.13 | 1.23 |
| 1 | A | 103 | TYR | C-O | -5.15 | 1.13 | 1.23 |
| 1 | D | 84 | LYS | C-N | -5.15 | 1.23 | 1.33 |
| 1 | D | 152 | TYR | CE1-CZ | -5.15 | 1.31 | 1.38 |
| 1 | C | 65 | ASP | CA-CB | -5.15 | 1.42 | 1.53 |
| 1 | D | 57 | GLY | N-CA | -5.14 | 1.38 | 1.46 |
| 1 | E | 86 | SER | N-CA | -5.14 | 1.36 | 1.46 |
| 1 | D | 107 | LEU | C-O | -5.13 | 1.13 | 1.23 |
| 1 | F | 89 | ASN | CG-ND2 | 5.12 | 1.45 | 1.32 |
| 1 | A | 14 | PRO | CG-CD | -5.12 | 1.33 | 1.50 |
| 1 | A | 140 | THR | C-O | -5.12 | 1.13 | 1.23 |
| 1 | A | 17 | LEU | CA-CB | -5.12 | 1.42 | 1.53 |
| 1 | C | 165 | PHE | CA-CB | -5.11 | 1.42 | 1.53 |
| 1 | D | 66 | GLY | N-CA | -5.11 | 1.38 | 1.46 |
| 1 | B | 184 | ARG | CZ-NH2 | 5.11 | 1.39 | 1.33 |
| 1 | D | 172 | TRP | CB-CG | -5.10 | 1.41 | 1.50 |
| 1 | B | 216 | VAL | CA-C | -5.10 | 1.39 | 1.52 |
| 1 | B | 95 | GLN | C-N | -5.09 | 1.24 | 1.34 |
| 1 | A | 128 | LEU | N-CA | -5.09 | 1.36 | 1.46 |
| 1 | E | 24 | GLU | CD-OE1 | 5.08 | 1.31 | 1.25 |
| 1 | F | 86 | SER | CB-OG | 5.08 | 1.48 | 1.42 |
| 1 | B | 59 | ARG | NE-CZ | 5.08 | 1.39 | 1.33 |
| 1 | D | 224 | ASN | CA-CB | 5.08 | 1.66 | 1.53 |
| 1 | C | 197 | THR | CB-OG1 | 5.07 | 1.53 | 1.43 |
| 1 | F | 110 | SER | CB-OG | -5.07 | 1.35 | 1.42 |
| 1 | A | 146 | SER | CA-CB | 5.07 | 1.60 | 1.52 |
| 1 | C | 224 | ASN | CB-CG | 5.07 | 1.62 | 1.51 |
| 1 | C | 59 | ARG | CZ-NH2 | 5.06 | 1.39 | 1.33 |
| 1 | E | 129 | TYR | CE2-CZ | 5.05 | 1.45 | 1.38 |
| 1 | A | 23 | LEU | CB-CG | -5.04 | 1.38 | 1.52 |
| 1 | C | 188 | GLN | CD-NE2 | 5.03 | 1.45 | 1.32 |
| 1 | D | 85 | GLY | N-CA | 5.03 | 1.53 | 1.46 |
| 1 | B | 107 | LEU | N-CA | 5.03 | 1.56 | 1.46 |
| 1 | D | 5 | PHE | CD1-CE1 | 5.02 | 1.49 | 1.39 |
| 1 | B | 63 | GLN | C-O | -5.02 | 1.13 | 1.23 |
| 1 | B | 97 | ASP | CA-CB | -5.02 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 125 | ASN | C-O | -5.01 | 1.13 | 1.23 |
| 1 | E | 157 | GLU | CB-CG | 5.01 | 1.61 | 1.52 |
| 1 | B | 191 | GLY | N-CA | -5.00 | 1.38 | 1.46 |
| 1 | F | 126 | SER | CB-OG | -5.00 | 1.35 | 1.42 |

All (5150) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 214 | ARG | NE-CZ-NH2 | 59.84 | 150.22 | 120.30 |
| 1 | E | 59 | ARG | NE-CZ-NH2 | -55.14 | 92.73 | 120.30 |
| 1 | B | 184 | ARG | NE-CZ-NH2 | -53.22 | 93.69 | 120.30 |
| 1 | F | 223 | ARG | NE-CZ-NH2 | -49.78 | 95.41 | 120.30 |
| 1 | A | 184 | ARG | NE-CZ-NH1 | 48.82 | 144.71 | 120.30 |
| 1 | A | 59 | ARG | NE-CZ-NH2 | -48.03 | 96.28 | 120.30 |
| 1 | C | 223 | ARG | NE-CZ-NH1 | -47.86 | 96.37 | 120.30 |
| 1 | F | 184 | ARG | NE-CZ-NH2 | -47.40 | 96.60 | 120.30 |
| 1 | F | 46 | ARG | NE-CZ-NH1 | 47.06 | 143.83 | 120.30 |
| 1 | A | 184 | ARG | NE-CZ-NH2 | -46.93 | 96.84 | 120.30 |
| 1 | A | 59 | ARG | NE-CZ-NH1 | 45.23 | 142.91 | 120.30 |
| 1 | E | 59 | ARG | NE-CZ-NH1 | 43.99 | 142.30 | 120.30 |
| 1 | A | 78 | ARG | NE-CZ-NH2 | 42.42 | 141.51 | 120.30 |
| 1 | F | 129 | TYR | CB-CG-CD2 | 41.91 | 146.15 | 121.00 |
| 1 | D | 59 | ARG | NE-CZ-NH1 | -41.20 | 99.70 | 120.30 |
| 1 | F | 129 | TYR | CB-CG-CD1 | -40.14 | 96.91 | 121.00 |
| 1 | D | 184 | ARG | NE-CZ-NH2 | -39.63 | 100.48 | 120.30 |
| 1 | E | 170 | ARG | NE-CZ-NH2 | 39.53 | 140.06 | 120.30 |
| 1 | A | 44 | ASP | CB-CG-OD1 | -37.95 | 84.14 | 118.30 |
| 1 | D | 214 | ARG | NE-CZ-NH2 | 37.90 | 139.25 | 120.30 |
| 1 | C | 159 | ASP | CB-CG-OD2 | 37.73 | 152.26 | 118.30 |
| 1 | A | 65 | ASP | CB-CG-OD2 | 37.37 | 151.93 | 118.30 |
| 1 | C | 59 | ARG | NE-CZ-NH2 | -36.93 | 101.84 | 120.30 |
| 1 | C | 168 | ASP | CB-CG-OD1 | -36.83 | 85.15 | 118.30 |
| 1 | E | 29 | ARG | CD-NE-CZ | 36.56 | 174.78 | 123.60 |
| 1 | D | 214 | ARG | CD-NE-CZ | 35.79 | 173.70 | 123.60 |
| 1 | F | 192 | ARG | CD-NE-CZ | 35.76 | 173.66 | 123.60 |
| 1 | D | 170 | ARG | NE-CZ-NH2 | 34.66 | 137.63 | 120.30 |
| 1 | C | 214 | ARG | NE-CZ-NH1 | -34.65 | 102.97 | 120.30 |
| 1 | D | 97 | ASP | CB-CG-OD2 | 34.19 | 149.07 | 118.30 |
| 1 | D | 97 | ASP | CB-CG-OD1 | -34.15 | 87.56 | 118.30 |
| 1 | B | 214 | ARG | CD-NE-CZ | 33.20 | 170.07 | 123.60 |
| 1 | A | 222 | ASP | CB-CG-OD2 | 33.16 | 148.15 | 118.30 |
| 1 | A | 170 | ARG | NE-CZ-NH2 | 33.01 | 136.81 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 153 | ARG | NE-CZ-NH2 | -32.57 | 104.01 | 120.30 |
| 1 | C | 167 | ARG | CD-NE-CZ | 32.51 | 169.12 | 123.60 |
| 1 | A | 153 | ARG | NE-CZ-NH2 | 31.88 | 136.24 | 120.30 |
| 1 | A | 170 | ARG | CD-NE-CZ | 31.85 | 168.19 | 123.60 |
| 1 | C | 170 | ARG | CD-NE-CZ | 31.51 | 167.72 | 123.60 |
| 1 | D | 167 | ARG | NE-CZ-NH1 | -31.49 | 104.55 | 120.30 |
| 1 | B | 193 | MET | CG-SD-CE | 31.36 | 150.38 | 100.20 |
| 1 | C | 97 | ASP | CB-CG-OD2 | 30.72 | 145.95 | 118.30 |
| 1 | A | 222 | ASP | CB-CG-OD1 | -30.63 | 90.74 | 118.30 |
| 1 | D | 174 | THR | CA-CB-CG2 | -30.62 | 69.54 | 112.40 |
| 1 | E | 157 | GLU | OE1-CD-OE2 | 30.46 | 159.85 | 123.30 |
| 1 | B | 192 | ARG | CD-NE-CZ | 30.33 | 166.06 | 123.60 |
| 1 | A | 214 | ARG | CD-NE-CZ | 30.23 | 165.93 | 123.60 |
| 1 | B | 128 | LEU | CB-CG-CD1 | 29.63 | 161.38 | 111.00 |
| 1 | A | 138 | PRO | CA-N-CD | -29.61 | 70.05 | 111.50 |
| 1 | A | 215 | TYR | CB-CG-CD2 | 29.11 | 138.47 | 121.00 |
| 1 | D | 212 | ALA | CB-CA-C | 29.06 | 153.69 | 110.10 |
| 1 | E | 167 | ARG | NE-CZ-NH1 | 28.99 | 134.79 | 120.30 |
| 1 | A | 98 | ARG | NE-CZ-NH2 | -28.48 | 106.06 | 120.30 |
| 1 | F | 109 | ASP | CA-CB-CG | 28.11 | 175.25 | 113.40 |
| 1 | D | 167 | ARG | NE-CZ-NH2 | 27.31 | 133.95 | 120.30 |
| 1 | D | 152 | TYR | CB-CG-CD1 | 27.28 | 137.37 | 121.00 |
| 1 | E | 98 | ARG | NE-CZ-NH1 | -27.24 | 106.68 | 120.30 |
| 1 | B | 59 | ARG | CA-CB-CG | 27.03 | 172.87 | 113.40 |
| 1 | B | 28 | PHE | CB-CG-CD1 | 26.99 | 139.69 | 120.80 |
| 1 | C | 60 | ALA | CA-C-N | 26.98 | 176.57 | 117.20 |
| 1 | D | 1 | ASN | OD1-CG-ND2 | -26.79 | 60.28 | 121.90 |
| 1 | E | 146 | SER | CA-C-N | 26.73 | 176.01 | 117.20 |
| 1 | B | 184 | ARG | NH1-CZ-NH2 | 26.52 | 148.57 | 119.40 |
| 1 | D | 46 | ARG | CD-NE-CZ | 26.43 | 160.61 | 123.60 |
| 1 | E | 228 | TYR | C-N-CA | 26.23 | 177.39 | 122.30 |
| 1 | B | 152 | TYR | CB-CG-CD2 | 26.06 | 136.63 | 121.00 |
| 1 | A | 78 | ARG | CA-CB-CG | 26.05 | 170.71 | 113.40 |
| 1 | C | 152 | TYR | CB-CG-CD2 | 26.00 | 136.60 | 121.00 |
| 1 | D | 128 | LEU | CA-C-N | 25.90 | 174.18 | 117.20 |
| 1 | C | 223 | ARG | NH1-CZ-NH2 | 25.88 | 147.87 | 119.40 |
| 1 | B | 214 | ARG | NE-CZ-NH2 | 25.85 | 133.23 | 120.30 |
| 1 | C | 168 | ASP | CB-CG-OD2 | -25.82 | 95.06 | 118.30 |
| 1 | C | 8 | SER | O-C-N | -25.72 | 81.54 | 122.70 |
| 1 | B | 167 | ARG | CA-CB-CG | 25.65 | 169.83 | 113.40 |
| 1 | A | 90 | TYR | CB-CG-CD1 | 25.65 | 136.39 | 121.00 |
| 1 | C | 215 | TYR | CB-CG-CD1 | -25.63 | 105.62 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 214 | ARG | CD-NE-CZ | 25.59 | 159.43 | 123.60 |
| 1 | E | 29 | ARG | NE-CZ-NH1 | 25.44 | 133.02 | 120.30 |
| 1 | F | 210 | ARG | CD-NE-CZ | 25.44 | 159.21 | 123.60 |
| 1 | B | 170 | ARG | CD-NE-CZ | 25.36 | 159.10 | 123.60 |
| 1 | F | 46 | ARG | NE-CZ-NH2 | -25.26 | 107.67 | 120.30 |
| 1 | B | 98 | ARG | NE-CZ-NH2 | 25.26 | 132.93 | 120.30 |
| 1 | D | 198 | ASN | N-CA-CB | -25.08 | 65.46 | 110.60 |
| 1 | D | 31 | THR | CA-CB-CG2 | 25.04 | 147.46 | 112.40 |
| 1 | A | 194 | ASP | CB-CG-OD2 | 24.88 | 140.69 | 118.30 |
| 1 | D | 1 | ASN | CB-CG-OD1 | 24.77 | 171.15 | 121.60 |
| 1 | E | 1 | ASN | CA-CB-CG | 24.77 | 167.89 | 113.40 |
| 1 | C | 210 | ARG | NE-CZ-NH1 | 24.73 | 132.67 | 120.30 |
| 1 | D | 128 | LEU | CA-C-O | -24.73 | 68.17 | 120.10 |
| 1 | A | 44 | ASP | CB-CG-OD2 | 24.72 | 140.55 | 118.30 |
| 1 | D | 152 | TYR | CB-CG-CD2 | -24.58 | 106.25 | 121.00 |
| 1 | B | 153 | ARG | NE-CZ-NH1 | -24.54 | 108.03 | 120.30 |
| 1 | D | 16 | THR | CA-CB-CG2 | -24.16 | 78.57 | 112.40 |
| 1 | F | 60 | ALA | CA-C-N | 24.16 | 170.35 | 117.20 |
| 1 | E | 129 | TYR | CG-CD1-CE1 | 24.06 | 140.54 | 121.30 |
| 1 | B | 230 | GLY | O-C-N | 23.98 | 161.07 | 122.70 |
| 1 | F | 9 | HIS | CA-CB-CG | 23.95 | 154.31 | 113.60 |
| 1 | D | 154 | LEU | CB-CG-CD1 | 23.91 | 151.65 | 111.00 |
| 1 | C | 132 | GLN | C-N-CA | 23.81 | 172.30 | 122.30 |
| 1 | F | 98 | ARG | NE-CZ-NH2 | -23.80 | 108.40 | 120.30 |
| 1 | F | 100 | VAL | CA-CB-CG2 | 23.76 | 146.54 | 110.90 |
| 1 | A | 157 | GLU | CG-CD-OE1 | 23.74 | 165.78 | 118.30 |
| 1 | B | 98 | ARG | CG-CD-NE | 23.67 | 161.51 | 111.80 |
| 1 | B | 28 | PHE | CB-CG-CD2 | -23.60 | 104.28 | 120.80 |
| 1 | B | 72 | THR | CA-CB-CG2 | 23.58 | 145.41 | 112.40 |
| 1 | E | 217 | PHE | CB-CG-CD1 | -23.46 | 104.38 | 120.80 |
| 1 | A | 19 | ALA | CB-CA-C | 23.45 | 145.27 | 110.10 |
| 1 | E | 138 | PRO | N-CA-CB | 23.43 | 131.42 | 103.30 |
| 1 | C | 159 | ASP | CB-CG-OD1 | -23.43 | 97.21 | 118.30 |
| 1 | C | 168 | ASP | OD1-CG-OD2 | -23.42 | 78.81 | 123.30 |
| 1 | D | 146 | SER | CA-C-N | 23.39 | 168.66 | 117.20 |
| 1 | D | 107 | LEU | CB-CG-CD1 | 23.30 | 150.61 | 111.00 |
| 1 | C | 170 | ARG | NE-CZ-NH1 | -23.26 | 108.67 | 120.30 |
| 1 | F | 166 | ASP | CB-CG-OD1 | 23.25 | 139.22 | 118.30 |
| 1 | B | 65 | ASP | CB-CG-OD2 | 23.24 | 139.22 | 118.30 |
| 1 | C | 138 | PRO | CA-N-CD | -23.21 | 79.01 | 111.50 |
| 1 | C | 117 | SER | C-N-CA | 23.17 | 179.63 | 121.70 |
| 1 | C | 153 | ARG | NH1-CZ-NH2 | 23.14 | 144.85 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 109 | ASP | CB-CG-OD2 | -23.07 | 97.54 | 118.30 |
| 1 | B | 55 | ALA | O-C-N | -23.02 | 85.86 | 122.70 |
| 1 | A | 129 | TYR | C-N-CA | 23.02 | 179.24 | 121.70 |
| 1 | F | 153 | ARG | NE-CZ-NH1 | -23.00 | 108.80 | 120.30 |
| 1 | B | 162 | LEU | CB-CG-CD1 | 22.92 | 149.97 | 111.00 |
| 1 | B | 64 | SER | N-CA-CB | -22.90 | 76.15 | 110.50 |
| 1 | F | 184 | ARG | NH1-CZ-NH2 | 22.87 | 144.55 | 119.40 |
| 1 | F | 90 | TYR | CB-CG-CD1 | 22.82 | 134.69 | 121.00 |
| 1 | C | 130 | SER | N-CA-CB | 22.80 | 144.70 | 110.50 |
| 1 | F | 92 | LEU | CB-CG-CD1 | 22.77 | 149.71 | 111.00 |
| 1 | C | 230 | GLY | CA-C-O | -22.76 | 79.63 | 120.60 |
| 1 | D | 20 | ALA | CB-CA-C | 22.76 | 144.25 | 110.10 |
| 1 | D | 99 | THR | CA-CB-CG2 | 22.69 | 144.16 | 112.40 |
| 1 | D | 72 | THR | CA-CB-CG2 | 22.65 | 144.11 | 112.40 |
| 1 | C | 59 | ARG | NE-CZ-NH1 | 22.64 | 131.62 | 120.30 |
| 1 | B | 59 | ARG | NE-CZ-NH2 | -22.57 | 109.01 | 120.30 |
| 1 | B | 228 | TYR | CB-CG-CD1 | 22.53 | 134.52 | 121.00 |
| 1 | B | 60 | ALA | CA-C-O | -22.49 | 72.87 | 120.10 |
| 1 | A | 210 | ARG | NE-CZ-NH1 | -22.45 | 109.07 | 120.30 |
| 1 | A | 228 | TYR | CB-CG-CD2 | 22.37 | 134.42 | 121.00 |
| 1 | D | 67 | LEU | CA-CB-CG | 22.31 | 166.62 | 115.30 |
| 1 | B | 67 | LEU | CB-CG-CD1 | -22.23 | 73.22 | 111.00 |
| 1 | E | 130 | SER | C-N-CA | 22.22 | 177.26 | 121.70 |
| 1 | D | 214 | ARG | CA-CB-CG | 22.20 | 162.23 | 113.40 |
| 1 | D | 185 | ALA | N-CA-CB | -22.14 | 79.10 | 110.10 |
| 1 | C | 215 | TYR | CB-CG-CD2 | 22.13 | 134.28 | 121.00 |
| 1 | B | 148 | GLN | CA-CB-CG | 22.12 | 162.07 | 113.40 |
| 1 | A | 167 | ARG | NE-CZ-NH1 | 22.09 | 131.35 | 120.30 |
| 1 | B | 126 | SER | N-CA-CB | -22.03 | 77.45 | 110.50 |
| 1 | D | 83 | THR | CA-C-N | 22.03 | 165.68 | 117.20 |
| 1 | C | 60 | ALA | O-C-N | -22.03 | 87.45 | 122.70 |
| 1 | E | 223 | ARG | NE-CZ-NH2 | 22.01 | 131.31 | 120.30 |
| 1 | E | 33 | GLN | C-N-CA | 21.96 | 176.60 | 121.70 |
| 1 | F | 1 | ASN | C-N-CA | 21.95 | 176.56 | 121.70 |
| 1 | A | 9 | HIS | N-CA-C | 21.88 | 170.07 | 111.00 |
| 1 | B | 87 | ILE | CA-CB-CG1 | 21.86 | 152.54 | 111.00 |
| 1 | F | 124 | GLY | C-N-CA | 21.79 | 176.16 | 121.70 |
| 1 | D | 109 | ASP | CB-CG-OD1 | -21.76 | 98.71 | 118.30 |
| 1 | F | 173 | SER | CA-CB-OG | 21.76 | 169.94 | 111.20 |
| 1 | F | 152 | TYR | CB-CG-CD1 | -21.75 | 107.95 | 121.00 |
| 1 | E | 217 | PHE | CB-CG-CD2 | 21.72 | 136.00 | 120.80 |
| 1 | B | 123 | ASN | C-N-CA | 21.67 | 167.80 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 170 | ARG | CA-CB-CG | 21.58 | 160.88 | 113.40 |
| 1 | A | 152 | TYR | CB-CG-CD2 | 21.57 | 133.94 | 121.00 |
| 1 | F | 128 | LEU | C-N-CA | 21.55 | 175.56 | 121.70 |
| 1 | A | 129 | TYR | CB-CG-CD2 | 21.43 | 133.85 | 121.00 |
| 1 | C | 145 | GLN | C-N-CA | 21.33 | 175.02 | 121.70 |
| 1 | D | 141 | LEU | C-N-CA | 21.32 | 175.00 | 121.70 |
| 1 | E | 113 | SER | CA-CB-OG | 21.32 | 168.76 | 111.20 |
| 1 | D | 193 | MET | C-N-CA | 21.31 | 174.98 | 121.70 |
| 1 | D | 209 | SER | N-CA-CB | -21.27 | 78.60 | 110.50 |
| 1 | E | 231 | ALA | N-CA-CB | 21.26 | 139.87 | 110.10 |
| 1 | F | 214 | ARG | CG-CD-NE | 21.24 | 156.41 | 111.80 |
| 1 | B | 60 | ALA | CA-C-N | 21.16 | 163.75 | 117.20 |
| 1 | B | 60 | ALA | N-CA-CB | 21.16 | 139.72 | 110.10 |
| 1 | B | 152 | TYR | CB-CG-CD1 | -21.14 | 108.32 | 121.00 |
| 1 | B | 109 | ASP | CB-CG-OD1 | -21.12 | 99.29 | 118.30 |
| 1 | B | 215 | TYR | CB-CG-CD1 | 20.99 | 133.59 | 121.00 |
| 1 | F | 210 | ARG | NE-CZ-NH1 | -20.88 | 109.86 | 120.30 |
| 1 | B | 47 | VAL | CA-CB-CG1 | -20.86 | 79.61 | 110.90 |
| 1 | B | 223 | ARG | NE-CZ-NH1 | -20.85 | 109.88 | 120.30 |
| 1 | D | 65 | ASP | CB-CG-OD2 | -20.84 | 99.54 | 118.30 |
| 1 | D | 202 | ALA | CB-CA-C | 20.79 | 141.28 | 110.10 |
| 1 | B | 109 | ASP | OD1-CG-OD2 | 20.76 | 162.74 | 123.30 |
| 1 | A | 153 | ARG | CD-NE-CZ | 20.68 | 152.55 | 123.60 |
| 1 | D | 29 | ARG | NE-CZ-NH1 | -20.68 | 109.96 | 120.30 |
| 1 | B | 5 | PHE | CE1-CZ-CE2 | -20.67 | 82.79 | 120.00 |
| 1 | F | 73 | ALA | C-N-CA | 20.67 | 173.38 | 121.70 |
| 1 | C | 184 | ARG | NE-CZ-NH1 | -20.66 | 109.97 | 120.30 |
| 1 | D | 76 | THR | C-N-CA | 20.51 | 172.99 | 121.70 |
| 1 | B | 56 | THR | C-N-CA | 20.41 | 165.16 | 122.30 |
| 1 | C | 128 | LEU | O-C-N | -20.31 | 90.20 | 122.70 |
| 1 | F | 193 | MET | C-N-CA | 20.24 | 172.29 | 121.70 |
| 1 | D | 60 | ALA | CA-C-O | -20.23 | 77.61 | 120.10 |
| 1 | D | 219 | LEU | CB-CG-CD2 | 20.21 | 145.37 | 111.00 |
| 1 | C | 190 | ASN | N-CA-CB | -20.15 | 74.32 | 110.60 |
| 1 | F | 154 | LEU | CA-CB-CG | 20.14 | 161.63 | 115.30 |
| 1 | C | 44 | ASP | N-CA-CB | -20.12 | 74.38 | 110.60 |
| 1 | A | 215 | TYR | CB-CG-CD1 | -20.10 | 108.94 | 121.00 |
| 1 | A | 131 | THR | CA-CB-OG1 | 20.08 | 151.17 | 109.00 |
| 1 | B | 193 | MET | C-N-CA | 20.08 | 171.89 | 121.70 |
| 1 | C | 230 | GLY | O-C-N | -20.06 | 90.61 | 122.70 |
| 1 | E | 33 | GLN | CG-CD-OE1 | 20.04 | 161.67 | 121.60 |
| 1 | D | 56 | THR | N-CA-CB | 20.00 | 148.31 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 203 | VAL | CG1-CB-CG2 | -19.97 | 78.95 | 110.90 |
| 1 | B | 137 | HIS | CA-C-O | -19.86 | 78.40 | 120.10 |
| 1 | F | 59 | ARG | NE-CZ-NH1 | 19.84 | 130.22 | 120.30 |
| 1 | F | 202 | ALA | CB-CA-C | 19.77 | 139.76 | 110.10 |
| 1 | C | 128 | LEU | CB-CG-CD2 | 19.74 | 144.56 | 111.00 |
| 1 | F | 128 | LEU | CB-CA-C | 19.67 | 147.57 | 110.20 |
| 1 | C | 123 | ASN | CA-CB-CG | 19.65 | 156.64 | 113.40 |
| 1 | F | 70 | ILE | CA-CB-CG1 | -19.59 | 73.78 | 111.00 |
| 1 | B | 30 | PHE | CB-CG-CD2 | -19.46 | 107.18 | 120.80 |
| 1 | E | 158 | THR | OG1-CB-CG2 | 19.45 | 154.73 | 110.00 |
| 1 | B | 22 | SER | N-CA-CB | -19.45 | 81.33 | 110.50 |
| 1 | B | 123 | ASN | CA-CB-CG | 19.40 | 156.07 | 113.40 |
| 1 | E | 35 | ASP | CB-CG-OD2 | 19.32 | 135.69 | 118.30 |
| 1 | B | 46 | ARG | NE-CZ-NH2 | -19.24 | 110.68 | 120.30 |
| 1 | A | 92 | LEU | N-CA-CB | 19.07 | 148.54 | 110.40 |
| 1 | B | 187 | LEU | O-C-N | 19.04 | 153.17 | 122.70 |
| 1 | C | 89 | ASN | CB-CG-OD1 | -19.02 | 83.56 | 121.60 |
| 1 | F | 223 | ARG | NH1-CZ-NH2 | 18.99 | 140.29 | 119.40 |
| 1 | F | 7 | LEU | CA-C-O | 18.99 | 159.98 | 120.10 |
| 1 | A | 221 | PRO | O-C-N | -18.97 | 92.34 | 122.70 |
| 1 | E | 138 | PRO | CA-N-CD | -18.95 | 84.96 | 111.50 |
| 1 | B | 228 | TYR | CG-CD2-CE2 | 18.95 | 136.46 | 121.30 |
| 1 | B | 154 | LEU | CA-CB-CG | 18.94 | 158.87 | 115.30 |
| 1 | F | 67 | LEU | CB-CG-CD1 | -18.94 | 78.80 | 111.00 |
| 1 | A | 100 | VAL | CG1-CB-CG2 | -18.93 | 80.61 | 110.90 |
| 1 | D | 174 | THR | CA-CB-OG1 | 18.91 | 148.71 | 109.00 |
| 1 | B | 64 | SER | O-C-N | -18.84 | 92.56 | 122.70 |
| 1 | B | 166 | ASP | CB-CG-OD1 | 18.82 | 135.24 | 118.30 |
| 1 | A | 170 | ARG | NH1-CZ-NH2 | -18.80 | 98.72 | 119.40 |
| 1 | C | 58 | CYS | CA-CB-SG | 18.79 | 147.81 | 114.00 |
| 1 | D | 144 | THR | N-CA-CB | 18.78 | 145.97 | 110.30 |
| 1 | A | 223 | ARG | CG-CD-NE | 18.77 | 151.21 | 111.80 |
| 1 | A | 40 | LEU | CB-CG-CD1 | 18.74 | 142.86 | 111.00 |
| 1 | D | 203 | VAL | CA-CB-CG1 | 18.73 | 138.99 | 110.90 |
| 1 | E | 76 | THR | CA-CB-OG1 | -18.71 | 69.72 | 109.00 |
| 1 | F | 97 | ASP | CB-CG-OD1 | -18.66 | 101.50 | 118.30 |
| 1 | B | 5 | PHE | CZ-CE2-CD2 | 18.66 | 142.49 | 120.10 |
| 1 | A | 157 | GLU | CG-CD-OE2 | -18.65 | 81.00 | 118.30 |
| 1 | E | 33 | GLN | O-C-N | -18.65 | 92.86 | 122.70 |
| 1 | F | 102 | ILE | CB-CG1-CD1 | 18.59 | 165.97 | 113.90 |
| 1 | C | 46 | ARG | CD-NE-CZ | 18.52 | 149.53 | 123.60 |
| 1 | A | 231 | ALA | C-N-CA | 18.52 | 168.00 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 222 | ASP | CB-CG-OD2 | 18.51 | 134.96 | 118.30 |
| 1 | B | 202 | ALA | CB-CA-C | 18.51 | 137.86 | 110.10 |
| 1 | C | 192 | ARG | CD-NE-CZ | 18.46 | 149.44 | 123.60 |
| 1 | F | 103 | TYR | O-C-N | -18.45 | 91.83 | 123.20 |
| 1 | A | 128 | LEU | CA-C-N | 18.44 | 157.77 | 117.20 |
| 1 | E | 98 | ARG | NH1-CZ-NH2 | 18.40 | 139.64 | 119.40 |
| 1 | B | 100 | VAL | O-C-N | -18.34 | 93.35 | 122.70 |
| 1 | C | 153 | ARG | NE-CZ-NH1 | -18.34 | 111.13 | 120.30 |
| 1 | A | 84 | LYS | CD-CE-NZ | 18.27 | 153.72 | 111.70 |
| 1 | B | 147 | LEU | CB-CG-CD1 | 18.26 | 142.04 | 111.00 |
| 1 | A | 169 | ASP | CA-CB-CG | 18.18 | 153.41 | 113.40 |
| 1 | A | 60 | ALA | CA-C-N | 18.18 | 157.19 | 117.20 |
| 1 | D | 6 | GLY | C-N-CA | 18.15 | 167.07 | 121.70 |
| 1 | F | 214 | ARG | O-C-N | -18.15 | 93.66 | 122.70 |
| 1 | F | 129 | TYR | N-CA-CB | -18.14 | 77.94 | 110.60 |
| 1 | B | 222 | ASP | C-N-CA | 18.11 | 166.99 | 121.70 |
| 1 | B | 137 | HIS | CA-C-N | 18.11 | 167.81 | 117.10 |
| 1 | A | 94 | LEU | CB-CG-CD2 | 18.06 | 141.70 | 111.00 |
| 1 | C | 132 | GLN | O-C-N | -18.00 | 92.60 | 123.20 |
| 1 | A | 159 | ASP | CB-CG-OD2 | 17.98 | 134.48 | 118.30 |
| 1 | E | 223 | ARG | CG-CD-NE | 17.96 | 149.51 | 111.80 |
| 1 | E | 223 | ARG | NE-CZ-NH1 | -17.89 | 111.36 | 120.30 |
| 1 | D | 167 | ARG | CG-CD-NE | 17.88 | 149.35 | 111.80 |
| 1 | D | 91 | VAL | CA-CB-CG1 | 17.83 | 137.65 | 110.90 |
| 1 | F | 202 | ALA | N-CA-CB | -17.80 | 85.18 | 110.10 |
| 1 | D | 8 | SER | N-CA-CB | -17.77 | 83.84 | 110.50 |
| 1 | C | 210 | ARG | CD-NE-CZ | -17.75 | 98.74 | 123.60 |
| 1 | F | 129 | TYR | CE1-CZ-OH | -17.72 | 72.27 | 120.10 |
| 1 | D | 126 | SER | CA-CB-OG | 17.70 | 159.00 | 111.20 |
| 1 | E | 109 | ASP | CB-CG-OD1 | 17.70 | 134.23 | 118.30 |
| 1 | A | 88 | GLY | CA-C-O | 17.67 | 152.40 | 120.60 |
| 1 | D | 105 | PRO | CA-N-CD | -17.65 | 86.79 | 111.50 |
| 1 | A | 123 | ASN | C-N-CA | 17.64 | 159.34 | 122.30 |
| 1 | A | 44 | ASP | CA-CB-CG | 17.59 | 152.10 | 113.40 |
| 1 | F | 72 | THR | CA-CB-CG2 | 17.59 | 137.03 | 112.40 |
| 1 | E | 125 | ASN | CA-CB-CG | 17.57 | 152.05 | 113.40 |
| 1 | A | 97 | ASP | CB-CG-OD2 | -17.56 | 102.49 | 118.30 |
| 1 | C | 210 | ARG | NE-CZ-NH2 | -17.56 | 111.52 | 120.30 |
| 1 | F | 196 | LEU | C-N-CA | 17.53 | 165.53 | 121.70 |
| 1 | D | 139 | GLN | CB-CG-CD | 17.52 | 157.16 | 111.60 |
| 1 | D | 153 | ARG | NE-CZ-NH2 | -17.50 | 111.55 | 120.30 |
| 1 | C | 175 | ASN | N-CA-CB | 17.47 | 142.04 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 5 | PHE | CB-CG-CD1 | 17.47 | 133.03 | 120.80 |
| 1 | D | 89 | ASN | O-C-N | -17.43 | 94.80 | 122.70 |
| 1 | A | 29 | ARG | CA-CB-CG | 17.43 | 151.75 | 113.40 |
| 1 | E | 20 | ALA | CB-CA-C | 17.41 | 136.22 | 110.10 |
| 1 | F | 8 | SER | C-N-CA | 17.41 | 165.22 | 121.70 |
| 1 | C | 163 | VAL | CG1-CB-CG2 | 17.40 | 138.74 | 110.90 |
| 1 | C | 124 | GLY | C-N-CA | 17.38 | 165.14 | 121.70 |
| 1 | D | 229 | GLY | CA-C-O | -17.37 | 89.34 | 120.60 |
| 1 | F | 203 | VAL | CA-CB-CG2 | 17.37 | 136.95 | 110.90 |
| 1 | F | 55 | ALA | CB-CA-C | 17.36 | 136.14 | 110.10 |
| 1 | C | 36 | CYS | CA-CB-SG | -17.35 | 82.78 | 114.00 |
| 1 | E | 175 | ASN | CA-CB-CG | 17.35 | 151.57 | 113.40 |
| 1 | B | 5 | PHE | CD1-CG-CD2 | -17.31 | 95.79 | 118.30 |
| 1 | B | 192 | ARG | NE-CZ-NH2 | 17.31 | 128.96 | 120.30 |
| 1 | D | 12 | SER | CB-CA-C | 17.29 | 142.95 | 110.10 |
| 1 | A | 208 | ASN | O-C-N | 17.29 | 150.36 | 122.70 |
| 1 | A | 14 | PRO | CA-N-CD | -17.28 | 87.31 | 111.50 |
| 1 | A | 18 | HIS | CA-C-O | 17.27 | 156.38 | 120.10 |
| 1 | D | 65 | ASP | CB-CG-OD1 | 17.25 | 133.83 | 118.30 |
| 1 | E | 60 | ALA | CA-C-N | 17.24 | 155.13 | 117.20 |
| 1 | A | 230 | GLY | C-N-CA | 17.23 | 164.78 | 121.70 |
| 1 | A | 124 | GLY | C-N-CA | 17.15 | 164.58 | 121.70 |
| 1 | B | 87 | ILE | CB-CG1-CD1 | 17.14 | 161.88 | 113.90 |
| 1 | A | 229 | GLY | C-N-CA | 17.11 | 158.24 | 122.30 |
| 1 | C | 214 | ARG | O-C-N | -17.10 | 95.34 | 122.70 |
| 1 | F | 104 | GLY | C-N-CD | -17.09 | 82.99 | 120.60 |
| 1 | D | 189 | PRO | N-CA-CB | 17.09 | 123.81 | 103.30 |
| 1 | A | 194 | ASP | OD1-CG-OD2 | -17.08 | 90.85 | 123.30 |
| 1 | D | 7 | LEU | CA-C-O | 17.05 | 155.91 | 120.10 |
| 1 | F | 104 | GLY | O-C-N | 17.04 | 153.48 | 121.10 |
| 1 | D | 107 | LEU | CB-CG-CD2 | -17.04 | 82.03 | 111.00 |
| 1 | E | 192 | ARG | NE-CZ-NH2 | -17.04 | 111.78 | 120.30 |
| 1 | D | 65 | ASP | N-CA-CB | -17.03 | 79.94 | 110.60 |
| 1 | D | 12 | SER | N-CA-CB | -17.03 | 84.96 | 110.50 |
| 1 | D | 171 | VAL | CA-CB-CG2 | 16.97 | 136.35 | 110.90 |
| 1 | D | 103 | TYR | CB-CG-CD1 | 16.95 | 131.17 | 121.00 |
| 1 | D | 166 | ASP | CB-CG-OD1 | 16.94 | 133.55 | 118.30 |
| 1 | D | 47 | VAL | CA-CB-CG1 | -16.93 | 85.50 | 110.90 |
| 1 | B | 210 | ARG | CA-C-O | -16.93 | 84.56 | 120.10 |
| 1 | F | 90 | TYR | CG-CD2-CE2 | 16.93 | 134.84 | 121.30 |
| 1 | E | 145 | GLN | CB-CG-CD | 16.92 | 155.59 | 111.60 |
| 1 | B | 124 | GLY | C-N-CA | 16.90 | 163.95 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 136 | ASN | CA-CB-CG | 16.89 | 150.56 | 113.40 |
| 1 | F | 7 | LEU | O-C-N | -16.88 | 95.70 | 122.70 |
| 1 | B | 167 | ARG | N-CA-CB | 16.87 | 140.97 | 110.60 |
| 1 | D | 51 | ASN | C-N-CA | 16.87 | 163.87 | 121.70 |
| 1 | D | 158 | THR | CA-C-N | 16.87 | 154.31 | 117.20 |
| 1 | E | 99 | THR | CA-CB-CG2 | 16.83 | 135.96 | 112.40 |
| 1 | D | 196 | LEU | CA-CB-CG | 16.83 | 154.00 | 115.30 |
| 1 | F | 154 | LEU | CB-CG-CD1 | 16.82 | 139.60 | 111.00 |
| 1 | D | 188 | GLN | O-C-N | -16.82 | 89.15 | 121.10 |
| 1 | B | 1 | ASN | CA-CB-CG | 16.81 | 150.39 | 113.40 |
| 1 | D | 169 | ASP | CB-CG-OD1 | -16.80 | 103.18 | 118.30 |
| 1 | F | 67 | LEU | CB-CG-CD2 | 16.78 | 139.53 | 111.00 |
| 1 | D | 106 | GLY | CA-C-N | 16.78 | 154.12 | 117.20 |
| 1 | E | 146 | SER | O-C-N | -16.75 | 95.90 | 122.70 |
| 1 | B | 105 | PRO | CA-N-CD | -16.74 | 88.06 | 111.50 |
| 1 | B | 143 | ALA | CA-C-N | 16.73 | 154.01 | 117.20 |
| 1 | C | 197 | THR | CA-CB-CG2 | 16.73 | 135.82 | 112.40 |
| 1 | B | 229 | GLY | CA-C-N | -16.73 | 82.75 | 116.20 |
| 1 | B | 124 | GLY | N-CA-C | 16.71 | 154.87 | 113.10 |
| 1 | C | 38 | LEU | O-C-N | -16.70 | 95.99 | 122.70 |
| 1 | C | 78 | ARG | NE-CZ-NH2 | 16.70 | 128.65 | 120.30 |
| 1 | E | 182 | GLY | C-N-CA | 16.69 | 163.42 | 121.70 |
| 1 | C | 132 | GLN | CA-CB-CG | 16.68 | 150.10 | 113.40 |
| 1 | A | 98 | ARG | NH1-CZ-NH2 | 16.68 | 137.74 | 119.40 |
| 1 | A | 182 | GLY | CA-C-O | -16.68 | 90.58 | 120.60 |
| 1 | B | 108 | TRP | O-C-N | -16.67 | 96.03 | 122.70 |
| 1 | D | 169 | ASP | CB-CG-OD2 | 16.67 | 133.30 | 118.30 |
| 1 | D | 56 | THR | C-N-CA | 16.67 | 157.30 | 122.30 |
| 1 | F | 189 | PRO | C-N-CA | 16.65 | 163.33 | 121.70 |
| 1 | F | 65 | ASP | N-CA-CB | -16.65 | 80.63 | 110.60 |
| 1 | C | 130 | SER | CA-C-O | 16.64 | 155.05 | 120.10 |
| 1 | E | 33 | GLN | CA-CB-CG | 16.63 | 149.98 | 113.40 |
| 1 | B | 201 | ILE | O-C-N | -16.63 | 96.10 | 122.70 |
| 1 | D | 129 | TYR | CZ-CE2-CD2 | -16.62 | 104.84 | 119.80 |
| 1 | A | 105 | PRO | CA-N-CD | -16.58 | 88.28 | 111.50 |
| 1 | E | 1 | ASN | OD1-CG-ND2 | -16.58 | 83.76 | 121.90 |
| 1 | B | 184 | ARG | CD-NE-CZ | 16.57 | 146.80 | 123.60 |
| 1 | E | 9 | HIS | C-N-CA | 16.56 | 163.09 | 121.70 |
| 1 | B | 107 | LEU | CA-C-N | 16.53 | 153.57 | 117.20 |
| 1 | B | 147 | LEU | CB-CG-CD2 | -16.53 | 82.90 | 111.00 |
| 1 | A | 128 | LEU | CA-C-O | -16.52 | 85.40 | 120.10 |
| 1 | B | 194 | ASP | CB-CG-OD2 | -16.50 | 103.45 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 128 | LEU | CB-CA-C | 16.50 | 141.54 | 110.20 |
| 1 | C | 78 | ARG | NE-CZ-NH1 | -16.49 | 112.06 | 120.30 |
| 1 | E | 167 | ARG | CD-NE-CZ | 16.47 | 146.66 | 123.60 |
| 1 | D | 64 | SER | CB-CA-C | 16.45 | 141.35 | 110.10 |
| 1 | E | 131 | THR | CA-C-O | 16.45 | 154.64 | 120.10 |
| 1 | D | 146 | SER | CA-C-O | -16.43 | 85.60 | 120.10 |
| 1 | D | 168 | ASP | CA-CB-CG | 16.43 | 149.53 | 113.40 |
| 1 | B | 89 | ASN | CB-CG-OD1 | -16.42 | 88.75 | 121.60 |
| 1 | D | 21 | GLN | CA-CB-CG | 16.42 | 149.52 | 113.40 |
| 1 | D | 89 | ASN | CB-CG-OD1 | -16.41 | 88.78 | 121.60 |
| 1 | F | 86 | SER | CA-C-O | -16.41 | 85.64 | 120.10 |
| 1 | D | 233 | TRP | CA-CB-CG | 16.41 | 144.87 | 113.70 |
| 1 | B | 21 | GLN | C-N-CA | 16.40 | 162.70 | 121.70 |
| 1 | E | 59 | ARG | CD-NE-CZ | 16.39 | 146.55 | 123.60 |
| 1 | E | 89 | ASN | CB-CG-OD1 | -16.36 | 88.89 | 121.60 |
| 1 | B | 54 | GLY | CA-C-O | -16.34 | 91.18 | 120.60 |
| 1 | A | 124 | GLY | N-CA-C | 16.29 | 153.83 | 113.10 |
| 1 | C | 150 | SER | N-CA-CB | 16.28 | 134.92 | 110.50 |
| 1 | C | 214 | ARG | CA-CB-CG | 16.25 | 149.16 | 113.40 |
| 1 | D | 124 | GLY | C-N-CA | 16.25 | 162.31 | 121.70 |
| 1 | E | 225 | LEU | N-CA-CB | -16.25 | 77.91 | 110.40 |
| 1 | B | 22 | SER | O-C-N | -16.24 | 96.72 | 122.70 |
| 1 | E | 128 | LEU | CB-CG-CD1 | 16.23 | 138.59 | 111.00 |
| 1 | A | 206 | SER | O-C-N | -16.21 | 95.64 | 123.20 |
| 1 | D | 210 | ARG | CA-CB-CG | 16.21 | 149.07 | 113.40 |
| 1 | B | 209 | SER | O-C-N | 16.15 | 148.54 | 122.70 |
| 1 | E | 128 | LEU | O-C-N | -16.14 | 96.88 | 122.70 |
| 1 | A | 143 | ALA | CB-CA-C | 16.14 | 134.30 | 110.10 |
| 1 | B | 142 | HIS | CA-CB-CG | 16.09 | 140.95 | 113.60 |
| 1 | A | 198 | ASN | C-N-CA | 16.09 | 161.91 | 121.70 |
| 1 | E | 59 | ARG | CA-CB-CG | 16.07 | 148.75 | 113.40 |
| 1 | F | 109 | ASP | CB-CG-OD1 | 16.05 | 132.75 | 118.30 |
| 1 | C | 174 | THR | O-C-N | -16.05 | 97.02 | 122.70 |
| 1 | F | 85 | GLY | O-C-N | -16.03 | 97.05 | 122.70 |
| 1 | D | 154 | LEU | CA-CB-CG | 16.02 | 152.15 | 115.30 |
| 1 | A | 180 | GLY | CA-C-O | -16.02 | 91.77 | 120.60 |
| 1 | F | 78 | ARG | CG-CD-NE | 16.02 | 145.44 | 111.80 |
| 1 | F | 111 | GLY | CA-C-O | 16.01 | 149.41 | 120.60 |
| 1 | B | 82 | GLY | CA-C-O | 15.98 | 149.37 | 120.60 |
| 1 | C | 152 | TYR | CG-CD2-CE2 | 15.97 | 134.08 | 121.30 |
| 1 | C | 206 | SER | O-C-N | -15.94 | 96.09 | 123.20 |
| 1 | C | 103 | TYR | CD1-CE1-CZ | -15.94 | 105.46 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 224 | ASN | C-N-CA | 15.92 | 161.50 | 121.70 |
| 1 | B | 5 | PHE | CB-CG-CD1 | 15.89 | 131.93 | 120.80 |
| 1 | D | 39 | VAL | CA-CB-CG2 | 15.89 | 134.74 | 110.90 |
| 1 | B | 230 | GLY | CA-C-N | -15.89 | 82.25 | 117.20 |
| 1 | A | 113 | SER | CA-C-O | 15.87 | 153.43 | 120.10 |
| 1 | B | 104 | GLY | C-N-CD | -15.87 | 85.70 | 120.60 |
| 1 | F | 194 | ASP | CB-CG-OD2 | 15.86 | 132.57 | 118.30 |
| 1 | D | 210 | ARG | CD-NE-CZ | 15.82 | 145.74 | 123.60 |
| 1 | E | 214 | ARG | O-C-N | -15.79 | 97.43 | 122.70 |
| 1 | C | 128 | LEU | C-N-CA | 15.79 | 161.18 | 121.70 |
| 1 | B | 91 | VAL | CA-CB-CG1 | 15.78 | 134.56 | 110.90 |
| 1 | A | 203 | VAL | CA-CB-CG1 | 15.76 | 134.54 | 110.90 |
| 1 | E | 158 | THR | CA-CB-CG2 | -15.74 | 90.36 | 112.40 |
| 1 | A | 129 | TYR | CD1-CE1-CZ | 15.74 | 133.97 | 119.80 |
| 1 | F | 8 | SER | CB-CA-C | 15.74 | 140.00 | 110.10 |
| 1 | D | 159 | ASP | CB-CG-OD1 | -15.72 | 104.15 | 118.30 |
| 1 | F | 24 | GLU | CA-CB-CG | 15.69 | 147.93 | 113.40 |
| 1 | F | 54 | GLY | O-C-N | -15.68 | 97.61 | 122.70 |
| 1 | A | 142 | HIS | O-C-N | -15.68 | 97.62 | 122.70 |
| 1 | C | 124 | GLY | N-CA-C | 15.67 | 152.28 | 113.10 |
| 1 | D | 214 | ARG | NH1-CZ-NH2 | -15.67 | 102.16 | 119.40 |
| 1 | B | 209 | SER | CA-C-O | -15.65 | 87.23 | 120.10 |
| 1 | A | 47 | VAL | CA-CB-CG1 | -15.65 | 87.43 | 110.90 |
| 1 | C | 40 | LEU | O-C-N | -15.65 | 97.66 | 122.70 |
| 1 | C | 212 | ALA | CB-CA-C | -15.65 | 86.63 | 110.10 |
| 1 | F | 32 | MET | CG-SD-CE | 15.64 | 125.22 | 100.20 |
| 1 | B | 222 | ASP | CA-C-N | 15.63 | 151.59 | 117.20 |
| 1 | B | 64 | SER | CB-CA-C | 15.63 | 139.79 | 110.10 |
| 1 | C | 28 | PHE | CD1-CE1-CZ | -15.62 | 101.36 | 120.10 |
| 1 | D | 217 | PHE | CB-CA-C | 15.60 | 141.60 | 110.40 |
| 1 | B | 5 | PHE | CD1-CE1-CZ | 15.58 | 138.80 | 120.10 |
| 1 | E | 35 | ASP | O-C-N | -15.57 | 97.79 | 122.70 |
| 1 | C | 228 | TYR | CB-CG-CD1 | 15.55 | 130.33 | 121.00 |
| 1 | F | 190 | ASN | OD1-CG-ND2 | -15.55 | 86.14 | 121.90 |
| 1 | D | 148 | GLN | O-C-N | -15.53 | 97.85 | 122.70 |
| 1 | A | 81 | SER | CA-C-N | 15.53 | 147.26 | 116.20 |
| 1 | E | 124 | GLY | C-N-CA | 15.53 | 160.52 | 121.70 |
| 1 | F | 128 | LEU | O-C-N | -15.53 | 97.86 | 122.70 |
| 1 | D | 35 | ASP | O-C-N | -15.52 | 97.87 | 122.70 |
| 1 | F | 109 | ASP | CB-CG-OD2 | -15.52 | 104.33 | 118.30 |
| 1 | D | 221 | PRO | O-C-N | -15.51 | 97.88 | 122.70 |
| 1 | F | 141 | LEU | N-CA-CB | -15.50 | 79.39 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 78 | ARG | CG-CD-NE | 15.49 | 144.33 | 111.80 |
| 1 | B | 71 | LEU | CB-CG-CD1 | -15.48 | 84.68 | 111.00 |
| 1 | A | 169 | ASP | CB-CG-OD2 | 15.48 | 132.23 | 118.30 |
| 1 | A | 145 | GLN | CA-CB-CG | 15.45 | 147.40 | 113.40 |
| 1 | C | 123 | ASN | C-N-CA | 15.43 | 154.71 | 122.30 |
| 1 | A | 170 | ARG | CB-CG-CD | 15.41 | 151.67 | 111.60 |
| 1 | A | 99 | THR | CA-CB-OG1 | -15.40 | 76.65 | 109.00 |
| 1 | C | 2 | ASN | CB-CG-ND2 | 15.40 | 153.67 | 116.70 |
| 1 | B | 5 | PHE | CB-CG-CD2 | 15.40 | 131.58 | 120.80 |
| 1 | F | 55 | ALA | O-C-N | -15.39 | 98.08 | 122.70 |
| 1 | B | 55 | ALA | CA-C-O | 15.38 | 152.41 | 120.10 |
| 1 | C | 61 | VAL | CB-CA-C | -15.38 | 82.17 | 111.40 |
| 1 | A | 55 | ALA | CB-CA-C | 15.36 | 133.13 | 110.10 |
| 1 | A | 214 | ARG | O-C-N | -15.35 | 98.14 | 122.70 |
| 1 | C | 13 | HIS | CA-C-O | -15.34 | 87.89 | 120.10 |
| 1 | C | 128 | LEU | CB-CA-C | 15.33 | 139.34 | 110.20 |
| 1 | C | 230 | GLY | CA-C-N | 15.32 | 150.91 | 117.20 |
| 1 | B | 107 | LEU | O-C-N | -15.32 | 98.19 | 122.70 |
| 1 | F | 210 | ARG | CA-C-N | 15.30 | 150.85 | 117.20 |
| 1 | E | 90 | TYR | CB-CG-CD2 | 15.28 | 130.17 | 121.00 |
| 1 | E | 146 | SER | CA-C-O | -15.28 | 88.02 | 120.10 |
| 1 | B | 192 | ARG | CG-CD-NE | 15.27 | 143.87 | 111.80 |
| 1 | B | 100 | VAL | CA-CB-CG2 | 15.26 | 133.78 | 110.90 |
| 1 | D | 213 | GLY | CA-C-O | -15.24 | 93.18 | 120.60 |
| 1 | B | 217 | PHE | O-C-N | 15.22 | 147.05 | 122.70 |
| 1 | F | 225 | LEU | N-CA-CB | 15.22 | 140.84 | 110.40 |
| 1 | A | 170 | ARG | O-C-N | -15.21 | 98.37 | 122.70 |
| 1 | D | 198 | ASN | CA-CB-CG | -15.21 | 79.94 | 113.40 |
| 1 | C | 189 | PRO | C-N-CA | 15.20 | 159.69 | 121.70 |
| 1 | B | 202 | ALA | O-C-N | -15.19 | 98.39 | 122.70 |
| 1 | E | 5 | PHE | CA-C-N | -15.18 | 85.84 | 116.20 |
| 1 | A | 174 | THR | CA-CB-CG2 | -15.17 | 91.17 | 112.40 |
| 1 | D | 130 | SER | C-N-CA | 15.16 | 159.59 | 121.70 |
| 1 | C | 210 | ARG | O-C-N | -15.15 | 98.45 | 122.70 |
| 1 | F | 131 | THR | N-CA-C | 15.15 | 151.90 | 111.00 |
| 1 | D | 224 | ASN | N-CA-CB | -15.14 | 83.35 | 110.60 |
| 1 | A | 33 | GLN | C-N-CA | 15.14 | 159.55 | 121.70 |
| 1 | F | 129 | TYR | OH-CZ-CE2 | 15.14 | 160.97 | 120.10 |
| 1 | F | 54 | GLY | C-N-CA | 15.13 | 159.53 | 121.70 |
| 1 | D | 106 | GLY | O-C-N | -15.10 | 98.54 | 122.70 |
| 1 | D | 1 | ASN | C-N-CA | 15.10 | 159.45 | 121.70 |
| 1 | F | 190 | ASN | O-C-N | -15.08 | 97.56 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 130 | SER | C-N-CA | 15.06 | 159.34 | 121.70 |
| 1 | A | 99 | THR | CA-CB-CG2 | 15.02 | 133.43 | 112.40 |
| 1 | F | 195 | VAL | CA-CB-CG1 | 15.01 | 133.41 | 110.90 |
| 1 | A | 166 | ASP | N-CA-CB | 14.99 | 137.59 | 110.60 |
| 1 | D | 83 | THR | CA-CB-CG2 | -14.99 | 91.41 | 112.40 |
| 1 | A | 61 | VAL | CA-CB-CG2 | -14.99 | 88.42 | 110.90 |
| 1 | D | 59 | ARG | NH1-CZ-NH2 | 14.99 | 135.88 | 119.40 |
| 1 | A | 113 | SER | O-C-N | -14.98 | 98.73 | 122.70 |
| 1 | A | 110 | SER | CA-C-O | 14.97 | 151.54 | 120.10 |
| 1 | E | 170 | ARG | NH1-CZ-NH2 | -14.96 | 102.94 | 119.40 |
| 1 | F | 101 | THR | N-CA-C | 14.93 | 151.31 | 111.00 |
| 1 | F | 153 | ARG | CG-CD-NE | 14.91 | 143.11 | 111.80 |
| 1 | E | 170 | ARG | CB-CG-CD | 14.90 | 150.35 | 111.60 |
| 1 | F | 26 | SER | C-N-CA | 14.87 | 158.88 | 121.70 |
| 1 | F | 152 | TYR | CB-CG-CD2 | 14.85 | 129.91 | 121.00 |
| 1 | F | 137 | HIS | CA-C-O | -14.84 | 88.93 | 120.10 |
| 1 | C | 41 | PHE | CB-CG-CD2 | -14.83 | 110.42 | 120.80 |
| 1 | A | 127 | ILE | CA-CB-CG1 | 14.83 | 139.17 | 111.00 |
| 1 | B | 19 | ALA | CB-CA-C | 14.78 | 132.26 | 110.10 |
| 1 | B | 22 | SER | CB-CA-C | -14.78 | 82.03 | 110.10 |
| 1 | D | 196 | LEU | C-N-CA | 14.77 | 158.62 | 121.70 |
| 1 | A | 7 | LEU | CA-C-N | 14.76 | 149.66 | 117.20 |
| 1 | A | 88 | GLY | N-CA-C | 14.76 | 149.99 | 113.10 |
| 1 | D | 62 | LEU | CA-C-O | 14.75 | 151.07 | 120.10 |
| 1 | C | 118 | VAL | C-N-CA | 14.74 | 158.56 | 121.70 |
| 1 | D | 34 | SER | N-CA-CB | 14.74 | 132.61 | 110.50 |
| 1 | F | 60 | ALA | CA-C-O | -14.73 | 89.17 | 120.10 |
| 1 | D | 223 | ARG | O-C-N | -14.72 | 99.14 | 122.70 |
| 1 | A | 92 | LEU | CA-CB-CG | 14.72 | 149.15 | 115.30 |
| 1 | A | 5 | PHE | CA-C-N | 14.71 | 145.62 | 116.20 |
| 1 | A | 164 | LEU | CB-CG-CD1 | 14.71 | 136.01 | 111.00 |
| 1 | F | 210 | ARG | NH1-CZ-NH2 | 14.71 | 135.58 | 119.40 |
| 1 | C | 206 | SER | C-N-CA | 14.70 | 153.18 | 122.30 |
| 1 | D | 75 | ASN | OD1-CG-ND2 | 14.71 | 155.72 | 121.90 |
| 1 | F | 60 | ALA | O-C-N | -14.70 | 99.18 | 122.70 |
| 1 | D | 193 | MET | CA-C-N | 14.70 | 149.53 | 117.20 |
| 1 | A | 193 | MET | CA-CB-CG | 14.69 | 138.28 | 113.30 |
| 1 | C | 217 | PHE | CB-CG-CD1 | 14.69 | 131.08 | 120.80 |
| 1 | D | 216 | VAL | CB-CA-C | 14.67 | 139.27 | 111.40 |
| 1 | A | 19 | ALA | CA-C-N | 14.65 | 149.44 | 117.20 |
| 1 | E | 102 | ILE | O-C-N | 14.65 | 146.15 | 122.70 |
| 1 | B | 59 | ARG | CB-CA-C | -14.64 | 81.12 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 86 | SER | N-CA-CB | -14.64 | 88.54 | 110.50 |
| 1 | C | 73 | ALA | CB-CA-C | 14.61 | 132.01 | 110.10 |
| 1 | D | 15 | GLN | CG-CD-OE1 | -14.60 | 92.40 | 121.60 |
| 1 | A | 68 | LEU | C-N-CA | 14.55 | 158.08 | 121.70 |
| 1 | E | 152 | TYR | CG-CD2-CE2 | 14.54 | 132.93 | 121.30 |
| 1 | C | 192 | ARG | NE-CZ-NH2 | -14.53 | 113.03 | 120.30 |
| 1 | A | 58 | CYS | N-CA-CB | -14.53 | 84.45 | 110.60 |
| 1 | A | 78 | ARG | NH1-CZ-NH2 | -14.53 | 103.42 | 119.40 |
| 1 | F | 136 | ASN | O-C-N | -14.52 | 99.47 | 122.70 |
| 1 | A | 20 | ALA | N-CA-CB | 14.51 | 130.42 | 110.10 |
| 1 | B | 7 | LEU | O-C-N | -14.49 | 99.52 | 122.70 |
| 1 | A | 135 | ASP | CB-CG-OD1 | -14.49 | 105.26 | 118.30 |
| 1 | D | 35 | ASP | CB-CG-OD2 | -14.49 | 105.26 | 118.30 |
| 1 | A | 94 | LEU | C-N-CA | 14.48 | 157.90 | 121.70 |
| 1 | D | 83 | THR | CA-C-O | -14.48 | 89.69 | 120.10 |
| 1 | C | 218 | VAL | CG1-CB-CG2 | -14.47 | 87.74 | 110.90 |
| 1 | F | 87 | ILE | CA-C-N | 14.47 | 145.15 | 116.20 |
| 1 | A | 146 | SER | N-CA-C | 14.47 | 150.07 | 111.00 |
| 1 | D | 104 | GLY | O-C-N | 14.45 | 148.55 | 121.10 |
| 1 | A | 167 | ARG | CD-NE-CZ | 14.44 | 143.81 | 123.60 |
| 1 | C | 105 | PRO | CA-N-CD | -14.44 | 91.29 | 111.50 |
| 1 | F | 26 | SER | CA-CB-OG | 14.43 | 150.16 | 111.20 |
| 1 | D | 91 | VAL | O-C-N | -14.42 | 99.63 | 122.70 |
| 1 | B | 205 | THR | CA-CB-CG2 | 14.41 | 132.58 | 112.40 |
| 1 | D | 46 | ARG | CB-CG-CD | 14.40 | 149.04 | 111.60 |
| 1 | C | 125 | ASN | CA-CB-CG | 14.40 | 145.08 | 113.40 |
| 1 | C | 37 | ASN | CB-CG-OD1 | -14.39 | 92.82 | 121.60 |
| 1 | C | 74 | GLN | OE1-CD-NE2 | 14.38 | 154.98 | 121.90 |
| 1 | D | 21 | GLN | CB-CG-CD | 14.38 | 148.99 | 111.60 |
| 1 | A | 210 | ARG | NH1-CZ-NH2 | 14.37 | 135.21 | 119.40 |
| 1 | C | 46 | ARG | NE-CZ-NH2 | 14.37 | 127.49 | 120.30 |
| 1 | D | 29 | ARG | NE-CZ-NH2 | 14.37 | 127.48 | 120.30 |
| 1 | D | 129 | TYR | CB-CG-CD1 | -14.37 | 112.38 | 121.00 |
| 1 | A | 200 | ASN | O-C-N | -14.37 | 99.72 | 122.70 |
| 1 | E | 193 | MET | CG-SD-CE | 14.37 | 123.18 | 100.20 |
| 1 | F | 83 | THR | O-C-N | -14.32 | 99.78 | 122.70 |
| 1 | D | 35 | ASP | CA-C-N | 14.32 | 148.71 | 117.20 |
| 1 | F | 78 | ARG | CB-CG-CD | 14.32 | 148.82 | 111.60 |
| 1 | C | 201 | ILE | O-C-N | -14.31 | 99.80 | 122.70 |
| 1 | E | 46 | ARG | CB-CA-C | 14.31 | 139.03 | 110.40 |
| 1 | D | 25 | LEU | CB-CG-CD2 | 14.31 | 135.32 | 111.00 |
| 1 | F | 164 | LEU | CA-C-O | -14.30 | 90.07 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 65 | ASP | CB-CG-OD2 | 14.29 | 131.17 | 118.30 |
| 1 | D | 213 | GLY | O-C-N | 14.24 | 145.49 | 122.70 |
| 1 | B | 100 | VAL | CA-C-O | 14.24 | 150.01 | 120.10 |
| 1 | F | 149 | LEU | N-CA-CB | 14.24 | 138.88 | 110.40 |
| 1 | B | 222 | ASP | CB-CG-OD2 | -14.24 | 105.49 | 118.30 |
| 1 | B | 129 | TYR | CB-CG-CD2 | -14.22 | 112.47 | 121.00 |
| 1 | B | 196 | LEU | CA-C-O | 14.22 | 149.97 | 120.10 |
| 1 | F | 195 | VAL | CB-CA-C | 14.22 | 138.42 | 111.40 |
| 1 | B | 73 | ALA | C-N-CA | 14.20 | 157.21 | 121.70 |
| 1 | D | 130 | SER | O-C-N | -14.20 | 99.98 | 122.70 |
| 1 | B | 183 | CYS | CA-CB-SG | 14.19 | 139.54 | 114.00 |
| 1 | D | 13 | HIS | CA-C-O | -14.19 | 90.31 | 120.10 |
| 1 | B | 105 | PRO | CA-C-O | -14.18 | 86.16 | 120.20 |
| 1 | A | 4 | LEU | CB-CA-C | 14.17 | 137.12 | 110.20 |
| 1 | E | 153 | ARG | CD-NE-CZ | 14.15 | 143.41 | 123.60 |
| 1 | D | 100 | VAL | CG1-CB-CG2 | -14.13 | 88.29 | 110.90 |
| 1 | E | 34 | SER | CB-CA-C | 14.12 | 136.93 | 110.10 |
| 1 | D | 76 | THR | O-C-N | -14.11 | 100.12 | 122.70 |
| 1 | A | 32 | MET | CG-SD-CE | -14.10 | 77.65 | 100.20 |
| 1 | D | 234 | THR | CA-CB-CG2 | 14.07 | 132.09 | 112.40 |
| 1 | B | 140 | THR | CA-CB-CG2 | 14.06 | 132.09 | 112.40 |
| 1 | B | 17 | LEU | CB-CG-CD1 | -14.04 | 87.12 | 111.00 |
| 1 | B | 203 | VAL | CA-CB-CG2 | 14.04 | 131.96 | 110.90 |
| 1 | E | 42 | ASP | CB-CG-OD2 | -14.03 | 105.68 | 118.30 |
| 1 | F | 166 | ASP | CB-CG-OD2 | -14.02 | 105.68 | 118.30 |
| 1 | F | 61 | VAL | CB-CA-C | -14.02 | 84.76 | 111.40 |
| 1 | D | 129 | TYR | CG-CD1-CE1 | -14.00 | 110.10 | 121.30 |
| 1 | C | 184 | ARG | NH1-CZ-NH2 | 13.99 | 134.79 | 119.40 |
| 1 | A | 94 | LEU | CA-CB-CG | 13.98 | 147.47 | 115.30 |
| 1 | D | 8 | SER | CB-CA-C | 13.98 | 136.67 | 110.10 |
| 1 | A | 48 | TRP | CG-CD1-NE1 | 13.98 | 124.08 | 110.10 |
| 1 | F | 129 | TYR | C-N-CA | 13.98 | 156.65 | 121.70 |
| 1 | A | 60 | ALA | O-C-N | -13.97 | 100.34 | 122.70 |
| 1 | D | 177 | ALA | N-CA-CB | 13.97 | 129.66 | 110.10 |
| 1 | D | 74 | GLN | CA-CB-CG | -13.97 | 82.67 | 113.40 |
| 1 | A | 187 | LEU | CA-CB-CG | 13.96 | 147.40 | 115.30 |
| 1 | B | 220 | GLN | CG-CD-NE2 | 13.96 | 150.20 | 116.70 |
| 1 | B | 64 | SER | CA-C-N | 13.95 | 147.90 | 117.20 |
| 1 | E | 129 | TYR | CB-CG-CD2 | 13.95 | 129.37 | 121.00 |
| 1 | E | 1 | ASN | O-C-N | -13.95 | 100.39 | 122.70 |
| 1 | D | 166 | ASP | CB-CG-OD2 | -13.94 | 105.75 | 118.30 |
| 1 | B | 9 | HIS | CB-CA-C | -13.91 | 82.58 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 184 | ARG | CD-NE-CZ | 13.90 | 143.06 | 123.60 |
| 1 | A | 95 | GLN | CB-CG-CD | 13.88 | 147.70 | 111.60 |
| 1 | B | 77 | ILE | CB-CA-C | -13.88 | 83.83 | 111.60 |
| 1 | C | 131 | THR | CA-CB-OG1 | 13.88 | 138.14 | 109.00 |
| 1 | D | 192 | ARG | CD-NE-CZ | 13.87 | 143.02 | 123.60 |
| 1 | D | 76 | THR | CA-CB-CG2 | 13.87 | 131.82 | 112.40 |
| 1 | D | 34 | SER | O-C-N | -13.87 | 100.52 | 122.70 |
| 1 | D | 15 | GLN | CG-CD-NE2 | 13.86 | 149.96 | 116.70 |
| 1 | E | 10 | GLU | CB-CA-C | 13.85 | 138.09 | 110.40 |
| 1 | F | 220 | GLN | CA-CB-CG | -13.84 | 82.95 | 113.40 |
| 1 | F | 8 | SER | N-CA-CB | -13.81 | 89.78 | 110.50 |
| 1 | D | 107 | LEU | CA-C-O | -13.80 | 91.13 | 120.10 |
| 1 | D | 226 | ALA | CB-CA-C | 13.79 | 130.79 | 110.10 |
| 1 | C | 28 | PHE | CG-CD1-CE1 | 13.79 | 135.97 | 120.80 |
| 1 | B | 215 | TYR | CB-CG-CD2 | -13.79 | 112.73 | 121.00 |
| 1 | A | 109 | ASP | N-CA-CB | 13.76 | 135.37 | 110.60 |
| 1 | A | 5 | PHE | CB-CG-CD2 | 13.75 | 130.43 | 120.80 |
| 1 | D | 224 | ASN | N-CA-C | 13.75 | 148.13 | 111.00 |
| 1 | A | 129 | TYR | CA-C-O | -13.74 | 91.25 | 120.10 |
| 1 | D | 223 | ARG | CG-CD-NE | 13.74 | 140.65 | 111.80 |
| 1 | E | 136 | ASN | N-CA-CB | 13.73 | 135.31 | 110.60 |
| 1 | F | 194 | ASP | CA-CB-CG | -13.72 | 83.21 | 113.40 |
| 1 | E | 128 | LEU | CD1-CG-CD2 | -13.71 | 69.35 | 110.50 |
| 1 | E | 64 | SER | O-C-N | -13.71 | 100.76 | 122.70 |
| 1 | E | 214 | ARG | CD-NE-CZ | 13.70 | 142.78 | 123.60 |
| 1 | F | 187 | LEU | CA-CB-CG | 13.70 | 146.81 | 115.30 |
| 1 | B | 109 | ASP | CB-CA-C | -13.69 | 83.02 | 110.40 |
| 1 | A | 19 | ALA | N-CA-CB | -13.68 | 90.95 | 110.10 |
| 1 | A | 62 | LEU | CA-CB-CG | 13.68 | 146.76 | 115.30 |
| 1 | A | 65 | ASP | OD1-CG-OD2 | -13.68 | 97.32 | 123.30 |
| 1 | F | 104 | GLY | C-N-CA | 13.65 | 179.33 | 122.00 |
| 1 | C | 62 | LEU | CB-CG-CD2 | 13.65 | 134.20 | 111.00 |
| 1 | A | 173 | SER | CA-C-N | 13.64 | 147.22 | 117.20 |
| 1 | D | 187 | LEU | N-CA-CB | 13.64 | 137.69 | 110.40 |
| 1 | D | 176 | THR | N-CA-CB | -13.64 | 84.38 | 110.30 |
| 1 | A | 7 | LEU | CB-CA-C | 13.63 | 136.10 | 110.20 |
| 1 | E | 188 | GLN | CA-CB-CG | -13.63 | 83.41 | 113.40 |
| 1 | A | 188 | GLN | CG-CD-NE2 | 13.62 | 149.39 | 116.70 |
| 1 | F | 210 | ARG | CA-C-O | -13.62 | 91.50 | 120.10 |
| 1 | B | 143 | ALA | CA-C-O | -13.62 | 91.50 | 120.10 |
| 1 | C | 71 | LEU | CB-CG-CD2 | -13.62 | 87.85 | 111.00 |
| 1 | F | 138 | PRO | N-CA-CB | 13.62 | 119.64 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 233 | TRP | CB-CG-CD2 | 13.60 | 144.28 | 126.60 |
| 1 | F | 192 | ARG | CA-CB-CG | 13.60 | 143.32 | 113.40 |
| 1 | D | 105 | PRO | CA-C-O | -13.60 | 87.56 | 120.20 |
| 1 | A | 131 | THR | N-CA-CB | 13.59 | 136.12 | 110.30 |
| 1 | D | 27 | SER | C-N-CA | 13.59 | 155.67 | 121.70 |
| 1 | D | 104 | GLY | C-N-CA | 13.57 | 178.98 | 122.00 |
| 1 | F | 59 | ARG | CD-NE-CZ | -13.56 | 104.62 | 123.60 |
| 1 | D | 3 | ILE | CA-CB-CG2 | -13.55 | 83.80 | 110.90 |
| 1 | D | 170 | ARG | NH1-CZ-NH2 | -13.55 | 104.50 | 119.40 |
| 1 | E | 159 | ASP | O-C-N | -13.54 | 101.03 | 122.70 |
| 1 | D | 130 | SER | CA-C-O | 13.54 | 148.54 | 120.10 |
| 1 | C | 234 | THR | O-C-N | -13.54 | 101.04 | 122.70 |
| 1 | D | 53 | ALA | N-CA-CB | 13.54 | 129.05 | 110.10 |
| 1 | B | 92 | LEU | N-CA-CB | 13.52 | 137.44 | 110.40 |
| 1 | E | 163 | VAL | O-C-N | 13.51 | 144.32 | 122.70 |
| 1 | B | 48 | TRP | N-CA-CB | -13.50 | 86.31 | 110.60 |
| 1 | B | 101 | THR | CA-CB-OG1 | -13.49 | 80.68 | 109.00 |
| 1 | A | 134 | ASN | CA-CB-CG | 13.48 | 143.06 | 113.40 |
| 1 | A | 212 | ALA | CB-CA-C | -13.48 | 89.88 | 110.10 |
| 1 | D | 42 | ASP | CB-CG-OD2 | -13.48 | 106.17 | 118.30 |
| 1 | F | 125 | ASN | CA-CB-CG | 13.47 | 143.04 | 113.40 |
| 1 | A | 110 | SER | C-N-CA | 13.46 | 150.58 | 122.30 |
| 1 | D | 217 | PHE | CB-CG-CD2 | 13.46 | 130.22 | 120.80 |
| 1 | D | 34 | SER | CA-CB-OG | -13.46 | 74.86 | 111.20 |
| 1 | C | 107 | LEU | CA-C-O | -13.46 | 91.84 | 120.10 |
| 1 | C | 127 | ILE | CA-CB-CG1 | 13.44 | 136.54 | 111.00 |
| 1 | E | 152 | TYR | CB-CG-CD1 | 13.44 | 129.06 | 121.00 |
| 1 | C | 188 | GLN | CA-CB-CG | -13.44 | 83.84 | 113.40 |
| 1 | E | 129 | TYR | CD1-CE1-CZ | -13.43 | 107.71 | 119.80 |
| 1 | A | 220 | GLN | CA-CB-CG | -13.43 | 83.85 | 113.40 |
| 1 | B | 78 | ARG | NE-CZ-NH2 | 13.43 | 127.01 | 120.30 |
| 1 | B | 146 | SER | CA-C-N | 13.40 | 146.69 | 117.20 |
| 1 | A | 8 | SER | C-N-CA | 13.39 | 155.18 | 121.70 |
| 1 | A | 29 | ARG | NE-CZ-NH1 | -13.37 | 113.61 | 120.30 |
| 1 | C | 58 | CYS | CB-CA-C | 13.35 | 137.11 | 110.40 |
| 1 | F | 224 | ASN | CA-C-N | 13.35 | 146.58 | 117.20 |
| 1 | C | 138 | PRO | C-N-CA | -13.34 | 88.35 | 121.70 |
| 1 | C | 20 | ALA | CB-CA-C | 13.34 | 130.11 | 110.10 |
| 1 | A | 1 | ASN | N-CA-CB | 13.32 | 134.59 | 110.60 |
| 1 | D | 196 | LEU | CB-CG-CD2 | 13.32 | 133.65 | 111.00 |
| 1 | F | 190 | ASN | CB-CG-ND2 | 13.32 | 148.66 | 116.70 |
| 1 | E | 62 | LEU | CB-CG-CD2 | 13.31 | 133.63 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 98 | ARG | NE-CZ-NH2 | -13.31 | 113.64 | 120.30 |
| 1 | B | 142 | HIS | CG-ND1-CE1 | 13.30 | 126.82 | 108.20 |
| 1 | E | 184 | ARG | NE-CZ-NH2 | -13.29 | 113.65 | 120.30 |
| 1 | A | 92 | LEU | O-C-N | -13.29 | 101.44 | 122.70 |
| 1 | C | 90 | TYR | CA-C-O | -13.28 | 92.22 | 120.10 |
| 1 | B | 15 | GLN | CA-CB-CG | 13.27 | 142.60 | 113.40 |
| 1 | B | 226 | ALA | N-CA-CB | 13.27 | 128.68 | 110.10 |
| 1 | B | 170 | ARG | NE-CZ-NH1 | 13.27 | 126.94 | 120.30 |
| 1 | B | 59 | ARG | NH1-CZ-NH2 | 13.27 | 133.99 | 119.40 |
| 1 | C | 197 | THR | CA-CB-OG1 | -13.25 | 81.18 | 109.00 |
| 1 | E | 222 | ASP | CB-CG-OD2 | 13.25 | 130.22 | 118.30 |
| 1 | B | 84 | LYS | CB-CG-CD | 13.24 | 146.02 | 111.60 |
| 1 | D | 19 | ALA | N-CA-CB | 13.23 | 128.63 | 110.10 |
| 1 | A | 128 | LEU | CB-CG-CD1 | 13.23 | 133.48 | 111.00 |
| 1 | A | 206 | SER | C-N-CA | 13.22 | 150.06 | 122.30 |
| 1 | A | 15 | GLN | CB-CA-C | 13.21 | 136.82 | 110.40 |
| 1 | E | 149 | LEU | C-N-CA | -13.21 | 88.67 | 121.70 |
| 1 | D | 212 | ALA | N-CA-CB | -13.21 | 91.61 | 110.10 |
| 1 | B | 194 | ASP | OD1-CG-OD2 | 13.20 | 148.38 | 123.30 |
| 1 | E | 128 | LEU | CB-CG-CD2 | 13.20 | 133.44 | 111.00 |
| 1 | A | 214 | ARG | CA-CB-CG | 13.20 | 142.43 | 113.40 |
| 1 | D | 96 | PRO | CA-C-N | 13.20 | 146.23 | 117.20 |
| 1 | D | 197 | THR | CA-CB-OG1 | -13.19 | 81.31 | 109.00 |
| 1 | E | 110 | SER | N-CA-CB | 13.18 | 130.27 | 110.50 |
| 1 | D | 196 | LEU | O-C-N | -13.17 | 101.63 | 122.70 |
| 1 | F | 234 | THR | OG1-CB-CG2 | -13.17 | 79.72 | 110.00 |
| 1 | C | 8 | SER | CA-C-O | 13.16 | 147.74 | 120.10 |
| 1 | D | 152 | TYR | OH-CZ-CE2 | -13.15 | 84.59 | 120.10 |
| 1 | B | 71 | LEU | C-N-CA | 13.14 | 154.55 | 121.70 |
| 1 | D | 138 | PRO | CA-N-CD | -13.14 | 93.11 | 111.50 |
| 1 | E | 215 | TYR | CB-CG-CD1 | -13.12 | 113.13 | 121.00 |
| 1 | A | 229 | GLY | CA-C-O | 13.11 | 144.20 | 120.60 |
| 1 | C | 167 | ARG | N-CA-C | -13.09 | 75.66 | 111.00 |
| 1 | B | 6 | GLY | O-C-N | -13.07 | 101.78 | 122.70 |
| 1 | D | 95 | GLN | CG-CD-OE1 | 13.07 | 147.74 | 121.60 |
| 1 | A | 14 | PRO | N-CD-CG | 13.06 | 122.80 | 103.20 |
| 1 | C | 45 | VAL | CA-CB-CG2 | 13.06 | 130.50 | 110.90 |
| 1 | F | 89 | ASN | CB-CG-OD1 | -13.06 | 95.48 | 121.60 |
| 1 | B | 21 | GLN | CG-CD-NE2 | 13.04 | 147.99 | 116.70 |
| 1 | B | 50 | SER | CB-CA-C | 13.03 | 134.85 | 110.10 |
| 1 | B | 62 | LEU | CB-CG-CD1 | 13.03 | 133.14 | 111.00 |
| 1 | B | 31 | THR | CA-CB-CG2 | 13.02 | 130.62 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 15 | GLN | CB-CA-C | 13.01 | 136.43 | 110.40 |
| 1 | B | 210 | ARG | O-C-N | 13.01 | 143.51 | 122.70 |
| 1 | E | 144 | THR | CA-CB-CG2 | -13.01 | 94.19 | 112.40 |
| 1 | C | 142 | HIS | O-C-N | -12.99 | 101.92 | 122.70 |
| 1 | D | 131 | THR | N-CA-C | 12.97 | 146.03 | 111.00 |
| 1 | A | 168 | ASP | CB-CG-OD1 | -12.97 | 106.63 | 118.30 |
| 1 | C | 112 | THR | CA-CB-CG2 | 12.97 | 130.56 | 112.40 |
| 1 | B | 220 | GLN | CG-CD-OE1 | -12.97 | 95.66 | 121.60 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 12.96 | 126.78 | 120.30 |
| 1 | B | 132 | GLN | CA-C-O | 12.96 | 147.32 | 120.10 |
| 1 | A | 88 | GLY | CA-C-N | -12.95 | 88.71 | 117.20 |
| 1 | A | 221 | PRO | N-CA-CB | -12.94 | 87.77 | 103.30 |
| 1 | C | 122 | ASN | CA-CB-CG | 12.94 | 141.86 | 113.40 |
| 1 | A | 221 | PRO | CB-CA-C | 12.93 | 144.32 | 112.00 |
| 1 | D | 194 | ASP | CB-CG-OD2 | 12.92 | 129.93 | 118.30 |
| 1 | C | 29 | ARG | NE-CZ-NH2 | 12.92 | 126.76 | 120.30 |
| 1 | D | 193 | MET | CA-CB-CG | 12.91 | 135.25 | 113.30 |
| 1 | A | 56 | THR | CA-C-O | 12.91 | 147.21 | 120.10 |
| 1 | A | 181 | THR | C-N-CA | -12.91 | 95.20 | 122.30 |
| 1 | D | 202 | ALA | CA-C-N | 12.90 | 145.59 | 117.20 |
| 1 | A | 92 | LEU | CB-CG-CD1 | -12.90 | 89.07 | 111.00 |
| 1 | B | 170 | ARG | NE-CZ-NH2 | -12.90 | 113.85 | 120.30 |
| 1 | C | 193 | MET | CG-SD-CE | -12.89 | 79.57 | 100.20 |
| 1 | E | 111 | GLY | O-C-N | 12.89 | 143.32 | 122.70 |
| 1 | E | 26 | SER | CA-C-N | 12.89 | 145.55 | 117.20 |
| 1 | B | 87 | ILE | CA-CB-CG2 | -12.88 | 85.14 | 110.90 |
| 1 | F | 101 | THR | CA-CB-OG1 | -12.88 | 81.96 | 109.00 |
| 1 | B | 89 | ASN | CB-CG-ND2 | 12.86 | 147.56 | 116.70 |
| 1 | D | 224 | ASN | CA-CB-CG | -12.86 | 85.11 | 113.40 |
| 1 | B | 73 | ALA | N-CA-CB | 12.85 | 128.09 | 110.10 |
| 1 | D | 107 | LEU | CB-CA-C | -12.84 | 85.80 | 110.20 |
| 1 | E | 166 | ASP | CB-CG-OD1 | -12.84 | 106.74 | 118.30 |
| 1 | B | 11 | GLY | C-N-CA | 12.83 | 153.78 | 121.70 |
| 1 | D | 13 | HIS | CA-CB-CG | -12.83 | 91.78 | 113.60 |
| 1 | B | 137 | HIS | N-CA-C | 12.83 | 145.63 | 111.00 |
| 1 | E | 210 | ARG | NE-CZ-NH1 | -12.82 | 113.89 | 120.30 |
| 1 | B | 139 | GLN | CG-CD-OE1 | 12.82 | 147.24 | 121.60 |
| 1 | B | 108 | TRP | CA-C-N | 12.82 | 145.40 | 117.20 |
| 1 | B | 217 | PHE | CA-C-O | -12.82 | 93.18 | 120.10 |
| 1 | B | 44 | ASP | CB-CG-OD1 | -12.81 | 106.77 | 118.30 |
| 1 | E | 87 | ILE | CG1-CB-CG2 | 12.80 | 139.56 | 111.40 |
| 1 | D | 101 | THR | CA-CB-OG1 | -12.79 | 82.13 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 191 | GLY | O-C-N | -12.79 | 102.23 | 122.70 |
| 1 | D | 189 | PRO | CA-N-CD | -12.79 | 93.59 | 111.50 |
| 1 | E | 160 | CYS | CA-CB-SG | 12.78 | 137.00 | 114.00 |
| 1 | D | 108 | TRP | CZ3-CH2-CZ2 | -12.77 | 106.27 | 121.60 |
| 1 | F | 125 | ASN | CA-C-N | 12.76 | 145.27 | 117.20 |
| 1 | A | 15 | GLN | CG-CD-NE2 | 12.75 | 147.30 | 116.70 |
| 1 | E | 105 | PRO | CA-N-CD | -12.75 | 93.66 | 111.50 |
| 1 | E | 7 | LEU | CA-C-N | 12.74 | 145.23 | 117.20 |
| 1 | B | 75 | ASN | O-C-N | 12.74 | 143.08 | 122.70 |
| 1 | C | 57 | GLY | O-C-N | 12.73 | 143.06 | 122.70 |
| 1 | A | 25 | LEU | CB-CG-CD2 | -12.72 | 89.38 | 111.00 |
| 1 | A | 190 | ASN | O-C-N | -12.71 | 101.59 | 123.20 |
| 1 | C | 44 | ASP | CB-CG-OD2 | -12.71 | 106.87 | 118.30 |
| 1 | F | 94 | LEU | CB-CG-CD2 | 12.71 | 132.60 | 111.00 |
| 1 | C | 166 | ASP | CB-CG-OD1 | -12.70 | 106.87 | 118.30 |
| 1 | F | 184 | ARG | N-CA-CB | 12.69 | 133.45 | 110.60 |
| 1 | B | 169 | ASP | CB-CG-OD1 | -12.69 | 106.88 | 118.30 |
| 1 | B | 194 | ASP | CB-CG-OD1 | -12.69 | 106.88 | 118.30 |
| 1 | F | 140 | THR | CA-CB-CG2 | 12.69 | 130.16 | 112.40 |
| 1 | B | 190 | ASN | CB-CG-ND2 | 12.68 | 147.12 | 116.70 |
| 1 | C | 103 | TYR | CG-CD1-CE1 | 12.67 | 131.44 | 121.30 |
| 1 | C | 107 | LEU | CB-CG-CD2 | -12.67 | 89.46 | 111.00 |
| 1 | D | 184 | ARG | NH1-CZ-NH2 | 12.66 | 133.33 | 119.40 |
| 1 | E | 5 | PHE | CA-C-O | 12.66 | 146.69 | 120.10 |
| 1 | F | 157 | GLU | OE1-CD-OE2 | -12.66 | 108.11 | 123.30 |
| 1 | A | 189 | PRO | N-CA-CB | 12.65 | 118.48 | 103.30 |
| 1 | D | 70 | ILE | CA-CB-CG1 | -12.64 | 86.97 | 111.00 |
| 1 | F | 230 | GLY | O-C-N | -12.63 | 102.49 | 122.70 |
| 1 | D | 88 | GLY | C-N-CA | 12.63 | 153.27 | 121.70 |
| 1 | A | 138 | PRO | N-CA-CB | 12.63 | 118.45 | 103.30 |
| 1 | D | 172 | TRP | CD1-CG-CD2 | -12.61 | 96.21 | 106.30 |
| 1 | A | 182 | GLY | O-C-N | 12.57 | 142.82 | 122.70 |
| 1 | B | 211 | SER | CA-C-O | -12.57 | 93.70 | 120.10 |
| 1 | B | 202 | ALA | CA-C-N | 12.56 | 144.84 | 117.20 |
| 1 | E | 33 | GLN | OE1-CD-NE2 | -12.56 | 93.02 | 121.90 |
| 1 | F | 100 | VAL | CG1-CB-CG2 | -12.56 | 90.81 | 110.90 |
| 1 | C | 232 | LEU | CA-C-N | 12.55 | 144.81 | 117.20 |
| 1 | D | 26 | SER | C-N-CA | 12.55 | 153.07 | 121.70 |
| 1 | D | 69 | VAL | CA-CB-CG1 | 12.54 | 129.71 | 110.90 |
| 1 | A | 129 | TYR | CA-C-N | 12.54 | 144.78 | 117.20 |
| 1 | A | 171 | VAL | CA-CB-CG2 | 12.53 | 129.69 | 110.90 |
| 1 | F | 214 | ARG | CB-CA-C | 12.53 | 135.45 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 48 | TRP | O-C-N | 12.52 | 142.73 | 122.70 |
| 1 | D | 232 | LEU | O-C-N | 12.51 | 142.72 | 122.70 |
| 1 | B | 214 | ARG | NH1-CZ-NH2 | -12.51 | 105.64 | 119.40 |
| 1 | C | 156 | MET | O-C-N | 12.51 | 142.71 | 122.70 |
| 1 | C | 25 | LEU | CB-CA-C | -12.51 | 86.44 | 110.20 |
| 1 | A | 15 | GLN | CA-CB-CG | 12.50 | 140.90 | 113.40 |
| 1 | B | 93 | VAL | O-C-N | 12.50 | 142.70 | 122.70 |
| 1 | E | 167 | ARG | NH1-CZ-NH2 | -12.49 | 105.66 | 119.40 |
| 1 | F | 106 | GLY | O-C-N | -12.48 | 102.73 | 122.70 |
| 1 | E | 103 | TYR | N-CA-CB | -12.48 | 88.13 | 110.60 |
| 1 | E | 156 | MET | CG-SD-CE | 12.48 | 120.16 | 100.20 |
| 1 | A | 15 | GLN | CG-CD-OE1 | -12.47 | 96.66 | 121.60 |
| 1 | A | 146 | SER | CA-CB-OG | -12.47 | 77.53 | 111.20 |
| 1 | A | 233 | TRP | CZ3-CH2-CZ2 | -12.47 | 106.64 | 121.60 |
| 1 | D | 60 | ALA | CA-C-N | 12.46 | 144.61 | 117.20 |
| 1 | C | 219 | LEU | O-C-N | -12.45 | 102.78 | 122.70 |
| 1 | D | 188 | GLN | OE1-CD-NE2 | -12.45 | 93.26 | 121.90 |
| 1 | A | 206 | SER | CA-C-N | 12.43 | 141.07 | 116.20 |
| 1 | B | 31 | THR | CA-CB-OG1 | -12.43 | 82.89 | 109.00 |
| 1 | A | 233 | TRP | CH2-CZ2-CE2 | 12.43 | 129.83 | 117.40 |
| 1 | F | 131 | THR | CA-C-O | 12.42 | 146.19 | 120.10 |
| 1 | F | 232 | LEU | CA-C-O | -12.42 | 94.02 | 120.10 |
| 1 | D | 192 | ARG | C-N-CA | 12.42 | 152.74 | 121.70 |
| 1 | B | 70 | ILE | CB-CA-C | -12.41 | 86.77 | 111.60 |
| 1 | D | 90 | TYR | CB-CG-CD1 | 12.41 | 128.45 | 121.00 |
| 1 | F | 125 | ASN | C-N-CA | 12.41 | 152.72 | 121.70 |
| 1 | A | 44 | ASP | CA-C-N | 12.40 | 144.47 | 117.20 |
| 1 | A | 20 | ALA | O-C-N | 12.39 | 142.52 | 122.70 |
| 1 | C | 130 | SER | O-C-N | -12.39 | 102.88 | 122.70 |
| 1 | D | 62 | LEU | CA-C-N | -12.39 | 89.95 | 117.20 |
| 1 | B | 81 | SER | N-CA-CB | -12.39 | 91.92 | 110.50 |
| 1 | D | 80 | SER | O-C-N | -12.38 | 102.89 | 122.70 |
| 1 | C | 38 | LEU | C-N-CA | 12.38 | 152.64 | 121.70 |
| 1 | B | 33 | GLN | CG-CD-NE2 | 12.37 | 146.39 | 116.70 |
| 1 | C | 32 | MET | CG-SD-CE | -12.37 | 80.41 | 100.20 |
| 1 | D | 223 | ARG | C-N-CA | 12.37 | 152.62 | 121.70 |
| 1 | E | 19 | ALA | CB-CA-C | 12.36 | 128.64 | 110.10 |
| 1 | F | 30 | PHE | C-N-CA | 12.36 | 152.61 | 121.70 |
| 1 | C | 170 | ARG | NE-CZ-NH2 | 12.35 | 126.47 | 120.30 |
| 1 | F | 90 | TYR | CD1-CG-CD2 | -12.34 | 104.33 | 117.90 |
| 1 | F | 143 | ALA | N-CA-CB | 12.34 | 127.37 | 110.10 |
| 1 | B | 71 | LEU | N-CA-CB | -12.33 | 85.73 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 42 | ASP | CB-CG-OD2 | 12.33 | 129.40 | 118.30 |
| 1 | E | 157 | GLU | CG-CD-OE2 | -12.33 | 93.64 | 118.30 |
| 1 | F | 176 | THR | CA-CB-CG2 | -12.33 | 95.14 | 112.40 |
| 1 | C | 106 | GLY | CA-C-O | 12.32 | 142.78 | 120.60 |
| 1 | E | 61 | VAL | CA-CB-CG2 | -12.32 | 92.42 | 110.90 |
| 1 | F | 192 | ARG | CB-CA-C | 12.31 | 135.02 | 110.40 |
| 1 | B | 224 | ASN | N-CA-CB | -12.31 | 88.44 | 110.60 |
| 1 | C | 158 | THR | CA-CB-CG2 | -12.30 | 95.18 | 112.40 |
| 1 | A | 42 | ASP | O-C-N | -12.30 | 103.02 | 122.70 |
| 1 | A | 145 | GLN | C-N-CA | 12.30 | 152.45 | 121.70 |
| 1 | B | 65 | ASP | OD1-CG-OD2 | -12.30 | 99.93 | 123.30 |
| 1 | C | 143 | ALA | CB-CA-C | 12.29 | 128.54 | 110.10 |
| 1 | D | 125 | ASN | O-C-N | -12.29 | 103.04 | 122.70 |
| 1 | F | 224 | ASN | O-C-N | -12.29 | 103.04 | 122.70 |
| 1 | A | 40 | LEU | CA-CB-CG | 12.27 | 143.52 | 115.30 |
| 1 | B | 234 | THR | C-N-CA | 12.27 | 152.37 | 121.70 |
| 1 | E | 129 | TYR | CZ-CE2-CD2 | 12.26 | 130.84 | 119.80 |
| 1 | F | 125 | ASN | O-C-N | -12.26 | 103.08 | 122.70 |
| 1 | D | 176 | THR | CA-C-N | 12.25 | 144.16 | 117.20 |
| 1 | B | 214 | ARG | N-CA-CB | -12.25 | 88.55 | 110.60 |
| 1 | E | 13 | HIS | CA-C-O | -12.25 | 94.37 | 120.10 |
| 1 | B | 139 | GLN | CB-CA-C | 12.24 | 134.87 | 110.40 |
| 1 | A | 72 | THR | CA-CB-CG2 | 12.23 | 129.52 | 112.40 |
| 1 | D | 136 | ASN | CA-C-N | 12.23 | 144.11 | 117.20 |
| 1 | A | 114 | ASN | CB-CG-OD1 | -12.23 | 97.14 | 121.60 |
| 1 | D | 46 | ARG | NE-CZ-NH1 | 12.23 | 126.41 | 120.30 |
| 1 | A | 129 | TYR | CD1-CG-CD2 | -12.23 | 104.45 | 117.90 |
| 1 | A | 181 | THR | N-CA-CB | 12.23 | 133.53 | 110.30 |
| 1 | D | 104 | GLY | C-N-CD | -12.21 | 93.74 | 120.60 |
| 1 | D | 129 | TYR | CA-C-N | 12.20 | 144.04 | 117.20 |
| 1 | B | 216 | VAL | CA-CB-CG2 | -12.19 | 92.62 | 110.90 |
| 1 | C | 137 | HIS | CB-CA-C | -12.18 | 86.03 | 110.40 |
| 1 | B | 105 | PRO | N-CD-CG | 12.18 | 121.47 | 103.20 |
| 1 | F | 193 | MET | CA-CB-CG | 12.18 | 134.00 | 113.30 |
| 1 | B | 56 | THR | CA-CB-OG1 | 12.18 | 134.57 | 109.00 |
| 1 | D | 131 | THR | CA-C-O | 12.17 | 145.66 | 120.10 |
| 1 | B | 194 | ASP | CA-CB-CG | -12.17 | 86.63 | 113.40 |
| 1 | D | 71 | LEU | O-C-N | 12.16 | 142.16 | 122.70 |
| 1 | A | 2 | ASN | CB-CG-OD1 | 12.16 | 145.92 | 121.60 |
| 1 | B | 125 | ASN | CA-C-N | 12.16 | 143.95 | 117.20 |
| 1 | E | 60 | ALA | CA-C-O | -12.16 | 94.57 | 120.10 |
| 1 | E | 185 | ALA | N-CA-CB | -12.15 | 93.08 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 223 | ARG | CA-C-N | 12.15 | 143.92 | 117.20 |
| 1 | D | 224 | ASN | OD1-CG-ND2 | 12.14 | 149.82 | 121.90 |
| 1 | F | 125 | ASN | CB-CG-OD1 | -12.13 | 97.33 | 121.60 |
| 1 | E | 18 | HIS | N-CA-CB | 12.13 | 132.43 | 110.60 |
| 1 | B | 126 | SER | O-C-N | -12.12 | 103.31 | 122.70 |
| 1 | A | 59 | ARG | N-CA-CB | 12.12 | 132.41 | 110.60 |
| 1 | D | 163 | VAL | CA-CB-CG1 | -12.11 | 92.73 | 110.90 |
| 1 | D | 60 | ALA | N-CA-CB | 12.10 | 127.04 | 110.10 |
| 1 | D | 72 | THR | CA-CB-OG1 | -12.10 | 83.59 | 109.00 |
| 1 | B | 27 | SER | CA-CB-OG | -12.09 | 78.56 | 111.20 |
| 1 | C | 128 | LEU | CD1-CG-CD2 | -12.09 | 74.23 | 110.50 |
| 1 | A | 125 | ASN | CB-CA-C | -12.08 | 86.25 | 110.40 |
| 1 | C | 232 | LEU | CA-C-O | -12.07 | 94.76 | 120.10 |
| 1 | C | 100 | VAL | CA-CB-CG1 | 12.06 | 128.99 | 110.90 |
| 1 | D | 32 | MET | N-CA-CB | 12.06 | 132.31 | 110.60 |
| 1 | E | 122 | ASN | CA-CB-CG | 12.06 | 139.93 | 113.40 |
| 1 | A | 2 | ASN | OD1-CG-ND2 | -12.05 | 94.19 | 121.90 |
| 1 | E | 40 | LEU | CA-CB-CG | 12.05 | 143.01 | 115.30 |
| 1 | C | 103 | TYR | C-N-CA | 12.04 | 147.59 | 122.30 |
| 1 | D | 146 | SER | N-CA-C | 12.03 | 143.48 | 111.00 |
| 1 | F | 29 | ARG | NE-CZ-NH1 | -12.03 | 114.28 | 120.30 |
| 1 | F | 192 | ARG | N-CA-CB | -12.03 | 88.95 | 110.60 |
| 1 | A | 180 | GLY | O-C-N | 12.03 | 141.94 | 122.70 |
| 1 | E | 137 | HIS | CB-CA-C | -12.02 | 86.36 | 110.40 |
| 1 | F | 138 | PRO | CA-CB-CG | -12.01 | 81.17 | 104.00 |
| 1 | E | 183 | CYS | CA-CB-SG | -12.01 | 92.38 | 114.00 |
| 1 | E | 168 | ASP | CB-CG-OD2 | 12.01 | 129.10 | 118.30 |
| 1 | D | 225 | LEU | CA-C-O | -12.00 | 94.90 | 120.10 |
| 1 | A | 128 | LEU | CB-CA-C | 11.99 | 132.98 | 110.20 |
| 1 | B | 45 | VAL | CB-CA-C | 11.99 | 134.18 | 111.40 |
| 1 | E | 138 | PRO | N-CD-CG | 11.98 | 121.17 | 103.20 |
| 1 | A | 169 | ASP | CB-CG-OD1 | -11.97 | 107.53 | 118.30 |
| 1 | B | 100 | VAL | CB-CA-C | 11.97 | 134.15 | 111.40 |
| 1 | D | 15 | GLN | CA-CB-CG | 11.97 | 139.74 | 113.40 |
| 1 | B | 29 | ARG | CD-NE-CZ | 11.96 | 140.35 | 123.60 |
| 1 | D | 61 | VAL | CB-CA-C | -11.96 | 88.69 | 111.40 |
| 1 | F | 73 | ALA | O-C-N | -11.95 | 103.58 | 122.70 |
| 1 | F | 219 | LEU | CB-CG-CD1 | 11.95 | 131.31 | 111.00 |
| 1 | A | 190 | ASN | C-N-CA | 11.95 | 147.39 | 122.30 |
| 1 | B | 112 | THR | C-N-CA | 11.94 | 151.54 | 121.70 |
| 1 | D | 34 | SER | CA-C-N | 11.93 | 143.44 | 117.20 |
| 1 | B | 86 | SER | O-C-N | -11.93 | 103.62 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 147 | LEU | CB-CG-CD2 | -11.93 | 90.72 | 111.00 |
| 1 | F | 183 | CYS | C-N-CA | 11.93 | 151.52 | 121.70 |
| 1 | D | 184 | ARG | O-C-N | -11.92 | 103.62 | 122.70 |
| 1 | D | 57 | GLY | CA-C-O | 11.91 | 142.04 | 120.60 |
| 1 | D | 123 | ASN | CA-CB-CG | 11.90 | 139.59 | 113.40 |
| 1 | D | 210 | ARG | CA-C-O | -11.90 | 95.11 | 120.10 |
| 1 | E | 129 | TYR | CA-C-N | 11.90 | 143.38 | 117.20 |
| 1 | A | 98 | ARG | CG-CD-NE | 11.89 | 136.77 | 111.80 |
| 1 | F | 83 | THR | CB-CA-C | 11.89 | 143.70 | 111.60 |
| 1 | D | 5 | PHE | CZ-CE2-CD2 | 11.88 | 134.36 | 120.10 |
| 1 | A | 108 | TRP | CA-C-O | -11.88 | 95.15 | 120.10 |
| 1 | E | 130 | SER | CA-C-O | -11.88 | 95.16 | 120.10 |
| 1 | E | 230 | GLY | CA-C-O | -11.88 | 99.22 | 120.60 |
| 1 | F | 16 | THR | CA-CB-CG2 | -11.88 | 95.78 | 112.40 |
| 1 | D | 156 | MET | CA-CB-CG | 11.87 | 133.48 | 113.30 |
| 1 | A | 137 | HIS | C-N-CA | 11.87 | 171.84 | 122.00 |
| 1 | F | 187 | LEU | CA-C-N | -11.87 | 91.10 | 117.20 |
| 1 | C | 218 | VAL | CA-CB-CG2 | 11.86 | 128.69 | 110.90 |
| 1 | B | 159 | ASP | CB-CG-OD2 | -11.86 | 107.63 | 118.30 |
| 1 | B | 222 | ASP | CA-C-O | -11.86 | 95.20 | 120.10 |
| 1 | C | 165 | PHE | CG-CD1-CE1 | 11.84 | 133.83 | 120.80 |
| 1 | D | 18 | HIS | CA-C-O | -11.84 | 95.24 | 120.10 |
| 1 | D | 194 | ASP | O-C-N | 11.83 | 141.63 | 122.70 |
| 1 | D | 139 | GLN | O-C-N | 11.83 | 141.63 | 122.70 |
| 1 | C | 97 | ASP | CB-CG-OD1 | -11.83 | 107.66 | 118.30 |
| 1 | A | 181 | THR | CA-CB-OG1 | -11.83 | 84.17 | 109.00 |
| 1 | F | 217 | PHE | N-CA-CB | -11.82 | 89.32 | 110.60 |
| 1 | F | 139 | GLN | CB-CA-C | 11.82 | 134.04 | 110.40 |
| 1 | E | 222 | ASP | CB-CG-OD1 | -11.81 | 107.67 | 118.30 |
| 1 | F | 84 | LYS | CB-CG-CD | 11.81 | 142.32 | 111.60 |
| 1 | B | 235 | THR | CA-C-O | 11.81 | 144.90 | 120.10 |
| 1 | D | 69 | VAL | CG1-CB-CG2 | -11.81 | 92.01 | 110.90 |
| 1 | C | 176 | THR | O-C-N | -11.80 | 103.82 | 122.70 |
| 1 | B | 138 | PRO | N-CA-CB | 11.80 | 117.45 | 103.30 |
| 1 | A | 90 | TYR | CA-CB-CG | -11.79 | 90.99 | 113.40 |
| 1 | A | 223 | ARG | NE-CZ-NH1 | -11.79 | 114.41 | 120.30 |
| 1 | B | 81 | SER | CA-C-N | 11.79 | 139.77 | 116.20 |
| 1 | F | 60 | ALA | N-CA-CB | 11.78 | 126.59 | 110.10 |
| 1 | F | 216 | VAL | O-C-N | -11.78 | 103.86 | 122.70 |
| 1 | A | 9 | HIS | CB-CA-C | -11.77 | 86.85 | 110.40 |
| 1 | F | 2 | ASN | CB-CA-C | -11.77 | 86.86 | 110.40 |
| 1 | A | 190 | ASN | N-CA-CB | -11.75 | 89.45 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 98 | ARG | CD-NE-CZ | -11.75 | 107.16 | 123.60 |
| 1 | A | 228 | TYR | CG-CD1-CE1 | 11.74 | 130.69 | 121.30 |
| 1 | B | 146 | SER | N-CA-CB | -11.74 | 92.88 | 110.50 |
| 1 | C | 19 | ALA | CA-C-N | 11.74 | 143.04 | 117.20 |
| 1 | B | 106 | GLY | CA-C-O | -11.74 | 99.47 | 120.60 |
| 1 | A | 171 | VAL | N-CA-CB | 11.74 | 137.32 | 111.50 |
| 1 | B | 109 | ASP | N-CA-CB | 11.74 | 131.73 | 110.60 |
| 1 | D | 169 | ASP | CA-C-N | -11.73 | 91.39 | 117.20 |
| 1 | B | 223 | ARG | NH1-CZ-NH2 | 11.73 | 132.30 | 119.40 |
| 1 | D | 229 | GLY | O-C-N | -11.73 | 103.26 | 123.20 |
| 1 | C | 138 | PRO | N-CA-CB | 11.73 | 117.37 | 103.30 |
| 1 | C | 174 | THR | C-N-CA | 11.71 | 150.99 | 121.70 |
| 1 | B | 125 | ASN | O-C-N | -11.71 | 103.96 | 122.70 |
| 1 | F | 29 | ARG | NE-CZ-NH2 | 11.71 | 126.15 | 120.30 |
| 1 | B | 137 | HIS | O-C-N | -11.70 | 98.87 | 121.10 |
| 1 | C | 162 | LEU | CB-CG-CD2 | 11.70 | 130.89 | 111.00 |
| 1 | D | 158 | THR | CA-C-O | -11.70 | 95.53 | 120.10 |
| 1 | A | 65 | ASP | CB-CA-C | 11.70 | 133.79 | 110.40 |
| 1 | D | 190 | ASN | CA-C-N | 11.69 | 139.58 | 116.20 |
| 1 | B | 195 | VAL | CA-C-O | -11.69 | 95.56 | 120.10 |
| 1 | E | 193 | MET | CA-CB-CG | 11.69 | 133.17 | 113.30 |
| 1 | A | 129 | TYR | CG-CD2-CE2 | 11.69 | 130.65 | 121.30 |
| 1 | B | 12 | SER | CA-CB-OG | 11.69 | 142.75 | 111.20 |
| 1 | D | 67 | LEU | CB-CG-CD1 | 11.68 | 130.86 | 111.00 |
| 1 | C | 139 | GLN | CB-CA-C | 11.68 | 133.76 | 110.40 |
| 1 | D | 16 | THR | C-N-CA | -11.67 | 92.53 | 121.70 |
| 1 | D | 7 | LEU | N-CA-CB | 11.66 | 133.72 | 110.40 |
| 1 | D | 7 | LEU | CA-C-N | -11.65 | 91.57 | 117.20 |
| 1 | C | 198 | ASN | CB-CG-OD1 | -11.65 | 98.31 | 121.60 |
| 1 | E | 20 | ALA | CA-C-O | 11.64 | 144.54 | 120.10 |
| 1 | E | 125 | ASN | CB-CA-C | -11.64 | 87.12 | 110.40 |
| 1 | D | 41 | PHE | CB-CG-CD1 | 11.63 | 128.94 | 120.80 |
| 1 | B | 190 | ASN | CA-C-N | 11.62 | 139.45 | 116.20 |
| 1 | D | 73 | ALA | N-CA-CB | 11.62 | 126.38 | 110.10 |
| 1 | A | 202 | ALA | N-CA-CB | -11.62 | 93.83 | 110.10 |
| 1 | B | 153 | ARG | NE-CZ-NH2 | 11.62 | 126.11 | 120.30 |
| 1 | F | 9 | HIS | CB-CA-C | -11.61 | 87.17 | 110.40 |
| 1 | D | 126 | SER | O-C-N | 11.61 | 141.27 | 122.70 |
| 1 | B | 23 | LEU | N-CA-CB | 11.61 | 133.61 | 110.40 |
| 1 | B | 101 | THR | CA-CB-CG2 | 11.59 | 128.63 | 112.40 |
| 1 | C | 222 | ASP | CA-C-N | 11.59 | 142.69 | 117.20 |
| 1 | C | 5 | PHE | CB-CG-CD2 | -11.58 | 112.69 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 47 | VAL | CA-CB-CG2 | 11.57 | 128.25 | 110.90 |
| 1 | E | 56 | THR | CA-CB-CG2 | -11.57 | 96.20 | 112.40 |
| 1 | D | 148 | GLN | CB-CG-CD | 11.57 | 141.68 | 111.60 |
| 1 | E | 154 | LEU | N-CA-CB | 11.56 | 133.52 | 110.40 |
| 1 | D | 141 | LEU | CB-CG-CD2 | -11.56 | 91.35 | 111.00 |
| 1 | E | 141 | LEU | CB-CG-CD2 | 11.55 | 130.63 | 111.00 |
| 1 | A | 90 | TYR | CG-CD1-CE1 | 11.55 | 130.54 | 121.30 |
| 1 | F | 50 | SER | O-C-N | -11.53 | 104.25 | 122.70 |
| 1 | F | 209 | SER | N-CA-CB | -11.53 | 93.21 | 110.50 |
| 1 | C | 60 | ALA | CA-C-O | -11.52 | 95.90 | 120.10 |
| 1 | E | 85 | GLY | C-N-CA | 11.52 | 150.50 | 121.70 |
| 1 | F | 37 | ASN | CB-CA-C | -11.52 | 87.36 | 110.40 |
| 1 | A | 26 | SER | CA-C-N | 11.52 | 142.54 | 117.20 |
| 1 | D | 151 | PRO | O-C-N | -11.51 | 104.28 | 122.70 |
| 1 | B | 231 | ALA | CB-CA-C | 11.51 | 127.36 | 110.10 |
| 1 | F | 210 | ARG | NE-CZ-NH2 | -11.50 | 114.55 | 120.30 |
| 1 | D | 26 | SER | CA-C-O | 11.49 | 144.24 | 120.10 |
| 1 | D | 27 | SER | O-C-N | -11.49 | 104.31 | 122.70 |
| 1 | A | 46 | ARG | NE-CZ-NH2 | -11.48 | 114.56 | 120.30 |
| 1 | E | 137 | HIS | N-CA-C | 11.48 | 142.01 | 111.00 |
| 1 | B | 45 | VAL | CA-CB-CG1 | 11.47 | 128.10 | 110.90 |
| 1 | B | 187 | LEU | CA-C-O | -11.46 | 96.02 | 120.10 |
| 1 | C | 172 | TRP | CH2-CZ2-CE2 | 11.47 | 128.87 | 117.40 |
| 1 | D | 78 | ARG | O-C-N | -11.46 | 104.36 | 122.70 |
| 1 | D | 144 | THR | CA-CB-OG1 | 11.46 | 133.07 | 109.00 |
| 1 | D | 184 | ARG | NE-CZ-NH1 | 11.46 | 126.03 | 120.30 |
| 1 | A | 75 | ASN | CB-CG-OD1 | -11.45 | 98.70 | 121.60 |
| 1 | C | 214 | ARG | NH1-CZ-NH2 | -11.45 | 106.80 | 119.40 |
| 1 | E | 131 | THR | OG1-CB-CG2 | 11.45 | 136.34 | 110.00 |
| 1 | D | 149 | LEU | C-N-CA | -11.45 | 93.08 | 121.70 |
| 1 | E | 167 | ARG | CG-CD-NE | 11.45 | 135.84 | 111.80 |
| 1 | E | 201 | ILE | CB-CG1-CD1 | 11.45 | 145.96 | 113.90 |
| 1 | C | 2 | ASN | CB-CG-OD1 | -11.44 | 98.71 | 121.60 |
| 1 | F | 149 | LEU | CA-C-O | -11.45 | 96.07 | 120.10 |
| 1 | C | 210 | ARG | CA-C-O | 11.44 | 144.12 | 120.10 |
| 1 | A | 120 | VAL | CA-CB-CG1 | 11.44 | 128.05 | 110.90 |
| 1 | B | 125 | ASN | CB-CG-ND2 | 11.43 | 144.14 | 116.70 |
| 1 | F | 31 | THR | CA-CB-OG1 | 11.43 | 133.00 | 109.00 |
| 1 | B | 98 | ARG | CA-CB-CG | 11.42 | 138.52 | 113.40 |
| 1 | E | 144 | THR | CA-CB-OG1 | 11.42 | 132.98 | 109.00 |
| 1 | F | 15 | GLN | CA-CB-CG | 11.42 | 138.52 | 113.40 |
| 1 | E | 157 | GLU | CA-C-N | 11.42 | 142.32 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 228 | TYR | O-C-N | -11.41 | 103.80 | 123.20 |
| 1 | F | 152 | TYR | CZ-CE2-CD2 | -11.41 | 109.53 | 119.80 |
| 1 | B | 192 | ARG | O-C-N | 11.40 | 140.93 | 122.70 |
| 1 | B | 223 | ARG | CD-NE-CZ | -11.40 | 107.64 | 123.60 |
| 1 | E | 103 | TYR | CB-CG-CD1 | 11.40 | 127.84 | 121.00 |
| 1 | D | 43 | SER | CB-CA-C | -11.39 | 88.45 | 110.10 |
| 1 | B | 149 | LEU | CB-CG-CD2 | 11.39 | 130.37 | 111.00 |
| 1 | B | 228 | TYR | CZ-CE2-CD2 | -11.39 | 109.55 | 119.80 |
| 1 | B | 85 | GLY | C-N-CA | 11.39 | 150.17 | 121.70 |
| 1 | B | 165 | PHE | N-CA-CB | -11.39 | 90.11 | 110.60 |
| 1 | D | 229 | GLY | N-CA-C | 11.38 | 141.56 | 113.10 |
| 1 | B | 216 | VAL | O-C-N | -11.38 | 104.49 | 122.70 |
| 1 | D | 58 | CYS | N-CA-CB | -11.38 | 90.11 | 110.60 |
| 1 | F | 67 | LEU | CA-CB-CG | 11.38 | 141.46 | 115.30 |
| 1 | B | 235 | THR | CA-CB-OG1 | 11.37 | 132.88 | 109.00 |
| 1 | A | 87 | ILE | O-C-N | -11.37 | 103.88 | 123.20 |
| 1 | C | 216 | VAL | CA-CB-CG2 | -11.36 | 93.86 | 110.90 |
| 1 | D | 83 | THR | O-C-N | -11.36 | 104.53 | 122.70 |
| 1 | F | 83 | THR | C-N-CA | 11.36 | 150.09 | 121.70 |
| 1 | A | 61 | VAL | CA-CB-CG1 | 11.35 | 127.92 | 110.90 |
| 1 | B | 223 | ARG | CA-CB-CG | 11.35 | 138.36 | 113.40 |
| 1 | D | 81 | SER | O-C-N | -11.35 | 103.91 | 123.20 |
| 1 | C | 152 | TYR | CD1-CG-CD2 | -11.34 | 105.43 | 117.90 |
| 1 | D | 142 | HIS | CA-C-N | 11.33 | 142.13 | 117.20 |
| 1 | B | 15 | GLN | CG-CD-OE1 | -11.33 | 98.94 | 121.60 |
| 1 | B | 104 | GLY | C-N-CA | 11.33 | 169.57 | 122.00 |
| 1 | A | 44 | ASP | N-CA-CB | 11.32 | 130.98 | 110.60 |
| 1 | C | 148 | GLN | CA-CB-CG | 11.32 | 138.31 | 113.40 |
| 1 | D | 184 | ARG | CD-NE-CZ | -11.32 | 107.75 | 123.60 |
| 1 | C | 136 | ASN | CB-CA-C | -11.32 | 87.77 | 110.40 |
| 1 | C | 46 | ARG | CA-C-N | 11.31 | 142.08 | 117.20 |
| 1 | D | 217 | PHE | CA-C-O | -11.31 | 96.35 | 120.10 |
| 1 | E | 60 | ALA | CB-CA-C | 11.31 | 127.06 | 110.10 |
| 1 | E | 58 | CYS | N-CA-CB | -11.30 | 90.25 | 110.60 |
| 1 | B | 198 | ASN | CA-CB-CG | -11.30 | 88.53 | 113.40 |
| 1 | D | 131 | THR | CA-CB-CG2 | -11.29 | 96.59 | 112.40 |
| 1 | F | 147 | LEU | CB-CG-CD1 | 11.29 | 130.19 | 111.00 |
| 1 | D | 163 | VAL | CG1-CB-CG2 | 11.29 | 128.96 | 110.90 |
| 1 | C | 89 | ASN | OD1-CG-ND2 | 11.28 | 147.85 | 121.90 |
| 1 | C | 219 | LEU | CA-CB-CG | 11.28 | 141.25 | 115.30 |
| 1 | D | 55 | ALA | N-CA-CB | 11.28 | 125.89 | 110.10 |
| 1 | D | 64 | SER | O-C-N | -11.28 | 104.65 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 233 | TRP | CB-CG-CD1 | -11.28 | 112.34 | 127.00 |
| 1 | C | 105 | PRO | N-CA-CB | 11.27 | 116.82 | 103.30 |
| 1 | A | 154 | LEU | CB-CG-CD2 | 11.27 | 130.16 | 111.00 |
| 1 | A | 90 | TYR | CB-CG-CD2 | -11.27 | 114.24 | 121.00 |
| 1 | E | 99 | THR | CA-CB-OG1 | -11.27 | 85.34 | 109.00 |
| 1 | A | 191 | GLY | C-N-CA | 11.26 | 149.85 | 121.70 |
| 1 | A | 196 | LEU | CB-CG-CD2 | -11.26 | 91.85 | 111.00 |
| 1 | A | 159 | ASP | O-C-N | -11.26 | 104.69 | 122.70 |
| 1 | D | 183 | CYS | C-N-CA | 11.25 | 149.82 | 121.70 |
| 1 | E | 62 | LEU | O-C-N | 11.24 | 140.69 | 122.70 |
| 1 | E | 232 | LEU | N-CA-CB | -11.24 | 87.91 | 110.40 |
| 1 | D | 100 | VAL | O-C-N | -11.24 | 104.71 | 122.70 |
| 1 | E | 169 | ASP | N-CA-CB | 11.24 | 130.83 | 110.60 |
| 1 | E | 225 | LEU | CB-CA-C | 11.24 | 131.56 | 110.20 |
| 1 | A | 193 | MET | CG-SD-CE | -11.24 | 82.22 | 100.20 |
| 1 | A | 95 | GLN | CG-CD-OE1 | 11.23 | 144.06 | 121.60 |
| 1 | F | 131 | THR | CB-CA-C | -11.23 | 81.29 | 111.60 |
| 1 | E | 100 | VAL | CA-CB-CG2 | 11.22 | 127.73 | 110.90 |
| 1 | A | 64 | SER | CA-CB-OG | -11.22 | 80.91 | 111.20 |
| 1 | A | 30 | PHE | C-N-CA | 11.22 | 149.75 | 121.70 |
| 1 | D | 234 | THR | C-N-CA | 11.22 | 149.74 | 121.70 |
| 1 | E | 137 | HIS | CA-C-O | -11.21 | 96.56 | 120.10 |
| 1 | F | 27 | SER | CA-CB-OG | -11.21 | 80.93 | 111.20 |
| 1 | B | 44 | ASP | CB-CG-OD2 | 11.21 | 128.39 | 118.30 |
| 1 | E | 123 | ASN | N-CA-C | 11.21 | 141.25 | 111.00 |
| 1 | B | 125 | ASN | CB-CG-OD1 | -11.20 | 99.20 | 121.60 |
| 1 | B | 224 | ASN | O-C-N | -11.20 | 104.78 | 122.70 |
| 1 | C | 99 | THR | O-C-N | -11.20 | 104.78 | 122.70 |
| 1 | A | 151 | PRO | N-CD-CG | -11.20 | 86.41 | 103.20 |
| 1 | E | 1 | ASN | CA-C-O | 11.19 | 143.60 | 120.10 |
| 1 | F | 5 | PHE | CB-CG-CD1 | 11.19 | 128.63 | 120.80 |
| 1 | A | 94 | LEU | CB-CG-CD1 | -11.19 | 91.98 | 111.00 |
| 1 | E | 103 | TYR | CA-CB-CG | 11.19 | 134.66 | 113.40 |
| 1 | D | 202 | ALA | O-C-N | -11.19 | 104.80 | 122.70 |
| 1 | B | 232 | LEU | O-C-N | -11.18 | 104.81 | 122.70 |
| 1 | C | 117 | SER | O-C-N | -11.18 | 104.81 | 122.70 |
| 1 | F | 5 | PHE | CD1-CG-CD2 | -11.18 | 103.77 | 118.30 |
| 1 | D | 216 | VAL | CA-CB-CG1 | -11.17 | 94.14 | 110.90 |
| 1 | F | 187 | LEU | O-C-N | 11.17 | 140.58 | 122.70 |
| 1 | B | 168 | ASP | CB-CA-C | 11.17 | 132.74 | 110.40 |
| 1 | B | 109 | ASP | O-C-N | 11.17 | 140.57 | 122.70 |
| 1 | D | 59 | ARG | CA-C-O | 11.17 | 143.55 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 188 | GLN | CG-CD-NE2 | 11.16 | 143.50 | 116.70 |
| 1 | A | 194 | ASP | CA-CB-CG | 11.15 | 137.93 | 113.40 |
| 1 | A | 214 | ARG | N-CA-CB | -11.14 | 90.54 | 110.60 |
| 1 | E | 159 | ASP | CB-CG-OD2 | 11.14 | 128.33 | 118.30 |
| 1 | A | 128 | LEU | CD1-CG-CD2 | -11.14 | 77.09 | 110.50 |
| 1 | F | 69 | VAL | CG1-CB-CG2 | -11.13 | 93.08 | 110.90 |
| 1 | B | 29 | ARG | N-CA-CB | 11.13 | 130.64 | 110.60 |
| 1 | B | 164 | LEU | CB-CA-C | -11.13 | 89.05 | 110.20 |
| 1 | C | 108 | TRP | CA-CB-CG | 11.13 | 134.85 | 113.70 |
| 1 | B | 138 | PRO | CA-N-CD | -11.12 | 95.93 | 111.50 |
| 1 | F | 214 | ARG | CA-C-N | 11.12 | 141.66 | 117.20 |
| 1 | F | 41 | PHE | CB-CG-CD1 | 11.11 | 128.58 | 120.80 |
| 1 | B | 181 | THR | CA-CB-CG2 | 11.11 | 127.95 | 112.40 |
| 1 | D | 158 | THR | O-C-N | -11.10 | 104.93 | 122.70 |
| 1 | F | 199 | GLN | O-C-N | -11.10 | 104.94 | 122.70 |
| 1 | E | 125 | ASN | N-CA-C | 11.10 | 140.97 | 111.00 |
| 1 | E | 129 | TYR | CG-CD2-CE2 | -11.10 | 112.42 | 121.30 |
| 1 | C | 197 | THR | OG1-CB-CG2 | -11.10 | 84.48 | 110.00 |
| 1 | A | 94 | LEU | CB-CA-C | -11.09 | 89.13 | 110.20 |
| 1 | E | 24 | GLU | O-C-N | -11.08 | 104.97 | 122.70 |
| 1 | C | 137 | HIS | N-CA-C | 11.08 | 140.91 | 111.00 |
| 1 | F | 46 | ARG | CG-CD-NE | 11.07 | 135.05 | 111.80 |
| 1 | B | 53 | ALA | CB-CA-C | 11.07 | 126.70 | 110.10 |
| 1 | C | 189 | PRO | O-C-N | -11.07 | 104.99 | 122.70 |
| 1 | C | 142 | HIS | CA-C-N | 11.07 | 141.54 | 117.20 |
| 1 | B | 124 | GLY | O-C-N | -11.06 | 105.01 | 122.70 |
| 1 | A | 137 | HIS | N-CA-CB | -11.05 | 90.71 | 110.60 |
| 1 | E | 46 | ARG | N-CA-CB | -11.05 | 90.72 | 110.60 |
| 1 | C | 98 | ARG | O-C-N | -11.04 | 105.03 | 122.70 |
| 1 | D | 217 | PHE | CD1-CE1-CZ | -11.04 | 106.85 | 120.10 |
| 1 | A | 196 | LEU | O-C-N | 11.04 | 140.36 | 122.70 |
| 1 | E | 122 | ASN | C-N-CA | 11.04 | 149.30 | 121.70 |
| 1 | E | 130 | SER | CA-C-N | 11.04 | 141.49 | 117.20 |
| 1 | C | 46 | ARG | C-N-CA | 11.04 | 149.29 | 121.70 |
| 1 | E | 34 | SER | CA-CB-OG | 11.04 | 141.00 | 111.20 |
| 1 | B | 149 | LEU | CB-CG-CD1 | -11.03 | 92.25 | 111.00 |
| 1 | C | 147 | LEU | N-CA-CB | 11.03 | 132.45 | 110.40 |
| 1 | F | 100 | VAL | CA-C-N | 11.02 | 141.45 | 117.20 |
| 1 | B | 69 | VAL | CA-CB-CG2 | 11.02 | 127.43 | 110.90 |
| 1 | B | 235 | THR | CA-CB-CG2 | -11.02 | 96.97 | 112.40 |
| 1 | C | 73 | ALA | N-CA-C | -11.02 | 81.26 | 111.00 |
| 1 | A | 194 | ASP | CB-CG-OD1 | 11.01 | 128.21 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 54 | GLY | CA-C-O | 11.01 | 140.42 | 120.60 |
| 1 | F | 209 | SER | CA-CB-OG | 11.01 | 140.93 | 111.20 |
| 1 | C | 60 | ALA | CB-CA-C | 11.01 | 126.61 | 110.10 |
| 1 | E | 62 | LEU | CA-C-N | -11.00 | 93.00 | 117.20 |
| 1 | F | 124 | GLY | O-C-N | -11.00 | 105.10 | 122.70 |
| 1 | B | 33 | GLN | OE1-CD-NE2 | -11.00 | 96.60 | 121.90 |
| 1 | F | 5 | PHE | CG-CD2-CE2 | 11.00 | 132.90 | 120.80 |
| 1 | D | 159 | ASP | CB-CG-OD2 | 11.00 | 128.20 | 118.30 |
| 1 | C | 95 | GLN | CG-CD-OE1 | 10.99 | 143.59 | 121.60 |
| 1 | F | 188 | GLN | CA-CB-CG | 10.99 | 137.59 | 113.40 |
| 1 | B | 90 | TYR | CE1-CZ-OH | 10.99 | 149.77 | 120.10 |
| 1 | B | 46 | ARG | NH1-CZ-NH2 | 10.99 | 131.49 | 119.40 |
| 1 | E | 105 | PRO | CA-CB-CG | -10.98 | 83.13 | 104.00 |
| 1 | F | 20 | ALA | CB-CA-C | 10.98 | 126.58 | 110.10 |
| 1 | F | 199 | GLN | CA-C-O | 10.98 | 143.16 | 120.10 |
| 1 | D | 167 | ARG | O-C-N | -10.98 | 105.13 | 122.70 |
| 1 | C | 46 | ARG | O-C-N | -10.98 | 105.14 | 122.70 |
| 1 | B | 8 | SER | CA-CB-OG | 10.97 | 140.82 | 111.20 |
| 1 | C | 38 | LEU | CA-C-N | 10.97 | 141.34 | 117.20 |
| 1 | A | 33 | GLN | CA-C-O | 10.97 | 143.13 | 120.10 |
| 1 | D | 6 | GLY | CA-C-O | -10.96 | 100.86 | 120.60 |
| 1 | F | 24 | GLU | N-CA-CB | -10.96 | 90.87 | 110.60 |
| 1 | A | 141 | LEU | CB-CG-CD1 | -10.96 | 92.37 | 111.00 |
| 1 | D | 146 | SER | O-C-N | -10.95 | 105.17 | 122.70 |
| 1 | C | 5 | PHE | CB-CG-CD1 | 10.95 | 128.46 | 120.80 |
| 1 | A | 56 | THR | CA-C-N | -10.94 | 94.32 | 116.20 |
| 1 | E | 155 | SER | N-CA-CB | -10.94 | 94.09 | 110.50 |
| 1 | A | 233 | TRP | CE3-CZ3-CH2 | 10.93 | 133.23 | 121.20 |
| 1 | B | 61 | VAL | CA-CB-CG2 | -10.93 | 94.51 | 110.90 |
| 1 | F | 28 | PHE | N-CA-CB | -10.92 | 90.94 | 110.60 |
| 1 | D | 210 | ARG | NE-CZ-NH1 | 10.92 | 125.76 | 120.30 |
| 1 | D | 53 | ALA | CB-CA-C | -10.92 | 93.73 | 110.10 |
| 1 | B | 189 | PRO | CB-CA-C | -10.91 | 84.72 | 112.00 |
| 1 | D | 125 | ASN | CB-CG-OD1 | -10.89 | 99.81 | 121.60 |
| 1 | C | 39 | VAL | O-C-N | -10.88 | 105.29 | 122.70 |
| 1 | E | 49 | ALA | N-CA-CB | 10.87 | 125.32 | 110.10 |
| 1 | A | 18 | HIS | O-C-N | -10.87 | 105.30 | 122.70 |
| 1 | B | 110 | SER | CA-C-O | -10.87 | 97.27 | 120.10 |
| 1 | F | 222 | ASP | CB-CA-C | -10.87 | 88.66 | 110.40 |
| 1 | D | 162 | LEU | O-C-N | -10.87 | 105.31 | 122.70 |
| 1 | E | 112 | THR | CA-C-N | 10.87 | 141.11 | 117.20 |
| 1 | F | 193 | MET | CA-C-N | 10.87 | 141.11 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 149 | LEU | CB-CA-C | -10.86 | 89.56 | 110.20 |
| 1 | D | 19 | ALA | C-N-CA | -10.86 | 94.54 | 121.70 |
| 1 | D | 200 | ASN | N-CA-CB | -10.86 | 91.05 | 110.60 |
| 1 | A | 71 | LEU | CA-C-N | -10.86 | 93.31 | 117.20 |
| 1 | D | 35 | ASP | CB-CG-OD1 | 10.86 | 128.07 | 118.30 |
| 1 | C | 221 | PRO | N-CA-CB | -10.86 | 90.27 | 103.30 |
| 1 | D | 107 | LEU | N-CA-CB | 10.85 | 132.10 | 110.40 |
| 1 | A | 30 | PHE | CB-CG-CD1 | -10.85 | 113.20 | 120.80 |
| 1 | A | 168 | ASP | CB-CG-OD2 | 10.85 | 128.06 | 118.30 |
| 1 | D | 30 | PHE | CD1-CE1-CZ | -10.85 | 107.08 | 120.10 |
| 1 | F | 192 | ARG | NE-CZ-NH1 | 10.85 | 125.72 | 120.30 |
| 1 | C | 127 | ILE | C-N-CA | 10.84 | 148.81 | 121.70 |
| 1 | A | 8 | SER | O-C-N | -10.84 | 105.36 | 122.70 |
| 1 | A | 191 | GLY | CA-C-O | 10.84 | 140.10 | 120.60 |
| 1 | C | 13 | HIS | CA-C-N | 10.83 | 147.43 | 117.10 |
| 1 | B | 169 | ASP | CA-C-O | 10.83 | 142.84 | 120.10 |
| 1 | D | 70 | ILE | N-CA-CB | -10.83 | 85.89 | 110.80 |
| 1 | D | 143 | ALA | CA-C-O | -10.83 | 97.36 | 120.10 |
| 1 | D | 36 | CYS | N-CA-CB | 10.83 | 130.09 | 110.60 |
| 1 | E | 63 | GLN | N-CA-C | 10.82 | 140.23 | 111.00 |
| 1 | C | 47 | VAL | CB-CA-C | -10.81 | 90.86 | 111.40 |
| 1 | D | 214 | ARG | CB-CA-C | 10.81 | 132.02 | 110.40 |
| 1 | A | 41 | PHE | CB-CA-C | -10.80 | 88.79 | 110.40 |
| 1 | B | 146 | SER | O-C-N | -10.80 | 105.42 | 122.70 |
| 1 | D | 31 | THR | CA-CB-OG1 | -10.79 | 86.33 | 109.00 |
| 1 | D | 92 | LEU | N-CA-CB | 10.79 | 131.99 | 110.40 |
| 1 | D | 30 | PHE | CB-CA-C | -10.78 | 88.84 | 110.40 |
| 1 | F | 153 | ARG | CA-CB-CG | 10.78 | 137.11 | 113.40 |
| 1 | A | 159 | ASP | OD1-CG-OD2 | -10.77 | 102.83 | 123.30 |
| 1 | D | 13 | HIS | CA-C-N | 10.77 | 147.26 | 117.10 |
| 1 | E | 141 | LEU | C-N-CA | 10.77 | 148.62 | 121.70 |
| 1 | B | 61 | VAL | CA-C-O | 10.77 | 142.71 | 120.10 |
| 1 | C | 12 | SER | CB-CA-C | 10.76 | 130.54 | 110.10 |
| 1 | A | 169 | ASP | O-C-N | 10.76 | 139.91 | 122.70 |
| 1 | F | 143 | ALA | O-C-N | 10.76 | 139.91 | 122.70 |
| 1 | D | 15 | GLN | CB-CA-C | 10.75 | 131.90 | 110.40 |
| 1 | E | 190 | ASN | O-C-N | -10.75 | 104.92 | 123.20 |
| 1 | A | 90 | TYR | O-C-N | -10.75 | 105.50 | 122.70 |
| 1 | C | 173 | SER | CB-CA-C | -10.75 | 89.67 | 110.10 |
| 1 | C | 201 | ILE | CA-CB-CG2 | 10.75 | 132.40 | 110.90 |
| 1 | E | 176 | THR | CA-CB-CG2 | -10.75 | 97.35 | 112.40 |
| 1 | F | 99 | THR | O-C-N | 10.75 | 139.89 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 79 | TRP | CB-CG-CD2 | 10.74 | 140.56 | 126.60 |
| 1 | C | 16 | THR | CA-C-O | -10.73 | 97.58 | 120.10 |
| 1 | B | 61 | VAL | CA-CB-CG1 | 10.72 | 126.98 | 110.90 |
| 1 | C | 148 | GLN | N-CA-CB | -10.72 | 91.30 | 110.60 |
| 1 | B | 165 | PHE | CB-CG-CD2 | 10.72 | 128.30 | 120.80 |
| 1 | C | 154 | LEU | CA-C-O | -10.71 | 97.61 | 120.10 |
| 1 | B | 83 | THR | CA-CB-CG2 | 10.71 | 127.39 | 112.40 |
| 1 | B | 72 | THR | C-N-CA | 10.69 | 148.44 | 121.70 |
| 1 | D | 222 | ASP | CA-CB-CG | 10.69 | 136.92 | 113.40 |
| 1 | E | 131 | THR | N-CA-C | 10.69 | 139.86 | 111.00 |
| 1 | A | 139 | GLN | N-CA-CB | -10.69 | 91.36 | 110.60 |
| 1 | B | 163 | VAL | O-C-N | -10.69 | 105.60 | 122.70 |
| 1 | D | 22 | SER | CB-CA-C | -10.68 | 89.80 | 110.10 |
| 1 | C | 125 | ASN | N-CA-C | 10.68 | 139.84 | 111.00 |
| 1 | C | 136 | ASN | N-CA-C | 10.68 | 139.83 | 111.00 |
| 1 | D | 89 | ASN | N-CA-CB | -10.68 | 91.38 | 110.60 |
| 1 | D | 72 | THR | N-CA-CB | -10.67 | 90.02 | 110.30 |
| 1 | A | 195 | VAL | CA-CB-CG1 | -10.67 | 94.89 | 110.90 |
| 1 | B | 197 | THR | CA-CB-CG2 | -10.67 | 97.46 | 112.40 |
| 1 | C | 196 | LEU | CA-CB-CG | 10.66 | 139.83 | 115.30 |
| 1 | D | 108 | TRP | CE2-CD2-CE3 | -10.66 | 105.91 | 118.70 |
| 1 | D | 192 | ARG | O-C-N | -10.65 | 105.65 | 122.70 |
| 1 | A | 86 | SER | N-CA-CB | -10.65 | 94.53 | 110.50 |
| 1 | A | 146 | SER | N-CA-CB | -10.63 | 94.56 | 110.50 |
| 1 | B | 5 | PHE | CB-CA-C | 10.62 | 131.64 | 110.40 |
| 1 | A | 86 | SER | CA-C-N | 10.62 | 140.56 | 117.20 |
| 1 | C | 186 | VAL | CB-CA-C | 10.61 | 131.56 | 111.40 |
| 1 | F | 212 | ALA | CB-CA-C | 10.61 | 126.02 | 110.10 |
| 1 | E | 194 | ASP | CB-CG-OD2 | 10.61 | 127.84 | 118.30 |
| 1 | F | 87 | ILE | O-C-N | -10.61 | 105.17 | 123.20 |
| 1 | F | 188 | GLN | CG-CD-OE1 | 10.60 | 142.80 | 121.60 |
| 1 | C | 90 | TYR | O-C-N | 10.60 | 139.65 | 122.70 |
| 1 | C | 9 | HIS | O-C-N | 10.59 | 139.64 | 122.70 |
| 1 | D | 1 | ASN | O-C-N | -10.59 | 105.76 | 122.70 |
| 1 | A | 173 | SER | CA-C-O | -10.58 | 97.88 | 120.10 |
| 1 | C | 45 | VAL | CG1-CB-CG2 | -10.58 | 93.98 | 110.90 |
| 1 | E | 232 | LEU | N-CA-C | 10.58 | 139.56 | 111.00 |
| 1 | A | 125 | ASN | N-CA-C | 10.57 | 139.55 | 111.00 |
| 1 | D | 98 | ARG | CD-NE-CZ | -10.57 | 108.80 | 123.60 |
| 1 | F | 64 | SER | CA-CB-OG | -10.57 | 82.65 | 111.20 |
| 1 | B | 76 | THR | CA-CB-CG2 | 10.57 | 127.20 | 112.40 |
| 1 | B | 9 | HIS | N-CA-CB | -10.57 | 91.57 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 209 | SER | N-CA-CB | -10.57 | 94.65 | 110.50 |
| 1 | A | 153 | ARG | NE-CZ-NH1 | -10.56 | 115.02 | 120.30 |
| 1 | B | 142 | HIS | N-CA-CB | -10.56 | 91.59 | 110.60 |
| 1 | A | 136 | ASN | N-CA-C | -10.56 | 82.49 | 111.00 |
| 1 | A | 137 | HIS | CB-CA-C | -10.56 | 89.29 | 110.40 |
| 1 | D | 219 | LEU | CD1-CG-CD2 | -10.54 | 78.87 | 110.50 |
| 1 | E | 128 | LEU | CA-C-N | 10.54 | 140.38 | 117.20 |
| 1 | D | 25 | LEU | N-CA-CB | 10.53 | 131.45 | 110.40 |
| 1 | A | 105 | PRO | C-N-CA | -10.52 | 100.21 | 122.30 |
| 1 | C | 228 | TYR | CG-CD2-CE2 | 10.52 | 129.72 | 121.30 |
| 1 | D | 152 | TYR | CE1-CZ-OH | 10.51 | 148.49 | 120.10 |
| 1 | A | 95 | GLN | OE1-CD-NE2 | -10.51 | 97.73 | 121.90 |
| 1 | A | 78 | ARG | NE-CZ-NH1 | -10.51 | 115.05 | 120.30 |
| 1 | C | 48 | TRP | CB-CG-CD2 | 10.51 | 140.26 | 126.60 |
| 1 | A | 93 | VAL | CA-C-O | -10.50 | 98.05 | 120.10 |
| 1 | A | 46 | ARG | CD-NE-CZ | 10.50 | 138.29 | 123.60 |
| 1 | D | 87 | ILE | CA-C-O | -10.49 | 98.07 | 120.10 |
| 1 | E | 1 | ASN | CB-CG-ND2 | 10.49 | 141.87 | 116.70 |
| 1 | A | 18 | HIS | C-N-CA | 10.49 | 147.92 | 121.70 |
| 1 | A | 131 | THR | OG1-CB-CG2 | -10.48 | 85.89 | 110.00 |
| 1 | E | 107 | LEU | CA-C-O | -10.48 | 98.09 | 120.10 |
| 1 | A | 7 | LEU | CA-C-O | -10.47 | 98.11 | 120.10 |
| 1 | B | 214 | ARG | CB-CA-C | 10.47 | 131.35 | 110.40 |
| 1 | D | 80 | SER | CA-C-N | 10.47 | 140.22 | 117.20 |
| 1 | E | 147 | LEU | O-C-N | -10.46 | 105.96 | 122.70 |
| 1 | F | 60 | ALA | CB-CA-C | 10.46 | 125.79 | 110.10 |
| 1 | B | 103 | TYR | CB-CG-CD2 | 10.46 | 127.28 | 121.00 |
| 1 | E | 20 | ALA | O-C-N | -10.46 | 105.96 | 122.70 |
| 1 | C | 1 | ASN | CA-CB-CG | 10.46 | 136.41 | 113.40 |
| 1 | A | 40 | LEU | O-C-N | 10.46 | 139.43 | 122.70 |
| 1 | C | 4 | LEU | CA-C-O | -10.46 | 98.14 | 120.10 |
| 1 | B | 4 | LEU | CA-C-N | 10.45 | 140.20 | 117.20 |
| 1 | E | 196 | LEU | CB-CG-CD2 | -10.45 | 93.23 | 111.00 |
| 1 | D | 101 | THR | N-CA-CB | -10.45 | 90.45 | 110.30 |
| 1 | A | 86 | SER | CA-C-O | -10.43 | 98.19 | 120.10 |
| 1 | E | 228 | TYR | CB-CG-CD2 | 10.43 | 127.26 | 121.00 |
| 1 | D | 193 | MET | O-C-N | -10.43 | 106.02 | 122.70 |
| 1 | E | 157 | GLU | CA-C-O | -10.43 | 98.20 | 120.10 |
| 1 | C | 105 | PRO | CA-CB-CG | -10.42 | 84.21 | 104.00 |
| 1 | C | 24 | GLU | O-C-N | -10.41 | 106.04 | 122.70 |
| 1 | C | 146 | SER | CA-C-O | -10.41 | 98.23 | 120.10 |
| 1 | A | 41 | PHE | CD1-CE1-CZ | -10.40 | 107.62 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 230 | GLY | N-CA-C | -10.40 | 87.09 | 113.10 |
| 1 | B | 193 | MET | O-C-N | -10.40 | 106.06 | 122.70 |
| 1 | D | 21 | GLN | N-CA-CB | -10.40 | 91.89 | 110.60 |
| 1 | F | 189 | PRO | CA-C-O | -10.40 | 95.25 | 120.20 |
| 1 | B | 128 | LEU | O-C-N | -10.38 | 106.09 | 122.70 |
| 1 | D | 27 | SER | CA-C-O | 10.38 | 141.89 | 120.10 |
| 1 | D | 105 | PRO | CA-C-N | 10.38 | 136.95 | 116.20 |
| 1 | D | 223 | ARG | NE-CZ-NH2 | 10.38 | 125.49 | 120.30 |
| 1 | D | 149 | LEU | N-CA-CB | 10.37 | 131.14 | 110.40 |
| 1 | D | 188 | GLN | N-CA-CB | -10.36 | 91.95 | 110.60 |
| 1 | E | 157 | GLU | CB-CG-CD | -10.36 | 86.23 | 114.20 |
| 1 | F | 98 | ARG | NH1-CZ-NH2 | 10.36 | 130.80 | 119.40 |
| 1 | D | 25 | LEU | O-C-N | 10.36 | 139.27 | 122.70 |
| 1 | A | 8 | SER | CA-C-O | 10.35 | 141.84 | 120.10 |
| 1 | C | 69 | VAL | CA-CB-CG1 | -10.35 | 95.38 | 110.90 |
| 1 | A | 198 | ASN | CA-CB-CG | -10.34 | 90.65 | 113.40 |
| 1 | D | 92 | LEU | CA-C-O | -10.33 | 98.41 | 120.10 |
| 1 | D | 160 | CYS | CA-CB-SG | 10.33 | 132.59 | 114.00 |
| 1 | F | 143 | ALA | CA-C-O | -10.33 | 98.41 | 120.10 |
| 1 | F | 61 | VAL | O-C-N | 10.32 | 139.22 | 122.70 |
| 1 | E | 58 | CYS | CA-C-O | 10.32 | 141.77 | 120.10 |
| 1 | D | 45 | VAL | N-CA-C | -10.31 | 83.15 | 111.00 |
| 1 | E | 149 | LEU | CB-CG-CD2 | 10.31 | 128.54 | 111.00 |
| 1 | E | 114 | ASN | CA-CB-CG | -10.31 | 90.71 | 113.40 |
| 1 | B | 137 | HIS | CB-CG-ND1 | 10.31 | 148.97 | 123.20 |
| 1 | A | 149 | LEU | C-N-CA | -10.31 | 95.94 | 121.70 |
| 1 | A | 48 | TRP | CE3-CZ3-CH2 | -10.30 | 109.86 | 121.20 |
| 1 | B | 105 | PRO | CB-CA-C | -10.30 | 86.24 | 112.00 |
| 1 | B | 71 | LEU | CA-CB-CG | 10.30 | 138.99 | 115.30 |
| 1 | A | 150 | SER | N-CA-CB | 10.30 | 125.95 | 110.50 |
| 1 | C | 9 | HIS | CA-CB-CG | 10.30 | 131.11 | 113.60 |
| 1 | D | 18 | HIS | CA-C-N | 10.30 | 139.86 | 117.20 |
| 1 | E | 2 | ASN | CB-CG-ND2 | 10.30 | 141.42 | 116.70 |
| 1 | E | 189 | PRO | CA-CB-CG | -10.30 | 84.43 | 104.00 |
| 1 | B | 31 | THR | OG1-CB-CG2 | 10.29 | 133.66 | 110.00 |
| 1 | B | 30 | PHE | O-C-N | -10.28 | 106.25 | 122.70 |
| 1 | E | 33 | GLN | CA-C-O | 10.28 | 141.69 | 120.10 |
| 1 | C | 227 | ILE | CA-CB-CG2 | -10.28 | 90.34 | 110.90 |
| 1 | D | 142 | HIS | N-CA-C | 10.28 | 138.75 | 111.00 |
| 1 | C | 48 | TRP | CB-CG-CD1 | -10.27 | 113.65 | 127.00 |
| 1 | C | 221 | PRO | CA-C-N | 10.27 | 139.79 | 117.20 |
| 1 | D | 204 | TRP | CB-CG-CD2 | 10.27 | 139.95 | 126.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 150 | SER | O-C-N | 10.26 | 140.60 | 121.10 |
| 1 | B | 150 | SER | CA-C-O | -10.26 | 98.55 | 120.10 |
| 1 | F | 30 | PHE | CB-CG-CD2 | -10.26 | 113.62 | 120.80 |
| 1 | E | 38 | LEU | CA-C-N | 10.25 | 139.74 | 117.20 |
| 1 | D | 219 | LEU | CA-CB-CG | 10.24 | 138.86 | 115.30 |
| 1 | C | 205 | THR | OG1-CB-CG2 | 10.24 | 133.55 | 110.00 |
| 1 | A | 107 | LEU | CA-C-O | -10.23 | 98.61 | 120.10 |
| 1 | C | 90 | TYR | CB-CG-CD2 | 10.23 | 127.14 | 121.00 |
| 1 | F | 226 | ALA | CB-CA-C | 10.23 | 125.44 | 110.10 |
| 1 | A | 176 | THR | N-CA-CB | -10.23 | 90.87 | 110.30 |
| 1 | C | 171 | VAL | CA-C-O | -10.23 | 98.62 | 120.10 |
| 1 | C | 184 | ARG | NE-CZ-NH2 | -10.21 | 115.19 | 120.30 |
| 1 | B | 42 | ASP | CA-C-N | 10.21 | 139.66 | 117.20 |
| 1 | F | 20 | ALA | O-C-N | -10.20 | 106.38 | 122.70 |
| 1 | C | 145 | GLN | CB-CA-C | 10.20 | 130.79 | 110.40 |
| 1 | E | 131 | THR | CB-CA-C | -10.20 | 84.07 | 111.60 |
| 1 | D | 223 | ARG | NE-CZ-NH1 | -10.19 | 115.20 | 120.30 |
| 1 | A | 72 | THR | CA-CB-OG1 | -10.19 | 87.61 | 109.00 |
| 1 | F | 9 | HIS | O-C-N | -10.18 | 106.42 | 122.70 |
| 1 | F | 63 | GLN | CG-CD-NE2 | 10.18 | 141.12 | 116.70 |
| 1 | A | 90 | TYR | CB-CA-C | -10.17 | 90.05 | 110.40 |
| 1 | E | 11 | GLY | O-C-N | -10.17 | 106.42 | 122.70 |
| 1 | F | 17 | LEU | O-C-N | 10.17 | 138.97 | 122.70 |
| 1 | C | 169 | ASP | CA-CB-CG | 10.16 | 135.76 | 113.40 |
| 1 | D | 194 | ASP | CB-CA-C | -10.16 | 90.08 | 110.40 |
| 1 | E | 211 | SER | CA-C-N | 10.16 | 139.56 | 117.20 |
| 1 | A | 103 | TYR | CB-CG-CD2 | -10.15 | 114.91 | 121.00 |
| 1 | E | 52 | THR | CA-CB-CG2 | 10.15 | 126.61 | 112.40 |
| 1 | F | 2 | ASN | N-CA-C | 10.15 | 138.40 | 111.00 |
| 1 | A | 36 | CYS | CA-CB-SG | -10.15 | 95.73 | 114.00 |
| 1 | D | 165 | PHE | CB-CG-CD2 | 10.15 | 127.90 | 120.80 |
| 1 | E | 233 | TRP | CD1-NE1-CE2 | -10.15 | 99.87 | 109.00 |
| 1 | D | 231 | ALA | CB-CA-C | -10.14 | 94.89 | 110.10 |
| 1 | A | 200 | ASN | CB-CG-OD1 | 10.14 | 141.88 | 121.60 |
| 1 | E | 51 | ASN | N-CA-CB | 10.14 | 128.85 | 110.60 |
| 1 | B | 174 | THR | CA-CB-CG2 | -10.14 | 98.21 | 112.40 |
| 1 | C | 216 | VAL | CA-CB-CG1 | 10.14 | 126.11 | 110.90 |
| 1 | E | 62 | LEU | CB-CA-C | -10.14 | 90.94 | 110.20 |
| 1 | B | 152 | TYR | CB-CA-C | -10.14 | 90.12 | 110.40 |
| 1 | D | 195 | VAL | CG1-CB-CG2 | 10.13 | 127.11 | 110.90 |
| 1 | E | 26 | SER | O-C-N | -10.13 | 106.49 | 122.70 |
| 1 | B | 82 | GLY | O-C-N | -10.13 | 106.49 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 195 | VAL | O-C-N | 10.11 | 138.88 | 122.70 |
| 1 | D | 105 | PRO | N-CD-CG | 10.11 | 118.37 | 103.20 |
| 1 | A | 90 | TYR | C-N-CA | 10.11 | 146.96 | 121.70 |
| 1 | D | 8 | SER | CA-CB-OG | 10.10 | 138.47 | 111.20 |
| 1 | D | 224 | ASN | CB-CG-OD1 | -10.10 | 101.40 | 121.60 |
| 1 | E | 38 | LEU | O-C-N | -10.09 | 106.55 | 122.70 |
| 1 | C | 205 | THR | CA-CB-CG2 | -10.09 | 98.28 | 112.40 |
| 1 | F | 31 | THR | N-CA-CB | -10.09 | 91.13 | 110.30 |
| 1 | D | 233 | TRP | CG-CD1-NE1 | 10.09 | 120.19 | 110.10 |
| 1 | A | 208 | ASN | CA-CB-CG | 10.08 | 135.58 | 113.40 |
| 1 | B | 13 | HIS | O-C-N | -10.08 | 101.95 | 121.10 |
| 1 | B | 71 | LEU | CA-C-N | 10.07 | 139.36 | 117.20 |
| 1 | C | 56 | THR | CA-C-N | -10.07 | 96.05 | 116.20 |
| 1 | E | 169 | ASP | CB-CG-OD2 | -10.07 | 109.23 | 118.30 |
| 1 | A | 110 | SER | O-C-N | -10.07 | 106.08 | 123.20 |
| 1 | D | 9 | HIS | CA-CB-CG | 10.07 | 130.72 | 113.60 |
| 1 | D | 13 | HIS | O-C-N | -10.06 | 101.99 | 121.10 |
| 1 | E | 61 | VAL | N-CA-C | 10.06 | 138.16 | 111.00 |
| 1 | E | 22 | SER | CA-CB-OG | -10.05 | 84.07 | 111.20 |
| 1 | D | 99 | THR | O-C-N | 10.04 | 138.77 | 122.70 |
| 1 | A | 128 | LEU | CA-CB-CG | 10.04 | 138.40 | 115.30 |
| 1 | B | 13 | HIS | N-CA-C | 10.04 | 138.12 | 111.00 |
| 1 | C | 25 | LEU | N-CA-CB | 10.04 | 130.48 | 110.40 |
| 1 | A | 49 | ALA | CB-CA-C | 10.04 | 125.16 | 110.10 |
| 1 | A | 90 | TYR | CA-C-N | 10.04 | 139.28 | 117.20 |
| 1 | B | 159 | ASP | C-N-CA | 10.04 | 146.79 | 121.70 |
| 1 | C | 98 | ARG | NE-CZ-NH2 | 10.04 | 125.32 | 120.30 |
| 1 | A | 15 | GLN | N-CA-C | -10.03 | 83.92 | 111.00 |
| 1 | D | 148 | GLN | CA-CB-CG | 10.02 | 135.45 | 113.40 |
| 1 | A | 81 | SER | O-C-N | -10.02 | 106.16 | 123.20 |
| 1 | D | 64 | SER | CA-C-O | 10.02 | 141.15 | 120.10 |
| 1 | E | 156 | MET | C-N-CA | -10.02 | 96.65 | 121.70 |
| 1 | B | 101 | THR | O-C-N | 10.02 | 138.73 | 122.70 |
| 1 | E | 167 | ARG | O-C-N | -10.01 | 106.68 | 122.70 |
| 1 | F | 14 | PRO | CA-N-CD | -10.01 | 97.49 | 111.50 |
| 1 | A | 217 | PHE | CA-C-O | -10.01 | 99.08 | 120.10 |
| 1 | A | 44 | ASP | CA-C-O | -10.01 | 99.09 | 120.10 |
| 1 | C | 112 | THR | O-C-N | -10.01 | 106.69 | 122.70 |
| 1 | A | 105 | PRO | N-CD-CG | 9.99 | 118.19 | 103.20 |
| 1 | B | 25 | LEU | N-CA-CB | 9.99 | 130.39 | 110.40 |
| 1 | F | 230 | GLY | N-CA-C | -9.99 | 88.12 | 113.10 |
| 1 | F | 84 | LYS | C-N-CA | 9.99 | 143.28 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 184 | ARG | CD-NE-CZ | 9.98 | 137.58 | 123.60 |
| 1 | C | 145 | GLN | CB-CG-CD | 9.98 | 137.56 | 111.60 |
| 1 | A | 104 | GLY | C-N-CA | 9.98 | 163.91 | 122.00 |
| 1 | D | 153 | ARG | N-CA-CB | -9.97 | 92.64 | 110.60 |
| 1 | F | 1 | ASN | OD1-CG-ND2 | 9.97 | 144.84 | 121.90 |
| 1 | F | 86 | SER | N-CA-CB | 9.97 | 125.46 | 110.50 |
| 1 | D | 142 | HIS | O-C-N | -9.97 | 106.75 | 122.70 |
| 1 | B | 150 | SER | CA-C-N | 9.96 | 144.99 | 117.10 |
| 1 | A | 109 | ASP | CB-CG-OD1 | 9.96 | 127.26 | 118.30 |
| 1 | A | 19 | ALA | O-C-N | -9.96 | 106.77 | 122.70 |
| 1 | A | 61 | VAL | N-CA-C | 9.96 | 137.88 | 111.00 |
| 1 | B | 214 | ARG | O-C-N | -9.95 | 106.78 | 122.70 |
| 1 | F | 46 | ARG | NH1-CZ-NH2 | -9.94 | 108.46 | 119.40 |
| 1 | A | 146 | SER | CB-CA-C | -9.94 | 91.21 | 110.10 |
| 1 | A | 77 | ILE | O-C-N | -9.94 | 106.80 | 122.70 |
| 1 | E | 100 | VAL | CA-CB-CG1 | -9.93 | 96.00 | 110.90 |
| 1 | E | 72 | THR | C-N-CA | 9.93 | 146.52 | 121.70 |
| 1 | B | 24 | GLU | OE1-CD-OE2 | 9.92 | 135.21 | 123.30 |
| 1 | B | 42 | ASP | CA-C-O | -9.92 | 99.28 | 120.10 |
| 1 | F | 110 | SER | CA-C-O | -9.91 | 99.28 | 120.10 |
| 1 | A | 198 | ASN | CB-CG-ND2 | 9.91 | 140.49 | 116.70 |
| 1 | E | 93 | VAL | CA-CB-CG1 | 9.91 | 125.77 | 110.90 |
| 1 | D | 109 | ASP | OD1-CG-OD2 | 9.91 | 142.13 | 123.30 |
| 1 | A | 178 | GLY | O-C-N | -9.91 | 106.85 | 122.70 |
| 1 | E | 139 | GLN | O-C-N | 9.91 | 138.55 | 122.70 |
| 1 | A | 218 | VAL | O-C-N | 9.90 | 138.54 | 122.70 |
| 1 | D | 154 | LEU | N-CA-CB | 9.90 | 130.20 | 110.40 |
| 1 | E | 158 | THR | CA-C-N | 9.90 | 138.98 | 117.20 |
| 1 | B | 5 | PHE | N-CA-CB | -9.90 | 92.78 | 110.60 |
| 1 | C | 27 | SER | O-C-N | -9.90 | 106.87 | 122.70 |
| 1 | C | 89 | ASN | CB-CA-C | -9.89 | 90.61 | 110.40 |
| 1 | D | 225 | LEU | CA-C-N | 9.88 | 138.95 | 117.20 |
| 1 | E | 43 | SER | C-N-CA | 9.88 | 146.41 | 121.70 |
| 1 | F | 55 | ALA | N-CA-CB | -9.88 | 96.26 | 110.10 |
| 1 | D | 27 | SER | CA-CB-OG | -9.88 | 84.52 | 111.20 |
| 1 | A | 48 | TRP | CZ3-CH2-CZ2 | 9.88 | 133.46 | 121.60 |
| 1 | A | 141 | LEU | CA-CB-CG | 9.88 | 138.03 | 115.30 |
| 1 | D | 94 | LEU | CB-CG-CD2 | 9.88 | 127.80 | 111.00 |
| 1 | F | 105 | PRO | CA-N-CD | -9.88 | 97.67 | 111.50 |
| 1 | B | 105 | PRO | C-N-CA | 9.88 | 143.04 | 122.30 |
| 1 | C | 143 | ALA | N-CA-CB | -9.88 | 96.27 | 110.10 |
| 1 | D | 172 | TRP | CG-CD1-NE1 | 9.88 | 119.98 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 235 | THR | CA-CB-OG1 | 9.88 | 129.74 | 109.00 |
| 1 | C | 67 | LEU | CA-CB-CG | 9.87 | 138.00 | 115.30 |
| 1 | E | 123 | ASN | CB-CA-C | -9.87 | 90.66 | 110.40 |
| 1 | D | 30 | PHE | CG-CD1-CE1 | 9.87 | 131.65 | 120.80 |
| 1 | E | 139 | GLN | CA-C-O | -9.86 | 99.39 | 120.10 |
| 1 | E | 43 | SER | CB-CA-C | 9.86 | 128.83 | 110.10 |
| 1 | A | 108 | TRP | CG-CD2-CE3 | -9.85 | 125.03 | 133.90 |
| 1 | F | 160 | CYS | CB-CA-C | 9.85 | 130.10 | 110.40 |
| 1 | B | 103 | TYR | CD1-CE1-CZ | -9.85 | 110.94 | 119.80 |
| 1 | E | 233 | TRP | CG-CD1-NE1 | 9.85 | 119.95 | 110.10 |
| 1 | E | 99 | THR | N-CA-C | 9.84 | 137.58 | 111.00 |
| 1 | F | 209 | SER | CB-CA-C | 9.84 | 128.80 | 110.10 |
| 1 | A | 94 | LEU | O-C-N | -9.84 | 106.96 | 122.70 |
| 1 | F | 73 | ALA | CA-C-O | 9.84 | 140.75 | 120.10 |
| 1 | A | 158 | THR | CA-CB-CG2 | -9.83 | 98.63 | 112.40 |
| 1 | A | 215 | TYR | O-C-N | -9.83 | 106.97 | 122.70 |
| 1 | B | 136 | ASN | CA-C-N | 9.83 | 138.82 | 117.20 |
| 1 | D | 8 | SER | C-N-CA | 9.82 | 146.24 | 121.70 |
| 1 | B | 148 | GLN | OE1-CD-NE2 | 9.81 | 144.46 | 121.90 |
| 1 | E | 38 | LEU | CB-CG-CD2 | -9.81 | 94.33 | 111.00 |
| 1 | A | 123 | ASN | CA-CB-CG | 9.81 | 134.97 | 113.40 |
| 1 | F | 8 | SER | CA-C-N | -9.81 | 95.62 | 117.20 |
| 1 | A | 139 | GLN | CB-CA-C | 9.80 | 130.01 | 110.40 |
| 1 | B | 149 | LEU | CB-CA-C | -9.80 | 91.58 | 110.20 |
| 1 | D | 5 | PHE | CE1-CZ-CE2 | -9.80 | 102.36 | 120.00 |
| 1 | E | 228 | TYR | O-C-N | -9.80 | 106.54 | 123.20 |
| 1 | D | 76 | THR | CA-C-N | 9.79 | 138.75 | 117.20 |
| 1 | A | 148 | GLN | O-C-N | -9.79 | 107.04 | 122.70 |
| 1 | B | 5 | PHE | CG-CD1-CE1 | 9.79 | 131.57 | 120.80 |
| 1 | C | 93 | VAL | CA-C-O | -9.79 | 99.54 | 120.10 |
| 1 | F | 139 | GLN | CG-CD-OE1 | 9.79 | 141.17 | 121.60 |
| 1 | F | 3 | ILE | O-C-N | 9.78 | 138.35 | 122.70 |
| 1 | D | 128 | LEU | N-CA-CB | 9.78 | 129.96 | 110.40 |
| 1 | E | 71 | LEU | CB-CG-CD1 | 9.78 | 127.62 | 111.00 |
| 1 | C | 40 | LEU | C-N-CA | 9.78 | 146.14 | 121.70 |
| 1 | B | 65 | ASP | N-CA-CB | -9.77 | 93.01 | 110.60 |
| 1 | D | 99 | THR | OG1-CB-CG2 | -9.77 | 87.52 | 110.00 |
| 1 | B | 129 | TYR | CB-CA-C | -9.76 | 90.88 | 110.40 |
| 1 | C | 99 | THR | CA-CB-OG1 | -9.76 | 88.50 | 109.00 |
| 1 | D | 101 | THR | N-CA-C | 9.76 | 137.35 | 111.00 |
| 1 | F | 97 | ASP | CB-CG-OD2 | 9.76 | 127.08 | 118.30 |
| 1 | E | 8 | SER | CA-C-N | -9.75 | 95.75 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 159 | ASP | CA-C-N | 9.75 | 138.64 | 117.20 |
| 1 | A | 122 | ASN | CA-CB-CG | 9.74 | 134.84 | 113.40 |
| 1 | B | 222 | ASP | CB-CG-OD1 | 9.74 | 127.07 | 118.30 |
| 1 | C | 228 | TYR | CA-C-O | 9.74 | 140.56 | 120.10 |
| 1 | F | 138 | PRO | CA-N-CD | -9.74 | 97.86 | 111.50 |
| 1 | E | 102 | ILE | C-N-CA | -9.74 | 97.35 | 121.70 |
| 1 | A | 60 | ALA | CA-C-O | -9.74 | 99.65 | 120.10 |
| 1 | A | 92 | LEU | CB-CA-C | -9.74 | 91.70 | 110.20 |
| 1 | F | 153 | ARG | NE-CZ-NH2 | 9.73 | 125.17 | 120.30 |
| 1 | A | 223 | ARG | CD-NE-CZ | -9.73 | 109.98 | 123.60 |
| 1 | A | 222 | ASP | N-CA-C | -9.72 | 84.74 | 111.00 |
| 1 | A | 49 | ALA | CA-C-O | -9.72 | 99.68 | 120.10 |
| 1 | C | 15 | GLN | CG-CD-OE1 | 9.72 | 141.03 | 121.60 |
| 1 | A | 153 | ARG | NH1-CZ-NH2 | -9.71 | 108.71 | 119.40 |
| 1 | F | 52 | THR | O-C-N | -9.71 | 107.17 | 122.70 |
| 1 | A | 48 | TRP | CD1-NE1-CE2 | -9.71 | 100.27 | 109.00 |
| 1 | B | 193 | MET | N-CA-CB | 9.71 | 128.07 | 110.60 |
| 1 | F | 129 | TYR | O-C-N | -9.71 | 107.17 | 122.70 |
| 1 | B | 220 | GLN | CA-CB-CG | 9.70 | 134.74 | 113.40 |
| 1 | E | 151 | PRO | N-CA-CB | -9.70 | 91.66 | 103.30 |
| 1 | F | 63 | GLN | CG-CD-OE1 | -9.69 | 102.21 | 121.60 |
| 1 | C | 221 | PRO | O-C-N | -9.69 | 107.19 | 122.70 |
| 1 | B | 167 | ARG | NE-CZ-NH2 | 9.69 | 125.14 | 120.30 |
| 1 | B | 216 | VAL | CG1-CB-CG2 | -9.69 | 95.40 | 110.90 |
| 1 | F | 137 | HIS | O-C-N | 9.69 | 139.51 | 121.10 |
| 1 | A | 100 | VAL | CA-C-O | -9.68 | 99.76 | 120.10 |
| 1 | F | 12 | SER | O-C-N | -9.68 | 107.21 | 122.70 |
| 1 | B | 200 | ASN | C-N-CA | 9.68 | 145.90 | 121.70 |
| 1 | D | 39 | VAL | CG1-CB-CG2 | -9.68 | 95.41 | 110.90 |
| 1 | E | 181 | THR | C-N-CA | -9.68 | 101.97 | 122.30 |
| 1 | D | 79 | TRP | CD1-NE1-CE2 | 9.68 | 117.71 | 109.00 |
| 1 | D | 158 | THR | OG1-CB-CG2 | 9.68 | 132.25 | 110.00 |
| 1 | F | 124 | GLY | CA-C-O | 9.68 | 138.02 | 120.60 |
| 1 | C | 145 | GLN | CA-CB-CG | 9.67 | 134.68 | 113.40 |
| 1 | D | 130 | SER | CA-CB-OG | 9.67 | 137.31 | 111.20 |
| 1 | A | 137 | HIS | CA-C-O | -9.67 | 99.80 | 120.10 |
| 1 | E | 34 | SER | CA-C-O | -9.66 | 99.81 | 120.10 |
| 1 | C | 178 | GLY | C-N-CA | 9.66 | 145.85 | 121.70 |
| 1 | D | 226 | ALA | N-CA-CB | 9.66 | 123.62 | 110.10 |
| 1 | F | 43 | SER | C-N-CA | 9.66 | 145.85 | 121.70 |
| 1 | F | 164 | LEU | CA-C-N | 9.65 | 138.44 | 117.20 |
| 1 | C | 157 | GLU | C-N-CA | 9.65 | 145.83 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 77 | ILE | CA-CB-CG1 | -9.64 | 92.68 | 111.00 |
| 1 | C | 124 | GLY | O-C-N | -9.64 | 107.28 | 122.70 |
| 1 | D | 226 | ALA | N-CA-C | -9.64 | 84.98 | 111.00 |
| 1 | D | 25 | LEU | C-N-CA | -9.63 | 97.62 | 121.70 |
| 1 | D | 73 | ALA | O-C-N | -9.63 | 107.28 | 122.70 |
| 1 | F | 31 | THR | CA-CB-CG2 | -9.63 | 98.91 | 112.40 |
| 1 | D | 78 | ARG | CB-CG-CD | -9.63 | 86.57 | 111.60 |
| 1 | D | 154 | LEU | CB-CG-CD2 | -9.62 | 94.64 | 111.00 |
| 1 | A | 121 | ALA | CB-CA-C | 9.62 | 124.53 | 110.10 |
| 1 | B | 191 | GLY | CA-C-O | -9.62 | 103.29 | 120.60 |
| 1 | C | 43 | SER | CB-CA-C | 9.62 | 128.38 | 110.10 |
| 1 | D | 164 | LEU | CB-CG-CD1 | 9.62 | 127.35 | 111.00 |
| 1 | F | 167 | ARG | CD-NE-CZ | 9.62 | 137.06 | 123.60 |
| 1 | B | 10 | GLU | CA-CB-CG | 9.62 | 134.56 | 113.40 |
| 1 | D | 86 | SER | CA-CB-OG | 9.62 | 137.16 | 111.20 |
| 1 | A | 70 | ILE | C-N-CA | 9.61 | 145.73 | 121.70 |
| 1 | F | 103 | TYR | CA-C-O | 9.61 | 140.28 | 120.10 |
| 1 | B | 75 | ASN | CA-CB-CG | -9.61 | 92.26 | 113.40 |
| 1 | C | 3 | ILE | O-C-N | 9.61 | 138.07 | 122.70 |
| 1 | D | 94 | LEU | CB-CG-CD1 | -9.61 | 94.67 | 111.00 |
| 1 | D | 130 | SER | CB-CA-C | 9.60 | 128.34 | 110.10 |
| 1 | A | 200 | ASN | CB-CA-C | 9.60 | 129.60 | 110.40 |
| 1 | D | 218 | VAL | CA-CB-CG2 | 9.60 | 125.30 | 110.90 |
| 1 | A | 2 | ASN | CB-CA-C | 9.60 | 129.59 | 110.40 |
| 1 | B | 190 | ASN | CA-C-O | -9.60 | 99.95 | 120.10 |
| 1 | D | 64 | SER | CA-CB-OG | -9.60 | 85.29 | 111.20 |
| 1 | E | 65 | ASP | CB-CG-OD1 | 9.59 | 126.93 | 118.30 |
| 1 | F | 110 | SER | CA-CB-OG | -9.59 | 85.30 | 111.20 |
| 1 | A | 3 | ILE | N-CA-CB | -9.59 | 88.75 | 110.80 |
| 1 | B | 169 | ASP | OD1-CG-OD2 | 9.59 | 141.52 | 123.30 |
| 1 | B | 79 | TRP | CD1-CG-CD2 | -9.58 | 98.63 | 106.30 |
| 1 | C | 64 | SER | N-CA-CB | -9.58 | 96.13 | 110.50 |
| 1 | F | 77 | ILE | N-CA-CB | -9.58 | 88.76 | 110.80 |
| 1 | C | 146 | SER | N-CA-CB | -9.58 | 96.13 | 110.50 |
| 1 | D | 52 | THR | CA-CB-CG2 | 9.58 | 125.81 | 112.40 |
| 1 | E | 161 | ASN | CB-CG-OD1 | -9.58 | 102.45 | 121.60 |
| 1 | E | 167 | ARG | CA-C-N | 9.57 | 138.26 | 117.20 |
| 1 | A | 19 | ALA | CA-C-O | -9.57 | 100.01 | 120.10 |
| 1 | B | 68 | LEU | CB-CA-C | 9.56 | 128.37 | 110.20 |
| 1 | B | 214 | ARG | CG-CD-NE | 9.55 | 131.86 | 111.80 |
| 1 | B | 225 | LEU | N-CA-CB | 9.55 | 129.51 | 110.40 |
| 1 | E | 137 | HIS | CB-CG-ND1 | 9.55 | 147.09 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 44 | ASP | CA-C-N | 9.55 | 138.22 | 117.20 |
| 1 | C | 99 | THR | N-CA-CB | -9.55 | 92.16 | 110.30 |
| 1 | D | 217 | PHE | CA-C-N | 9.55 | 138.21 | 117.20 |
| 1 | F | 180 | GLY | CA-C-O | -9.54 | 103.43 | 120.60 |
| 1 | A | 20 | ALA | CA-C-N | -9.54 | 96.22 | 117.20 |
| 1 | D | 230 | GLY | CA-C-N | 9.54 | 138.18 | 117.20 |
| 1 | B | 129 | TYR | CB-CG-CD1 | 9.52 | 126.71 | 121.00 |
| 1 | B | 106 | GLY | CA-C-N | 9.52 | 138.14 | 117.20 |
| 1 | C | 77 | ILE | CG1-CB-CG2 | -9.52 | 90.46 | 111.40 |
| 1 | C | 118 | VAL | O-C-N | -9.51 | 107.49 | 122.70 |
| 1 | C | 41 | PHE | CB-CA-C | -9.51 | 91.39 | 110.40 |
| 1 | F | 72 | THR | CA-CB-OG1 | -9.51 | 89.04 | 109.00 |
| 1 | A | 188 | GLN | CG-CD-OE1 | -9.50 | 102.59 | 121.60 |
| 1 | F | 59 | ARG | NH1-CZ-NH2 | -9.50 | 108.95 | 119.40 |
| 1 | C | 165 | PHE | CB-CG-CD1 | 9.48 | 127.44 | 120.80 |
| 1 | A | 158 | THR | CA-C-O | -9.48 | 100.19 | 120.10 |
| 1 | C | 196 | LEU | CB-CG-CD2 | 9.48 | 127.11 | 111.00 |
| 1 | E | 71 | LEU | CA-C-O | 9.48 | 140.00 | 120.10 |
| 1 | A | 222 | ASP | N-CA-CB | 9.47 | 127.65 | 110.60 |
| 1 | C | 195 | VAL | CG1-CB-CG2 | -9.47 | 95.75 | 110.90 |
| 1 | E | 5 | PHE | C-N-CA | -9.47 | 102.42 | 122.30 |
| 1 | F | 53 | ALA | N-CA-CB | -9.47 | 96.85 | 110.10 |
| 1 | A | 224 | ASN | C-N-CA | -9.46 | 98.04 | 121.70 |
| 1 | C | 145 | GLN | O-C-N | -9.46 | 107.56 | 122.70 |
| 1 | A | 104 | GLY | C-N-CD | -9.46 | 99.79 | 120.60 |
| 1 | F | 105 | PRO | N-CD-CG | 9.46 | 117.39 | 103.20 |
| 1 | A | 209 | SER | CA-CB-OG | -9.46 | 85.67 | 111.20 |
| 1 | A | 179 | LYS | O-C-N | 9.45 | 139.26 | 123.20 |
| 1 | B | 49 | ALA | CB-CA-C | -9.45 | 95.93 | 110.10 |
| 1 | B | 152 | TYR | CE1-CZ-OH | -9.45 | 94.59 | 120.10 |
| 1 | B | 56 | THR | N-CA-C | 9.45 | 136.50 | 111.00 |
| 1 | B | 142 | HIS | CA-C-N | 9.45 | 137.98 | 117.20 |
| 1 | D | 164 | LEU | CA-C-O | -9.45 | 100.26 | 120.10 |
| 1 | D | 63 | GLN | CA-CB-CG | -9.44 | 92.63 | 113.40 |
| 1 | C | 74 | GLN | CG-CD-NE2 | -9.44 | 94.05 | 116.70 |
| 1 | A | 215 | TYR | CG-CD2-CE2 | 9.43 | 128.85 | 121.30 |
| 1 | E | 8 | SER | N-CA-CB | 9.43 | 124.64 | 110.50 |
| 1 | A | 136 | ASN | CB-CA-C | 9.42 | 129.25 | 110.40 |
| 1 | E | 139 | GLN | OE1-CD-NE2 | 9.41 | 143.55 | 121.90 |
| 1 | F | 180 | GLY | CA-C-N | 9.41 | 137.91 | 117.20 |
| 1 | F | 12 | SER | CA-C-O | 9.39 | 139.82 | 120.10 |
| 1 | A | 139 | GLN | O-C-N | 9.39 | 137.72 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 196 | LEU | CA-CB-CG | 9.38 | 136.88 | 115.30 |
| 1 | B | 94 | LEU | CB-CG-CD2 | -9.39 | 95.04 | 111.00 |
| 1 | B | 108 | TRP | CB-CA-C | 9.39 | 129.17 | 110.40 |
| 1 | B | 10 | GLU | C-N-CA | -9.38 | 102.59 | 122.30 |
| 1 | D | 156 | MET | CB-CA-C | -9.38 | 91.63 | 110.40 |
| 1 | D | 217 | PHE | CG-CD2-CE2 | 9.38 | 131.12 | 120.80 |
| 1 | B | 84 | LYS | CB-CA-C | -9.37 | 91.66 | 110.40 |
| 1 | D | 59 | ARG | O-C-N | -9.37 | 107.71 | 122.70 |
| 1 | F | 174 | THR | CA-CB-CG2 | -9.37 | 99.29 | 112.40 |
| 1 | A | 157 | GLU | N-CA-CB | -9.37 | 93.74 | 110.60 |
| 1 | A | 179 | LYS | CA-C-O | -9.37 | 100.43 | 120.10 |
| 1 | C | 228 | TYR | CB-CG-CD2 | -9.37 | 115.38 | 121.00 |
| 1 | E | 14 | PRO | CA-N-CD | -9.36 | 98.39 | 111.50 |
| 1 | A | 204 | TRP | CE2-CD2-CG | 9.36 | 114.79 | 107.30 |
| 1 | F | 65 | ASP | C-N-CA | 9.36 | 141.95 | 122.30 |
| 1 | A | 63 | GLN | CB-CA-C | -9.36 | 91.69 | 110.40 |
| 1 | B | 70 | ILE | CA-C-O | 9.35 | 139.74 | 120.10 |
| 1 | F | 47 | VAL | CA-C-O | -9.35 | 100.46 | 120.10 |
| 1 | F | 55 | ALA | CA-C-N | 9.35 | 137.77 | 117.20 |
| 1 | A | 204 | TRP | CB-CG-CD2 | 9.34 | 138.75 | 126.60 |
| 1 | D | 165 | PHE | CB-CG-CD1 | -9.34 | 114.26 | 120.80 |
| 1 | D | 181 | THR | N-CA-C | -9.34 | 85.78 | 111.00 |
| 1 | E | 159 | ASP | C-N-CA | 9.34 | 145.05 | 121.70 |
| 1 | D | 190 | ASN | O-C-N | -9.34 | 107.33 | 123.20 |
| 1 | C | 222 | ASP | CA-C-O | -9.33 | 100.50 | 120.10 |
| 1 | B | 30 | PHE | CA-CB-CG | -9.33 | 91.51 | 113.90 |
| 1 | F | 160 | CYS | CA-C-O | 9.33 | 139.69 | 120.10 |
| 1 | C | 125 | ASN | N-CA-CB | -9.32 | 93.82 | 110.60 |
| 1 | E | 124 | GLY | N-CA-C | 9.32 | 136.41 | 113.10 |
| 1 | F | 138 | PRO | C-N-CA | -9.32 | 98.39 | 121.70 |
| 1 | F | 192 | ARG | O-C-N | -9.32 | 107.78 | 122.70 |
| 1 | D | 100 | VAL | CA-CB-CG2 | 9.31 | 124.87 | 110.90 |
| 1 | F | 16 | THR | OG1-CB-CG2 | 9.31 | 131.42 | 110.00 |
| 1 | F | 34 | SER | CA-CB-OG | -9.31 | 86.05 | 111.20 |
| 1 | A | 226 | ALA | O-C-N | 9.31 | 137.59 | 122.70 |
| 1 | A | 104 | GLY | O-C-N | 9.30 | 138.77 | 121.10 |
| 1 | D | 71 | LEU | N-CA-CB | -9.30 | 91.80 | 110.40 |
| 1 | A | 26 | SER | N-CA-CB | -9.30 | 96.55 | 110.50 |
| 1 | A | 208 | ASN | CA-C-O | -9.30 | 100.57 | 120.10 |
| 1 | D | 202 | ALA | N-CA-CB | -9.30 | 97.08 | 110.10 |
| 1 | A | 41 | PHE | CG-CD2-CE2 | -9.29 | 110.58 | 120.80 |
| 1 | F | 92 | LEU | CA-C-O | -9.29 | 100.58 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 102 | ILE | CG1-CB-CG2 | -9.29 | 90.96 | 111.40 |
| 1 | F | 165 | PHE | CA-CB-CG | 9.29 | 136.20 | 113.90 |
| 1 | A | 41 | PHE | CB-CG-CD2 | -9.29 | 114.30 | 120.80 |
| 1 | A | 195 | VAL | CG1-CB-CG2 | 9.29 | 125.76 | 110.90 |
| 1 | C | 65 | ASP | CA-C-N | 9.29 | 134.78 | 116.20 |
| 1 | F | 84 | LYS | CA-CB-CG | 9.29 | 133.83 | 113.40 |
| 1 | F | 152 | TYR | N-CA-C | 9.29 | 136.08 | 111.00 |
| 1 | B | 24 | GLU | CA-C-O | -9.29 | 100.60 | 120.10 |
| 1 | F | 199 | GLN | C-N-CA | 9.29 | 144.91 | 121.70 |
| 1 | C | 89 | ASN | O-C-N | 9.28 | 137.55 | 122.70 |
| 1 | C | 200 | ASN | CB-CG-ND2 | 9.28 | 138.97 | 116.70 |
| 1 | D | 232 | LEU | CB-CG-CD1 | -9.28 | 95.23 | 111.00 |
| 1 | B | 68 | LEU | C-N-CA | -9.27 | 98.52 | 121.70 |
| 1 | A | 210 | ARG | NE-CZ-NH2 | -9.27 | 115.67 | 120.30 |
| 1 | D | 35 | ASP | C-N-CA | 9.27 | 144.88 | 121.70 |
| 1 | C | 29 | ARG | CB-CG-CD | 9.27 | 135.69 | 111.60 |
| 1 | A | 184 | ARG | CA-C-O | 9.27 | 139.56 | 120.10 |
| 1 | C | 213 | GLY | CA-C-O | -9.27 | 103.92 | 120.60 |
| 1 | F | 78 | ARG | CA-C-O | 9.27 | 139.56 | 120.10 |
| 1 | A | 184 | ARG | CB-CG-CD | 9.26 | 135.68 | 111.60 |
| 1 | A | 218 | VAL | CA-CB-CG1 | -9.26 | 97.01 | 110.90 |
| 1 | A | 196 | LEU | CD1-CG-CD2 | 9.26 | 138.28 | 110.50 |
| 1 | D | 56 | THR | O-C-N | -9.26 | 107.46 | 123.20 |
| 1 | C | 158 | THR | OG1-CB-CG2 | -9.26 | 88.71 | 110.00 |
| 1 | D | 16 | THR | CA-C-O | -9.25 | 100.67 | 120.10 |
| 1 | E | 127 | ILE | CG1-CB-CG2 | 9.25 | 131.76 | 111.40 |
| 1 | D | 37 | ASN | CA-CB-CG | -9.25 | 93.06 | 113.40 |
| 1 | F | 146 | SER | CA-C-N | 9.24 | 137.54 | 117.20 |
| 1 | B | 33 | GLN | CA-CB-CG | 9.24 | 133.73 | 113.40 |
| 1 | D | 129 | TYR | CA-CB-CG | 9.24 | 130.96 | 113.40 |
| 1 | C | 211 | SER | CA-C-N | 9.24 | 137.53 | 117.20 |
| 1 | D | 5 | PHE | N-CA-CB | -9.24 | 93.97 | 110.60 |
| 1 | A | 48 | TRP | CB-CG-CD2 | 9.24 | 138.61 | 126.60 |
| 1 | C | 153 | ARG | CA-CB-CG | -9.24 | 93.08 | 113.40 |
| 1 | C | 205 | THR | O-C-N | -9.24 | 107.92 | 122.70 |
| 1 | C | 227 | ILE | N-CA-CB | 9.24 | 132.05 | 110.80 |
| 1 | F | 144 | THR | CA-CB-CG2 | 9.24 | 125.33 | 112.40 |
| 1 | A | 204 | TRP | CD1-CG-CD2 | -9.23 | 98.91 | 106.30 |
| 1 | D | 158 | THR | CA-CB-CG2 | -9.23 | 99.48 | 112.40 |
| 1 | D | 129 | TYR | CE1-CZ-CE2 | 9.23 | 134.57 | 119.80 |
| 1 | A | 48 | TRP | CD1-CG-CD2 | -9.23 | 98.92 | 106.30 |
| 1 | F | 143 | ALA | CB-CA-C | -9.23 | 96.26 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 108 | TRP | CD1-CG-CD2 | -9.22 | 98.92 | 106.30 |
| 1 | D | 235 | THR | CA-CB-OG1 | 9.22 | 128.37 | 109.00 |
| 1 | D | 47 | VAL | CG1-CB-CG2 | -9.22 | 96.15 | 110.90 |
| 1 | A | 18 | HIS | CA-C-N | -9.21 | 96.93 | 117.20 |
| 1 | A | 118 | VAL | N-CA-CB | -9.21 | 91.23 | 111.50 |
| 1 | E | 147 | LEU | N-CA-C | 9.21 | 135.88 | 111.00 |
| 1 | E | 99 | THR | O-C-N | -9.21 | 107.96 | 122.70 |
| 1 | F | 152 | TYR | CB-CA-C | -9.21 | 91.98 | 110.40 |
| 1 | B | 211 | SER | O-C-N | 9.21 | 137.43 | 122.70 |
| 1 | C | 186 | VAL | CA-CB-CG2 | -9.20 | 97.10 | 110.90 |
| 1 | C | 192 | ARG | NH1-CZ-NH2 | 9.20 | 129.52 | 119.40 |
| 1 | D | 26 | SER | O-C-N | -9.20 | 107.98 | 122.70 |
| 1 | F | 176 | THR | CA-C-O | 9.20 | 139.42 | 120.10 |
| 1 | C | 50 | SER | N-CA-CB | -9.20 | 96.71 | 110.50 |
| 1 | D | 24 | GLU | CA-C-N | 9.20 | 137.43 | 117.20 |
| 1 | B | 30 | PHE | CB-CG-CD1 | 9.19 | 127.23 | 120.80 |
| 1 | D | 129 | TYR | CA-C-O | -9.19 | 100.81 | 120.10 |
| 1 | E | 21 | GLN | N-CA-CB | -9.19 | 94.06 | 110.60 |
| 1 | A | 87 | ILE | CB-CA-C | 9.19 | 129.97 | 111.60 |
| 1 | F | 128 | LEU | N-CA-C | -9.18 | 86.21 | 111.00 |
| 1 | C | 29 | ARG | N-CA-CB | -9.18 | 94.08 | 110.60 |
| 1 | F | 5 | PHE | CB-CG-CD2 | 9.18 | 127.22 | 120.80 |
| 1 | D | 38 | LEU | CB-CG-CD2 | -9.18 | 95.40 | 111.00 |
| 1 | D | 229 | GLY | CA-C-N | 9.17 | 134.54 | 116.20 |
| 1 | E | 206 | SER | O-C-N | -9.17 | 107.61 | 123.20 |
| 1 | C | 223 | ARG | NE-CZ-NH2 | -9.17 | 115.72 | 120.30 |
| 1 | D | 86 | SER | N-CA-CB | 9.17 | 124.25 | 110.50 |
| 1 | F | 22 | SER | CA-C-O | 9.17 | 139.35 | 120.10 |
| 1 | B | 53 | ALA | CA-C-N | 9.16 | 134.53 | 116.20 |
| 1 | D | 54 | GLY | C-N-CA | 9.16 | 144.60 | 121.70 |
| 1 | F | 86 | SER | CA-C-N | 9.16 | 137.35 | 117.20 |
| 1 | D | 9 | HIS | CB-CA-C | -9.16 | 92.08 | 110.40 |
| 1 | C | 43 | SER | O-C-N | -9.15 | 108.05 | 122.70 |
| 1 | C | 156 | MET | CG-SD-CE | 9.15 | 114.85 | 100.20 |
| 1 | C | 87 | ILE | C-N-CA | -9.15 | 103.08 | 122.30 |
| 1 | C | 114 | ASN | N-CA-CB | -9.14 | 94.14 | 110.60 |
| 1 | F | 84 | LYS | CB-CA-C | -9.14 | 92.11 | 110.40 |
| 1 | D | 5 | PHE | CB-CG-CD1 | 9.14 | 127.20 | 120.80 |
| 1 | C | 41 | PHE | CD1-CE1-CZ | -9.14 | 109.14 | 120.10 |
| 1 | C | 65 | ASP | CB-CG-OD1 | -9.14 | 110.08 | 118.30 |
| 1 | A | 183 | CYS | CB-CA-C | 9.13 | 128.67 | 110.40 |
| 1 | B | 194 | ASP | CB-CA-C | -9.13 | 92.13 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 43 | SER | CA-CB-OG | -9.14 | 86.53 | 111.20 |
| 1 | F | 192 | ARG | C-N-CA | 9.13 | 144.54 | 121.70 |
| 1 | C | 37 | ASN | C-N-CA | 9.13 | 144.53 | 121.70 |
| 1 | A | 118 | VAL | O-C-N | -9.12 | 108.10 | 122.70 |
| 1 | A | 157 | GLU | CA-C-O | -9.12 | 100.94 | 120.10 |
| 1 | C | 150 | SER | CA-CB-OG | -9.12 | 86.56 | 111.20 |
| 1 | B | 24 | GLU | CA-C-N | 9.12 | 137.27 | 117.20 |
| 1 | A | 154 | LEU | C-N-CA | -9.12 | 98.90 | 121.70 |
| 1 | A | 213 | GLY | N-CA-C | -9.12 | 90.31 | 113.10 |
| 1 | B | 212 | ALA | CB-CA-C | 9.12 | 123.78 | 110.10 |
| 1 | C | 160 | CYS | N-CA-CB | 9.12 | 127.01 | 110.60 |
| 1 | C | 164 | LEU | CB-CA-C | -9.11 | 92.89 | 110.20 |
| 1 | F | 1 | ASN | O-C-N | -9.11 | 108.12 | 122.70 |
| 1 | A | 92 | LEU | C-N-CA | 9.11 | 144.47 | 121.70 |
| 1 | E | 69 | VAL | O-C-N | 9.11 | 137.27 | 122.70 |
| 1 | D | 136 | ASN | N-CA-CB | 9.10 | 126.98 | 110.60 |
| 1 | B | 130 | SER | CB-CA-C | 9.10 | 127.39 | 110.10 |
| 1 | D | 12 | SER | CA-CB-OG | 9.09 | 135.74 | 111.20 |
| 1 | C | 71 | LEU | CB-CG-CD1 | 9.09 | 126.45 | 111.00 |
| 1 | F | 13 | HIS | CA-CB-CG | -9.09 | 98.15 | 113.60 |
| 1 | D | 58 | CYS | CA-CB-SG | -9.09 | 97.64 | 114.00 |
| 1 | B | 152 | TYR | OH-CZ-CE2 | 9.08 | 144.62 | 120.10 |
| 1 | C | 101 | THR | N-CA-CB | -9.08 | 93.04 | 110.30 |
| 1 | C | 128 | LEU | CB-CG-CD1 | 9.08 | 126.44 | 111.00 |
| 1 | D | 217 | PHE | CZ-CE2-CD2 | -9.08 | 109.20 | 120.10 |
| 1 | A | 227 | ILE | C-N-CA | 9.08 | 144.40 | 121.70 |
| 1 | B | 14 | PRO | C-N-CA | -9.08 | 99.00 | 121.70 |
| 1 | D | 210 | ARG | NH1-CZ-NH2 | -9.08 | 109.41 | 119.40 |
| 1 | F | 168 | ASP | CB-CG-OD1 | 9.08 | 126.47 | 118.30 |
| 1 | F | 217 | PHE | CA-C-N | 9.08 | 137.17 | 117.20 |
| 1 | A | 113 | SER | C-N-CA | 9.07 | 144.38 | 121.70 |
| 1 | E | 214 | ARG | NE-CZ-NH2 | 9.07 | 124.84 | 120.30 |
| 1 | F | 192 | ARG | NE-CZ-NH2 | 9.07 | 124.84 | 120.30 |
| 1 | F | 61 | VAL | N-CA-CB | 9.07 | 131.45 | 111.50 |
| 1 | A | 5 | PHE | CA-C-O | -9.07 | 101.06 | 120.10 |
| 1 | D | 125 | ASN | N-CA-C | 9.07 | 135.48 | 111.00 |
| 1 | D | 196 | LEU | CA-C-O | 9.07 | 139.14 | 120.10 |
| 1 | E | 210 | ARG | CA-C-O | 9.06 | 139.14 | 120.10 |
| 1 | A | 39 | VAL | CA-CB-CG1 | 9.06 | 124.49 | 110.90 |
| 1 | B | 91 | VAL | CA-CB-CG2 | -9.06 | 97.31 | 110.90 |
| 1 | B | 104 | GLY | CA-C-N | -9.06 | 91.73 | 117.10 |
| 1 | F | 201 | ILE | CA-C-O | -9.06 | 101.07 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 17 | LEU | CA-CB-CG | 9.06 | 136.13 | 115.30 |
| 1 | F | 104 | GLY | CA-C-N | -9.06 | 91.74 | 117.10 |
| 1 | F | 192 | ARG | NH1-CZ-NH2 | -9.06 | 109.44 | 119.40 |
| 1 | E | 235 | THR | CA-CB-CG2 | -9.05 | 99.72 | 112.40 |
| 1 | B | 217 | PHE | CD1-CE1-CZ | -9.05 | 109.24 | 120.10 |
| 1 | C | 46 | ARG | NH1-CZ-NH2 | -9.05 | 109.44 | 119.40 |
| 1 | C | 125 | ASN | CB-CA-C | -9.05 | 92.30 | 110.40 |
| 1 | B | 46 | ARG | CD-NE-CZ | 9.05 | 136.27 | 123.60 |
| 1 | C | 182 | GLY | CA-C-O | -9.05 | 104.31 | 120.60 |
| 1 | D | 105 | PRO | C-N-CA | 9.05 | 141.30 | 122.30 |
| 1 | C | 83 | THR | N-CA-CB | 9.05 | 127.49 | 110.30 |
| 1 | C | 94 | LEU | CA-C-O | -9.05 | 101.10 | 120.10 |
| 1 | B | 159 | ASP | OD1-CG-OD2 | 9.04 | 140.48 | 123.30 |
| 1 | F | 6 | GLY | O-C-N | -9.04 | 108.23 | 122.70 |
| 1 | A | 217 | PHE | CB-CG-CD2 | 9.04 | 127.13 | 120.80 |
| 1 | C | 10 | GLU | N-CA-CB | -9.03 | 94.34 | 110.60 |
| 1 | B | 6 | GLY | CA-C-N | 9.03 | 137.06 | 117.20 |
| 1 | C | 67 | LEU | CB-CA-C | 9.03 | 127.35 | 110.20 |
| 1 | F | 20 | ALA | CA-C-O | 9.02 | 139.05 | 120.10 |
| 1 | A | 228 | TYR | CG-CD2-CE2 | 9.02 | 128.52 | 121.30 |
| 1 | F | 167 | ARG | NE-CZ-NH1 | -9.02 | 115.79 | 120.30 |
| 1 | B | 24 | GLU | CA-CB-CG | 9.02 | 133.24 | 113.40 |
| 1 | B | 79 | TRP | CA-C-O | -9.02 | 101.16 | 120.10 |
| 1 | C | 183 | CYS | N-CA-CB | -9.02 | 94.37 | 110.60 |
| 1 | B | 138 | PRO | C-N-CA | -9.01 | 99.17 | 121.70 |
| 1 | C | 93 | VAL | CA-C-N | 9.01 | 137.03 | 117.20 |
| 1 | B | 25 | LEU | C-N-CA | 9.01 | 144.22 | 121.70 |
| 1 | F | 29 | ARG | CA-C-O | 9.01 | 139.02 | 120.10 |
| 1 | D | 108 | TRP | CH2-CZ2-CE2 | 9.01 | 126.41 | 117.40 |
| 1 | D | 186 | VAL | C-N-CA | -9.00 | 99.19 | 121.70 |
| 1 | F | 223 | ARG | CG-CD-NE | 9.00 | 130.70 | 111.80 |
| 1 | C | 166 | ASP | OD1-CG-OD2 | 9.00 | 140.40 | 123.30 |
| 1 | E | 211 | SER | CA-CB-OG | 9.00 | 135.50 | 111.20 |
| 1 | B | 101 | THR | N-CA-C | 9.00 | 135.29 | 111.00 |
| 1 | C | 206 | SER | CA-C-O | 9.00 | 138.99 | 120.10 |
| 1 | B | 19 | ALA | N-CA-CB | -8.99 | 97.51 | 110.10 |
| 1 | E | 139 | GLN | CG-CD-OE1 | -8.99 | 103.62 | 121.60 |
| 1 | C | 102 | ILE | CA-CB-CG2 | 8.99 | 128.88 | 110.90 |
| 1 | D | 192 | ARG | CB-CA-C | 8.99 | 128.37 | 110.40 |
| 1 | C | 41 | PHE | CZ-CE2-CD2 | -8.98 | 109.32 | 120.10 |
| 1 | D | 190 | ASN | N-CA-CB | -8.98 | 94.43 | 110.60 |
| 1 | F | 136 | ASN | CA-C-N | 8.98 | 136.96 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 176 | THR | OG1-CB-CG2 | -8.98 | 89.35 | 110.00 |
| 1 | D | 1 | ASN | CA-CB-CG | 8.98 | 133.15 | 113.40 |
| 1 | E | 165 | PHE | CB-CG-CD1 | 8.98 | 127.08 | 120.80 |
| 1 | A | 83 | THR | OG1-CB-CG2 | 8.97 | 130.64 | 110.00 |
| 1 | C | 198 | ASN | CB-CG-ND2 | 8.97 | 138.23 | 116.70 |
| 1 | F | 151 | PRO | C-N-CA | 8.97 | 144.13 | 121.70 |
| 1 | C | 146 | SER | CB-CA-C | -8.97 | 93.06 | 110.10 |
| 1 | C | 228 | TYR | N-CA-CB | 8.97 | 126.75 | 110.60 |
| 1 | B | 195 | VAL | CA-C-N | 8.97 | 136.93 | 117.20 |
| 1 | E | 218 | VAL | CA-C-O | -8.97 | 101.27 | 120.10 |
| 1 | C | 225 | LEU | CB-CG-CD2 | -8.96 | 95.76 | 111.00 |
| 1 | E | 230 | GLY | O-C-N | 8.96 | 137.04 | 122.70 |
| 1 | B | 209 | SER | CB-CA-C | -8.96 | 93.08 | 110.10 |
| 1 | B | 192 | ARG | NH1-CZ-NH2 | -8.96 | 109.55 | 119.40 |
| 1 | C | 194 | ASP | CA-CB-CG | 8.95 | 133.10 | 113.40 |
| 1 | D | 70 | ILE | CB-CG1-CD1 | -8.96 | 88.83 | 113.90 |
| 1 | F | 187 | LEU | N-CA-CB | 8.96 | 128.31 | 110.40 |
| 1 | E | 48 | TRP | CD1-NE1-CE2 | 8.95 | 117.06 | 109.00 |
| 1 | F | 146 | SER | N-CA-C | 8.95 | 135.16 | 111.00 |
| 1 | A | 129 | TYR | CE1-CZ-CE2 | -8.95 | 105.49 | 119.80 |
| 1 | B | 90 | TYR | OH-CZ-CE2 | -8.95 | 95.94 | 120.10 |
| 1 | B | 228 | TYR | CB-CG-CD2 | -8.95 | 115.63 | 121.00 |
| 1 | E | 199 | GLN | CB-CA-C | -8.95 | 92.51 | 110.40 |
| 1 | B | 28 | PHE | CA-CB-CG | 8.94 | 135.36 | 113.90 |
| 1 | C | 90 | TYR | CG-CD1-CE1 | 8.94 | 128.45 | 121.30 |
| 1 | A | 199 | GLN | CA-CB-CG | 8.94 | 133.06 | 113.40 |
| 1 | E | 126 | SER | CA-CB-OG | 8.94 | 135.34 | 111.20 |
| 1 | C | 97 | ASP | OD1-CG-OD2 | -8.94 | 106.32 | 123.30 |
| 1 | F | 39 | VAL | CA-CB-CG1 | 8.94 | 124.31 | 110.90 |
| 1 | A | 219 | LEU | N-CA-C | -8.93 | 86.88 | 111.00 |
| 1 | F | 42 | ASP | CB-CG-OD2 | 8.93 | 126.34 | 118.30 |
| 1 | A | 68 | LEU | CA-C-N | 8.93 | 136.84 | 117.20 |
| 1 | C | 182 | GLY | CA-C-N | 8.92 | 136.83 | 117.20 |
| 1 | C | 130 | SER | CA-C-N | -8.92 | 97.58 | 117.20 |
| 1 | F | 19 | ALA | N-CA-CB | 8.92 | 122.59 | 110.10 |
| 1 | C | 165 | PHE | CD1-CG-CD2 | -8.92 | 106.71 | 118.30 |
| 1 | E | 210 | ARG | CD-NE-CZ | -8.92 | 111.11 | 123.60 |
| 1 | B | 78 | ARG | NE-CZ-NH1 | -8.92 | 115.84 | 120.30 |
| 1 | E | 192 | ARG | CB-CA-C | 8.91 | 128.23 | 110.40 |
| 1 | C | 10 | GLU | CA-C-N | 8.91 | 134.02 | 116.20 |
| 1 | A | 233 | TRP | O-C-N | -8.91 | 108.45 | 122.70 |
| 1 | E | 29 | ARG | NH1-CZ-NH2 | -8.91 | 109.60 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 151 | PRO | C-N-CA | 8.91 | 143.97 | 121.70 |
| 1 | A | 214 | ARG | NE-CZ-NH2 | 8.90 | 124.75 | 120.30 |
| 1 | E | 138 | PRO | CA-C-N | -8.90 | 97.61 | 117.20 |
| 1 | B | 222 | ASP | O-C-N | -8.90 | 108.46 | 122.70 |
| 1 | D | 39 | VAL | CB-CA-C | -8.90 | 94.49 | 111.40 |
| 1 | C | 129 | TYR | O-C-N | -8.89 | 108.47 | 122.70 |
| 1 | A | 29 | ARG | NE-CZ-NH2 | 8.89 | 124.75 | 120.30 |
| 1 | E | 3 | ILE | CG1-CB-CG2 | -8.89 | 91.84 | 111.40 |
| 1 | A | 36 | CYS | N-CA-CB | 8.89 | 126.60 | 110.60 |
| 1 | B | 79 | TRP | CD1-NE1-CE2 | -8.89 | 101.00 | 109.00 |
| 1 | A | 48 | TRP | CA-C-O | -8.88 | 101.44 | 120.10 |
| 1 | F | 95 | GLN | CG-CD-NE2 | 8.88 | 138.03 | 116.70 |
| 1 | E | 184 | ARG | NH1-CZ-NH2 | 8.88 | 129.17 | 119.40 |
| 1 | C | 49 | ALA | CA-C-N | 8.88 | 136.73 | 117.20 |
| 1 | A | 12 | SER | N-CA-C | -8.88 | 87.03 | 111.00 |
| 1 | B | 55 | ALA | N-CA-CB | -8.87 | 97.68 | 110.10 |
| 1 | E | 64 | SER | N-CA-CB | 8.86 | 123.79 | 110.50 |
| 1 | F | 37 | ASN | CA-CB-CG | 8.86 | 132.89 | 113.40 |
| 1 | C | 214 | ARG | N-CA-CB | -8.86 | 94.66 | 110.60 |
| 1 | E | 28 | PHE | CB-CG-CD2 | 8.86 | 127.00 | 120.80 |
| 1 | A | 150 | SER | CA-C-O | -8.85 | 101.52 | 120.10 |
| 1 | C | 52 | THR | CA-CB-CG2 | 8.85 | 124.79 | 112.40 |
| 1 | A | 174 | THR | CA-C-O | 8.85 | 138.68 | 120.10 |
| 1 | B | 22 | SER | CA-CB-OG | -8.85 | 87.31 | 111.20 |
| 1 | C | 128 | LEU | CA-C-O | 8.84 | 138.67 | 120.10 |
| 1 | F | 35 | ASP | N-CA-CB | 8.84 | 126.52 | 110.60 |
| 1 | D | 177 | ALA | O-C-N | 8.84 | 138.23 | 123.20 |
| 1 | F | 76 | THR | CA-CB-CG2 | 8.84 | 124.78 | 112.40 |
| 1 | A | 137 | HIS | CB-CG-CD2 | -8.84 | 103.40 | 130.80 |
| 1 | E | 26 | SER | CA-CB-OG | 8.84 | 135.06 | 111.20 |
| 1 | D | 57 | GLY | O-C-N | -8.84 | 108.56 | 122.70 |
| 1 | D | 175 | ASN | CA-CB-CG | 8.84 | 132.84 | 113.40 |
| 1 | F | 139 | GLN | N-CA-CB | -8.84 | 94.70 | 110.60 |
| 1 | C | 224 | ASN | OD1-CG-ND2 | 8.83 | 142.22 | 121.90 |
| 1 | E | 29 | ARG | CG-CD-NE | 8.83 | 130.34 | 111.80 |
| 1 | D | 42 | ASP | OD1-CG-OD2 | 8.82 | 140.06 | 123.30 |
| 1 | A | 222 | ASP | CA-C-O | -8.82 | 101.58 | 120.10 |
| 1 | D | 198 | ASN | OD1-CG-ND2 | 8.82 | 142.18 | 121.90 |
| 1 | C | 40 | LEU | CA-CB-CG | 8.81 | 135.56 | 115.30 |
| 1 | D | 99 | THR | N-CA-C | -8.80 | 87.24 | 111.00 |
| 1 | B | 86 | SER | CA-CB-OG | 8.80 | 134.96 | 111.20 |
| 1 | C | 133 | GLY | CA-C-O | 8.80 | 136.44 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 203 | VAL | CG1-CB-CG2 | 8.80 | 124.98 | 110.90 |
| 1 | C | 168 | ASP | CA-C-N | 8.79 | 136.54 | 117.20 |
| 1 | C | 19 | ALA | CA-C-O | -8.79 | 101.65 | 120.10 |
| 1 | C | 103 | TYR | CA-C-N | 8.79 | 133.78 | 116.20 |
| 1 | D | 31 | THR | N-CA-CB | 8.79 | 126.99 | 110.30 |
| 1 | F | 153 | ARG | CD-NE-CZ | 8.78 | 135.90 | 123.60 |
| 1 | B | 69 | VAL | CA-CB-CG1 | 8.78 | 124.07 | 110.90 |
| 1 | C | 176 | THR | N-CA-CB | -8.78 | 93.61 | 110.30 |
| 1 | F | 185 | ALA | CB-CA-C | 8.78 | 123.27 | 110.10 |
| 1 | C | 205 | THR | N-CA-CB | -8.78 | 93.62 | 110.30 |
| 1 | C | 10 | GLU | CB-CA-C | 8.77 | 127.94 | 110.40 |
| 1 | A | 77 | ILE | CG1-CB-CG2 | -8.77 | 92.11 | 111.40 |
| 1 | A | 145 | GLN | CG-CD-OE1 | -8.77 | 104.06 | 121.60 |
| 1 | A | 215 | TYR | CA-CB-CG | -8.77 | 96.74 | 113.40 |
| 1 | D | 143 | ALA | CA-C-N | 8.77 | 136.49 | 117.20 |
| 1 | D | 163 | VAL | CA-CB-CG2 | -8.77 | 97.75 | 110.90 |
| 1 | F | 64 | SER | O-C-N | -8.76 | 108.69 | 122.70 |
| 1 | F | 50 | SER | N-CA-CB | -8.76 | 97.37 | 110.50 |
| 1 | C | 233 | TRP | CD1-CG-CD2 | -8.75 | 99.30 | 106.30 |
| 1 | E | 148 | GLN | N-CA-CB | -8.75 | 94.84 | 110.60 |
| 1 | D | 125 | ASN | N-CA-CB | -8.75 | 94.85 | 110.60 |
| 1 | C | 228 | TYR | CD1-CE1-CZ | 8.75 | 127.67 | 119.80 |
| 1 | E | 33 | GLN | CB-CG-CD | 8.75 | 134.35 | 111.60 |
| 1 | F | 87 | ILE | N-CA-C | 8.74 | 134.60 | 111.00 |
| 1 | D | 221 | PRO | CB-CA-C | 8.74 | 133.85 | 112.00 |
| 1 | B | 203 | VAL | CB-CA-C | 8.74 | 128.00 | 111.40 |
| 1 | C | 19 | ALA | CB-CA-C | 8.74 | 123.21 | 110.10 |
| 1 | A | 108 | TRP | CE3-CZ3-CH2 | 8.73 | 130.81 | 121.20 |
| 1 | C | 165 | PHE | N-CA-CB | -8.73 | 94.88 | 110.60 |
| 1 | E | 173 | SER | CA-CB-OG | -8.73 | 87.62 | 111.20 |
| 1 | D | 214 | ARG | O-C-N | -8.73 | 108.73 | 122.70 |
| 1 | D | 188 | GLN | CA-CB-CG | 8.73 | 132.60 | 113.40 |
| 1 | F | 202 | ALA | O-C-N | -8.73 | 108.74 | 122.70 |
| 1 | A | 34 | SER | CB-CA-C | 8.72 | 126.67 | 110.10 |
| 1 | A | 32 | MET | N-CA-CB | 8.71 | 126.28 | 110.60 |
| 1 | B | 22 | SER | N-CA-C | 8.71 | 134.53 | 111.00 |
| 1 | C | 16 | THR | CB-CA-C | -8.71 | 88.08 | 111.60 |
| 1 | E | 98 | ARG | CG-CD-NE | -8.71 | 93.50 | 111.80 |
| 1 | F | 30 | PHE | N-CA-CB | -8.71 | 94.92 | 110.60 |
| 1 | A | 160 | CYS | CA-C-O | -8.71 | 101.82 | 120.10 |
| 1 | A | 3 | ILE | CA-CB-CG2 | -8.70 | 93.49 | 110.90 |
| 1 | B | 13 | HIS | CA-CB-CG | -8.70 | 98.81 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 103 | TYR | CB-CG-CD1 | 8.70 | 126.22 | 121.00 |
| 1 | D | 30 | PHE | CB-CG-CD2 | -8.70 | 114.71 | 120.80 |
| 1 | D | 157 | GLU | CG-CD-OE2 | -8.70 | 100.90 | 118.30 |
| 1 | E | 142 | HIS | N-CA-C | 8.70 | 134.48 | 111.00 |
| 1 | D | 95 | GLN | OE1-CD-NE2 | -8.69 | 101.90 | 121.90 |
| 1 | E | 125 | ASN | C-N-CA | 8.70 | 143.44 | 121.70 |
| 1 | B | 205 | THR | CA-CB-OG1 | -8.68 | 90.77 | 109.00 |
| 1 | C | 137 | HIS | CA-C-O | -8.68 | 101.87 | 120.10 |
| 1 | D | 64 | SER | CA-C-N | -8.68 | 98.09 | 117.20 |
| 1 | F | 98 | ARG | CB-CA-C | 8.68 | 127.77 | 110.40 |
| 1 | D | 232 | LEU | CA-CB-CG | 8.68 | 135.26 | 115.30 |
| 1 | A | 228 | TYR | CD1-CG-CD2 | -8.68 | 108.35 | 117.90 |
| 1 | A | 62 | LEU | CB-CG-CD1 | -8.68 | 96.25 | 111.00 |
| 1 | A | 82 | GLY | CA-C-N | -8.68 | 98.11 | 117.20 |
| 1 | C | 69 | VAL | CG1-CB-CG2 | -8.68 | 97.02 | 110.90 |
| 1 | D | 69 | VAL | O-C-N | -8.68 | 108.82 | 122.70 |
| 1 | B | 112 | THR | O-C-N | -8.67 | 108.82 | 122.70 |
| 1 | F | 8 | SER | O-C-N | 8.67 | 136.57 | 122.70 |
| 1 | A | 160 | CYS | N-CA-CB | 8.67 | 126.20 | 110.60 |
| 1 | E | 228 | TYR | CB-CG-CD1 | -8.67 | 115.80 | 121.00 |
| 1 | C | 24 | GLU | CA-C-N | 8.66 | 136.26 | 117.20 |
| 1 | B | 88 | GLY | C-N-CA | 8.66 | 143.35 | 121.70 |
| 1 | C | 158 | THR | N-CA-CB | 8.66 | 126.75 | 110.30 |
| 1 | E | 150 | SER | CA-CB-OG | -8.66 | 87.82 | 111.20 |
| 1 | F | 146 | SER | CA-C-O | -8.66 | 101.91 | 120.10 |
| 1 | C | 200 | ASN | CB-CG-OD1 | -8.66 | 104.28 | 121.60 |
| 1 | F | 127 | ILE | N-CA-CB | 8.65 | 130.70 | 110.80 |
| 1 | B | 110 | SER | CA-CB-OG | -8.65 | 87.84 | 111.20 |
| 1 | B | 229 | GLY | CA-C-O | 8.65 | 136.17 | 120.60 |
| 1 | F | 28 | PHE | CB-CA-C | 8.65 | 127.69 | 110.40 |
| 1 | D | 184 | ARG | C-N-CA | 8.64 | 143.31 | 121.70 |
| 1 | E | 129 | TYR | O-C-N | -8.64 | 108.87 | 122.70 |
| 1 | C | 107 | LEU | O-C-N | 8.64 | 136.53 | 122.70 |
| 1 | E | 61 | VAL | CA-C-O | 8.64 | 138.24 | 120.10 |
| 1 | F | 225 | LEU | CB-CA-C | -8.64 | 93.79 | 110.20 |
| 1 | F | 157 | GLU | CG-CD-OE1 | 8.64 | 135.57 | 118.30 |
| 1 | D | 210 | ARG | NE-CZ-NH2 | 8.63 | 124.62 | 120.30 |
| 1 | F | 141 | LEU | CA-C-N | 8.63 | 136.18 | 117.20 |
| 1 | D | 223 | ARG | CD-NE-CZ | -8.62 | 111.53 | 123.60 |
| 1 | D | 230 | GLY | O-C-N | -8.62 | 108.90 | 122.70 |
| 1 | A | 143 | ALA | N-CA-C | -8.62 | 87.73 | 111.00 |
| 1 | F | 166 | ASP | CA-CB-CG | 8.62 | 132.36 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 104 | GLY | O-C-N | 8.61 | 137.46 | 121.10 |
| 1 | B | 169 | ASP | CB-CG-OD2 | -8.61 | 110.55 | 118.30 |
| 1 | B | 83 | THR | OG1-CB-CG2 | -8.61 | 90.20 | 110.00 |
| 1 | C | 139 | GLN | CG-CD-NE2 | 8.61 | 137.36 | 116.70 |
| 1 | A | 65 | ASP | CB-CG-OD1 | -8.61 | 110.56 | 118.30 |
| 1 | B | 55 | ALA | N-CA-C | 8.61 | 134.24 | 111.00 |
| 1 | C | 207 | GLY | CA-C-N | 8.60 | 136.13 | 117.20 |
| 1 | D | 10 | GLU | C-N-CA | -8.60 | 104.24 | 122.30 |
| 1 | D | 208 | ASN | CB-CG-ND2 | -8.60 | 96.06 | 116.70 |
| 1 | E | 168 | ASP | OD1-CG-OD2 | -8.59 | 106.97 | 123.30 |
| 1 | F | 150 | SER | CB-CA-C | 8.59 | 126.42 | 110.10 |
| 1 | E | 87 | ILE | N-CA-C | 8.59 | 134.19 | 111.00 |
| 1 | F | 87 | ILE | CG1-CB-CG2 | 8.59 | 130.29 | 111.40 |
| 1 | A | 174 | THR | CA-C-N | -8.58 | 98.32 | 117.20 |
| 1 | B | 61 | VAL | CA-C-N | -8.58 | 98.32 | 117.20 |
| 1 | C | 127 | ILE | CG1-CB-CG2 | -8.58 | 92.52 | 111.40 |
| 1 | E | 56 | THR | N-CA-CB | 8.58 | 126.61 | 110.30 |
| 1 | F | 70 | ILE | CA-C-O | 8.58 | 138.12 | 120.10 |
| 1 | D | 46 | ARG | N-CA-CB | -8.58 | 95.16 | 110.60 |
| 1 | F | 18 | HIS | CA-C-O | -8.58 | 102.08 | 120.10 |
| 1 | A | 157 | GLU | OE1-CD-OE2 | -8.57 | 113.01 | 123.30 |
| 1 | C | 30 | PHE | CB-CA-C | 8.57 | 127.55 | 110.40 |
| 1 | B | 1 | ASN | N-CA-C | -8.57 | 87.86 | 111.00 |
| 1 | B | 191 | GLY | C-N-CA | -8.57 | 100.28 | 121.70 |
| 1 | B | 203 | VAL | CG1-CB-CG2 | -8.57 | 97.19 | 110.90 |
| 1 | A | 46 | ARG | CB-CG-CD | 8.57 | 133.87 | 111.60 |
| 1 | C | 174 | THR | CA-CB-OG1 | -8.57 | 91.01 | 109.00 |
| 1 | E | 129 | TYR | CD1-CG-CD2 | -8.56 | 108.48 | 117.90 |
| 1 | C | 10 | GLU | OE1-CD-OE2 | -8.56 | 113.03 | 123.30 |
| 1 | B | 70 | ILE | CA-CB-CG2 | 8.56 | 128.02 | 110.90 |
| 1 | F | 68 | LEU | N-CA-CB | 8.56 | 127.52 | 110.40 |
| 1 | F | 217 | PHE | CA-C-O | -8.56 | 102.13 | 120.10 |
| 1 | E | 162 | LEU | CB-CA-C | 8.56 | 126.46 | 110.20 |
| 1 | F | 69 | VAL | CA-CB-CG1 | 8.55 | 123.73 | 110.90 |
| 1 | F | 129 | TYR | CA-C-N | 8.55 | 136.01 | 117.20 |
| 1 | B | 83 | THR | N-CA-CB | -8.55 | 94.06 | 110.30 |
| 1 | E | 89 | ASN | CB-CG-ND2 | 8.55 | 137.22 | 116.70 |
| 1 | C | 80 | SER | N-CA-CB | 8.55 | 123.32 | 110.50 |
| 1 | E | 142 | HIS | N-CA-CB | -8.54 | 95.23 | 110.60 |
| 1 | C | 234 | THR | CA-C-N | 8.54 | 135.98 | 117.20 |
| 1 | E | 7 | LEU | O-C-N | -8.54 | 109.04 | 122.70 |
| 1 | F | 230 | GLY | CA-C-N | 8.54 | 135.98 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 235 | THR | CA-C-O | 8.54 | 138.03 | 120.10 |
| 1 | A | 1 | ASN | CB-CG-OD1 | -8.53 | 104.53 | 121.60 |
| 1 | A | 63 | GLN | N-CA-C | 8.53 | 134.03 | 111.00 |
| 1 | A | 166 | ASP | CA-C-O | -8.53 | 102.19 | 120.10 |
| 1 | F | 152 | TYR | CA-C-O | -8.53 | 102.19 | 120.10 |
| 1 | C | 36 | CYS | CB-CA-C | -8.52 | 93.36 | 110.40 |
| 1 | D | 45 | VAL | C-N-CA | 8.52 | 143.00 | 121.70 |
| 1 | A | 214 | ARG | CA-C-O | 8.52 | 137.98 | 120.10 |
| 1 | B | 225 | LEU | CB-CG-CD1 | -8.52 | 96.52 | 111.00 |
| 1 | B | 79 | TRP | O-C-N | 8.51 | 136.32 | 122.70 |
| 1 | A | 128 | LEU | O-C-N | -8.51 | 109.08 | 122.70 |
| 1 | E | 154 | LEU | CB-CA-C | -8.51 | 94.03 | 110.20 |
| 1 | F | 234 | THR | CA-CB-OG1 | 8.51 | 126.87 | 109.00 |
| 1 | A | 78 | ARG | CG-CD-NE | 8.50 | 129.66 | 111.80 |
| 1 | F | 3 | ILE | CB-CA-C | -8.50 | 94.60 | 111.60 |
| 1 | A | 216 | VAL | CA-CB-CG2 | 8.50 | 123.65 | 110.90 |
| 1 | A | 42 | ASP | CA-C-N | 8.49 | 135.89 | 117.20 |
| 1 | E | 38 | LEU | C-N-CA | 8.49 | 142.93 | 121.70 |
| 1 | A | 138 | PRO | CA-CB-CG | -8.49 | 87.87 | 104.00 |
| 1 | A | 107 | LEU | CA-C-N | 8.49 | 135.87 | 117.20 |
| 1 | A | 152 | TYR | CG-CD2-CE2 | 8.48 | 128.09 | 121.30 |
| 1 | B | 28 | PHE | N-CA-CB | -8.48 | 95.33 | 110.60 |
| 1 | B | 48 | TRP | CB-CA-C | -8.48 | 93.44 | 110.40 |
| 1 | A | 87 | ILE | CA-CB-CG2 | -8.48 | 93.94 | 110.90 |
| 1 | A | 128 | LEU | C-N-CA | 8.48 | 142.90 | 121.70 |
| 1 | D | 28 | PHE | N-CA-CB | -8.47 | 95.35 | 110.60 |
| 1 | E | 208 | ASN | O-C-N | 8.47 | 136.26 | 122.70 |
| 1 | A | 235 | THR | N-CA-CB | -8.47 | 94.20 | 110.30 |
| 1 | D | 69 | VAL | CA-C-N | 8.47 | 135.84 | 117.20 |
| 1 | D | 179 | LYS | CA-C-N | 8.47 | 133.14 | 116.20 |
| 1 | C | 41 | PHE | CE1-CZ-CE2 | 8.47 | 135.24 | 120.00 |
| 1 | D | 3 | ILE | C-N-CA | 8.47 | 142.87 | 121.70 |
| 1 | B | 21 | GLN | CG-CD-OE1 | -8.46 | 104.67 | 121.60 |
| 1 | C | 43 | SER | CA-CB-OG | 8.46 | 134.06 | 111.20 |
| 1 | A | 91 | VAL | C-N-CA | 8.46 | 142.84 | 121.70 |
| 1 | A | 225 | LEU | CB-CA-C | 8.46 | 126.27 | 110.20 |
| 1 | B | 145 | GLN | CB-CG-CD | 8.46 | 133.59 | 111.60 |
| 1 | C | 29 | ARG | C-N-CA | -8.46 | 100.56 | 121.70 |
| 1 | F | 19 | ALA | CA-C-O | -8.46 | 102.34 | 120.10 |
| 1 | D | 63 | GLN | C-N-CA | -8.45 | 100.57 | 121.70 |
| 1 | A | 78 | ARG | CD-NE-CZ | -8.45 | 111.77 | 123.60 |
| 1 | A | 5 | PHE | O-C-N | -8.45 | 108.84 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 22 | SER | CB-CA-C | -8.45 | 94.04 | 110.10 |
| 1 | E | 63 | GLN | CB-CA-C | -8.45 | 93.50 | 110.40 |
| 1 | F | 203 | VAL | CA-C-O | -8.45 | 102.36 | 120.10 |
| 1 | D | 232 | LEU | CA-C-O | -8.45 | 102.36 | 120.10 |
| 1 | C | 195 | VAL | CA-CB-CG1 | 8.44 | 123.57 | 110.90 |
| 1 | C | 139 | GLN | CA-CB-CG | 8.44 | 131.97 | 113.40 |
| 1 | C | 10 | GLU | C-N-CA | -8.44 | 104.58 | 122.30 |
| 1 | D | 233 | TRP | CD1-NE1-CE2 | -8.44 | 101.41 | 109.00 |
| 1 | B | 138 | PRO | CA-C-O | 8.44 | 140.45 | 120.20 |
| 1 | A | 37 | ASN | CB-CG-OD1 | -8.44 | 104.73 | 121.60 |
| 1 | B | 158 | THR | C-N-CA | 8.44 | 142.79 | 121.70 |
| 1 | D | 192 | ARG | CA-C-N | 8.44 | 135.76 | 117.20 |
| 1 | B | 30 | PHE | CD1-CE1-CZ | -8.43 | 109.98 | 120.10 |
| 1 | D | 172 | TRP | CE2-CD2-CG | 8.43 | 114.05 | 107.30 |
| 1 | C | 65 | ASP | CA-C-O | -8.43 | 102.39 | 120.10 |
| 1 | A | 135 | ASP | OD1-CG-OD2 | 8.43 | 139.31 | 123.30 |
| 1 | B | 194 | ASP | N-CA-C | 8.43 | 133.75 | 111.00 |
| 1 | C | 185 | ALA | CB-CA-C | -8.43 | 97.46 | 110.10 |
| 1 | E | 59 | ARG | CG-CD-NE | -8.43 | 94.10 | 111.80 |
| 1 | F | 44 | ASP | CA-CB-CG | -8.43 | 94.86 | 113.40 |
| 1 | E | 120 | VAL | CA-CB-CG1 | 8.42 | 123.53 | 110.90 |
| 1 | B | 10 | GLU | CB-CA-C | 8.42 | 127.24 | 110.40 |
| 1 | D | 30 | PHE | CG-CD2-CE2 | -8.42 | 111.54 | 120.80 |
| 1 | F | 72 | THR | O-C-N | 8.42 | 136.17 | 122.70 |
| 1 | A | 74 | GLN | N-CA-CB | -8.41 | 95.45 | 110.60 |
| 1 | C | 66 | GLY | C-N-CA | -8.41 | 100.66 | 121.70 |
| 1 | D | 208 | ASN | OD1-CG-ND2 | 8.41 | 141.25 | 121.90 |
| 1 | F | 194 | ASP | N-CA-C | 8.41 | 133.72 | 111.00 |
| 1 | B | 172 | TRP | CH2-CZ2-CE2 | 8.41 | 125.81 | 117.40 |
| 1 | D | 145 | GLN | C-N-CA | 8.41 | 142.72 | 121.70 |
| 1 | F | 13 | HIS | C-N-CD | -8.41 | 102.11 | 120.60 |
| 1 | E | 212 | ALA | CB-CA-C | -8.40 | 97.50 | 110.10 |
| 1 | C | 42 | ASP | N-CA-C | -8.39 | 88.33 | 111.00 |
| 1 | A | 137 | HIS | N-CA-C | 8.39 | 133.66 | 111.00 |
| 1 | A | 198 | ASN | CB-CA-C | -8.39 | 93.62 | 110.40 |
| 1 | B | 109 | ASP | CA-CB-CG | -8.38 | 94.95 | 113.40 |
| 1 | B | 223 | ARG | CB-CG-CD | -8.38 | 89.80 | 111.60 |
| 1 | D | 146 | SER | N-CA-CB | -8.38 | 97.92 | 110.50 |
| 1 | B | 11 | GLY | O-C-N | 8.38 | 136.11 | 122.70 |
| 1 | D | 138 | PRO | C-N-CA | -8.38 | 100.76 | 121.70 |
| 1 | B | 107 | LEU | CA-C-O | -8.38 | 102.51 | 120.10 |
| 1 | B | 110 | SER | CB-CA-C | -8.37 | 94.19 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 214 | ARG | C-N-CA | 8.37 | 142.64 | 121.70 |
| 1 | C | 192 | ARG | CB-CG-CD | 8.37 | 133.37 | 111.60 |
| 1 | D | 21 | GLN | CB-CA-C | 8.37 | 127.13 | 110.40 |
| 1 | E | 173 | SER | CB-CA-C | -8.36 | 94.21 | 110.10 |
| 1 | B | 228 | TYR | N-CA-CB | 8.36 | 125.65 | 110.60 |
| 1 | E | 156 | MET | CA-CB-CG | 8.36 | 127.51 | 113.30 |
| 1 | A | 187 | LEU | CB-CA-C | -8.36 | 94.32 | 110.20 |
| 1 | F | 235 | THR | CA-C-O | 8.36 | 137.66 | 120.10 |
| 1 | B | 41 | PHE | CB-CG-CD1 | 8.36 | 126.65 | 120.80 |
| 1 | B | 201 | ILE | C-N-CA | 8.35 | 142.58 | 121.70 |
| 1 | E | 114 | ASN | CB-CG-OD1 | -8.35 | 104.90 | 121.60 |
| 1 | C | 207 | GLY | N-CA-C | 8.35 | 133.97 | 113.10 |
| 1 | E | 161 | ASN | CB-CA-C | 8.35 | 127.10 | 110.40 |
| 1 | B | 99 | THR | N-CA-CB | 8.35 | 126.16 | 110.30 |
| 1 | C | 197 | THR | CA-C-N | -8.35 | 98.84 | 117.20 |
| 1 | D | 90 | TYR | CA-C-O | -8.35 | 102.57 | 120.10 |
| 1 | E | 200 | ASN | N-CA-CB | 8.35 | 125.62 | 110.60 |
| 1 | A | 125 | ASN | CA-CB-CG | 8.34 | 131.76 | 113.40 |
| 1 | A | 38 | LEU | CA-CB-CG | -8.34 | 96.11 | 115.30 |
| 1 | A | 7 | LEU | CB-CG-CD1 | 8.34 | 125.18 | 111.00 |
| 1 | D | 137 | HIS | CB-CA-C | -8.34 | 93.72 | 110.40 |
| 1 | E | 85 | GLY | N-CA-C | -8.34 | 92.25 | 113.10 |
| 1 | C | 119 | VAL | CA-CB-CG1 | 8.34 | 123.41 | 110.90 |
| 1 | E | 149 | LEU | O-C-N | 8.34 | 136.04 | 122.70 |
| 1 | A | 184 | ARG | N-CA-CB | 8.33 | 125.60 | 110.60 |
| 1 | F | 195 | VAL | N-CA-CB | 8.33 | 129.83 | 111.50 |
| 1 | D | 61 | VAL | N-CA-C | 8.33 | 133.49 | 111.00 |
| 1 | E | 202 | ALA | C-N-CA | 8.33 | 142.52 | 121.70 |
| 1 | E | 152 | TYR | CD1-CG-CD2 | -8.32 | 108.75 | 117.90 |
| 1 | F | 26 | SER | O-C-N | -8.32 | 109.39 | 122.70 |
| 1 | D | 42 | ASP | N-CA-CB | 8.32 | 125.57 | 110.60 |
| 1 | C | 173 | SER | CA-CB-OG | -8.32 | 88.74 | 111.20 |
| 1 | F | 125 | ASN | N-CA-CB | -8.32 | 95.63 | 110.60 |
| 1 | C | 27 | SER | CA-C-O | 8.31 | 137.56 | 120.10 |
| 1 | F | 223 | ARG | C-N-CA | 8.31 | 142.49 | 121.70 |
| 1 | B | 68 | LEU | CB-CG-CD2 | 8.31 | 125.13 | 111.00 |
| 1 | D | 136 | ASN | CA-C-O | -8.31 | 102.65 | 120.10 |
| 1 | E | 73 | ALA | C-N-CA | 8.31 | 142.48 | 121.70 |
| 1 | B | 196 | LEU | O-C-N | -8.31 | 109.41 | 122.70 |
| 1 | E | 109 | ASP | O-C-N | 8.31 | 135.99 | 122.70 |
| 1 | F | 215 | TYR | CD1-CE1-CZ | -8.31 | 112.32 | 119.80 |
| 1 | E | 216 | VAL | O-C-N | -8.30 | 109.41 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 228 | TYR | CA-C-O | -8.30 | 102.66 | 120.10 |
| 1 | A | 188 | GLN | N-CA-C | 8.30 | 133.41 | 111.00 |
| 1 | A | 28 | PHE | CB-CG-CD1 | 8.30 | 126.61 | 120.80 |
| 1 | C | 11 | GLY | CA-C-N | 8.30 | 135.46 | 117.20 |
| 1 | F | 169 | ASP | CB-CA-C | 8.30 | 127.00 | 110.40 |
| 1 | C | 25 | LEU | CB-CG-CD2 | -8.30 | 96.89 | 111.00 |
| 1 | D | 28 | PHE | CB-CG-CD2 | 8.30 | 126.61 | 120.80 |
| 1 | E | 105 | PRO | N-CA-CB | 8.29 | 113.25 | 103.30 |
| 1 | E | 205 | THR | CA-CB-CG2 | -8.29 | 100.79 | 112.40 |
| 1 | F | 17 | LEU | CB-CG-CD2 | -8.29 | 96.90 | 111.00 |
| 1 | F | 105 | PRO | N-CA-C | 8.29 | 133.67 | 112.10 |
| 1 | C | 2 | ASN | O-C-N | -8.29 | 109.43 | 122.70 |
| 1 | F | 196 | LEU | N-CA-C | 8.29 | 133.39 | 111.00 |
| 1 | F | 234 | THR | CA-CB-CG2 | 8.29 | 124.00 | 112.40 |
| 1 | B | 56 | THR | O-C-N | -8.29 | 109.11 | 123.20 |
| 1 | D | 183 | CYS | CA-CB-SG | 8.29 | 128.92 | 114.00 |
| 1 | F | 144 | THR | N-CA-CB | 8.29 | 126.04 | 110.30 |
| 1 | C | 50 | SER | CA-C-N | 8.28 | 135.42 | 117.20 |
| 1 | F | 206 | SER | O-C-N | -8.29 | 109.11 | 123.20 |
| 1 | D | 173 | SER | CB-CA-C | -8.28 | 94.36 | 110.10 |
| 1 | A | 143 | ALA | CA-C-N | 8.28 | 135.42 | 117.20 |
| 1 | A | 98 | ARG | NE-CZ-NH1 | -8.28 | 116.16 | 120.30 |
| 1 | A | 145 | GLN | CB-CA-C | 8.28 | 126.95 | 110.40 |
| 1 | D | 100 | VAL | CA-C-N | 8.28 | 135.41 | 117.20 |
| 1 | A | 170 | ARG | NE-CZ-NH1 | 8.27 | 124.44 | 120.30 |
| 1 | D | 77 | ILE | CA-CB-CG1 | 8.27 | 126.72 | 111.00 |
| 1 | B | 38 | LEU | O-C-N | 8.27 | 135.93 | 122.70 |
| 1 | E | 150 | SER | N-CA-CB | 8.27 | 122.90 | 110.50 |
| 1 | B | 108 | TRP | C-N-CA | 8.26 | 142.36 | 121.70 |
| 1 | C | 141 | LEU | CA-CB-CG | 8.26 | 134.31 | 115.30 |
| 1 | A | 17 | LEU | CB-CG-CD1 | -8.26 | 96.96 | 111.00 |
| 1 | B | 124 | GLY | CA-C-O | 8.26 | 135.47 | 120.60 |
| 1 | C | 22 | SER | C-N-CA | 8.26 | 142.35 | 121.70 |
| 1 | E | 229 | GLY | C-N-CA | -8.26 | 104.95 | 122.30 |
| 1 | B | 131 | THR | OG1-CB-CG2 | -8.26 | 91.01 | 110.00 |
| 1 | E | 30 | PHE | C-N-CA | 8.26 | 142.34 | 121.70 |
| 1 | B | 213 | GLY | O-C-N | -8.26 | 109.49 | 122.70 |
| 1 | F | 214 | ARG | CA-CB-CG | 8.26 | 131.57 | 113.40 |
| 1 | D | 204 | TRP | CB-CG-CD1 | -8.26 | 116.27 | 127.00 |
| 1 | F | 232 | LEU | N-CA-C | 8.25 | 133.28 | 111.00 |
| 1 | D | 139 | GLN | CA-CB-CG | 8.25 | 131.55 | 113.40 |
| 1 | F | 195 | VAL | CA-C-O | -8.25 | 102.77 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 149 | LEU | CB-CA-C | -8.25 | 94.53 | 110.20 |
| 1 | A | 194 | ASP | C-N-CA | -8.25 | 101.09 | 121.70 |
| 1 | C | 131 | THR | OG1-CB-CG2 | -8.25 | 91.03 | 110.00 |
| 1 | B | 2 | ASN | CA-CB-CG | 8.24 | 131.54 | 113.40 |
| 1 | E | 123 | ASN | C-N-CA | 8.24 | 139.61 | 122.30 |
| 1 | E | 233 | TRP | CA-C-O | -8.24 | 102.78 | 120.10 |
| 1 | F | 37 | ASN | OD1-CG-ND2 | 8.24 | 140.86 | 121.90 |
| 1 | F | 196 | LEU | CB-CA-C | -8.24 | 94.54 | 110.20 |
| 1 | A | 33 | GLN | CA-C-N | -8.24 | 99.07 | 117.20 |
| 1 | A | 227 | ILE | CG1-CB-CG2 | -8.24 | 93.27 | 111.40 |
| 1 | C | 206 | SER | N-CA-CB | -8.24 | 98.14 | 110.50 |
| 1 | D | 155 | SER | CA-CB-OG | -8.24 | 88.96 | 111.20 |
| 1 | F | 175 | ASN | N-CA-CB | 8.24 | 125.42 | 110.60 |
| 1 | B | 55 | ALA | CB-CA-C | 8.23 | 122.44 | 110.10 |
| 1 | C | 204 | TRP | CZ3-CH2-CZ2 | -8.23 | 111.73 | 121.60 |
| 1 | B | 107 | LEU | N-CA-CB | 8.22 | 126.85 | 110.40 |
| 1 | B | 159 | ASP | O-C-N | -8.22 | 109.54 | 122.70 |
| 1 | C | 154 | LEU | CA-C-N | 8.22 | 135.29 | 117.20 |
| 1 | D | 194 | ASP | CA-CB-CG | -8.22 | 95.31 | 113.40 |
| 1 | A | 152 | TYR | CB-CG-CD1 | -8.22 | 116.07 | 121.00 |
| 1 | E | 1 | ASN | CB-CA-C | 8.22 | 126.83 | 110.40 |
| 1 | B | 137 | HIS | CB-CA-C | -8.21 | 93.97 | 110.40 |
| 1 | A | 219 | LEU | CA-CB-CG | 8.21 | 134.19 | 115.30 |
| 1 | C | 95 | GLN | CG-CD-NE2 | -8.21 | 96.99 | 116.70 |
| 1 | D | 114 | ASN | CA-CB-CG | 8.21 | 131.47 | 113.40 |
| 1 | E | 15 | GLN | CB-CA-C | 8.21 | 126.82 | 110.40 |
| 1 | C | 143 | ALA | N-CA-C | -8.21 | 88.84 | 111.00 |
| 1 | D | 2 | ASN | CB-CA-C | -8.21 | 93.99 | 110.40 |
| 1 | B | 129 | TYR | N-CA-C | 8.20 | 133.15 | 111.00 |
| 1 | B | 217 | PHE | N-CA-CB | -8.20 | 95.84 | 110.60 |
| 1 | E | 233 | TRP | CD1-CG-CD2 | -8.20 | 99.74 | 106.30 |
| 1 | C | 27 | SER | CB-CA-C | 8.20 | 125.68 | 110.10 |
| 1 | E | 198 | ASN | N-CA-CB | -8.20 | 95.85 | 110.60 |
| 1 | E | 233 | TRP | O-C-N | 8.20 | 135.81 | 122.70 |
| 1 | F | 94 | LEU | N-CA-C | -8.19 | 88.89 | 111.00 |
| 1 | F | 165 | PHE | CA-C-O | -8.19 | 102.91 | 120.10 |
| 1 | F | 224 | ASN | CB-CA-C | 8.19 | 126.78 | 110.40 |
| 1 | A | 167 | ARG | CA-C-N | 8.18 | 135.20 | 117.20 |
| 1 | E | 233 | TRP | CA-CB-CG | 8.18 | 129.25 | 113.70 |
| 1 | F | 145 | GLN | OE1-CD-NE2 | 8.18 | 140.71 | 121.90 |
| 1 | D | 125 | ASN | CB-CA-C | -8.17 | 94.06 | 110.40 |
| 1 | E | 136 | ASN | O-C-N | -8.17 | 109.63 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 5 | PHE | N-CA-CB | 8.17 | 125.30 | 110.60 |
| 1 | E | 113 | SER | N-CA-CB | 8.17 | 122.75 | 110.50 |
| 1 | C | 28 | PHE | CB-CA-C | 8.16 | 126.72 | 110.40 |
| 1 | C | 190 | ASN | CB-CG-OD1 | -8.16 | 105.28 | 121.60 |
| 1 | B | 26 | SER | N-CA-CB | -8.16 | 98.27 | 110.50 |
| 1 | C | 6 | GLY | CA-C-O | -8.15 | 105.93 | 120.60 |
| 1 | D | 128 | LEU | CB-CG-CD2 | 8.15 | 124.86 | 111.00 |
| 1 | C | 198 | ASN | N-CA-CB | -8.15 | 95.93 | 110.60 |
| 1 | E | 194 | ASP | OD1-CG-OD2 | -8.15 | 107.82 | 123.30 |
| 1 | E | 71 | LEU | CA-C-N | -8.15 | 99.28 | 117.20 |
| 1 | B | 55 | ALA | C-N-CA | 8.14 | 142.06 | 121.70 |
| 1 | D | 176 | THR | O-C-N | -8.14 | 109.67 | 122.70 |
| 1 | B | 209 | SER | C-N-CA | -8.14 | 101.34 | 121.70 |
| 1 | B | 64 | SER | CA-CB-OG | -8.14 | 89.22 | 111.20 |
| 1 | E | 5 | PHE | CG-CD2-CE2 | 8.14 | 129.75 | 120.80 |
| 1 | D | 16 | THR | CB-CA-C | -8.14 | 89.63 | 111.60 |
| 1 | C | 48 | TRP | CA-C-O | -8.14 | 103.02 | 120.10 |
| 1 | C | 150 | SER | CA-C-O | -8.14 | 103.01 | 120.10 |
| 1 | F | 131 | THR | OG1-CB-CG2 | 8.14 | 128.71 | 110.00 |
| 1 | A | 170 | ARG | CB-CA-C | 8.13 | 126.67 | 110.40 |
| 1 | B | 69 | VAL | N-CA-CB | 8.13 | 129.39 | 111.50 |
| 1 | C | 38 | LEU | CB-CG-CD1 | 8.13 | 124.83 | 111.00 |
| 1 | B | 175 | ASN | C-N-CA | 8.13 | 142.03 | 121.70 |
| 1 | D | 108 | TRP | CD1-CG-CD2 | -8.13 | 99.80 | 106.30 |
| 1 | F | 63 | GLN | CB-CG-CD | 8.13 | 132.74 | 111.60 |
| 1 | D | 108 | TRP | CG-CD1-NE1 | 8.13 | 118.23 | 110.10 |
| 1 | A | 121 | ALA | C-N-CA | 8.12 | 142.01 | 121.70 |
| 1 | F | 214 | ARG | NE-CZ-NH1 | 8.13 | 124.36 | 120.30 |
| 1 | B | 57 | GLY | O-C-N | -8.12 | 109.70 | 122.70 |
| 1 | B | 80 | SER | CB-CA-C | -8.12 | 94.67 | 110.10 |
| 1 | E | 153 | ARG | NE-CZ-NH2 | 8.12 | 124.36 | 120.30 |
| 1 | B | 155 | SER | C-N-CA | 8.12 | 141.99 | 121.70 |
| 1 | C | 138 | PRO | CB-CA-C | -8.11 | 91.72 | 112.00 |
| 1 | B | 148 | GLN | CB-CG-CD | 8.11 | 132.69 | 111.60 |
| 1 | C | 61 | VAL | N-CA-CB | 8.11 | 129.35 | 111.50 |
| 1 | A | 108 | TRP | CD2-CE3-CZ3 | -8.11 | 108.26 | 118.80 |
| 1 | E | 81 | SER | C-N-CA | -8.11 | 105.27 | 122.30 |
| 1 | A | 89 | ASN | N-CA-CB | -8.11 | 96.01 | 110.60 |
| 1 | B | 21 | GLN | N-CA-CB | 8.11 | 125.19 | 110.60 |
| 1 | C | 29 | ARG | CD-NE-CZ | 8.11 | 134.95 | 123.60 |
| 1 | D | 32 | MET | C-N-CA | -8.11 | 101.44 | 121.70 |
| 1 | E | 87 | ILE | CA-CB-CG2 | -8.11 | 94.69 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 128 | LEU | CA-C-O | 8.11 | 137.12 | 120.10 |
| 1 | F | 232 | LEU | CA-C-N | 8.11 | 135.03 | 117.20 |
| 1 | B | 29 | ARG | CG-CD-NE | 8.10 | 128.82 | 111.80 |
| 1 | A | 108 | TRP | CA-C-N | 8.10 | 135.03 | 117.20 |
| 1 | D | 61 | VAL | C-N-CA | 8.10 | 141.96 | 121.70 |
| 1 | B | 40 | LEU | CB-CG-CD2 | -8.10 | 97.23 | 111.00 |
| 1 | B | 54 | GLY | O-C-N | 8.10 | 135.66 | 122.70 |
| 1 | E | 31 | THR | O-C-N | -8.10 | 109.74 | 122.70 |
| 1 | F | 163 | VAL | CA-CB-CG2 | -8.10 | 98.75 | 110.90 |
| 1 | B | 138 | PRO | CA-C-N | -8.10 | 99.39 | 117.20 |
| 1 | B | 227 | ILE | CB-CG1-CD1 | -8.10 | 91.23 | 113.90 |
| 1 | A | 157 | GLU | CA-C-N | 8.09 | 135.00 | 117.20 |
| 1 | D | 131 | THR | N-CA-CB | -8.09 | 94.93 | 110.30 |
| 1 | E | 193 | MET | CB-CG-SD | -8.09 | 88.13 | 112.40 |
| 1 | B | 212 | ALA | O-C-N | 8.09 | 136.95 | 123.20 |
| 1 | C | 84 | LYS | CD-CE-NZ | 8.09 | 130.30 | 111.70 |
| 1 | D | 45 | VAL | O-C-N | -8.09 | 109.76 | 122.70 |
| 1 | D | 8 | SER | CA-C-N | -8.09 | 99.41 | 117.20 |
| 1 | B | 189 | PRO | C-N-CA | 8.08 | 141.90 | 121.70 |
| 1 | A | 28 | PHE | CZ-CE2-CD2 | -8.08 | 110.41 | 120.10 |
| 1 | D | 178 | GLY | CA-C-O | 8.08 | 135.14 | 120.60 |
| 1 | A | 166 | ASP | CB-CA-C | -8.07 | 94.26 | 110.40 |
| 1 | F | 144 | THR | CA-C-N | 8.07 | 134.96 | 117.20 |
| 1 | D | 108 | TRP | CD1-NE1-CE2 | -8.07 | 101.74 | 109.00 |
| 1 | D | 214 | ARG | CB-CG-CD | 8.07 | 132.58 | 111.60 |
| 1 | D | 75 | ASN | CB-CG-OD1 | -8.06 | 105.48 | 121.60 |
| 1 | A | 25 | LEU | CD1-CG-CD2 | 8.06 | 134.68 | 110.50 |
| 1 | C | 147 | LEU | CB-CA-C | -8.06 | 94.89 | 110.20 |
| 1 | B | 129 | TYR | CG-CD1-CE1 | -8.06 | 114.85 | 121.30 |
| 1 | D | 40 | LEU | O-C-N | 8.05 | 135.59 | 122.70 |
| 1 | A | 200 | ASN | OD1-CG-ND2 | -8.05 | 103.38 | 121.90 |
| 1 | A | 70 | ILE | O-C-N | -8.05 | 109.82 | 122.70 |
| 1 | A | 186 | VAL | CG1-CB-CG2 | -8.05 | 98.02 | 110.90 |
| 1 | F | 155 | SER | O-C-N | -8.05 | 109.82 | 122.70 |
| 1 | B | 4 | LEU | CA-C-O | -8.05 | 103.20 | 120.10 |
| 1 | B | 235 | THR | N-CA-CB | -8.05 | 95.01 | 110.30 |
| 1 | C | 98 | ARG | CD-NE-CZ | -8.05 | 112.33 | 123.60 |
| 1 | E | 76 | THR | N-CA-CB | -8.05 | 95.01 | 110.30 |
| 1 | F | 69 | VAL | CA-CB-CG2 | 8.05 | 122.97 | 110.90 |
| 1 | F | 234 | THR | C-N-CA | 8.05 | 141.82 | 121.70 |
| 1 | D | 79 | TRP | CH2-CZ2-CE2 | 8.04 | 125.44 | 117.40 |
| 1 | F | 204 | TRP | CD1-CG-CD2 | -8.04 | 99.86 | 106.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 158 | THR | CA-C-N | 8.04 | 134.89 | 117.20 |
| 1 | F | 127 | ILE | CA-CB-CG1 | 8.04 | 126.27 | 111.00 |
| 1 | D | 14 | PRO | O-C-N | 8.04 | 135.56 | 122.70 |
| 1 | E | 193 | MET | C-N-CA | 8.04 | 141.79 | 121.70 |
| 1 | F | 98 | ARG | O-C-N | -8.04 | 109.84 | 122.70 |
| 1 | C | 46 | ARG | N-CA-CB | 8.03 | 125.06 | 110.60 |
| 1 | A | 28 | PHE | CG-CD2-CE2 | 8.03 | 129.63 | 120.80 |
| 1 | C | 213 | GLY | CA-C-N | 8.03 | 134.86 | 117.20 |
| 1 | A | 190 | ASN | CA-C-O | 8.03 | 136.96 | 120.10 |
| 1 | B | 98 | ARG | NH1-CZ-NH2 | -8.03 | 110.57 | 119.40 |
| 1 | E | 28 | PHE | N-CA-CB | -8.03 | 96.15 | 110.60 |
| 1 | C | 77 | ILE | CB-CG1-CD1 | 8.02 | 136.36 | 113.90 |
| 1 | C | 196 | LEU | C-N-CA | 8.02 | 141.75 | 121.70 |
| 1 | A | 156 | MET | CA-CB-CG | 8.02 | 126.93 | 113.30 |
| 1 | E | 44 | ASP | N-CA-C | -8.02 | 89.35 | 111.00 |
| 1 | F | 84 | LYS | CA-C-N | 8.02 | 132.23 | 116.20 |
| 1 | A | 149 | LEU | CB-CA-C | -8.01 | 94.98 | 110.20 |
| 1 | A | 101 | THR | CA-CB-CG2 | 8.01 | 123.62 | 112.40 |
| 1 | B | 201 | ILE | CA-C-N | 8.00 | 134.81 | 117.20 |
| 1 | F | 18 | HIS | CA-C-N | 8.00 | 134.81 | 117.20 |
| 1 | B | 131 | THR | N-CA-CB | 7.99 | 125.49 | 110.30 |
| 1 | E | 214 | ARG | CA-CB-CG | 7.99 | 130.98 | 113.40 |
| 1 | A | 176 | THR | CA-CB-OG1 | 7.99 | 125.78 | 109.00 |
| 1 | F | 220 | GLN | OE1-CD-NE2 | -7.99 | 103.53 | 121.90 |
| 1 | A | 114 | ASN | CB-CA-C | -7.99 | 94.43 | 110.40 |
| 1 | C | 44 | ASP | CA-CB-CG | -7.99 | 95.83 | 113.40 |
| 1 | E | 157 | GLU | CA-CB-CG | -7.98 | 95.83 | 113.40 |
| 1 | F | 157 | GLU | O-C-N | 7.98 | 135.47 | 122.70 |
| 1 | C | 157 | GLU | CB-CA-C | 7.98 | 126.36 | 110.40 |
| 1 | C | 43 | SER | N-CA-CB | -7.98 | 98.54 | 110.50 |
| 1 | E | 60 | ALA | O-C-N | -7.98 | 109.94 | 122.70 |
| 1 | A | 33 | GLN | OE1-CD-NE2 | 7.97 | 140.24 | 121.90 |
| 1 | B | 177 | ALA | CA-C-O | 7.97 | 136.83 | 120.10 |
| 1 | D | 59 | ARG | NE-CZ-NH2 | 7.97 | 124.28 | 120.30 |
| 1 | E | 5 | PHE | CB-CA-C | 7.96 | 126.33 | 110.40 |
| 1 | C | 56 | THR | CA-C-O | 7.96 | 136.82 | 120.10 |
| 1 | D | 112 | THR | C-N-CA | 7.96 | 141.60 | 121.70 |
| 1 | B | 101 | THR | CA-C-O | -7.96 | 103.39 | 120.10 |
| 1 | E | 197 | THR | CA-CB-OG1 | -7.96 | 92.29 | 109.00 |
| 1 | B | 32 | MET | CB-CA-C | 7.96 | 126.31 | 110.40 |
| 1 | B | 218 | VAL | CA-CB-CG2 | -7.96 | 98.97 | 110.90 |
| 1 | C | 58 | CYS | CA-C-O | 7.96 | 136.81 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 188 | GLN | N-CA-C | 7.96 | 132.48 | 111.00 |
| 1 | F | 107 | LEU | CB-CA-C | 7.95 | 125.31 | 110.20 |
| 1 | B | 16 | THR | C-N-CA | -7.95 | 101.83 | 121.70 |
| 1 | D | 111 | GLY | C-N-CA | 7.95 | 141.57 | 121.70 |
| 1 | E | 196 | LEU | N-CA-CB | -7.94 | 94.51 | 110.40 |
| 1 | D | 168 | ASP | N-CA-CB | 7.94 | 124.89 | 110.60 |
| 1 | F | 222 | ASP | CB-CG-OD2 | -7.94 | 111.16 | 118.30 |
| 1 | B | 190 | ASN | OD1-CG-ND2 | -7.93 | 103.65 | 121.90 |
| 1 | F | 83 | THR | CA-CB-OG1 | 7.93 | 125.66 | 109.00 |
| 1 | D | 57 | GLY | C-N-CA | 7.93 | 141.53 | 121.70 |
| 1 | C | 51 | ASN | CB-CA-C | 7.93 | 126.26 | 110.40 |
| 1 | D | 42 | ASP | CB-CA-C | -7.93 | 94.54 | 110.40 |
| 1 | C | 22 | SER | O-C-N | -7.93 | 110.01 | 122.70 |
| 1 | A | 155 | SER | O-C-N | 7.93 | 135.38 | 122.70 |
| 1 | C | 121 | ALA | CB-CA-C | 7.93 | 121.99 | 110.10 |
| 1 | F | 223 | ARG | NE-CZ-NH1 | 7.93 | 124.26 | 120.30 |
| 1 | B | 108 | TRP | CG-CD1-NE1 | 7.92 | 118.02 | 110.10 |
| 1 | C | 180 | GLY | N-CA-C | 7.92 | 132.91 | 113.10 |
| 1 | F | 34 | SER | C-N-CA | 7.92 | 141.51 | 121.70 |
| 1 | B | 40 | LEU | CB-CG-CD1 | 7.92 | 124.47 | 111.00 |
| 1 | E | 195 | VAL | CA-CB-CG1 | -7.92 | 99.02 | 110.90 |
| 1 | B | 42 | ASP | CA-CB-CG | 7.92 | 130.82 | 113.40 |
| 1 | D | 110 | SER | CA-CB-OG | -7.92 | 89.82 | 111.20 |
| 1 | F | 87 | ILE | CB-CA-C | -7.92 | 95.77 | 111.60 |
| 1 | C | 232 | LEU | N-CA-CB | -7.91 | 94.57 | 110.40 |
| 1 | D | 189 | PRO | CA-CB-CG | -7.91 | 88.97 | 104.00 |
| 1 | D | 76 | THR | OG1-CB-CG2 | -7.91 | 91.80 | 110.00 |
| 1 | B | 69 | VAL | CG1-CB-CG2 | -7.91 | 98.24 | 110.90 |
| 1 | F | 61 | VAL | CA-C-N | -7.90 | 99.82 | 117.20 |
| 1 | F | 81 | SER | CA-CB-OG | 7.90 | 132.54 | 111.20 |
| 1 | E | 47 | VAL | CB-CA-C | -7.90 | 96.39 | 111.40 |
| 1 | C | 233 | TRP | CG-CD1-NE1 | 7.89 | 117.99 | 110.10 |
| 1 | D | 187 | LEU | CB-CA-C | -7.89 | 95.20 | 110.20 |
| 1 | E | 41 | PHE | N-CA-CB | -7.89 | 96.39 | 110.60 |
| 1 | D | 148 | GLN | CB-CA-C | 7.89 | 126.18 | 110.40 |
| 1 | A | 127 | ILE | CA-CB-CG2 | -7.89 | 95.13 | 110.90 |
| 1 | F | 154 | LEU | N-CA-CB | 7.88 | 126.17 | 110.40 |
| 1 | F | 20 | ALA | N-CA-CB | -7.88 | 99.06 | 110.10 |
| 1 | A | 3 | ILE | CG1-CB-CG2 | 7.88 | 128.74 | 111.40 |
| 1 | C | 90 | TYR | CD1-CE1-CZ | -7.88 | 112.71 | 119.80 |
| 1 | A | 87 | ILE | CB-CG1-CD1 | -7.88 | 91.84 | 113.90 |
| 1 | C | 39 | VAL | CA-C-N | 7.88 | 134.53 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 218 | VAL | CA-CB-CG2 | 7.88 | 122.72 | 110.90 |
| 1 | B | 128 | LEU | CB-CG-CD2 | -7.88 | 97.61 | 111.00 |
| 1 | B | 227 | ILE | CB-CA-C | 7.87 | 127.35 | 111.60 |
| 1 | C | 211 | SER | CA-C-O | -7.87 | 103.57 | 120.10 |
| 1 | D | 193 | MET | CA-C-O | -7.87 | 103.57 | 120.10 |
| 1 | A | 97 | ASP | CA-C-N | 7.87 | 134.51 | 117.20 |
| 1 | E | 26 | SER | N-CA-CB | -7.87 | 98.70 | 110.50 |
| 1 | A | 102 | ILE | CB-CG1-CD1 | 7.87 | 135.92 | 113.90 |
| 1 | F | 206 | SER | CB-CA-C | 7.87 | 125.04 | 110.10 |
| 1 | B | 74 | GLN | CB-CA-C | -7.86 | 94.67 | 110.40 |
| 1 | C | 46 | ARG | CB-CA-C | -7.86 | 94.67 | 110.40 |
| 1 | E | 35 | ASP | OD1-CG-OD2 | -7.86 | 108.36 | 123.30 |
| 1 | B | 41 | PHE | CA-C-N | 7.86 | 134.49 | 117.20 |
| 1 | B | 136 | ASN | CB-CA-C | -7.86 | 94.68 | 110.40 |
| 1 | E | 102 | ILE | CA-CB-CG2 | 7.86 | 126.62 | 110.90 |
| 1 | D | 129 | TYR | C-N-CA | 7.86 | 141.35 | 121.70 |
| 1 | C | 16 | THR | O-C-N | 7.86 | 135.27 | 122.70 |
| 1 | C | 166 | ASP | CA-C-N | 7.86 | 134.49 | 117.20 |
| 1 | D | 96 | PRO | CA-C-O | -7.86 | 101.35 | 120.20 |
| 1 | F | 48 | TRP | CD1-NE1-CE2 | 7.86 | 116.07 | 109.00 |
| 1 | B | 47 | VAL | N-CA-CB | 7.85 | 128.77 | 111.50 |
| 1 | A | 86 | SER | C-N-CA | -7.85 | 102.08 | 121.70 |
| 1 | B | 38 | LEU | CA-C-O | -7.85 | 103.62 | 120.10 |
| 1 | D | 9 | HIS | N-CA-C | 7.85 | 132.19 | 111.00 |
| 1 | A | 192 | ARG | CB-CG-CD | 7.85 | 132.00 | 111.60 |
| 1 | A | 35 | ASP | C-N-CA | 7.84 | 141.31 | 121.70 |
| 1 | D | 9 | HIS | O-C-N | -7.84 | 110.16 | 122.70 |
| 1 | D | 216 | VAL | CA-CB-CG2 | 7.84 | 122.66 | 110.90 |
| 1 | E | 170 | ARG | O-C-N | 7.84 | 135.25 | 122.70 |
| 1 | E | 223 | ARG | CA-CB-CG | 7.84 | 130.65 | 113.40 |
| 1 | A | 139 | GLN | CA-C-N | -7.84 | 99.96 | 117.20 |
| 1 | C | 172 | TRP | CD1-NE1-CE2 | -7.84 | 101.95 | 109.00 |
| 1 | F | 130 | SER | CA-CB-OG | -7.84 | 90.04 | 111.20 |
| 1 | E | 146 | SER | N-CA-C | 7.83 | 132.15 | 111.00 |
| 1 | A | 155 | SER | CB-CA-C | 7.83 | 124.98 | 110.10 |
| 1 | F | 8 | SER | CA-CB-OG | 7.83 | 132.35 | 111.20 |
| 1 | B | 223 | ARG | CG-CD-NE | 7.83 | 128.24 | 111.80 |
| 1 | D | 2 | ASN | N-CA-C | 7.83 | 132.13 | 111.00 |
| 1 | D | 22 | SER | O-C-N | 7.83 | 135.23 | 122.70 |
| 1 | D | 224 | ASN | CA-C-N | 7.83 | 134.42 | 117.20 |
| 1 | B | 226 | ALA | CB-CA-C | 7.83 | 121.84 | 110.10 |
| 1 | E | 125 | ASN | O-C-N | -7.82 | 110.18 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 10 | GLU | N-CA-CB | -7.82 | 96.52 | 110.60 |
| 1 | F | 101 | THR | OG1-CB-CG2 | 7.82 | 127.98 | 110.00 |
| 1 | A | 40 | LEU | CB-CA-C | -7.82 | 95.35 | 110.20 |
| 1 | A | 65 | ASP | N-CA-C | -7.82 | 89.89 | 111.00 |
| 1 | D | 87 | ILE | CB-CA-C | -7.82 | 95.96 | 111.60 |
| 1 | E | 41 | PHE | CZ-CE2-CD2 | -7.82 | 110.72 | 120.10 |
| 1 | E | 71 | LEU | CB-CG-CD2 | -7.82 | 97.71 | 111.00 |
| 1 | A | 118 | VAL | C-N-CA | 7.81 | 141.24 | 121.70 |
| 1 | D | 107 | LEU | O-C-N | 7.81 | 135.20 | 122.70 |
| 1 | F | 85 | GLY | CA-C-N | 7.81 | 134.39 | 117.20 |
| 1 | A | 2 | ASN | N-CA-CB | -7.81 | 96.54 | 110.60 |
| 1 | F | 89 | ASN | CB-CA-C | -7.81 | 94.79 | 110.40 |
| 1 | B | 93 | VAL | CA-C-O | -7.80 | 103.72 | 120.10 |
| 1 | E | 22 | SER | N-CA-CB | 7.80 | 122.20 | 110.50 |
| 1 | D | 1 | ASN | CA-C-O | 7.80 | 136.48 | 120.10 |
| 1 | F | 220 | GLN | CA-C-O | 7.79 | 136.47 | 120.10 |
| 1 | D | 143 | ALA | C-N-CA | 7.79 | 141.18 | 121.70 |
| 1 | D | 149 | LEU | CB-CG-CD2 | 7.79 | 124.25 | 111.00 |
| 1 | A | 235 | THR | CA-C-O | 7.79 | 136.46 | 120.10 |
| 1 | C | 149 | LEU | C-N-CA | -7.79 | 102.22 | 121.70 |
| 1 | F | 201 | ILE | CA-CB-CG2 | -7.79 | 95.32 | 110.90 |
| 1 | F | 152 | TYR | CE1-CZ-OH | -7.79 | 99.08 | 120.10 |
| 1 | F | 231 | ALA | C-N-CA | 7.79 | 141.17 | 121.70 |
| 1 | C | 10 | GLU | CA-C-O | -7.79 | 103.75 | 120.10 |
| 1 | E | 192 | ARG | NH1-CZ-NH2 | 7.79 | 127.97 | 119.40 |
| 1 | B | 152 | TYR | CG-CD2-CE2 | 7.78 | 127.53 | 121.30 |
| 1 | C | 74 | GLN | C-N-CA | 7.78 | 141.16 | 121.70 |
| 1 | B | 38 | LEU | CD1-CG-CD2 | 7.78 | 133.85 | 110.50 |
| 1 | A | 109 | ASP | OD1-CG-OD2 | -7.78 | 108.52 | 123.30 |
| 1 | D | 123 | ASN | C-N-CA | 7.78 | 138.63 | 122.30 |
| 1 | E | 228 | TYR | CA-C-O | 7.78 | 136.43 | 120.10 |
| 1 | B | 30 | PHE | CA-C-N | 7.78 | 134.30 | 117.20 |
| 1 | A | 50 | SER | CA-C-O | 7.77 | 136.42 | 120.10 |
| 1 | E | 73 | ALA | CB-CA-C | 7.77 | 121.75 | 110.10 |
| 1 | A | 90 | TYR | CD1-CG-CD2 | -7.77 | 109.36 | 117.90 |
| 1 | B | 164 | LEU | CB-CG-CD2 | 7.77 | 124.21 | 111.00 |
| 1 | B | 75 | ASN | CA-C-O | -7.76 | 103.80 | 120.10 |
| 1 | F | 70 | ILE | N-CA-CB | -7.76 | 92.94 | 110.80 |
| 1 | E | 190 | ASN | C-N-CA | 7.76 | 138.60 | 122.30 |
| 1 | B | 225 | LEU | CA-C-O | -7.76 | 103.80 | 120.10 |
| 1 | E | 48 | TRP | NE1-CE2-CD2 | -7.76 | 99.54 | 107.30 |
| 1 | A | 34 | SER | CA-CB-OG | 7.76 | 132.15 | 111.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 34 | SER | CB-CA-C | 7.76 | 124.84 | 110.10 |
| 1 | C | 53 | ALA | O-C-N | -7.76 | 110.01 | 123.20 |
| 1 | C | 72 | THR | OG1-CB-CG2 | -7.76 | 92.16 | 110.00 |
| 1 | B | 127 | ILE | C-N-CA | 7.75 | 141.09 | 121.70 |
| 1 | A | 170 | ARG | CA-CB-CG | 7.75 | 130.46 | 113.40 |
| 1 | F | 99 | THR | N-CA-C | -7.75 | 90.07 | 111.00 |
| 1 | A | 166 | ASP | CA-CB-CG | 7.75 | 130.45 | 113.40 |
| 1 | B | 50 | SER | CA-C-N | 7.75 | 134.25 | 117.20 |
| 1 | C | 94 | LEU | N-CA-CB | -7.75 | 94.90 | 110.40 |
| 1 | D | 234 | THR | OG1-CB-CG2 | -7.75 | 92.18 | 110.00 |
| 1 | B | 142 | HIS | ND1-CG-CD2 | -7.75 | 95.16 | 106.00 |
| 1 | F | 190 | ASN | CA-C-O | 7.75 | 136.37 | 120.10 |
| 1 | C | 41 | PHE | CB-CG-CD1 | 7.74 | 126.22 | 120.80 |
| 1 | C | 61 | VAL | N-CA-C | 7.74 | 131.91 | 111.00 |
| 1 | A | 68 | LEU | CA-C-O | -7.74 | 103.84 | 120.10 |
| 1 | E | 197 | THR | C-N-CA | 7.74 | 141.05 | 121.70 |
| 1 | E | 34 | SER | N-CA-CB | -7.74 | 98.89 | 110.50 |
| 1 | D | 7 | LEU | O-C-N | -7.74 | 110.32 | 122.70 |
| 1 | D | 217 | PHE | CA-CB-CG | -7.74 | 95.33 | 113.90 |
| 1 | B | 67 | LEU | O-C-N | -7.74 | 110.32 | 122.70 |
| 1 | A | 14 | PRO | CA-CB-CG | -7.74 | 89.30 | 104.00 |
| 1 | D | 193 | MET | N-CA-C | -7.74 | 90.11 | 111.00 |
| 1 | A | 75 | ASN | OD1-CG-ND2 | 7.73 | 139.69 | 121.90 |
| 1 | D | 107 | LEU | CA-CB-CG | 7.73 | 133.08 | 115.30 |
| 1 | D | 227 | ILE | CA-CB-CG2 | 7.73 | 126.36 | 110.90 |
| 1 | A | 48 | TRP | CD2-CE3-CZ3 | 7.73 | 128.85 | 118.80 |
| 1 | D | 4 | LEU | CB-CA-C | -7.73 | 95.51 | 110.20 |
| 1 | C | 193 | MET | C-N-CA | 7.73 | 141.02 | 121.70 |
| 1 | E | 13 | HIS | N-CA-CB | -7.73 | 96.69 | 110.60 |
| 1 | B | 129 | TYR | OH-CZ-CE2 | -7.72 | 99.24 | 120.10 |
| 1 | F | 50 | SER | CB-CA-C | -7.72 | 95.42 | 110.10 |
| 1 | A | 28 | PHE | O-C-N | 7.72 | 135.06 | 122.70 |
| 1 | C | 44 | ASP | CB-CA-C | -7.72 | 94.95 | 110.40 |
| 1 | D | 205 | THR | O-C-N | -7.72 | 110.34 | 122.70 |
| 1 | F | 182 | GLY | CA-C-O | 7.72 | 134.50 | 120.60 |
| 1 | E | 168 | ASP | CB-CA-C | 7.72 | 125.84 | 110.40 |
| 1 | F | 191 | GLY | C-N-CA | -7.72 | 102.40 | 121.70 |
| 1 | A | 60 | ALA | CB-CA-C | 7.71 | 121.67 | 110.10 |
| 1 | B | 137 | HIS | N-CA-CB | -7.71 | 96.71 | 110.60 |
| 1 | F | 75 | ASN | OD1-CG-ND2 | 7.71 | 139.64 | 121.90 |
| 1 | B | 130 | SER | N-CA-C | -7.71 | 90.18 | 111.00 |
| 1 | D | 24 | GLU | N-CA-CB | -7.71 | 96.72 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 17 | LEU | O-C-N | -7.71 | 110.37 | 122.70 |
| 1 | E | 189 | PRO | CB-CA-C | 7.71 | 131.27 | 112.00 |
| 1 | C | 227 | ILE | CA-C-O | -7.71 | 103.92 | 120.10 |
| 1 | D | 160 | CYS | C-N-CA | 7.70 | 140.96 | 121.70 |
| 1 | E | 45 | VAL | N-CA-CB | 7.70 | 128.45 | 111.50 |
| 1 | B | 30 | PHE | CG-CD2-CE2 | -7.70 | 112.33 | 120.80 |
| 1 | E | 168 | ASP | N-CA-CB | 7.70 | 124.46 | 110.60 |
| 1 | A | 13 | HIS | CA-CB-CG | 7.70 | 126.69 | 113.60 |
| 1 | C | 87 | ILE | O-C-N | 7.70 | 136.29 | 123.20 |
| 1 | C | 132 | GLN | CB-CA-C | 7.70 | 125.80 | 110.40 |
| 1 | E | 32 | MET | CA-C-N | 7.70 | 134.14 | 117.20 |
| 1 | A | 2 | ASN | CA-CB-CG | -7.70 | 96.47 | 113.40 |
| 1 | A | 69 | VAL | O-C-N | 7.70 | 135.02 | 122.70 |
| 1 | A | 74 | GLN | CG-CD-OE1 | -7.70 | 106.20 | 121.60 |
| 1 | A | 223 | ARG | O-C-N | -7.70 | 110.39 | 122.70 |
| 1 | E | 107 | LEU | CB-CG-CD2 | -7.70 | 97.92 | 111.00 |
| 1 | F | 149 | LEU | CA-CB-CG | -7.69 | 97.61 | 115.30 |
| 1 | E | 151 | PRO | C-N-CA | 7.69 | 140.93 | 121.70 |
| 1 | A | 119 | VAL | N-CA-C | 7.69 | 131.76 | 111.00 |
| 1 | F | 79 | TRP | CB-CG-CD2 | 7.68 | 136.59 | 126.60 |
| 1 | A | 31 | THR | CA-CB-CG2 | 7.68 | 123.16 | 112.40 |
| 1 | E | 72 | THR | CA-C-N | -7.68 | 100.30 | 117.20 |
| 1 | A | 224 | ASN | CA-C-O | 7.68 | 136.23 | 120.10 |
| 1 | C | 122 | ASN | C-N-CA | 7.68 | 140.90 | 121.70 |
| 1 | C | 11 | GLY | CA-C-O | -7.68 | 106.78 | 120.60 |
| 1 | E | 138 | PRO | CB-CA-C | -7.67 | 92.81 | 112.00 |
| 1 | F | 47 | VAL | CA-CB-CG2 | -7.67 | 99.39 | 110.90 |
| 1 | D | 74 | GLN | CB-CA-C | -7.67 | 95.06 | 110.40 |
| 1 | C | 160 | CYS | CA-C-O | -7.67 | 104.00 | 120.10 |
| 1 | C | 219 | LEU | CA-C-O | 7.67 | 136.20 | 120.10 |
| 1 | E | 156 | MET | O-C-N | 7.67 | 134.97 | 122.70 |
| 1 | C | 30 | PHE | CD1-CE1-CZ | 7.66 | 129.30 | 120.10 |
| 1 | D | 103 | TYR | CB-CG-CD2 | -7.66 | 116.40 | 121.00 |
| 1 | F | 107 | LEU | CB-CG-CD2 | 7.66 | 124.03 | 111.00 |
| 1 | C | 85 | GLY | CA-C-O | -7.66 | 106.81 | 120.60 |
| 1 | E | 92 | LEU | CA-CB-CG | 7.66 | 132.92 | 115.30 |
| 1 | C | 83 | THR | N-CA-C | -7.66 | 90.31 | 111.00 |
| 1 | E | 97 | ASP | CA-CB-CG | 7.66 | 130.25 | 113.40 |
| 1 | B | 103 | TYR | N-CA-CB | 7.66 | 124.38 | 110.60 |
| 1 | C | 88 | GLY | N-CA-C | 7.66 | 132.24 | 113.10 |
| 1 | B | 221 | PRO | N-CD-CG | -7.65 | 91.72 | 103.20 |
| 1 | A | 207 | GLY | N-CA-C | 7.65 | 132.23 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 10 | GLU | CG-CD-OE2 | 7.65 | 133.60 | 118.30 |
| 1 | A | 10 | GLU | CG-CD-OE2 | -7.65 | 103.00 | 118.30 |
| 1 | A | 192 | ARG | N-CA-CB | -7.65 | 96.83 | 110.60 |
| 1 | B | 36 | CYS | CA-C-N | 7.65 | 134.03 | 117.20 |
| 1 | D | 128 | LEU | CB-CG-CD1 | 7.65 | 124.00 | 111.00 |
| 1 | A | 48 | TRP | O-C-N | 7.64 | 134.93 | 122.70 |
| 1 | C | 164 | LEU | CA-C-O | -7.64 | 104.05 | 120.10 |
| 1 | B | 29 | ARG | CA-C-N | -7.64 | 100.39 | 117.20 |
| 1 | E | 123 | ASN | CA-CB-CG | 7.64 | 130.21 | 113.40 |
| 1 | A | 102 | ILE | CA-CB-CG2 | 7.64 | 126.17 | 110.90 |
| 1 | D | 39 | VAL | C-N-CA | 7.64 | 140.79 | 121.70 |
| 1 | D | 87 | ILE | N-CA-C | 7.64 | 131.62 | 111.00 |
| 1 | A | 129 | TYR | N-CA-CB | 7.63 | 124.34 | 110.60 |
| 1 | C | 233 | TRP | CD2-CE3-CZ3 | -7.63 | 108.88 | 118.80 |
| 1 | D | 173 | SER | C-N-CA | 7.63 | 140.78 | 121.70 |
| 1 | C | 183 | CYS | CB-CA-C | 7.63 | 125.66 | 110.40 |
| 1 | E | 7 | LEU | C-N-CA | 7.63 | 140.77 | 121.70 |
| 1 | B | 192 | ARG | C-N-CA | -7.63 | 102.63 | 121.70 |
| 1 | F | 49 | ALA | CB-CA-C | -7.63 | 98.66 | 110.10 |
| 1 | D | 59 | ARG | CA-CB-CG | 7.63 | 130.18 | 113.40 |
| 1 | E | 46 | ARG | NE-CZ-NH1 | -7.62 | 116.49 | 120.30 |
| 1 | B | 98 | ARG | NE-CZ-NH1 | -7.62 | 116.49 | 120.30 |
| 1 | A | 82 | GLY | C-N-CA | -7.62 | 102.65 | 121.70 |
| 1 | D | 203 | VAL | N-CA-CB | 7.62 | 128.27 | 111.50 |
| 1 | D | 224 | ASN | O-C-N | -7.62 | 110.51 | 122.70 |
| 1 | E | 103 | TYR | CG-CD1-CE1 | 7.62 | 127.40 | 121.30 |
| 1 | F | 78 | ARG | CA-C-N | -7.62 | 100.43 | 117.20 |
| 1 | F | 43 | SER | O-C-N | -7.62 | 110.51 | 122.70 |
| 1 | A | 110 | SER | CA-C-N | -7.62 | 100.96 | 116.20 |
| 1 | B | 50 | SER | O-C-N | -7.62 | 110.51 | 122.70 |
| 1 | E | 34 | SER | N-CA-C | -7.62 | 90.43 | 111.00 |
| 1 | F | 131 | THR | CA-CB-OG1 | -7.62 | 93.00 | 109.00 |
| 1 | F | 165 | PHE | CD1-CE1-CZ | -7.62 | 110.96 | 120.10 |
| 1 | B | 208 | ASN | CA-C-N | -7.61 | 100.45 | 117.20 |
| 1 | F | 149 | LEU | C-N-CA | -7.61 | 102.67 | 121.70 |
| 1 | C | 142 | HIS | CA-CB-CG | 7.61 | 126.54 | 113.60 |
| 1 | C | 94 | LEU | CA-C-N | 7.60 | 133.93 | 117.20 |
| 1 | E | 169 | ASP | C-N-CA | 7.60 | 140.71 | 121.70 |
| 1 | A | 32 | MET | CB-CA-C | -7.60 | 95.20 | 110.40 |
| 1 | A | 40 | LEU | CA-C-O | -7.60 | 104.15 | 120.10 |
| 1 | C | 172 | TRP | CZ3-CH2-CZ2 | -7.60 | 112.48 | 121.60 |
| 1 | F | 36 | CYS | CA-CB-SG | -7.60 | 100.33 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 170 | ARG | CA-C-O | -7.60 | 104.15 | 120.10 |
| 1 | A | 87 | ILE | CG1-CB-CG2 | -7.59 | 94.69 | 111.40 |
| 1 | B | 128 | LEU | CB-CA-C | 7.59 | 124.62 | 110.20 |
| 1 | D | 79 | TRP | CA-C-O | -7.59 | 104.16 | 120.10 |
| 1 | E | 19 | ALA | O-C-N | -7.59 | 110.55 | 122.70 |
| 1 | C | 113 | SER | CB-CA-C | 7.59 | 124.52 | 110.10 |
| 1 | D | 89 | ASN | OD1-CG-ND2 | 7.59 | 139.36 | 121.90 |
| 1 | B | 61 | VAL | N-CA-C | 7.59 | 131.49 | 111.00 |
| 1 | B | 149 | LEU | CA-CB-CG | -7.58 | 97.85 | 115.30 |
| 1 | C | 167 | ARG | CG-CD-NE | 7.58 | 127.73 | 111.80 |
| 1 | E | 99 | THR | N-CA-CB | -7.58 | 95.89 | 110.30 |
| 1 | E | 148 | GLN | CA-CB-CG | 7.58 | 130.08 | 113.40 |
| 1 | B | 5 | PHE | CA-CB-CG | 7.58 | 132.08 | 113.90 |
| 1 | E | 28 | PHE | CD1-CG-CD2 | -7.58 | 108.45 | 118.30 |
| 1 | B | 224 | ASN | CB-CA-C | 7.58 | 125.55 | 110.40 |
| 1 | D | 217 | PHE | CB-CG-CD1 | -7.57 | 115.50 | 120.80 |
| 1 | D | 91 | VAL | CG1-CB-CG2 | -7.57 | 98.79 | 110.90 |
| 1 | E | 112 | THR | O-C-N | -7.57 | 110.59 | 122.70 |
| 1 | F | 39 | VAL | O-C-N | 7.57 | 134.81 | 122.70 |
| 1 | F | 190 | ASN | N-CA-CB | -7.57 | 96.98 | 110.60 |
| 1 | C | 186 | VAL | N-CA-CB | -7.56 | 94.86 | 111.50 |
| 1 | F | 213 | GLY | CA-C-O | -7.56 | 106.99 | 120.60 |
| 1 | D | 154 | LEU | CD1-CG-CD2 | -7.56 | 87.82 | 110.50 |
| 1 | A | 176 | THR | N-CA-C | -7.56 | 90.59 | 111.00 |
| 1 | D | 33 | GLN | CA-C-N | 7.56 | 133.83 | 117.20 |
| 1 | D | 195 | VAL | O-C-N | -7.56 | 110.61 | 122.70 |
| 1 | B | 142 | HIS | ND1-CE1-NE2 | -7.55 | 93.28 | 109.90 |
| 1 | F | 53 | ALA | CA-C-N | 7.55 | 131.30 | 116.20 |
| 1 | B | 63 | GLN | CA-C-N | -7.55 | 100.59 | 117.20 |
| 1 | B | 196 | LEU | CA-C-N | -7.54 | 100.61 | 117.20 |
| 1 | D | 206 | SER | CA-C-N | 7.54 | 131.29 | 116.20 |
| 1 | E | 162 | LEU | CB-CG-CD1 | -7.54 | 98.18 | 111.00 |
| 1 | B | 36 | CYS | CA-C-O | -7.54 | 104.26 | 120.10 |
| 1 | E | 9 | HIS | CA-C-N | -7.54 | 100.61 | 117.20 |
| 1 | B | 184 | ARG | O-C-N | -7.54 | 110.64 | 122.70 |
| 1 | E | 3 | ILE | CB-CG1-CD1 | -7.54 | 92.79 | 113.90 |
| 1 | E | 146 | SER | CB-CA-C | -7.54 | 95.78 | 110.10 |
| 1 | D | 88 | GLY | CA-C-O | -7.54 | 107.03 | 120.60 |
| 1 | D | 227 | ILE | CA-C-O | -7.54 | 104.28 | 120.10 |
| 1 | F | 222 | ASP | CB-CG-OD1 | -7.54 | 111.52 | 118.30 |
| 1 | B | 33 | GLN | N-CA-CB | 7.53 | 124.16 | 110.60 |
| 1 | E | 169 | ASP | OD1-CG-OD2 | 7.53 | 137.61 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 148 | GLN | CB-CG-CD | 7.53 | 131.18 | 111.60 |
| 1 | D | 181 | THR | N-CA-CB | -7.53 | 95.99 | 110.30 |
| 1 | A | 149 | LEU | N-CA-CB | 7.53 | 125.46 | 110.40 |
| 1 | A | 152 | TYR | O-C-N | 7.53 | 134.75 | 122.70 |
| 1 | B | 68 | LEU | CB-CG-CD1 | 7.53 | 123.80 | 111.00 |
| 1 | D | 24 | GLU | CA-C-O | -7.53 | 104.29 | 120.10 |
| 1 | D | 46 | ARG | CA-C-N | 7.53 | 133.76 | 117.20 |
| 1 | E | 216 | VAL | CA-CB-CG1 | -7.53 | 99.61 | 110.90 |
| 1 | D | 198 | ASN | O-C-N | -7.52 | 110.66 | 122.70 |
| 1 | E | 138 | PRO | CA-CB-CG | -7.52 | 89.71 | 104.00 |
| 1 | C | 137 | HIS | CG-ND1-CE1 | -7.52 | 95.93 | 105.70 |
| 1 | C | 118 | VAL | CA-C-O | 7.52 | 135.88 | 120.10 |
| 1 | D | 7 | LEU | CB-CG-CD2 | -7.51 | 98.22 | 111.00 |
| 1 | D | 157 | GLU | N-CA-CB | -7.51 | 97.08 | 110.60 |
| 1 | B | 149 | LEU | C-N-CA | -7.51 | 102.92 | 121.70 |
| 1 | F | 222 | ASP | CA-C-N | 7.51 | 133.73 | 117.20 |
| 1 | A | 82 | GLY | CA-C-O | 7.51 | 134.12 | 120.60 |
| 1 | D | 71 | LEU | CA-C-O | -7.51 | 104.33 | 120.10 |
| 1 | E | 2 | ASN | CB-CG-OD1 | -7.51 | 106.58 | 121.60 |
| 1 | C | 199 | GLN | O-C-N | -7.51 | 110.69 | 122.70 |
| 1 | A | 53 | ALA | C-N-CA | 7.51 | 138.07 | 122.30 |
| 1 | E | 53 | ALA | CB-CA-C | 7.51 | 121.36 | 110.10 |
| 1 | C | 155 | SER | CA-CB-OG | -7.50 | 90.94 | 111.20 |
| 1 | D | 79 | TRP | CZ3-CH2-CZ2 | -7.50 | 112.59 | 121.60 |
| 1 | F | 193 | MET | CA-C-O | -7.50 | 104.34 | 120.10 |
| 1 | F | 195 | VAL | N-CA-C | -7.50 | 90.74 | 111.00 |
| 1 | F | 217 | PHE | CA-CB-CG | -7.50 | 95.89 | 113.90 |
| 1 | A | 3 | ILE | CB-CG1-CD1 | -7.50 | 92.90 | 113.90 |
| 1 | A | 70 | ILE | CA-CB-CG2 | 7.50 | 125.90 | 110.90 |
| 1 | B | 161 | ASN | OD1-CG-ND2 | 7.50 | 139.15 | 121.90 |
| 1 | B | 89 | ASN | C-N-CA | 7.50 | 140.45 | 121.70 |
| 1 | A | 165 | PHE | CB-CG-CD2 | 7.50 | 126.05 | 120.80 |
| 1 | B | 63 | GLN | CG-CD-OE1 | 7.50 | 136.59 | 121.60 |
| 1 | C | 186 | VAL | C-N-CA | 7.50 | 140.44 | 121.70 |
| 1 | D | 139 | GLN | N-CA-CB | 7.49 | 124.09 | 110.60 |
| 1 | D | 192 | ARG | N-CA-CB | -7.49 | 97.11 | 110.60 |
| 1 | E | 210 | ARG | CB-CA-C | 7.49 | 125.39 | 110.40 |
| 1 | D | 108 | TRP | CE2-CD2-CG | 7.49 | 113.29 | 107.30 |
| 1 | D | 107 | LEU | CD1-CG-CD2 | -7.49 | 88.03 | 110.50 |
| 1 | E | 54 | GLY | CA-C-N | 7.49 | 133.67 | 117.20 |
| 1 | F | 7 | LEU | CA-C-N | -7.49 | 100.73 | 117.20 |
| 1 | C | 200 | ASN | O-C-N | -7.48 | 110.73 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 17 | LEU | N-CA-CB | 7.48 | 125.36 | 110.40 |
| 1 | C | 184 | ARG | CA-CB-CG | -7.48 | 96.95 | 113.40 |
| 1 | A | 47 | VAL | CA-C-N | 7.48 | 133.65 | 117.20 |
| 1 | F | 5 | PHE | C-N-CA | 7.48 | 138.00 | 122.30 |
| 1 | E | 18 | HIS | C-N-CA | -7.47 | 103.02 | 121.70 |
| 1 | D | 210 | ARG | O-C-N | 7.47 | 134.65 | 122.70 |
| 1 | D | 75 | ASN | CB-CG-ND2 | -7.46 | 98.78 | 116.70 |
| 1 | D | 169 | ASP | CA-C-O | 7.46 | 135.77 | 120.10 |
| 1 | B | 67 | LEU | CA-C-N | 7.46 | 133.62 | 117.20 |
| 1 | F | 149 | LEU | O-C-N | 7.46 | 134.64 | 122.70 |
| 1 | E | 175 | ASN | CA-C-O | 7.46 | 135.77 | 120.10 |
| 1 | D | 174 | THR | N-CA-CB | 7.46 | 124.47 | 110.30 |
| 1 | D | 217 | PHE | O-C-N | -7.46 | 110.77 | 122.70 |
| 1 | E | 5 | PHE | CA-CB-CG | 7.46 | 131.80 | 113.90 |
| 1 | E | 128 | LEU | CA-CB-CG | 7.46 | 132.46 | 115.30 |
| 1 | B | 74 | GLN | CG-CD-OE1 | -7.46 | 106.69 | 121.60 |
| 1 | A | 79 | TRP | CA-C-O | -7.46 | 104.44 | 120.10 |
| 1 | D | 17 | LEU | CB-CA-C | 7.45 | 124.36 | 110.20 |
| 1 | D | 181 | THR | CB-CA-C | 7.45 | 131.72 | 111.60 |
| 1 | E | 166 | ASP | CB-CA-C | 7.45 | 125.31 | 110.40 |
| 1 | F | 25 | LEU | CB-CA-C | -7.45 | 96.04 | 110.20 |
| 1 | A | 130 | SER | N-CA-CB | -7.45 | 99.32 | 110.50 |
| 1 | D | 226 | ALA | CA-C-O | 7.45 | 135.75 | 120.10 |
| 1 | F | 149 | LEU | CB-CG-CD2 | 7.45 | 123.67 | 111.00 |
| 1 | D | 78 | ARG | CA-C-O | 7.45 | 135.74 | 120.10 |
| 1 | A | 131 | THR | CA-C-O | 7.45 | 135.74 | 120.10 |
| 1 | E | 65 | ASP | N-CA-CB | -7.45 | 97.20 | 110.60 |
| 1 | E | 84 | LYS | CA-CB-CG | 7.45 | 129.78 | 113.40 |
| 1 | F | 97 | ASP | N-CA-CB | -7.45 | 97.20 | 110.60 |
| 1 | D | 38 | LEU | CA-CB-CG | -7.44 | 98.18 | 115.30 |
| 1 | D | 147 | LEU | O-C-N | -7.44 | 110.80 | 122.70 |
| 1 | E | 68 | LEU | CB-CG-CD1 | -7.44 | 98.35 | 111.00 |
| 1 | A | 83 | THR | CA-C-O | -7.44 | 104.48 | 120.10 |
| 1 | A | 214 | ARG | CB-CG-CD | 7.44 | 130.94 | 111.60 |
| 1 | B | 5 | PHE | O-C-N | -7.44 | 110.56 | 123.20 |
| 1 | B | 93 | VAL | CA-CB-CG1 | 7.44 | 122.06 | 110.90 |
| 1 | D | 141 | LEU | CA-C-O | -7.44 | 104.48 | 120.10 |
| 1 | E | 61 | VAL | CG1-CB-CG2 | -7.44 | 99.00 | 110.90 |
| 1 | F | 7 | LEU | CA-CB-CG | -7.44 | 98.19 | 115.30 |
| 1 | A | 1 | ASN | CB-CG-ND2 | 7.44 | 134.55 | 116.70 |
| 1 | B | 41 | PHE | N-CA-CB | -7.43 | 97.22 | 110.60 |
| 1 | D | 125 | ASN | CA-C-O | 7.43 | 135.71 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 188 | GLN | O-C-N | -7.43 | 106.98 | 121.10 |
| 1 | F | 216 | VAL | CA-C-O | 7.42 | 135.69 | 120.10 |
| 1 | A | 91 | VAL | CB-CA-C | 7.42 | 125.49 | 111.40 |
| 1 | A | 105 | PRO | O-C-N | 7.42 | 135.81 | 123.20 |
| 1 | D | 106 | GLY | CA-C-O | -7.42 | 107.25 | 120.60 |
| 1 | A | 76 | THR | CA-C-O | -7.42 | 104.52 | 120.10 |
| 1 | A | 126 | SER | N-CA-CB | 7.42 | 121.62 | 110.50 |
| 1 | F | 90 | TYR | CG-CD1-CE1 | 7.42 | 127.23 | 121.30 |
| 1 | C | 215 | TYR | CZ-CE2-CD2 | -7.42 | 113.13 | 119.80 |
| 1 | D | 6 | GLY | O-C-N | 7.42 | 134.56 | 122.70 |
| 1 | B | 215 | TYR | CB-CA-C | -7.41 | 95.58 | 110.40 |
| 1 | C | 152 | TYR | CD1-CE1-CZ | 7.41 | 126.47 | 119.80 |
| 1 | D | 69 | VAL | CA-CB-CG2 | 7.41 | 122.01 | 110.90 |
| 1 | E | 28 | PHE | CG-CD2-CE2 | 7.41 | 128.95 | 120.80 |
| 1 | B | 221 | PRO | C-N-CA | 7.40 | 140.20 | 121.70 |
| 1 | C | 131 | THR | N-CA-C | -7.40 | 91.01 | 111.00 |
| 1 | B | 165 | PHE | CG-CD1-CE1 | 7.40 | 128.94 | 120.80 |
| 1 | D | 142 | HIS | CB-CA-C | -7.40 | 95.61 | 110.40 |
| 1 | D | 151 | PRO | CA-C-N | 7.40 | 133.47 | 117.20 |
| 1 | B | 30 | PHE | C-N-CA | 7.39 | 140.19 | 121.70 |
| 1 | F | 137 | HIS | CB-CA-C | -7.39 | 95.61 | 110.40 |
| 1 | A | 80 | SER | CB-CA-C | -7.39 | 96.05 | 110.10 |
| 1 | B | 32 | MET | C-N-CA | -7.39 | 103.22 | 121.70 |
| 1 | C | 140 | THR | CA-CB-CG2 | 7.39 | 122.75 | 112.40 |
| 1 | E | 179 | LYS | O-C-N | -7.39 | 110.64 | 123.20 |
| 1 | F | 228 | TYR | CG-CD1-CE1 | 7.39 | 127.21 | 121.30 |
| 1 | A | 155 | SER | CA-C-N | -7.38 | 100.96 | 117.20 |
| 1 | B | 84 | LYS | C-N-CA | 7.38 | 137.81 | 122.30 |
| 1 | D | 112 | THR | N-CA-CB | -7.38 | 96.27 | 110.30 |
| 1 | E | 72 | THR | CA-C-O | 7.38 | 135.61 | 120.10 |
| 1 | F | 222 | ASP | OD1-CG-OD2 | 7.38 | 137.32 | 123.30 |
| 1 | E | 23 | LEU | N-CA-CB | 7.37 | 125.15 | 110.40 |
| 1 | E | 110 | SER | CB-CA-C | -7.37 | 96.09 | 110.10 |
| 1 | C | 103 | TYR | CE1-CZ-CE2 | 7.37 | 131.59 | 119.80 |
| 1 | E | 222 | ASP | CA-C-O | -7.37 | 104.62 | 120.10 |
| 1 | A | 137 | HIS | CB-CG-ND1 | 7.37 | 141.62 | 123.20 |
| 1 | C | 181 | THR | CA-CB-OG1 | -7.37 | 93.53 | 109.00 |
| 1 | E | 37 | ASN | CB-CG-ND2 | -7.37 | 99.02 | 116.70 |
| 1 | E | 232 | LEU | C-N-CA | -7.37 | 103.28 | 121.70 |
| 1 | D | 28 | PHE | CG-CD1-CE1 | 7.37 | 128.90 | 120.80 |
| 1 | B | 85 | GLY | N-CA-C | -7.36 | 94.69 | 113.10 |
| 1 | B | 172 | TRP | CZ3-CH2-CZ2 | -7.36 | 112.77 | 121.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 140 | THR | N-CA-C | 7.36 | 130.88 | 111.00 |
| 1 | E | 222 | ASP | O-C-N | 7.36 | 134.48 | 122.70 |
| 1 | E | 114 | ASN | OD1-CG-ND2 | 7.36 | 138.83 | 121.90 |
| 1 | F | 108 | TRP | CA-C-N | 7.36 | 133.40 | 117.20 |
| 1 | B | 146 | SER | N-CA-C | 7.36 | 130.88 | 111.00 |
| 1 | D | 75 | ASN | CA-CB-CG | -7.36 | 97.21 | 113.40 |
| 1 | A | 24 | GLU | CG-CD-OE1 | 7.36 | 133.02 | 118.30 |
| 1 | B | 31 | THR | CB-CA-C | -7.36 | 91.73 | 111.60 |
| 1 | B | 209 | SER | N-CA-C | 7.36 | 130.87 | 111.00 |
| 1 | D | 29 | ARG | CB-CA-C | -7.36 | 95.68 | 110.40 |
| 1 | D | 112 | THR | CA-CB-CG2 | -7.36 | 102.10 | 112.40 |
| 1 | E | 1 | ASN | N-CA-CB | 7.36 | 123.84 | 110.60 |
| 1 | A | 66 | GLY | CA-C-O | -7.35 | 107.36 | 120.60 |
| 1 | B | 165 | PHE | CA-C-O | -7.35 | 104.66 | 120.10 |
| 1 | D | 89 | ASN | CA-C-N | 7.35 | 133.37 | 117.20 |
| 1 | A | 166 | ASP | CB-CG-OD1 | -7.35 | 111.68 | 118.30 |
| 1 | C | 132 | GLN | CG-CD-NE2 | 7.35 | 134.34 | 116.70 |
| 1 | C | 59 | ARG | CA-CB-CG | 7.34 | 129.56 | 113.40 |
| 1 | D | 167 | ARG | CD-NE-CZ | -7.34 | 113.32 | 123.60 |
| 1 | F | 44 | ASP | CA-C-O | 7.34 | 135.52 | 120.10 |
| 1 | C | 48 | TRP | CH2-CZ2-CE2 | -7.34 | 110.06 | 117.40 |
| 1 | E | 58 | CYS | O-C-N | -7.34 | 110.95 | 122.70 |
| 1 | F | 61 | VAL | N-CA-C | 7.34 | 130.82 | 111.00 |
| 1 | F | 188 | GLN | CA-C-O | 7.34 | 135.52 | 120.10 |
| 1 | F | 193 | MET | O-C-N | -7.34 | 110.95 | 122.70 |
| 1 | F | 219 | LEU | CA-C-O | -7.34 | 104.68 | 120.10 |
| 1 | A | 59 | ARG | CD-NE-CZ | 7.34 | 133.88 | 123.60 |
| 1 | B | 163 | VAL | CA-C-O | 7.34 | 135.51 | 120.10 |
| 1 | B | 228 | TYR | CD1-CG-CD2 | -7.33 | 109.83 | 117.90 |
| 1 | E | 122 | ASN | O-C-N | -7.33 | 110.96 | 122.70 |
| 1 | E | 199 | GLN | C-N-CA | 7.33 | 140.03 | 121.70 |
| 1 | F | 204 | TRP | CB-CG-CD1 | 7.33 | 136.53 | 127.00 |
| 1 | B | 167 | ARG | NE-CZ-NH1 | -7.33 | 116.64 | 120.30 |
| 1 | D | 140 | THR | CA-C-O | 7.33 | 135.48 | 120.10 |
| 1 | E | 166 | ASP | OD1-CG-OD2 | 7.33 | 137.22 | 123.30 |
| 1 | F | 13 | HIS | CB-CA-C | 7.33 | 125.05 | 110.40 |
| 1 | A | 41 | PHE | O-C-N | 7.32 | 134.42 | 122.70 |
| 1 | B | 30 | PHE | CB-CA-C | -7.32 | 95.76 | 110.40 |
| 1 | B | 7 | LEU | C-N-CA | 7.32 | 140.00 | 121.70 |
| 1 | C | 193 | MET | CB-CA-C | 7.32 | 125.04 | 110.40 |
| 1 | F | 157 | GLU | CA-CB-CG | 7.32 | 129.50 | 113.40 |
| 1 | F | 224 | ASN | CA-CB-CG | -7.32 | 97.29 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 196 | LEU | CB-CA-C | -7.32 | 96.30 | 110.20 |
| 1 | F | 228 | TYR | CB-CG-CD1 | 7.32 | 125.39 | 121.00 |
| 1 | C | 170 | ARG | CB-CG-CD | 7.31 | 130.61 | 111.60 |
| 1 | A | 39 | VAL | N-CA-CB | -7.31 | 95.42 | 111.50 |
| 1 | C | 13 | HIS | O-C-N | -7.31 | 107.22 | 121.10 |
| 1 | D | 167 | ARG | CB-CA-C | 7.31 | 125.01 | 110.40 |
| 1 | C | 18 | HIS | CA-CB-CG | 7.31 | 126.02 | 113.60 |
| 1 | D | 85 | GLY | CA-C-N | 7.31 | 133.27 | 117.20 |
| 1 | F | 183 | CYS | O-C-N | -7.31 | 111.01 | 122.70 |
| 1 | B | 24 | GLU | N-CA-CB | -7.30 | 97.45 | 110.60 |
| 1 | D | 107 | LEU | CA-C-N | 7.30 | 133.27 | 117.20 |
| 1 | A | 94 | LEU | N-CA-C | -7.30 | 91.28 | 111.00 |
| 1 | D | 45 | VAL | N-CA-CB | 7.30 | 127.56 | 111.50 |
| 1 | D | 106 | GLY | N-CA-C | -7.30 | 94.85 | 113.10 |
| 1 | A | 120 | VAL | CA-C-N | 7.30 | 133.26 | 117.20 |
| 1 | F | 129 | TYR | CA-CB-CG | 7.30 | 127.27 | 113.40 |
| 1 | B | 199 | GLN | O-C-N | -7.30 | 111.03 | 122.70 |
| 1 | C | 132 | GLN | CB-CG-CD | 7.29 | 130.57 | 111.60 |
| 1 | B | 206 | SER | CA-CB-OG | 7.29 | 130.89 | 111.20 |
| 1 | E | 197 | THR | CA-CB-CG2 | 7.29 | 122.61 | 112.40 |
| 1 | F | 128 | LEU | CB-CG-CD2 | 7.29 | 123.40 | 111.00 |
| 1 | F | 204 | TRP | CG-CD2-CE3 | -7.29 | 127.34 | 133.90 |
| 1 | E | 235 | THR | CA-C-O | 7.29 | 135.41 | 120.10 |
| 1 | D | 37 | ASN | CB-CG-OD1 | -7.29 | 107.02 | 121.60 |
| 1 | A | 59 | ARG | O-C-N | 7.29 | 134.36 | 122.70 |
| 1 | B | 39 | VAL | C-N-CA | 7.29 | 139.91 | 121.70 |
| 1 | B | 131 | THR | C-N-CA | -7.29 | 103.49 | 121.70 |
| 1 | B | 187 | LEU | N-CA-CB | 7.29 | 124.97 | 110.40 |
| 1 | C | 157 | GLU | OE1-CD-OE2 | 7.29 | 132.04 | 123.30 |
| 1 | B | 226 | ALA | O-C-N | 7.28 | 134.35 | 122.70 |
| 1 | B | 18 | HIS | O-C-N | -7.28 | 111.05 | 122.70 |
| 1 | C | 20 | ALA | CA-C-O | 7.28 | 135.39 | 120.10 |
| 1 | D | 69 | VAL | CB-CA-C | 7.28 | 125.23 | 111.40 |
| 1 | E | 144 | THR | N-CA-CB | 7.28 | 124.13 | 110.30 |
| 1 | A | 83 | THR | CA-CB-CG2 | -7.28 | 102.21 | 112.40 |
| 1 | B | 92 | LEU | CA-C-O | -7.28 | 104.82 | 120.10 |
| 1 | C | 118 | VAL | N-CA-C | 7.27 | 130.64 | 111.00 |
| 1 | D | 67 | LEU | CA-C-N | 7.27 | 133.20 | 117.20 |
| 1 | E | 12 | SER | CA-C-N | -7.27 | 101.20 | 117.20 |
| 1 | E | 158 | THR | CA-C-O | -7.27 | 104.83 | 120.10 |
| 1 | C | 164 | LEU | O-C-N | 7.27 | 134.33 | 122.70 |
| 1 | E | 25 | LEU | CD1-CG-CD2 | -7.27 | 88.69 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 224 | ASN | N-CA-CB | -7.27 | 97.51 | 110.60 |
| 1 | B | 13 | HIS | N-CA-CB | -7.27 | 97.52 | 110.60 |
| 1 | C | 131 | THR | CB-CA-C | 7.27 | 131.22 | 111.60 |
| 1 | C | 229 | GLY | N-CA-C | 7.27 | 131.27 | 113.10 |
| 1 | C | 90 | TYR | N-CA-CB | -7.26 | 97.52 | 110.60 |
| 1 | A | 84 | LYS | CB-CA-C | 7.26 | 124.93 | 110.40 |
| 1 | F | 14 | PRO | N-CA-CB | 7.26 | 112.01 | 103.30 |
| 1 | F | 100 | VAL | CA-C-O | -7.26 | 104.86 | 120.10 |
| 1 | B | 230 | GLY | CA-C-O | -7.25 | 107.54 | 120.60 |
| 1 | C | 121 | ALA | C-N-CA | 7.25 | 139.84 | 121.70 |
| 1 | F | 77 | ILE | CA-CB-CG1 | 7.25 | 124.78 | 111.00 |
| 1 | C | 108 | TRP | CB-CG-CD2 | -7.25 | 117.17 | 126.60 |
| 1 | D | 62 | LEU | N-CA-CB | 7.25 | 124.90 | 110.40 |
| 1 | B | 136 | ASN | N-CA-CB | 7.25 | 123.65 | 110.60 |
| 1 | F | 155 | SER | CA-CB-OG | -7.25 | 91.63 | 111.20 |
| 1 | E | 9 | HIS | N-CA-CB | -7.25 | 97.56 | 110.60 |
| 1 | E | 173 | SER | O-C-N | -7.25 | 111.11 | 122.70 |
| 1 | A | 31 | THR | C-N-CA | 7.24 | 139.81 | 121.70 |
| 1 | E | 119 | VAL | O-C-N | -7.24 | 111.11 | 122.70 |
| 1 | B | 71 | LEU | CA-C-O | -7.24 | 104.90 | 120.10 |
| 1 | B | 234 | THR | CA-CB-CG2 | 7.24 | 122.54 | 112.40 |
| 1 | C | 57 | GLY | C-N-CA | -7.24 | 103.60 | 121.70 |
| 1 | D | 25 | LEU | CB-CG-CD1 | -7.24 | 98.69 | 111.00 |
| 1 | B | 6 | GLY | C-N-CA | 7.23 | 139.78 | 121.70 |
| 1 | E | 114 | ASN | N-CA-C | 7.23 | 130.53 | 111.00 |
| 1 | C | 147 | LEU | CA-C-N | -7.23 | 101.29 | 117.20 |
| 1 | F | 145 | GLN | CG-CD-OE1 | -7.23 | 107.14 | 121.60 |
| 1 | D | 211 | SER | N-CA-C | 7.23 | 130.51 | 111.00 |
| 1 | E | 230 | GLY | N-CA-C | -7.22 | 95.04 | 113.10 |
| 1 | E | 79 | TRP | O-C-N | 7.22 | 134.26 | 122.70 |
| 1 | C | 109 | ASP | CA-CB-CG | 7.22 | 129.28 | 113.40 |
| 1 | D | 91 | VAL | CB-CA-C | 7.22 | 125.12 | 111.40 |
| 1 | A | 81 | SER | CB-CA-C | 7.22 | 123.81 | 110.10 |
| 1 | C | 228 | TYR | C-N-CA | 7.21 | 137.45 | 122.30 |
| 1 | F | 62 | LEU | CA-C-N | -7.21 | 101.33 | 117.20 |
| 1 | C | 147 | LEU | O-C-N | 7.21 | 134.24 | 122.70 |
| 1 | A | 165 | PHE | CD1-CG-CD2 | -7.21 | 108.92 | 118.30 |
| 1 | D | 167 | ARG | CA-C-O | 7.21 | 135.25 | 120.10 |
| 1 | A | 26 | SER | O-C-N | -7.21 | 111.17 | 122.70 |
| 1 | E | 195 | VAL | CG1-CB-CG2 | 7.21 | 122.43 | 110.90 |
| 1 | E | 215 | TYR | CB-CG-CD2 | 7.21 | 125.33 | 121.00 |
| 1 | B | 147 | LEU | CB-CA-C | -7.21 | 96.51 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 193 | MET | N-CA-CB | 7.20 | 123.57 | 110.60 |
| 1 | A | 166 | ASP | O-C-N | 7.20 | 134.22 | 122.70 |
| 1 | A | 152 | TYR | CD1-CG-CD2 | -7.20 | 109.98 | 117.90 |
| 1 | B | 69 | VAL | O-C-N | 7.20 | 134.22 | 122.70 |
| 1 | D | 229 | GLY | C-N-CA | 7.20 | 137.41 | 122.30 |
| 1 | E | 220 | GLN | CA-CB-CG | -7.20 | 97.56 | 113.40 |
| 1 | B | 73 | ALA | CA-C-N | 7.20 | 133.03 | 117.20 |
| 1 | B | 54 | GLY | CA-C-N | 7.20 | 133.03 | 117.20 |
| 1 | B | 224 | ASN | CA-C-N | 7.20 | 133.03 | 117.20 |
| 1 | D | 152 | TYR | CZ-CE2-CD2 | -7.20 | 113.32 | 119.80 |
| 1 | A | 218 | VAL | CA-C-O | -7.19 | 105.00 | 120.10 |
| 1 | B | 56 | THR | CA-C-N | 7.19 | 130.58 | 116.20 |
| 1 | F | 160 | CYS | CA-C-N | -7.18 | 101.40 | 117.20 |
| 1 | A | 111 | GLY | CA-C-N | 7.18 | 133.00 | 117.20 |
| 1 | C | 117 | SER | CA-C-O | 7.18 | 135.19 | 120.10 |
| 1 | D | 208 | ASN | CA-C-N | -7.18 | 101.40 | 117.20 |
| 1 | E | 149 | LEU | CA-CB-CG | -7.18 | 98.78 | 115.30 |
| 1 | D | 44 | ASP | O-C-N | -7.18 | 111.21 | 122.70 |
| 1 | F | 59 | ARG | CG-CD-NE | 7.18 | 126.87 | 111.80 |
| 1 | C | 67 | LEU | O-C-N | 7.18 | 134.18 | 122.70 |
| 1 | C | 171 | VAL | CA-C-N | 7.18 | 132.99 | 117.20 |
| 1 | A | 71 | LEU | CA-C-O | 7.17 | 135.16 | 120.10 |
| 1 | A | 81 | SER | CA-C-O | -7.17 | 105.05 | 120.10 |
| 1 | C | 216 | VAL | C-N-CA | 7.17 | 139.62 | 121.70 |
| 1 | D | 177 | ALA | CA-C-N | -7.17 | 101.87 | 116.20 |
| 1 | E | 7 | LEU | CA-C-O | -7.17 | 105.05 | 120.10 |
| 1 | C | 71 | LEU | CA-C-N | -7.17 | 101.44 | 117.20 |
| 1 | E | 216 | VAL | CA-CB-CG2 | 7.16 | 121.65 | 110.90 |
| 1 | C | 64 | SER | CA-CB-OG | 7.16 | 130.54 | 111.20 |
| 1 | A | 33 | GLN | CG-CD-NE2 | -7.16 | 99.52 | 116.70 |
| 1 | D | 137 | HIS | N-CA-CB | 7.16 | 123.49 | 110.60 |
| 1 | A | 72 | THR | C-N-CA | 7.16 | 139.60 | 121.70 |
| 1 | B | 73 | ALA | N-CA-C | -7.16 | 91.67 | 111.00 |
| 1 | A | 52 | THR | CA-CB-CG2 | 7.16 | 122.42 | 112.40 |
| 1 | A | 171 | VAL | CA-C-O | -7.16 | 105.07 | 120.10 |
| 1 | C | 217 | PHE | CB-CG-CD2 | -7.16 | 115.79 | 120.80 |
| 1 | F | 128 | LEU | CB-CG-CD1 | 7.16 | 123.17 | 111.00 |
| 1 | B | 185 | ALA | C-N-CA | 7.16 | 139.59 | 121.70 |
| 1 | F | 210 | ARG | CB-CG-CD | -7.16 | 93.00 | 111.60 |
| 1 | C | 181 | THR | CA-CB-CG2 | 7.15 | 122.42 | 112.40 |
| 1 | D | 147 | LEU | CA-CB-CG | 7.15 | 131.75 | 115.30 |
| 1 | B | 186 | VAL | CG1-CB-CG2 | -7.15 | 99.46 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 4 | LEU | CA-CB-CG | 7.15 | 131.74 | 115.30 |
| 1 | F | 101 | THR | N-CA-CB | -7.15 | 96.72 | 110.30 |
| 1 | C | 66 | GLY | CA-C-N | -7.14 | 101.48 | 117.20 |
| 1 | F | 139 | GLN | CB-CG-CD | 7.14 | 130.17 | 111.60 |
| 1 | C | 17 | LEU | CA-C-N | 7.14 | 132.91 | 117.20 |
| 1 | C | 152 | TYR | CA-CB-CG | 7.14 | 126.97 | 113.40 |
| 1 | C | 167 | ARG | N-CA-CB | 7.14 | 123.45 | 110.60 |
| 1 | B | 81 | SER | CA-C-O | -7.14 | 105.11 | 120.10 |
| 1 | C | 131 | THR | CA-CB-CG2 | 7.14 | 122.39 | 112.40 |
| 1 | F | 59 | ARG | CA-C-N | -7.14 | 101.49 | 117.20 |
| 1 | B | 203 | VAL | N-CA-C | -7.14 | 91.73 | 111.00 |
| 1 | F | 23 | LEU | N-CA-CB | -7.14 | 96.12 | 110.40 |
| 1 | A | 233 | TRP | CB-CG-CD2 | 7.14 | 135.88 | 126.60 |
| 1 | C | 50 | SER | O-C-N | -7.13 | 111.28 | 122.70 |
| 1 | C | 214 | ARG | C-N-CA | 7.13 | 139.54 | 121.70 |
| 1 | A | 167 | ARG | NH1-CZ-NH2 | -7.13 | 111.56 | 119.40 |
| 1 | B | 128 | LEU | CA-C-O | 7.13 | 135.07 | 120.10 |
| 1 | A | 225 | LEU | C-N-CA | -7.13 | 103.88 | 121.70 |
| 1 | C | 233 | TRP | CE3-CZ3-CH2 | 7.12 | 129.04 | 121.20 |
| 1 | F | 203 | VAL | CG1-CB-CG2 | -7.12 | 99.50 | 110.90 |
| 1 | F | 215 | TYR | CG-CD2-CE2 | -7.12 | 115.60 | 121.30 |
| 1 | B | 160 | CYS | CA-CB-SG | -7.12 | 101.18 | 114.00 |
| 1 | B | 159 | ASP | CB-CG-OD1 | -7.12 | 111.89 | 118.30 |
| 1 | E | 8 | SER | CA-C-O | 7.12 | 135.05 | 120.10 |
| 1 | A | 145 | GLN | CG-CD-NE2 | 7.12 | 133.78 | 116.70 |
| 1 | C | 36 | CYS | N-CA-C | 7.12 | 130.22 | 111.00 |
| 1 | F | 138 | PRO | CB-CA-C | -7.11 | 94.21 | 112.00 |
| 1 | C | 57 | GLY | CA-C-O | -7.11 | 107.80 | 120.60 |
| 1 | C | 113 | SER | N-CA-CB | -7.11 | 99.83 | 110.50 |
| 1 | D | 197 | THR | N-CA-C | 7.11 | 130.20 | 111.00 |
| 1 | A | 59 | ARG | CA-CB-CG | 7.11 | 129.03 | 113.40 |
| 1 | C | 5 | PHE | CZ-CE2-CD2 | 7.11 | 128.63 | 120.10 |
| 1 | C | 136 | ASN | CA-C-O | 7.11 | 135.02 | 120.10 |
| 1 | C | 156 | MET | CA-C-O | -7.10 | 105.18 | 120.10 |
| 1 | C | 224 | ASN | CA-CB-CG | -7.10 | 97.79 | 113.40 |
| 1 | F | 79 | TRP | CD1-NE1-CE2 | -7.10 | 102.61 | 109.00 |
| 1 | D | 178 | GLY | O-C-N | -7.09 | 111.35 | 122.70 |
| 1 | D | 222 | ASP | CB-CG-OD1 | -7.09 | 111.91 | 118.30 |
| 1 | F | 52 | THR | C-N-CA | 7.09 | 139.44 | 121.70 |
| 1 | F | 154 | LEU | CD1-CG-CD2 | -7.09 | 89.22 | 110.50 |
| 1 | C | 175 | ASN | C-N-CA | 7.09 | 139.43 | 121.70 |
| 1 | D | 64 | SER | N-CA-CB | -7.09 | 99.86 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 144 | THR | OG1-CB-CG2 | -7.09 | 93.69 | 110.00 |
| 1 | F | 30 | PHE | CD1-CE1-CZ | -7.09 | 111.59 | 120.10 |
| 1 | A | 3 | ILE | O-C-N | -7.09 | 111.36 | 122.70 |
| 1 | E | 65 | ASP | CB-CG-OD2 | -7.09 | 111.92 | 118.30 |
| 1 | E | 209 | SER | N-CA-C | -7.09 | 91.86 | 111.00 |
| 1 | F | 234 | THR | CA-C-N | 7.09 | 132.80 | 117.20 |
| 1 | B | 160 | CYS | N-CA-CB | 7.09 | 123.36 | 110.60 |
| 1 | B | 130 | SER | O-C-N | -7.09 | 111.36 | 122.70 |
| 1 | B | 202 | ALA | N-CA-C | -7.09 | 91.87 | 111.00 |
| 1 | D | 14 | PRO | CA-C-O | -7.09 | 103.19 | 120.20 |
| 1 | C | 216 | VAL | O-C-N | -7.08 | 111.36 | 122.70 |
| 1 | F | 196 | LEU | CB-CG-CD1 | 7.08 | 123.04 | 111.00 |
| 1 | B | 233 | TRP | CD2-CE2-CZ2 | 7.08 | 130.80 | 122.30 |
| 1 | C | 228 | TYR | OH-CZ-CE2 | 7.08 | 139.21 | 120.10 |
| 1 | A | 93 | VAL | CG1-CB-CG2 | 7.08 | 122.22 | 110.90 |
| 1 | C | 149 | LEU | O-C-N | 7.08 | 134.02 | 122.70 |
| 1 | D | 209 | SER | N-CA-C | 7.08 | 130.11 | 111.00 |
| 1 | E | 52 | THR | CA-C-N | 7.08 | 132.77 | 117.20 |
| 1 | F | 167 | ARG | NE-CZ-NH2 | 7.08 | 123.84 | 120.30 |
| 1 | A | 176 | THR | CB-CA-C | 7.07 | 130.70 | 111.60 |
| 1 | D | 5 | PHE | CD1-CE1-CZ | 7.07 | 128.59 | 120.10 |
| 1 | D | 144 | THR | CA-CB-CG2 | 7.07 | 122.30 | 112.40 |
| 1 | C | 207 | GLY | CA-C-O | -7.07 | 107.88 | 120.60 |
| 1 | B | 175 | ASN | CB-CA-C | 7.07 | 124.53 | 110.40 |
| 1 | F | 108 | TRP | CB-CA-C | 7.07 | 124.54 | 110.40 |
| 1 | E | 221 | PRO | O-C-N | 7.06 | 134.00 | 122.70 |
| 1 | C | 146 | SER | N-CA-C | 7.06 | 130.07 | 111.00 |
| 1 | D | 144 | THR | N-CA-C | -7.06 | 91.93 | 111.00 |
| 1 | C | 98 | ARG | CG-CD-NE | -7.06 | 96.97 | 111.80 |
| 1 | D | 91 | VAL | CA-C-N | 7.06 | 132.73 | 117.20 |
| 1 | B | 103 | TYR | CG-CD1-CE1 | 7.06 | 126.94 | 121.30 |
| 1 | A | 172 | TRP | CD2-CE3-CZ3 | 7.06 | 127.97 | 118.80 |
| 1 | D | 44 | ASP | CB-CA-C | 7.06 | 124.51 | 110.40 |
| 1 | D | 84 | LYS | CA-CB-CG | 7.05 | 128.92 | 113.40 |
| 1 | C | 192 | ARG | CA-CB-CG | 7.05 | 128.92 | 113.40 |
| 1 | D | 199 | GLN | CA-C-N | 7.05 | 132.71 | 117.20 |
| 1 | D | 204 | TRP | CA-CB-CG | 7.05 | 127.09 | 113.70 |
| 1 | B | 196 | LEU | CB-CA-C | -7.04 | 96.82 | 110.20 |
| 1 | C | 36 | CYS | O-C-N | 7.04 | 133.97 | 122.70 |
| 1 | B | 89 | ASN | CA-C-N | 7.04 | 132.69 | 117.20 |
| 1 | E | 63 | GLN | CG-CD-NE2 | -7.04 | 99.81 | 116.70 |
| 1 | E | 6 | GLY | O-C-N | 7.03 | 133.96 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 2 | ASN | OD1-CG-ND2 | -7.03 | 105.73 | 121.90 |
| 1 | C | 86 | SER | CA-CB-OG | -7.03 | 92.21 | 111.20 |
| 1 | C | 216 | VAL | CA-C-N | 7.03 | 132.66 | 117.20 |
| 1 | E | 28 | PHE | CG-CD1-CE1 | 7.03 | 128.53 | 120.80 |
| 1 | E | 27 | SER | CA-CB-OG | -7.02 | 92.23 | 111.20 |
| 1 | C | 48 | TRP | CB-CA-C | 7.02 | 124.45 | 110.40 |
| 1 | C | 126 | SER | O-C-N | 7.02 | 133.93 | 122.70 |
| 1 | D | 154 | LEU | O-C-N | -7.02 | 111.46 | 122.70 |
| 1 | E | 37 | ASN | OD1-CG-ND2 | 7.02 | 138.05 | 121.90 |
| 1 | F | 100 | VAL | CA-CB-CG1 | -7.02 | 100.37 | 110.90 |
| 1 | A | 62 | LEU | CB-CG-CD2 | 7.02 | 122.94 | 111.00 |
| 1 | F | 142 | HIS | CA-CB-CG | -7.02 | 101.67 | 113.60 |
| 1 | B | 61 | VAL | CB-CA-C | -7.02 | 98.06 | 111.40 |
| 1 | D | 101 | THR | OG1-CB-CG2 | 7.02 | 126.15 | 110.00 |
| 1 | F | 141 | LEU | CB-CA-C | 7.02 | 123.54 | 110.20 |
| 1 | F | 142 | HIS | CG-ND1-CE1 | 7.02 | 118.03 | 108.20 |
| 1 | F | 159 | ASP | CB-CG-OD2 | -7.02 | 111.98 | 118.30 |
| 1 | B | 147 | LEU | O-C-N | 7.02 | 133.93 | 122.70 |
| 1 | D | 148 | GLN | CA-C-O | 7.02 | 134.84 | 120.10 |
| 1 | A | 164 | LEU | C-N-CA | -7.02 | 104.16 | 121.70 |
| 1 | F | 87 | ILE | CA-CB-CG1 | -7.02 | 97.67 | 111.00 |
| 1 | B | 59 | ARG | NE-CZ-NH1 | -7.01 | 116.79 | 120.30 |
| 1 | D | 200 | ASN | CB-CA-C | 7.01 | 124.42 | 110.40 |
| 1 | F | 215 | TYR | CG-CD1-CE1 | 7.01 | 126.91 | 121.30 |
| 1 | B | 127 | ILE | CA-CB-CG2 | -7.01 | 96.88 | 110.90 |
| 1 | E | 74 | GLN | CA-CB-CG | 7.01 | 128.82 | 113.40 |
| 1 | E | 219 | LEU | CB-CA-C | -7.01 | 96.88 | 110.20 |
| 1 | E | 5 | PHE | CB-CG-CD2 | -7.01 | 115.89 | 120.80 |
| 1 | F | 151 | PRO | O-C-N | -7.01 | 111.48 | 122.70 |
| 1 | A | 129 | TYR | CZ-CE2-CD2 | 7.00 | 126.11 | 119.80 |
| 1 | A | 172 | TRP | CE3-CZ3-CH2 | -7.00 | 113.50 | 121.20 |
| 1 | B | 50 | SER | N-CA-CB | -7.00 | 100.00 | 110.50 |
| 1 | C | 79 | TRP | N-CA-CB | -7.00 | 98.00 | 110.60 |
| 1 | B | 200 | ASN | N-CA-C | 7.00 | 129.90 | 111.00 |
| 1 | E | 43 | SER | O-C-N | -7.00 | 111.51 | 122.70 |
| 1 | A | 229 | GLY | O-C-N | -6.99 | 111.32 | 123.20 |
| 1 | C | 116 | GLY | C-N-CA | 6.99 | 139.17 | 121.70 |
| 1 | E | 107 | LEU | CA-C-N | 6.99 | 132.57 | 117.20 |
| 1 | F | 79 | TRP | CE3-CZ3-CH2 | -6.99 | 113.51 | 121.20 |
| 1 | F | 147 | LEU | CA-C-N | -6.99 | 101.83 | 117.20 |
| 1 | A | 4 | LEU | CA-C-O | -6.99 | 105.43 | 120.10 |
| 1 | C | 123 | ASN | N-CA-C | 6.99 | 129.86 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 188 | GLN | CA-C-N | 6.98 | 136.65 | 117.10 |
| 1 | F | 39 | VAL | CA-C-N | -6.98 | 101.85 | 117.20 |
| 1 | D | 84 | LYS | CB-CA-C | -6.98 | 96.45 | 110.40 |
| 1 | D | 101 | THR | CA-C-N | 6.98 | 132.55 | 117.20 |
| 1 | E | 92 | LEU | N-CA-CB | 6.98 | 124.36 | 110.40 |
| 1 | A | 67 | LEU | CB-CG-CD2 | -6.97 | 99.14 | 111.00 |
| 1 | D | 148 | GLN | C-N-CA | 6.97 | 139.14 | 121.70 |
| 1 | F | 77 | ILE | O-C-N | -6.97 | 111.54 | 122.70 |
| 1 | A | 137 | HIS | CG-CD2-NE2 | -6.97 | 95.96 | 109.20 |
| 1 | B | 110 | SER | CA-C-N | 6.97 | 130.14 | 116.20 |
| 1 | B | 144 | THR | OG1-CB-CG2 | -6.97 | 93.97 | 110.00 |
| 1 | C | 166 | ASP | CA-CB-CG | 6.97 | 128.73 | 113.40 |
| 1 | A | 185 | ALA | CA-C-N | -6.96 | 101.88 | 117.20 |
| 1 | D | 97 | ASP | CA-C-N | 6.96 | 132.52 | 117.20 |
| 1 | F | 220 | GLN | CG-CD-NE2 | 6.96 | 133.41 | 116.70 |
| 1 | C | 159 | ASP | OD1-CG-OD2 | -6.96 | 110.08 | 123.30 |
| 1 | B | 42 | ASP | CB-CG-OD1 | -6.96 | 112.04 | 118.30 |
| 1 | C | 141 | LEU | CA-C-O | -6.96 | 105.49 | 120.10 |
| 1 | E | 7 | LEU | CB-CA-C | -6.96 | 96.98 | 110.20 |
| 1 | E | 145 | GLN | O-C-N | 6.96 | 133.83 | 122.70 |
| 1 | F | 43 | SER | CA-C-O | 6.96 | 134.71 | 120.10 |
| 1 | F | 103 | TYR | N-CA-CB | 6.96 | 123.12 | 110.60 |
| 1 | B | 3 | ILE | CB-CG1-CD1 | -6.96 | 94.43 | 113.90 |
| 1 | B | 212 | ALA | CA-C-O | -6.96 | 105.49 | 120.10 |
| 1 | B | 17 | LEU | O-C-N | -6.95 | 111.58 | 122.70 |
| 1 | B | 73 | ALA | CA-C-O | -6.95 | 105.50 | 120.10 |
| 1 | F | 184 | ARG | CB-CA-C | -6.95 | 96.50 | 110.40 |
| 1 | D | 161 | ASN | CB-CA-C | -6.95 | 96.50 | 110.40 |
| 1 | A | 93 | VAL | O-C-N | 6.95 | 133.81 | 122.70 |
| 1 | B | 92 | LEU | N-CA-C | -6.95 | 92.25 | 111.00 |
| 1 | B | 103 | TYR | CZ-CE2-CD2 | -6.95 | 113.55 | 119.80 |
| 1 | D | 37 | ASN | CA-C-N | -6.95 | 101.92 | 117.20 |
| 1 | F | 194 | ASP | OD1-CG-OD2 | -6.95 | 110.10 | 123.30 |
| 1 | A | 142 | HIS | ND1-CG-CD2 | -6.94 | 96.28 | 106.00 |
| 1 | B | 2 | ASN | N-CA-C | 6.94 | 129.75 | 111.00 |
| 1 | A | 160 | CYS | O-C-N | 6.94 | 133.81 | 122.70 |
| 1 | E | 214 | ARG | NH1-CZ-NH2 | -6.94 | 111.76 | 119.40 |
| 1 | F | 16 | THR | N-CA-C | 6.94 | 129.75 | 111.00 |
| 1 | B | 184 | ARG | CB-CA-C | -6.94 | 96.52 | 110.40 |
| 1 | C | 64 | SER | CA-C-O | 6.94 | 134.67 | 120.10 |
| 1 | F | 141 | LEU | C-N-CA | 6.94 | 139.05 | 121.70 |
| 1 | C | 29 | ARG | NH1-CZ-NH2 | -6.94 | 111.77 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 50 | SER | CB-CA-C | 6.94 | 123.28 | 110.10 |
| 1 | F | 17 | LEU | CB-CA-C | -6.94 | 97.02 | 110.20 |
| 1 | F | 28 | PHE | CD1-CE1-CZ | 6.94 | 128.42 | 120.10 |
| 1 | D | 137 | HIS | CB-CG-ND1 | -6.93 | 105.86 | 123.20 |
| 1 | B | 21 | GLN | CB-CG-CD | 6.93 | 129.62 | 111.60 |
| 1 | B | 84 | LYS | CA-C-N | 6.93 | 130.07 | 116.20 |
| 1 | B | 225 | LEU | CA-CB-CG | -6.93 | 99.36 | 115.30 |
| 1 | E | 42 | ASP | N-CA-C | -6.93 | 92.28 | 111.00 |
| 1 | F | 136 | ASN | N-CA-C | 6.93 | 129.72 | 111.00 |
| 1 | D | 6 | GLY | N-CA-C | -6.93 | 95.78 | 113.10 |
| 1 | D | 207 | GLY | CA-C-O | 6.93 | 133.07 | 120.60 |
| 1 | E | 123 | ASN | N-CA-CB | -6.93 | 98.13 | 110.60 |
| 1 | B | 76 | THR | CA-C-O | -6.92 | 105.56 | 120.10 |
| 1 | E | 47 | VAL | CA-C-O | -6.92 | 105.56 | 120.10 |
| 1 | F | 129 | TYR | CB-CA-C | 6.92 | 124.25 | 110.40 |
| 1 | F | 158 | THR | CA-CB-CG2 | -6.92 | 102.71 | 112.40 |
| 1 | E | 12 | SER | O-C-N | 6.92 | 133.77 | 122.70 |
| 1 | F | 126 | SER | N-CA-CB | -6.92 | 100.12 | 110.50 |
| 1 | E | 190 | ASN | CA-C-N | 6.92 | 130.03 | 116.20 |
| 1 | A | 69 | VAL | CB-CA-C | -6.91 | 98.27 | 111.40 |
| 1 | A | 86 | SER | N-CA-C | 6.91 | 129.67 | 111.00 |
| 1 | F | 2 | ASN | N-CA-CB | -6.91 | 98.16 | 110.60 |
| 1 | F | 92 | LEU | N-CA-CB | 6.91 | 124.23 | 110.40 |
| 1 | C | 173 | SER | N-CA-CB | 6.91 | 120.87 | 110.50 |
| 1 | D | 233 | TRP | CZ3-CH2-CZ2 | 6.91 | 129.89 | 121.60 |
| 1 | C | 160 | CYS | CA-C-N | 6.91 | 132.40 | 117.20 |
| 1 | B | 34 | SER | N-CA-CB | 6.91 | 120.86 | 110.50 |
| 1 | F | 28 | PHE | CA-C-O | 6.91 | 134.60 | 120.10 |
| 1 | B | 72 | THR | CA-C-O | -6.90 | 105.60 | 120.10 |
| 1 | B | 195 | VAL | CA-CB-CG1 | 6.90 | 121.25 | 110.90 |
| 1 | D | 221 | PRO | CA-C-N | 6.90 | 132.38 | 117.20 |
| 1 | F | 80 | SER | N-CA-CB | 6.90 | 120.86 | 110.50 |
| 1 | A | 9 | HIS | CA-CB-CG | 6.90 | 125.33 | 113.60 |
| 1 | C | 49 | ALA | CA-C-O | -6.90 | 105.61 | 120.10 |
| 1 | C | 1 | ASN | N-CA-CB | 6.90 | 123.02 | 110.60 |
| 1 | E | 66 | GLY | C-N-CA | -6.90 | 104.46 | 121.70 |
| 1 | A | 63 | GLN | CA-C-O | -6.90 | 105.62 | 120.10 |
| 1 | D | 138 | PRO | O-C-N | -6.89 | 111.67 | 122.70 |
| 1 | D | 109 | ASP | N-CA-C | 6.89 | 129.61 | 111.00 |
| 1 | E | 51 | ASN | CB-CA-C | -6.89 | 96.63 | 110.40 |
| 1 | D | 112 | THR | N-CA-C | 6.88 | 129.59 | 111.00 |
| 1 | F | 208 | ASN | CB-CA-C | -6.88 | 96.63 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 91 | VAL | C-N-CA | 6.88 | 138.90 | 121.70 |
| 1 | B | 191 | GLY | O-C-N | 6.88 | 133.71 | 122.70 |
| 1 | B | 1 | ASN | CB-CG-OD1 | 6.87 | 135.35 | 121.60 |
| 1 | B | 234 | THR | O-C-N | -6.87 | 111.70 | 122.70 |
| 1 | E | 227 | ILE | O-C-N | -6.87 | 111.70 | 122.70 |
| 1 | D | 108 | TRP | CE3-CZ3-CH2 | 6.87 | 128.76 | 121.20 |
| 1 | E | 198 | ASN | CB-CG-ND2 | -6.87 | 100.21 | 116.70 |
| 1 | D | 3 | ILE | CG1-CB-CG2 | -6.87 | 96.29 | 111.40 |
| 1 | C | 33 | GLN | O-C-N | 6.86 | 133.68 | 122.70 |
| 1 | D | 2 | ASN | O-C-N | -6.86 | 111.72 | 122.70 |
| 1 | C | 150 | SER | O-C-N | 6.86 | 134.14 | 121.10 |
| 1 | D | 108 | TRP | O-C-N | -6.86 | 111.72 | 122.70 |
| 1 | F | 141 | LEU | CB-CG-CD2 | 6.86 | 122.66 | 111.00 |
| 1 | C | 152 | TYR | OH-CZ-CE2 | 6.86 | 138.62 | 120.10 |
| 1 | B | 141 | LEU | C-N-CA | 6.85 | 138.83 | 121.70 |
| 1 | B | 210 | ARG | CG-CD-NE | 6.85 | 126.19 | 111.80 |
| 1 | E | 204 | TRP | O-C-N | 6.85 | 133.66 | 122.70 |
| 1 | F | 165 | PHE | CB-CG-CD1 | 6.85 | 125.60 | 120.80 |
| 1 | E | 161 | ASN | O-C-N | 6.85 | 133.66 | 122.70 |
| 1 | A | 202 | ALA | CB-CA-C | 6.85 | 120.38 | 110.10 |
| 1 | B | 137 | HIS | CB-CG-CD2 | -6.85 | 109.57 | 130.80 |
| 1 | C | 23 | LEU | CA-CB-CG | -6.85 | 99.55 | 115.30 |
| 1 | E | 201 | ILE | N-CA-CB | -6.85 | 95.05 | 110.80 |
| 1 | A | 208 | ASN | C-N-CA | -6.85 | 104.58 | 121.70 |
| 1 | A | 35 | ASP | CB-CG-OD2 | 6.84 | 124.46 | 118.30 |
| 1 | D | 178 | GLY | C-N-CA | 6.84 | 138.81 | 121.70 |
| 1 | A | 16 | THR | N-CA-C | 6.84 | 129.48 | 111.00 |
| 1 | D | 88 | GLY | CA-C-N | 6.84 | 132.25 | 117.20 |
| 1 | A | 72 | THR | OG1-CB-CG2 | -6.84 | 94.26 | 110.00 |
| 1 | A | 123 | ASN | N-CA-C | 6.84 | 129.47 | 111.00 |
| 1 | A | 173 | SER | N-CA-CB | -6.84 | 100.24 | 110.50 |
| 1 | A | 159 | ASP | N-CA-CB | 6.84 | 122.91 | 110.60 |
| 1 | E | 154 | LEU | O-C-N | 6.84 | 133.64 | 122.70 |
| 1 | F | 62 | LEU | CA-C-O | 6.83 | 134.45 | 120.10 |
| 1 | A | 162 | LEU | N-CA-CB | -6.83 | 96.74 | 110.40 |
| 1 | C | 47 | VAL | CA-C-O | -6.83 | 105.76 | 120.10 |
| 1 | B | 5 | PHE | CA-C-O | 6.83 | 134.44 | 120.10 |
| 1 | A | 104 | GLY | CA-C-N | -6.83 | 97.99 | 117.10 |
| 1 | B | 79 | TRP | CB-CA-C | -6.83 | 96.75 | 110.40 |
| 1 | A | 142 | HIS | N-CA-C | 6.82 | 129.42 | 111.00 |
| 1 | A | 220 | GLN | CA-C-O | -6.82 | 105.77 | 120.10 |
| 1 | C | 161 | ASN | C-N-CA | -6.82 | 104.66 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 201 | ILE | N-CA-CB | -6.82 | 95.12 | 110.80 |
| 1 | A | 40 | LEU | CD1-CG-CD2 | -6.81 | 90.07 | 110.50 |
| 1 | B | 140 | THR | CA-CB-OG1 | -6.81 | 94.70 | 109.00 |
| 1 | C | 158 | THR | CA-CB-OG1 | 6.81 | 123.30 | 109.00 |
| 1 | D | 73 | ALA | C-N-CA | 6.81 | 138.72 | 121.70 |
| 1 | A | 228 | TYR | CB-CG-CD1 | -6.81 | 116.92 | 121.00 |
| 1 | D | 28 | PHE | CB-CA-C | 6.81 | 124.02 | 110.40 |
| 1 | A | 26 | SER | CA-C-O | -6.80 | 105.81 | 120.10 |
| 1 | F | 211 | SER | CB-CA-C | -6.80 | 97.17 | 110.10 |
| 1 | D | 46 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | A | 13 | HIS | CA-C-O | -6.80 | 105.82 | 120.10 |
| 1 | F | 20 | ALA | C-N-CA | 6.80 | 138.70 | 121.70 |
| 1 | F | 166 | ASP | CB-CA-C | 6.80 | 124.00 | 110.40 |
| 1 | F | 193 | MET | CB-CG-SD | -6.80 | 92.00 | 112.40 |
| 1 | C | 146 | SER | C-N-CA | 6.80 | 138.69 | 121.70 |
| 1 | B | 136 | ASN | O-C-N | -6.80 | 111.83 | 122.70 |
| 1 | B | 188 | GLN | CA-CB-CG | 6.80 | 128.35 | 113.40 |
| 1 | B | 195 | VAL | CG1-CB-CG2 | -6.79 | 100.03 | 110.90 |
| 1 | C | 190 | ASN | CB-CA-C | 6.79 | 123.99 | 110.40 |
| 1 | B | 105 | PRO | N-CA-CB | 6.79 | 111.45 | 103.30 |
| 1 | F | 67 | LEU | CA-C-O | -6.79 | 105.84 | 120.10 |
| 1 | B | 2 | ASN | CB-CA-C | -6.79 | 96.83 | 110.40 |
| 1 | D | 129 | TYR | CD1-CG-CD2 | 6.79 | 125.36 | 117.90 |
| 1 | D | 192 | ARG | CG-CD-NE | 6.79 | 126.05 | 111.80 |
| 1 | C | 159 | ASP | N-CA-CB | 6.78 | 122.81 | 110.60 |
| 1 | D | 32 | MET | CA-CB-CG | 6.78 | 124.83 | 113.30 |
| 1 | D | 56 | THR | CB-CA-C | -6.78 | 93.28 | 111.60 |
| 1 | E | 188 | GLN | CA-C-N | 6.78 | 136.09 | 117.10 |
| 1 | F | 32 | MET | CA-C-O | -6.78 | 105.85 | 120.10 |
| 1 | C | 187 | LEU | CB-CG-CD1 | 6.78 | 122.53 | 111.00 |
| 1 | A | 112 | THR | OG1-CB-CG2 | -6.78 | 94.41 | 110.00 |
| 1 | A | 142 | HIS | CA-C-N | 6.78 | 132.11 | 117.20 |
| 1 | B | 126 | SER | CA-C-O | 6.78 | 134.33 | 120.10 |
| 1 | D | 32 | MET | CB-CA-C | -6.78 | 96.85 | 110.40 |
| 1 | A | 87 | ILE | CA-C-N | 6.78 | 129.75 | 116.20 |
| 1 | D | 221 | PRO | C-N-CA | 6.78 | 138.64 | 121.70 |
| 1 | A | 62 | LEU | N-CA-CB | 6.77 | 123.95 | 110.40 |
| 1 | C | 130 | SER | C-N-CA | 6.77 | 138.63 | 121.70 |
| 1 | D | 176 | THR | CA-C-O | -6.77 | 105.88 | 120.10 |
| 1 | E | 234 | THR | CA-CB-CG2 | 6.77 | 121.88 | 112.40 |
| 1 | C | 172 | TRP | NE1-CE2-CD2 | 6.77 | 114.07 | 107.30 |
| 1 | A | 228 | TYR | CD1-CE1-CZ | -6.77 | 113.71 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 141 | LEU | CB-CG-CD2 | 6.77 | 122.50 | 111.00 |
| 1 | D | 74 | GLN | CG-CD-OE1 | -6.76 | 108.07 | 121.60 |
| 1 | D | 84 | LYS | CA-C-N | 6.76 | 129.73 | 116.20 |
| 1 | B | 125 | ASN | N-CA-C | 6.76 | 129.26 | 111.00 |
| 1 | B | 158 | THR | CA-CB-CG2 | -6.76 | 102.93 | 112.40 |
| 1 | D | 183 | CYS | N-CA-C | 6.76 | 129.26 | 111.00 |
| 1 | D | 211 | SER | N-CA-CB | -6.76 | 100.36 | 110.50 |
| 1 | E | 152 | TYR | CA-CB-CG | 6.76 | 126.24 | 113.40 |
| 1 | F | 186 | VAL | CA-C-O | -6.76 | 105.91 | 120.10 |
| 1 | F | 40 | LEU | O-C-N | 6.76 | 133.51 | 122.70 |
| 1 | D | 84 | LYS | N-CA-CB | 6.76 | 122.76 | 110.60 |
| 1 | E | 78 | ARG | CB-CA-C | -6.76 | 96.89 | 110.40 |
| 1 | F | 201 | ILE | CA-C-N | 6.75 | 132.06 | 117.20 |
| 1 | C | 46 | ARG | CB-CG-CD | 6.75 | 129.16 | 111.60 |
| 1 | A | 217 | PHE | C-N-CA | 6.75 | 138.58 | 121.70 |
| 1 | C | 72 | THR | C-N-CA | -6.75 | 104.82 | 121.70 |
| 1 | B | 128 | LEU | N-CA-C | -6.75 | 92.78 | 111.00 |
| 1 | D | 218 | VAL | CA-CB-CG1 | -6.75 | 100.78 | 110.90 |
| 1 | E | 233 | TRP | N-CA-CB | 6.75 | 122.75 | 110.60 |
| 1 | C | 146 | SER | O-C-N | 6.75 | 133.50 | 122.70 |
| 1 | E | 145 | GLN | N-CA-C | -6.74 | 92.80 | 111.00 |
| 1 | F | 89 | ASN | N-CA-C | 6.74 | 129.20 | 111.00 |
| 1 | D | 3 | ILE | CA-C-O | -6.74 | 105.95 | 120.10 |
| 1 | E | 171 | VAL | CA-CB-CG1 | 6.74 | 121.01 | 110.90 |
| 1 | A | 44 | ASP | N-CA-C | -6.74 | 92.82 | 111.00 |
| 1 | C | 214 | ARG | CA-C-N | 6.74 | 132.02 | 117.20 |
| 1 | D | 73 | ALA | CB-CA-C | -6.73 | 100.01 | 110.10 |
| 1 | D | 87 | ILE | C-N-CA | -6.73 | 108.17 | 122.30 |
| 1 | F | 125 | ASN | CB-CG-ND2 | 6.72 | 132.84 | 116.70 |
| 1 | A | 231 | ALA | O-C-N | -6.72 | 111.94 | 122.70 |
| 1 | F | 99 | THR | CA-CB-CG2 | -6.72 | 102.99 | 112.40 |
| 1 | F | 232 | LEU | CA-CB-CG | 6.72 | 130.76 | 115.30 |
| 1 | F | 1 | ASN | CA-C-O | 6.72 | 134.21 | 120.10 |
| 1 | B | 15 | GLN | CG-CD-NE2 | 6.72 | 132.82 | 116.70 |
| 1 | C | 106 | GLY | CA-C-N | -6.72 | 102.42 | 117.20 |
| 1 | A | 152 | TYR | CG-CD1-CE1 | 6.71 | 126.67 | 121.30 |
| 1 | C | 119 | VAL | CB-CA-C | 6.71 | 124.16 | 111.40 |
| 1 | C | 168 | ASP | CA-C-O | -6.71 | 106.00 | 120.10 |
| 1 | E | 129 | TYR | N-CA-C | 6.71 | 129.12 | 111.00 |
| 1 | F | 201 | ILE | CA-CB-CG1 | 6.71 | 123.75 | 111.00 |
| 1 | B | 44 | ASP | CA-CB-CG | 6.71 | 128.16 | 113.40 |
| 1 | A | 62 | LEU | CB-CA-C | -6.71 | 97.46 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 162 | LEU | N-CA-CB | -6.70 | 96.99 | 110.40 |
| 1 | B | 76 | THR | CA-C-N | 6.70 | 131.94 | 117.20 |
| 1 | E | 209 | SER | C-N-CA | 6.70 | 138.45 | 121.70 |
| 1 | A | 8 | SER | N-CA-CB | -6.70 | 100.45 | 110.50 |
| 1 | A | 70 | ILE | CA-C-O | 6.70 | 134.17 | 120.10 |
| 1 | F | 204 | TRP | CE2-CD2-CG | 6.70 | 112.66 | 107.30 |
| 1 | E | 119 | VAL | N-CA-C | 6.70 | 129.08 | 111.00 |
| 1 | E | 163 | VAL | CA-C-O | -6.70 | 106.04 | 120.10 |
| 1 | C | 144 | THR | OG1-CB-CG2 | 6.69 | 125.40 | 110.00 |
| 1 | D | 190 | ASN | CB-CG-OD1 | 6.69 | 134.99 | 121.60 |
| 1 | F | 181 | THR | CA-C-N | 6.69 | 129.59 | 116.20 |
| 1 | C | 98 | ARG | NE-CZ-NH1 | -6.69 | 116.95 | 120.30 |
| 1 | E | 232 | LEU | CD1-CG-CD2 | -6.69 | 90.43 | 110.50 |
| 1 | D | 139 | GLN | CA-C-N | -6.69 | 102.48 | 117.20 |
| 1 | C | 37 | ASN | CA-C-O | -6.69 | 106.06 | 120.10 |
| 1 | F | 165 | PHE | N-CA-CB | -6.69 | 98.56 | 110.60 |
| 1 | D | 25 | LEU | CA-C-O | -6.69 | 106.06 | 120.10 |
| 1 | D | 167 | ARG | C-N-CA | 6.69 | 138.41 | 121.70 |
| 1 | A | 21 | GLN | O-C-N | 6.68 | 133.39 | 122.70 |
| 1 | D | 96 | PRO | O-C-N | -6.68 | 112.01 | 122.70 |
| 1 | D | 222 | ASP | CB-CA-C | -6.68 | 97.03 | 110.40 |
| 1 | B | 123 | ASN | O-C-N | -6.68 | 111.84 | 123.20 |
| 1 | D | 92 | LEU | CA-C-N | 6.68 | 131.89 | 117.20 |
| 1 | A | 42 | ASP | CA-CB-CG | -6.68 | 98.71 | 113.40 |
| 1 | A | 189 | PRO | CA-N-CD | -6.68 | 102.15 | 111.50 |
| 1 | D | 204 | TRP | CA-C-O | -6.68 | 106.08 | 120.10 |
| 1 | D | 112 | THR | O-C-N | -6.67 | 112.02 | 122.70 |
| 1 | B | 212 | ALA | N-CA-CB | -6.67 | 100.76 | 110.10 |
| 1 | C | 113 | SER | C-N-CA | 6.67 | 138.38 | 121.70 |
| 1 | C | 174 | THR | N-CA-CB | 6.67 | 122.98 | 110.30 |
| 1 | F | 145 | GLN | CA-CB-CG | -6.67 | 98.72 | 113.40 |
| 1 | C | 228 | TYR | CA-C-N | -6.67 | 102.87 | 116.20 |
| 1 | D | 177 | ALA | N-CA-C | -6.67 | 93.00 | 111.00 |
| 1 | F | 155 | SER | CA-C-O | 6.67 | 134.10 | 120.10 |
| 1 | C | 127 | ILE | CA-CB-CG2 | -6.67 | 97.57 | 110.90 |
| 1 | C | 139 | GLN | CB-CG-CD | 6.67 | 128.93 | 111.60 |
| 1 | A | 92 | LEU | CA-C-N | 6.66 | 131.86 | 117.20 |
| 1 | C | 201 | ILE | C-N-CA | 6.66 | 138.36 | 121.70 |
| 1 | B | 11 | GLY | CA-C-N | -6.66 | 102.54 | 117.20 |
| 1 | C | 26 | SER | CA-C-N | 6.66 | 131.86 | 117.20 |
| 1 | C | 204 | TRP | CH2-CZ2-CE2 | 6.66 | 124.06 | 117.40 |
| 1 | D | 188 | GLN | CA-C-O | 6.66 | 134.09 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 202 | ALA | O-C-N | -6.66 | 112.04 | 122.70 |
| 1 | F | 25 | LEU | CB-CG-CD1 | -6.66 | 99.68 | 111.00 |
| 1 | A | 102 | ILE | C-N-CA | -6.66 | 105.06 | 121.70 |
| 1 | B | 6 | GLY | N-CA-C | -6.66 | 96.46 | 113.10 |
| 1 | D | 164 | LEU | CB-CA-C | -6.66 | 97.56 | 110.20 |
| 1 | F | 48 | TRP | O-C-N | 6.66 | 133.35 | 122.70 |
| 1 | F | 61 | VAL | C-N-CA | -6.66 | 105.06 | 121.70 |
| 1 | F | 74 | GLN | CB-CA-C | -6.66 | 97.09 | 110.40 |
| 1 | F | 110 | SER | C-N-CA | -6.66 | 108.32 | 122.30 |
| 1 | A | 165 | PHE | CG-CD1-CE1 | 6.65 | 128.12 | 120.80 |
| 1 | C | 170 | ARG | CA-C-O | -6.65 | 106.13 | 120.10 |
| 1 | D | 95 | GLN | N-CA-CB | -6.65 | 98.63 | 110.60 |
| 1 | E | 194 | ASP | CB-CG-OD1 | 6.65 | 124.29 | 118.30 |
| 1 | A | 66 | GLY | CA-C-N | 6.64 | 131.82 | 117.20 |
| 1 | D | 20 | ALA | N-CA-CB | -6.64 | 100.80 | 110.10 |
| 1 | A | 138 | PRO | O-C-N | -6.64 | 112.07 | 122.70 |
| 1 | B | 226 | ALA | CA-C-N | -6.64 | 102.59 | 117.20 |
| 1 | B | 144 | THR | O-C-N | -6.64 | 112.08 | 122.70 |
| 1 | D | 228 | TYR | C-N-CA | 6.64 | 136.24 | 122.30 |
| 1 | A | 34 | SER | O-C-N | -6.64 | 112.08 | 122.70 |
| 1 | A | 143 | ALA | N-CA-CB | -6.63 | 100.81 | 110.10 |
| 1 | B | 40 | LEU | CB-CA-C | -6.63 | 97.60 | 110.20 |
| 1 | F | 210 | ARG | CA-CB-CG | -6.63 | 98.81 | 113.40 |
| 1 | B | 219 | LEU | CA-CB-CG | 6.63 | 130.54 | 115.30 |
| 1 | A | 186 | VAL | C-N-CA | -6.62 | 105.14 | 121.70 |
| 1 | E | 199 | GLN | N-CA-CB | -6.62 | 98.68 | 110.60 |
| 1 | E | 35 | ASP | C-N-CA | 6.62 | 138.26 | 121.70 |
| 1 | B | 29 | ARG | O-C-N | 6.62 | 133.29 | 122.70 |
| 1 | C | 214 | ARG | CG-CD-NE | 6.62 | 125.70 | 111.80 |
| 1 | E | 16 | THR | CB-CA-C | -6.62 | 93.72 | 111.60 |
| 1 | E | 67 | LEU | C-N-CA | -6.62 | 105.15 | 121.70 |
| 1 | A | 195 | VAL | CA-C-N | -6.62 | 102.64 | 117.20 |
| 1 | A | 227 | ILE | CA-C-N | 6.62 | 131.76 | 117.20 |
| 1 | B | 144 | THR | CA-CB-CG2 | 6.62 | 121.66 | 112.40 |
| 1 | A | 97 | ASP | CA-C-O | -6.62 | 106.21 | 120.10 |
| 1 | C | 46 | ARG | CG-CD-NE | 6.62 | 125.69 | 111.80 |
| 1 | D | 33 | GLN | CA-C-O | -6.61 | 106.21 | 120.10 |
| 1 | D | 217 | PHE | N-CA-CB | -6.61 | 98.70 | 110.60 |
| 1 | E | 79 | TRP | CD1-NE1-CE2 | -6.61 | 103.05 | 109.00 |
| 1 | E | 170 | ARG | NE-CZ-NH1 | -6.61 | 116.99 | 120.30 |
| 1 | E | 235 | THR | N-CA-CB | -6.61 | 97.73 | 110.30 |
| 1 | E | 171 | VAL | CA-C-N | 6.61 | 131.75 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 63 | GLN | N-CA-C | 6.61 | 128.85 | 111.00 |
| 1 | C | 119 | VAL | C-N-CA | 6.61 | 138.23 | 121.70 |
| 1 | A | 138 | PRO | CA-C-N | 6.61 | 131.74 | 117.20 |
| 1 | F | 216 | VAL | C-N-CA | 6.61 | 138.22 | 121.70 |
| 1 | A | 156 | MET | CG-SD-CE | 6.60 | 110.77 | 100.20 |
| 1 | B | 1 | ASN | C-N-CA | 6.60 | 138.21 | 121.70 |
| 1 | B | 53 | ALA | CA-C-O | -6.60 | 106.24 | 120.10 |
| 1 | F | 223 | ARG | CA-CB-CG | -6.60 | 98.88 | 113.40 |
| 1 | E | 27 | SER | CB-CA-C | -6.60 | 97.57 | 110.10 |
| 1 | F | 155 | SER | C-N-CA | 6.60 | 138.19 | 121.70 |
| 1 | F | 181 | THR | CA-CB-CG2 | -6.60 | 103.16 | 112.40 |
| 1 | C | 69 | VAL | CA-CB-CG2 | -6.59 | 101.01 | 110.90 |
| 1 | E | 2 | ASN | N-CA-CB | -6.59 | 98.73 | 110.60 |
| 1 | C | 153 | ARG | CB-CG-CD | -6.59 | 94.46 | 111.60 |
| 1 | F | 30 | PHE | CG-CD2-CE2 | -6.59 | 113.55 | 120.80 |
| 1 | D | 137 | HIS | C-N-CD | -6.59 | 106.10 | 120.60 |
| 1 | B | 82 | GLY | CA-C-N | -6.59 | 102.71 | 117.20 |
| 1 | C | 113 | SER | N-CA-C | -6.59 | 93.22 | 111.00 |
| 1 | E | 23 | LEU | N-CA-C | -6.59 | 93.22 | 111.00 |
| 1 | F | 222 | ASP | CA-CB-CG | 6.59 | 127.89 | 113.40 |
| 1 | B | 108 | TRP | CE3-CZ3-CH2 | 6.58 | 128.44 | 121.20 |
| 1 | B | 162 | LEU | C-N-CA | -6.58 | 105.24 | 121.70 |
| 1 | A | 29 | ARG | CB-CA-C | -6.58 | 97.23 | 110.40 |
| 1 | F | 186 | VAL | CA-CB-CG1 | 6.58 | 120.77 | 110.90 |
| 1 | E | 18 | HIS | CA-C-O | -6.58 | 106.28 | 120.10 |
| 1 | F | 39 | VAL | CG1-CB-CG2 | -6.58 | 100.38 | 110.90 |
| 1 | B | 188 | GLN | CA-C-N | 6.58 | 135.51 | 117.10 |
| 1 | F | 209 | SER | CA-C-O | -6.58 | 106.29 | 120.10 |
| 1 | D | 152 | TYR | CG-CD2-CE2 | 6.57 | 126.56 | 121.30 |
| 1 | E | 192 | ARG | CD-NE-CZ | 6.57 | 132.80 | 123.60 |
| 1 | E | 47 | VAL | CG1-CB-CG2 | -6.57 | 100.39 | 110.90 |
| 1 | E | 154 | LEU | CA-CB-CG | 6.57 | 130.40 | 115.30 |
| 1 | D | 92 | LEU | CB-CA-C | -6.57 | 97.73 | 110.20 |
| 1 | E | 99 | THR | CA-C-O | 6.57 | 133.89 | 120.10 |
| 1 | F | 235 | THR | CA-CB-OG1 | 6.57 | 122.79 | 109.00 |
| 1 | C | 86 | SER | CA-C-O | -6.56 | 106.32 | 120.10 |
| 1 | C | 109 | ASP | CB-CG-OD2 | 6.56 | 124.21 | 118.30 |
| 1 | C | 126 | SER | N-CA-CB | 6.56 | 120.34 | 110.50 |
| 1 | C | 190 | ASN | CB-CG-ND2 | 6.56 | 132.45 | 116.70 |
| 1 | A | 130 | SER | CA-C-N | 6.56 | 131.63 | 117.20 |
| 1 | B | 111 | GLY | CA-C-N | 6.56 | 131.63 | 117.20 |
| 1 | A | 30 | PHE | CA-CB-CG | 6.56 | 129.64 | 113.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 103 | TYR | N-CA-CB | -6.55 | 98.80 | 110.60 |
| 1 | D | 152 | TYR | CB-CA-C | -6.55 | 97.29 | 110.40 |
| 1 | B | 37 | ASN | CA-C-O | -6.55 | 106.34 | 120.10 |
| 1 | A | 7 | LEU | O-C-N | -6.55 | 112.22 | 122.70 |
| 1 | C | 107 | LEU | CB-CA-C | 6.55 | 122.65 | 110.20 |
| 1 | A | 89 | ASN | CA-C-O | -6.55 | 106.35 | 120.10 |
| 1 | C | 107 | LEU | CA-C-N | 6.55 | 131.61 | 117.20 |
| 1 | D | 198 | ASN | CB-CG-OD1 | -6.55 | 108.50 | 121.60 |
| 1 | E | 30 | PHE | CA-CB-CG | 6.55 | 129.62 | 113.90 |
| 1 | F | 68 | LEU | CA-C-N | -6.55 | 102.79 | 117.20 |
| 1 | C | 165 | PHE | CB-CG-CD2 | 6.55 | 125.38 | 120.80 |
| 1 | E | 184 | ARG | NE-CZ-NH1 | -6.54 | 117.03 | 120.30 |
| 1 | F | 1 | ASN | N-CA-C | 6.54 | 128.67 | 111.00 |
| 1 | F | 74 | GLN | OE1-CD-NE2 | 6.54 | 136.95 | 121.90 |
| 1 | A | 30 | PHE | CB-CG-CD2 | 6.54 | 125.38 | 120.80 |
| 1 | A | 200 | ASN | CA-C-O | 6.54 | 133.84 | 120.10 |
| 1 | D | 168 | ASP | CA-C-O | 6.54 | 133.84 | 120.10 |
| 1 | F | 165 | PHE | CA-C-N | 6.54 | 131.60 | 117.20 |
| 1 | C | 3 | ILE | CG1-CB-CG2 | -6.54 | 97.01 | 111.40 |
| 1 | C | 174 | THR | CA-C-O | 6.54 | 133.84 | 120.10 |
| 1 | D | 141 | LEU | N-CA-CB | -6.54 | 97.32 | 110.40 |
| 1 | B | 144 | THR | CA-CB-OG1 | 6.54 | 122.73 | 109.00 |
| 1 | A | 48 | TRP | CH2-CZ2-CE2 | -6.54 | 110.86 | 117.40 |
| 1 | C | 10 | GLU | CB-CG-CD | 6.54 | 131.85 | 114.20 |
| 1 | C | 163 | VAL | CA-CB-CG2 | -6.54 | 101.09 | 110.90 |
| 1 | A | 63 | GLN | CA-CB-CG | -6.54 | 99.02 | 113.40 |
| 1 | A | 165 | PHE | CZ-CE2-CD2 | 6.54 | 127.94 | 120.10 |
| 1 | A | 130 | SER | N-CA-C | 6.53 | 128.63 | 111.00 |
| 1 | A | 1 | ASN | N-CA-C | -6.53 | 93.38 | 111.00 |
| 1 | B | 139 | GLN | OE1-CD-NE2 | -6.53 | 106.89 | 121.90 |
| 1 | E | 69 | VAL | CB-CA-C | -6.53 | 99.00 | 111.40 |
| 1 | F | 44 | ASP | CB-CG-OD1 | -6.52 | 112.43 | 118.30 |
| 1 | D | 188 | GLN | CB-CA-C | 6.52 | 123.44 | 110.40 |
| 1 | D | 206 | SER | CA-C-O | -6.52 | 106.41 | 120.10 |
| 1 | A | 187 | LEU | CB-CG-CD1 | 6.52 | 122.08 | 111.00 |
| 1 | C | 48 | TRP | CD2-CE2-CZ2 | 6.51 | 130.12 | 122.30 |
| 1 | A | 219 | LEU | CB-CG-CD2 | 6.51 | 122.07 | 111.00 |
| 1 | B | 97 | ASP | CA-C-N | 6.51 | 131.53 | 117.20 |
| 1 | F | 225 | LEU | CB-CG-CD2 | -6.51 | 99.93 | 111.00 |
| 1 | A | 13 | HIS | CB-CG-ND1 | 6.51 | 139.47 | 123.20 |
| 1 | C | 195 | VAL | N-CA-C | -6.51 | 93.43 | 111.00 |
| 1 | A | 78 | ARG | O-C-N | -6.51 | 112.29 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 103 | TYR | OH-CZ-CE2 | -6.51 | 102.53 | 120.10 |
| 1 | B | 132 | GLN | N-CA-C | 6.50 | 128.56 | 111.00 |
| 1 | D | 48 | TRP | N-CA-C | -6.50 | 93.45 | 111.00 |
| 1 | A | 127 | ILE | O-C-N | -6.50 | 112.31 | 122.70 |
| 1 | C | 184 | ARG | CA-C-O | 6.50 | 133.74 | 120.10 |
| 1 | D | 131 | THR | OG1-CB-CG2 | 6.50 | 124.94 | 110.00 |
| 1 | C | 42 | ASP | CA-C-O | -6.49 | 106.46 | 120.10 |
| 1 | A | 74 | GLN | CB-CA-C | -6.49 | 97.42 | 110.40 |
| 1 | D | 59 | ARG | CG-CD-NE | -6.49 | 98.17 | 111.80 |
| 1 | E | 107 | LEU | CB-CG-CD1 | 6.49 | 122.03 | 111.00 |
| 1 | E | 223 | ARG | CB-CG-CD | 6.49 | 128.47 | 111.60 |
| 1 | C | 98 | ARG | CA-C-O | 6.49 | 133.72 | 120.10 |
| 1 | A | 56 | THR | CA-CB-CG2 | -6.49 | 103.32 | 112.40 |
| 1 | A | 225 | LEU | CA-C-O | 6.49 | 133.72 | 120.10 |
| 1 | D | 24 | GLU | C-N-CA | 6.48 | 137.91 | 121.70 |
| 1 | A | 127 | ILE | CA-C-N | 6.48 | 131.46 | 117.20 |
| 1 | B | 16 | THR | CB-CA-C | -6.48 | 94.09 | 111.60 |
| 1 | C | 40 | LEU | CD1-CG-CD2 | -6.48 | 91.05 | 110.50 |
| 1 | C | 56 | THR | C-N-CA | 6.48 | 135.91 | 122.30 |
| 1 | C | 132 | GLN | OE1-CD-NE2 | -6.48 | 106.99 | 121.90 |
| 1 | F | 21 | GLN | O-C-N | 6.48 | 133.07 | 122.70 |
| 1 | F | 198 | ASN | N-CA-CB | -6.48 | 98.93 | 110.60 |
| 1 | A | 47 | VAL | N-CA-C | 6.48 | 128.50 | 111.00 |
| 1 | A | 228 | TYR | CE1-CZ-OH | -6.48 | 102.61 | 120.10 |
| 1 | C | 100 | VAL | N-CA-C | -6.48 | 93.50 | 111.00 |
| 1 | C | 234 | THR | OG1-CB-CG2 | -6.48 | 95.10 | 110.00 |
| 1 | F | 129 | TYR | N-CA-C | 6.48 | 128.49 | 111.00 |
| 1 | B | 169 | ASP | CA-CB-CG | -6.47 | 99.16 | 113.40 |
| 1 | C | 48 | TRP | CE3-CZ3-CH2 | 6.47 | 128.32 | 121.20 |
| 1 | C | 56 | THR | N-CA-CB | 6.47 | 122.60 | 110.30 |
| 1 | E | 31 | THR | CA-C-O | 6.47 | 133.69 | 120.10 |
| 1 | F | 86 | SER | O-C-N | 6.47 | 133.06 | 122.70 |
| 1 | F | 152 | TYR | CE1-CZ-CE2 | 6.47 | 130.16 | 119.80 |
| 1 | F | 154 | LEU | CA-C-N | 6.47 | 131.44 | 117.20 |
| 1 | C | 92 | LEU | CA-C-N | 6.47 | 131.44 | 117.20 |
| 1 | A | 220 | GLN | CA-C-N | 6.47 | 135.21 | 117.10 |
| 1 | C | 206 | SER | CA-CB-OG | 6.47 | 128.66 | 111.20 |
| 1 | A | 231 | ALA | CB-CA-C | -6.47 | 100.40 | 110.10 |
| 1 | B | 72 | THR | OG1-CB-CG2 | -6.47 | 95.13 | 110.00 |
| 1 | A | 147 | LEU | C-N-CA | 6.46 | 137.86 | 121.70 |
| 1 | B | 97 | ASP | CA-CB-CG | 6.46 | 127.62 | 113.40 |
| 1 | B | 62 | LEU | CB-CA-C | -6.46 | 97.92 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 130 | SER | N-CA-CB | -6.46 | 100.81 | 110.50 |
| 1 | F | 37 | ASN | O-C-N | 6.46 | 133.04 | 122.70 |
| 1 | D | 154 | LEU | C-N-CA | 6.46 | 137.85 | 121.70 |
| 1 | C | 137 | HIS | C-N-CA | 6.46 | 149.12 | 122.00 |
| 1 | E | 181 | THR | N-CA-CB | 6.46 | 122.57 | 110.30 |
| 1 | E | 198 | ASN | CB-CG-OD1 | 6.46 | 134.51 | 121.60 |
| 1 | A | 186 | VAL | CA-CB-CG2 | 6.45 | 120.58 | 110.90 |
| 1 | D | 172 | TRP | CB-CG-CD2 | 6.45 | 134.99 | 126.60 |
| 1 | E | 157 | GLU | C-N-CA | -6.45 | 105.58 | 121.70 |
| 1 | E | 217 | PHE | CA-C-O | -6.45 | 106.56 | 120.10 |
| 1 | D | 138 | PRO | CA-CB-CG | -6.45 | 91.75 | 104.00 |
| 1 | E | 161 | ASN | N-CA-CB | -6.45 | 98.99 | 110.60 |
| 1 | D | 185 | ALA | O-C-N | 6.45 | 133.01 | 122.70 |
| 1 | E | 232 | LEU | CA-C-O | -6.45 | 106.56 | 120.10 |
| 1 | F | 68 | LEU | CA-C-O | 6.45 | 133.64 | 120.10 |
| 1 | D | 228 | TYR | CA-C-O | -6.44 | 106.57 | 120.10 |
| 1 | D | 63 | GLN | CG-CD-OE1 | -6.44 | 108.71 | 121.60 |
| 1 | F | 103 | TYR | CG-CD2-CE2 | 6.44 | 126.45 | 121.30 |
| 1 | B | 18 | HIS | C-N-CA | -6.44 | 105.60 | 121.70 |
| 1 | F | 172 | TRP | N-CA-CB | -6.44 | 99.01 | 110.60 |
| 1 | B | 111 | GLY | C-N-CA | 6.44 | 137.79 | 121.70 |
| 1 | B | 214 | ARG | CB-CG-CD | 6.44 | 128.34 | 111.60 |
| 1 | C | 47 | VAL | CA-C-N | 6.44 | 131.37 | 117.20 |
| 1 | F | 103 | TYR | CB-CG-CD2 | 6.44 | 124.86 | 121.00 |
| 1 | E | 58 | CYS | CA-CB-SG | -6.44 | 102.42 | 114.00 |
| 1 | B | 181 | THR | C-N-CA | -6.43 | 108.79 | 122.30 |
| 1 | A | 204 | TRP | CA-C-O | 6.43 | 133.60 | 120.10 |
| 1 | B | 58 | CYS | CA-C-O | -6.43 | 106.60 | 120.10 |
| 1 | E | 193 | MET | N-CA-C | -6.43 | 93.64 | 111.00 |
| 1 | C | 44 | ASP | CA-C-N | 6.43 | 131.34 | 117.20 |
| 1 | E | 219 | LEU | CB-CG-CD2 | 6.43 | 121.93 | 111.00 |
| 1 | C | 166 | ASP | CB-CG-OD2 | -6.43 | 112.52 | 118.30 |
| 1 | A | 77 | ILE | CA-C-N | 6.42 | 131.33 | 117.20 |
| 1 | C | 46 | ARG | CA-CB-CG | 6.42 | 127.53 | 113.40 |
| 1 | C | 196 | LEU | CB-CA-C | -6.42 | 97.99 | 110.20 |
| 1 | A | 169 | ASP | N-CA-CB | 6.42 | 122.16 | 110.60 |
| 1 | A | 167 | ARG | NE-CZ-NH2 | -6.42 | 117.09 | 120.30 |
| 1 | D | 172 | TRP | CD1-NE1-CE2 | -6.42 | 103.22 | 109.00 |
| 1 | F | 186 | VAL | C-N-CA | -6.42 | 105.65 | 121.70 |
| 1 | C | 37 | ASN | OD1-CG-ND2 | 6.42 | 136.66 | 121.90 |
| 1 | D | 51 | ASN | N-CA-CB | -6.42 | 99.05 | 110.60 |
| 1 | F | 15 | GLN | O-C-N | -6.42 | 112.43 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 188 | GLN | CA-C-O | -6.42 | 106.63 | 120.10 |
| 1 | E | 87 | ILE | C-N-CA | 6.42 | 135.77 | 122.30 |
| 1 | C | 117 | SER | N-CA-C | 6.41 | 128.32 | 111.00 |
| 1 | D | 32 | MET | CA-C-O | 6.41 | 133.57 | 120.10 |
| 1 | D | 92 | LEU | N-CA-C | -6.41 | 93.68 | 111.00 |
| 1 | D | 217 | PHE | CG-CD1-CE1 | 6.41 | 127.85 | 120.80 |
| 1 | E | 70 | ILE | CA-CB-CG2 | -6.41 | 98.08 | 110.90 |
| 1 | B | 192 | ARG | CA-C-O | -6.41 | 106.64 | 120.10 |
| 1 | C | 140 | THR | CA-CB-OG1 | -6.41 | 95.54 | 109.00 |
| 1 | D | 17 | LEU | N-CA-CB | 6.41 | 123.22 | 110.40 |
| 1 | F | 105 | PRO | CA-C-N | 6.41 | 129.02 | 116.20 |
| 1 | D | 39 | VAL | CA-CB-CG1 | -6.41 | 101.29 | 110.90 |
| 1 | D | 143 | ALA | CB-CA-C | 6.41 | 119.71 | 110.10 |
| 1 | A | 205 | THR | O-C-N | -6.40 | 112.46 | 122.70 |
| 1 | A | 22 | SER | CA-CB-OG | 6.40 | 128.48 | 111.20 |
| 1 | F | 22 | SER | O-C-N | -6.40 | 112.46 | 122.70 |
| 1 | B | 71 | LEU | CB-CG-CD2 | -6.40 | 100.12 | 111.00 |
| 1 | A | 97 | ASP | CA-CB-CG | 6.40 | 127.47 | 113.40 |
| 1 | E | 36 | CYS | CA-C-O | -6.40 | 106.67 | 120.10 |
| 1 | B | 142 | HIS | N-CA-C | 6.40 | 128.27 | 111.00 |
| 1 | A | 198 | ASN | CB-CG-OD1 | -6.39 | 108.81 | 121.60 |
| 1 | B | 228 | TYR | CA-C-N | 6.39 | 128.99 | 116.20 |
| 1 | D | 33 | GLN | O-C-N | -6.39 | 112.47 | 122.70 |
| 1 | E | 94 | LEU | CB-CA-C | -6.39 | 98.05 | 110.20 |
| 1 | A | 51 | ASN | CB-CG-ND2 | 6.39 | 132.04 | 116.70 |
| 1 | B | 232 | LEU | CA-C-O | 6.39 | 133.53 | 120.10 |
| 1 | D | 147 | LEU | C-N-CA | 6.39 | 137.68 | 121.70 |
| 1 | E | 175 | ASN | CB-CG-OD1 | 6.39 | 134.39 | 121.60 |
| 1 | D | 104 | GLY | CA-C-O | -6.39 | 109.10 | 120.60 |
| 1 | A | 45 | VAL | CA-C-N | -6.39 | 103.15 | 117.20 |
| 1 | A | 103 | TYR | O-C-N | -6.39 | 112.34 | 123.20 |
| 1 | E | 152 | TYR | CD1-CE1-CZ | 6.38 | 125.55 | 119.80 |
| 1 | E | 152 | TYR | N-CA-CB | 6.38 | 122.09 | 110.60 |
| 1 | E | 137 | HIS | CB-CG-CD2 | -6.38 | 111.01 | 130.80 |
| 1 | B | 58 | CYS | N-CA-C | 6.38 | 128.23 | 111.00 |
| 1 | B | 217 | PHE | CA-CB-CG | -6.38 | 98.58 | 113.90 |
| 1 | E | 215 | TYR | O-C-N | 6.38 | 132.91 | 122.70 |
| 1 | F | 5 | PHE | CG-CD1-CE1 | 6.38 | 127.82 | 120.80 |
| 1 | F | 14 | PRO | O-C-N | -6.38 | 112.49 | 122.70 |
| 1 | D | 216 | VAL | N-CA-CB | -6.38 | 97.47 | 111.50 |
| 1 | C | 145 | GLN | OE1-CD-NE2 | -6.37 | 107.24 | 121.90 |
| 1 | E | 28 | PHE | O-C-N | -6.37 | 112.50 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 141 | LEU | O-C-N | -6.37 | 112.50 | 122.70 |
| 1 | B | 206 | SER | O-C-N | -6.37 | 112.37 | 123.20 |
| 1 | C | 122 | ASN | N-CA-CB | 6.37 | 122.07 | 110.60 |
| 1 | F | 186 | VAL | O-C-N | 6.37 | 132.89 | 122.70 |
| 1 | B | 21 | GLN | OE1-CD-NE2 | -6.37 | 107.26 | 121.90 |
| 1 | D | 99 | THR | CA-C-N | -6.37 | 103.19 | 117.20 |
| 1 | E | 147 | LEU | CB-CA-C | -6.37 | 98.11 | 110.20 |
| 1 | B | 219 | LEU | CB-CA-C | -6.36 | 98.11 | 110.20 |
| 1 | E | 211 | SER | O-C-N | -6.36 | 112.52 | 122.70 |
| 1 | D | 58 | CYS | CA-C-O | -6.36 | 106.74 | 120.10 |
| 1 | C | 59 | ARG | NH1-CZ-NH2 | 6.36 | 126.39 | 119.40 |
| 1 | A | 195 | VAL | CB-CA-C | 6.36 | 123.47 | 111.40 |
| 1 | C | 158 | THR | O-C-N | -6.36 | 112.53 | 122.70 |
| 1 | E | 78 | ARG | CB-CG-CD | 6.35 | 128.12 | 111.60 |
| 1 | F | 92 | LEU | O-C-N | 6.35 | 132.87 | 122.70 |
| 1 | D | 225 | LEU | CA-CB-CG | -6.35 | 100.69 | 115.30 |
| 1 | E | 159 | ASP | OD1-CG-OD2 | -6.35 | 111.23 | 123.30 |
| 1 | E | 188 | GLN | CA-C-O | -6.35 | 106.76 | 120.10 |
| 1 | C | 233 | TRP | CG-CD2-CE3 | -6.35 | 128.19 | 133.90 |
| 1 | F | 30 | PHE | CA-CB-CG | -6.35 | 98.66 | 113.90 |
| 1 | A | 53 | ALA | CA-C-O | 6.35 | 133.43 | 120.10 |
| 1 | B | 219 | LEU | CA-C-N | 6.35 | 131.17 | 117.20 |
| 1 | E | 48 | TRP | CA-C-N | 6.35 | 131.17 | 117.20 |
| 1 | E | 51 | ASN | CA-CB-CG | 6.35 | 127.36 | 113.40 |
| 1 | F | 150 | SER | CA-C-O | -6.35 | 106.77 | 120.10 |
| 1 | F | 168 | ASP | CA-CB-CG | 6.35 | 127.37 | 113.40 |
| 1 | A | 119 | VAL | O-C-N | -6.35 | 112.55 | 122.70 |
| 1 | D | 190 | ASN | OD1-CG-ND2 | -6.35 | 107.30 | 121.90 |
| 1 | A | 198 | ASN | CA-C-O | 6.34 | 133.42 | 120.10 |
| 1 | D | 207 | GLY | N-CA-C | 6.34 | 128.96 | 113.10 |
| 1 | A | 163 | VAL | N-CA-CB | 6.34 | 125.44 | 111.50 |
| 1 | D | 200 | ASN | CA-CB-CG | -6.34 | 99.46 | 113.40 |
| 1 | B | 225 | LEU | CB-CG-CD2 | 6.34 | 121.77 | 111.00 |
| 1 | C | 166 | ASP | O-C-N | -6.34 | 112.56 | 122.70 |
| 1 | E | 169 | ASP | CA-CB-CG | 6.34 | 127.34 | 113.40 |
| 1 | E | 211 | SER | CA-C-O | -6.33 | 106.80 | 120.10 |
| 1 | F | 10 | GLU | CG-CD-OE1 | 6.33 | 130.97 | 118.30 |
| 1 | A | 77 | ILE | N-CA-C | 6.33 | 128.10 | 111.00 |
| 1 | F | 52 | THR | CB-CA-C | -6.33 | 94.51 | 111.60 |
| 1 | E | 1 | ASN | CB-CG-OD1 | 6.33 | 134.26 | 121.60 |
| 1 | E | 46 | ARG | NE-CZ-NH2 | 6.33 | 123.46 | 120.30 |
| 1 | A | 56 | THR | N-CA-CB | 6.33 | 122.32 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 93 | VAL | CA-C-O | -6.33 | 106.81 | 120.10 |
| 1 | B | 87 | ILE | O-C-N | -6.33 | 112.45 | 123.20 |
| 1 | C | 205 | THR | CB-CA-C | -6.33 | 94.52 | 111.60 |
| 1 | F | 108 | TRP | CA-C-O | -6.33 | 106.82 | 120.10 |
| 1 | D | 165 | PHE | N-CA-CB | 6.32 | 121.98 | 110.60 |
| 1 | F | 50 | SER | C-N-CA | 6.32 | 137.49 | 121.70 |
| 1 | B | 142 | HIS | O-C-N | -6.32 | 112.60 | 122.70 |
| 1 | C | 167 | ARG | CA-C-O | -6.32 | 106.84 | 120.10 |
| 1 | C | 201 | ILE | CA-CB-CG1 | -6.32 | 99.00 | 111.00 |
| 1 | F | 33 | GLN | CA-C-O | -6.32 | 106.84 | 120.10 |
| 1 | F | 189 | PRO | CA-C-N | 6.32 | 131.10 | 117.20 |
| 1 | A | 199 | GLN | C-N-CA | 6.31 | 137.48 | 121.70 |
| 1 | D | 108 | TRP | CA-C-N | 6.31 | 131.08 | 117.20 |
| 1 | B | 17 | LEU | CA-C-N | 6.31 | 131.08 | 117.20 |
| 1 | C | 217 | PHE | CG-CD2-CE2 | 6.31 | 127.74 | 120.80 |
| 1 | F | 79 | TRP | CB-CA-C | -6.31 | 97.78 | 110.40 |
| 1 | F | 151 | PRO | CB-CA-C | 6.31 | 127.77 | 112.00 |
| 1 | A | 175 | ASN | OD1-CG-ND2 | 6.30 | 136.40 | 121.90 |
| 1 | A | 219 | LEU | CB-CA-C | -6.30 | 98.22 | 110.20 |
| 1 | F | 165 | PHE | CG-CD1-CE1 | 6.30 | 127.73 | 120.80 |
| 1 | F | 108 | TRP | CG-CD2-CE3 | -6.30 | 128.23 | 133.90 |
| 1 | A | 105 | PRO | N-CA-CB | 6.30 | 110.86 | 103.30 |
| 1 | C | 52 | THR | CA-C-N | 6.30 | 131.06 | 117.20 |
| 1 | A | 107 | LEU | CB-CA-C | 6.30 | 122.16 | 110.20 |
| 1 | D | 83 | THR | OG1-CB-CG2 | 6.30 | 124.48 | 110.00 |
| 1 | E | 81 | SER | O-C-N | 6.29 | 133.90 | 123.20 |
| 1 | F | 62 | LEU | N-CA-CB | 6.29 | 122.99 | 110.40 |
| 1 | B | 109 | ASP | C-N-CA | 6.29 | 137.43 | 121.70 |
| 1 | B | 112 | THR | CA-C-N | 6.29 | 131.04 | 117.20 |
| 1 | D | 75 | ASN | CB-CA-C | -6.29 | 97.82 | 110.40 |
| 1 | F | 56 | THR | CB-CA-C | -6.29 | 94.62 | 111.60 |
| 1 | B | 108 | TRP | CE2-CD2-CG | 6.29 | 112.33 | 107.30 |
| 1 | F | 129 | TYR | CZ-CE2-CD2 | -6.29 | 114.14 | 119.80 |
| 1 | C | 145 | GLN | N-CA-CB | -6.29 | 99.29 | 110.60 |
| 1 | E | 149 | LEU | N-CA-CB | 6.29 | 122.97 | 110.40 |
| 1 | A | 97 | ASP | N-CA-CB | -6.28 | 99.29 | 110.60 |
| 1 | C | 16 | THR | C-N-CA | -6.28 | 105.99 | 121.70 |
| 1 | F | 235 | THR | N-CA-CB | -6.28 | 98.36 | 110.30 |
| 1 | C | 5 | PHE | CA-C-O | 6.28 | 133.29 | 120.10 |
| 1 | D | 9 | HIS | CA-C-N | 6.28 | 131.02 | 117.20 |
| 1 | A | 76 | THR | CA-C-N | 6.28 | 131.01 | 117.20 |
| 1 | A | 118 | VAL | CA-CB-CG1 | 6.28 | 120.32 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 169 | ASP | O-C-N | -6.28 | 112.65 | 122.70 |
| 1 | B | 137 | HIS | C-N-CD | 6.28 | 141.58 | 128.40 |
| 1 | F | 2 | ASN | OD1-CG-ND2 | 6.28 | 136.34 | 121.90 |
| 1 | B | 141 | LEU | CD1-CG-CD2 | -6.28 | 91.67 | 110.50 |
| 1 | C | 176 | THR | CA-C-N | 6.28 | 131.00 | 117.20 |
| 1 | C | 96 | PRO | C-N-CA | 6.27 | 137.39 | 121.70 |
| 1 | F | 192 | ARG | CG-CD-NE | 6.27 | 124.97 | 111.80 |
| 1 | A | 129 | TYR | N-CA-C | -6.27 | 94.06 | 111.00 |
| 1 | E | 218 | VAL | C-N-CA | 6.27 | 137.38 | 121.70 |
| 1 | F | 206 | SER | C-N-CA | 6.27 | 135.47 | 122.30 |
| 1 | B | 107 | LEU | CB-CG-CD1 | 6.27 | 121.66 | 111.00 |
| 1 | C | 232 | LEU | CB-CA-C | -6.26 | 98.30 | 110.20 |
| 1 | C | 73 | ALA | N-CA-CB | 6.26 | 118.87 | 110.10 |
| 1 | C | 229 | GLY | C-N-CA | 6.26 | 135.45 | 122.30 |
| 1 | A | 104 | GLY | CA-C-O | -6.26 | 109.33 | 120.60 |
| 1 | C | 62 | LEU | CA-C-O | 6.26 | 133.24 | 120.10 |
| 1 | C | 161 | ASN | CB-CG-ND2 | 6.26 | 131.72 | 116.70 |
| 1 | A | 78 | ARG | CB-CG-CD | 6.26 | 127.87 | 111.60 |
| 1 | B | 190 | ASN | CB-CG-OD1 | -6.26 | 109.09 | 121.60 |
| 1 | E | 145 | GLN | CG-CD-NE2 | 6.26 | 131.71 | 116.70 |
| 1 | E | 138 | PRO | O-C-N | 6.25 | 132.71 | 122.70 |
| 1 | B | 46 | ARG | CG-CD-NE | -6.25 | 98.68 | 111.80 |
| 1 | C | 181 | THR | C-N-CA | -6.25 | 109.18 | 122.30 |
| 1 | F | 105 | PRO | C-N-CA | 6.25 | 135.42 | 122.30 |
| 1 | E | 168 | ASP | CB-CG-OD1 | 6.25 | 123.92 | 118.30 |
| 1 | F | 45 | VAL | N-CA-C | -6.25 | 94.14 | 111.00 |
| 1 | F | 24 | GLU | CA-C-O | -6.24 | 106.99 | 120.10 |
| 1 | D | 169 | ASP | O-C-N | 6.24 | 132.69 | 122.70 |
| 1 | A | 147 | LEU | CA-C-N | 6.24 | 130.93 | 117.20 |
| 1 | B | 70 | ILE | CG1-CB-CG2 | -6.24 | 97.67 | 111.40 |
| 1 | C | 184 | ARG | N-CA-C | -6.24 | 94.15 | 111.00 |
| 1 | C | 132 | GLN | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 1 | B | 54 | GLY | C-N-CA | -6.24 | 106.11 | 121.70 |
| 1 | D | 40 | LEU | CA-CB-CG | -6.23 | 100.96 | 115.30 |
| 1 | F | 68 | LEU | CD1-CG-CD2 | 6.23 | 129.20 | 110.50 |
| 1 | A | 117 | SER | N-CA-C | 6.23 | 127.83 | 111.00 |
| 1 | B | 22 | SER | CA-C-N | 6.23 | 130.91 | 117.20 |
| 1 | D | 204 | TRP | N-CA-CB | 6.23 | 121.82 | 110.60 |
| 1 | E | 74 | GLN | CB-CA-C | -6.23 | 97.94 | 110.40 |
| 1 | A | 140 | THR | CA-C-N | -6.22 | 103.51 | 117.20 |
| 1 | A | 206 | SER | CA-CB-OG | 6.22 | 128.00 | 111.20 |
| 1 | D | 33 | GLN | OE1-CD-NE2 | 6.22 | 136.22 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 67 | LEU | N-CA-CB | 6.22 | 122.85 | 110.40 |
| 1 | A | 194 | ASP | CA-C-O | 6.22 | 133.17 | 120.10 |
| 1 | D | 45 | VAL | CA-C-N | -6.22 | 103.51 | 117.20 |
| 1 | A | 22 | SER | N-CA-CB | -6.22 | 101.17 | 110.50 |
| 1 | C | 176 | THR | CA-CB-OG1 | 6.22 | 122.06 | 109.00 |
| 1 | E | 35 | ASP | CA-C-N | 6.22 | 130.89 | 117.20 |
| 1 | B | 230 | GLY | C-N-CA | 6.22 | 137.25 | 121.70 |
| 1 | D | 89 | ASN | N-CA-C | 6.22 | 127.79 | 111.00 |
| 1 | B | 79 | TRP | CH2-CZ2-CE2 | 6.22 | 123.62 | 117.40 |
| 1 | E | 194 | ASP | N-CA-CB | -6.22 | 99.41 | 110.60 |
| 1 | A | 185 | ALA | CB-CA-C | 6.21 | 119.42 | 110.10 |
| 1 | C | 192 | ARG | CB-CA-C | 6.21 | 122.83 | 110.40 |
| 1 | C | 185 | ALA | N-CA-CB | 6.21 | 118.80 | 110.10 |
| 1 | F | 74 | GLN | N-CA-C | 6.21 | 127.77 | 111.00 |
| 1 | D | 33 | GLN | N-CA-C | 6.21 | 127.77 | 111.00 |
| 1 | A | 93 | VAL | CA-CB-CG1 | 6.21 | 120.21 | 110.90 |
| 1 | A | 188 | GLN | OE1-CD-NE2 | -6.21 | 107.62 | 121.90 |
| 1 | A | 209 | SER | N-CA-CB | -6.21 | 101.19 | 110.50 |
| 1 | F | 89 | ASN | OD1-CG-ND2 | 6.21 | 136.17 | 121.90 |
| 1 | A | 155 | SER | C-N-CA | -6.20 | 106.19 | 121.70 |
| 1 | B | 164 | LEU | N-CA-CB | 6.20 | 122.80 | 110.40 |
| 1 | A | 109 | ASP | CB-CA-C | -6.20 | 98.00 | 110.40 |
| 1 | A | 85 | GLY | CA-C-N | -6.20 | 103.56 | 117.20 |
| 1 | B | 220 | GLN | CA-C-O | 6.20 | 133.12 | 120.10 |
| 1 | A | 18 | HIS | N-CA-CB | 6.20 | 121.75 | 110.60 |
| 1 | B | 16 | THR | O-C-N | 6.20 | 132.62 | 122.70 |
| 1 | C | 25 | LEU | N-CA-C | -6.20 | 94.27 | 111.00 |
| 1 | B | 165 | PHE | C-N-CA | -6.20 | 106.21 | 121.70 |
| 1 | C | 25 | LEU | C-N-CA | 6.20 | 137.19 | 121.70 |
| 1 | C | 170 | ARG | CA-C-N | 6.20 | 130.83 | 117.20 |
| 1 | A | 222 | ASP | C-N-CA | -6.19 | 106.22 | 121.70 |
| 1 | D | 30 | PHE | CA-CB-CG | -6.19 | 99.04 | 113.90 |
| 1 | F | 51 | ASN | OD1-CG-ND2 | -6.19 | 107.67 | 121.90 |
| 1 | B | 213 | GLY | CA-C-O | 6.19 | 131.74 | 120.60 |
| 1 | E | 235 | THR | OG1-CB-CG2 | -6.19 | 95.77 | 110.00 |
| 1 | F | 74 | GLN | C-N-CA | 6.19 | 137.17 | 121.70 |
| 1 | A | 105 | PRO | N-CA-C | -6.19 | 96.02 | 112.10 |
| 1 | C | 91 | VAL | CA-C-N | 6.19 | 130.81 | 117.20 |
| 1 | A | 221 | PRO | CA-C-N | 6.18 | 130.81 | 117.20 |
| 1 | B | 15 | GLN | O-C-N | 6.18 | 132.60 | 122.70 |
| 1 | B | 215 | TYR | CE1-CZ-OH | 6.18 | 136.80 | 120.10 |
| 1 | E | 140 | THR | C-N-CA | -6.18 | 106.24 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 83 | THR | CA-C-N | 6.18 | 130.81 | 117.20 |
| 1 | B | 13 | HIS | CA-C-O | -6.18 | 107.11 | 120.10 |
| 1 | B | 63 | GLN | CB-CA-C | -6.18 | 98.03 | 110.40 |
| 1 | C | 38 | LEU | CD1-CG-CD2 | -6.18 | 91.95 | 110.50 |
| 1 | A | 7 | LEU | N-CA-CB | -6.18 | 98.04 | 110.40 |
| 1 | E | 10 | GLU | CA-C-O | -6.18 | 107.12 | 120.10 |
| 1 | B | 217 | PHE | CB-CA-C | 6.18 | 122.76 | 110.40 |
| 1 | E | 114 | ASN | CB-CA-C | -6.18 | 98.04 | 110.40 |
| 1 | D | 215 | TYR | CA-C-O | -6.18 | 107.13 | 120.10 |
| 1 | E | 119 | VAL | C-N-CA | 6.18 | 137.14 | 121.70 |
| 1 | C | 28 | PHE | CB-CG-CD2 | 6.17 | 125.12 | 120.80 |
| 1 | B | 79 | TRP | CB-CG-CD1 | -6.17 | 118.97 | 127.00 |
| 1 | A | 197 | THR | C-N-CA | 6.17 | 137.13 | 121.70 |
| 1 | F | 206 | SER | CA-C-N | 6.17 | 128.54 | 116.20 |
| 1 | B | 169 | ASP | C-N-CA | 6.17 | 137.12 | 121.70 |
| 1 | F | 7 | LEU | CB-CG-CD1 | 6.17 | 121.49 | 111.00 |
| 1 | A | 56 | THR | CA-CB-OG1 | 6.17 | 121.95 | 109.00 |
| 1 | A | 195 | VAL | N-CA-C | -6.17 | 94.35 | 111.00 |
| 1 | D | 97 | ASP | CA-CB-CG | 6.17 | 126.96 | 113.40 |
| 1 | E | 105 | PRO | O-C-N | 6.17 | 133.68 | 123.20 |
| 1 | C | 187 | LEU | O-C-N | -6.17 | 112.84 | 122.70 |
| 1 | F | 106 | GLY | CA-C-N | 6.17 | 130.76 | 117.20 |
| 1 | A | 228 | TYR | OH-CZ-CE2 | 6.16 | 136.74 | 120.10 |
| 1 | D | 87 | ILE | CA-C-N | 6.16 | 128.52 | 116.20 |
| 1 | F | 105 | PRO | CB-CG-CD | -6.16 | 82.47 | 106.50 |
| 1 | D | 65 | ASP | CB-CA-C | 6.16 | 122.72 | 110.40 |
| 1 | D | 71 | LEU | CB-CG-CD2 | -6.16 | 100.53 | 111.00 |
| 1 | A | 2 | ASN | O-C-N | -6.16 | 112.84 | 122.70 |
| 1 | A | 162 | LEU | CB-CA-C | 6.16 | 121.90 | 110.20 |
| 1 | B | 79 | TRP | CG-CD1-NE1 | 6.16 | 116.26 | 110.10 |
| 1 | E | 34 | SER | CA-C-N | 6.16 | 130.75 | 117.20 |
| 1 | E | 67 | LEU | O-C-N | 6.16 | 132.55 | 122.70 |
| 1 | F | 143 | ALA | N-CA-C | -6.16 | 94.38 | 111.00 |
| 1 | D | 31 | THR | OG1-CB-CG2 | -6.16 | 95.84 | 110.00 |
| 1 | F | 142 | HIS | ND1-CE1-NE2 | -6.16 | 96.36 | 109.90 |
| 1 | C | 41 | PHE | N-CA-CB | -6.15 | 99.53 | 110.60 |
| 1 | B | 193 | MET | N-CA-C | -6.15 | 94.40 | 111.00 |
| 1 | C | 209 | SER | O-C-N | -6.15 | 112.86 | 122.70 |
| 1 | A | 134 | ASN | N-CA-CB | 6.15 | 121.67 | 110.60 |
| 1 | B | 9 | HIS | CA-CB-CG | 6.14 | 124.05 | 113.60 |
| 1 | C | 222 | ASP | CB-CG-OD1 | -6.14 | 112.77 | 118.30 |
| 1 | F | 229 | GLY | CA-C-O | -6.14 | 109.54 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 45 | VAL | CA-CB-CG1 | 6.14 | 120.11 | 110.90 |
| 1 | A | 99 | THR | OG1-CB-CG2 | 6.14 | 124.13 | 110.00 |
| 1 | B | 166 | ASP | OD1-CG-OD2 | -6.14 | 111.63 | 123.30 |
| 1 | F | 11 | GLY | O-C-N | -6.14 | 112.88 | 122.70 |
| 1 | F | 40 | LEU | CA-CB-CG | -6.14 | 101.18 | 115.30 |
| 1 | E | 70 | ILE | CA-C-O | -6.14 | 107.21 | 120.10 |
| 1 | E | 129 | TYR | CA-C-O | -6.14 | 107.21 | 120.10 |
| 1 | C | 82 | GLY | CA-C-O | 6.14 | 131.64 | 120.60 |
| 1 | F | 215 | TYR | CA-CB-CG | -6.14 | 101.74 | 113.40 |
| 1 | E | 206 | SER | N-CA-CB | -6.13 | 101.30 | 110.50 |
| 1 | A | 232 | LEU | CA-C-O | -6.13 | 107.23 | 120.10 |
| 1 | A | 75 | ASN | N-CA-CB | 6.13 | 121.63 | 110.60 |
| 1 | A | 171 | VAL | N-CA-C | -6.13 | 94.45 | 111.00 |
| 1 | F | 183 | CYS | CB-CA-C | 6.13 | 122.66 | 110.40 |
| 1 | B | 18 | HIS | CG-ND1-CE1 | -6.13 | 97.73 | 105.70 |
| 1 | F | 32 | MET | CA-C-N | 6.13 | 130.68 | 117.20 |
| 1 | A | 31 | THR | O-C-N | -6.12 | 112.90 | 122.70 |
| 1 | B | 162 | LEU | CD1-CG-CD2 | -6.12 | 92.13 | 110.50 |
| 1 | B | 181 | THR | OG1-CB-CG2 | -6.12 | 95.92 | 110.00 |
| 1 | A | 175 | ASN | CB-CG-ND2 | -6.12 | 102.01 | 116.70 |
| 1 | B | 147 | LEU | CD1-CG-CD2 | -6.12 | 92.14 | 110.50 |
| 1 | B | 222 | ASP | CB-CA-C | -6.12 | 98.16 | 110.40 |
| 1 | C | 184 | ARG | CG-CD-NE | -6.12 | 98.94 | 111.80 |
| 1 | D | 145 | GLN | CA-C-N | -6.12 | 103.73 | 117.20 |
| 1 | D | 184 | ARG | CA-C-O | 6.12 | 132.96 | 120.10 |
| 1 | D | 228 | TYR | CG-CD1-CE1 | -6.12 | 116.40 | 121.30 |
| 1 | F | 196 | LEU | O-C-N | -6.12 | 112.91 | 122.70 |
| 1 | A | 229 | GLY | CA-C-N | -6.12 | 103.96 | 116.20 |
| 1 | B | 111 | GLY | O-C-N | -6.12 | 112.91 | 122.70 |
| 1 | F | 101 | THR | CA-C-O | -6.12 | 107.25 | 120.10 |
| 1 | B | 194 | ASP | CA-C-N | -6.12 | 103.74 | 117.20 |
| 1 | B | 216 | VAL | CB-CA-C | 6.12 | 123.02 | 111.40 |
| 1 | A | 144 | THR | CA-C-O | -6.11 | 107.26 | 120.10 |
| 1 | C | 152 | TYR | CB-CG-CD1 | -6.11 | 117.33 | 121.00 |
| 1 | D | 73 | ALA | CA-C-N | 6.11 | 130.65 | 117.20 |
| 1 | C | 205 | THR | CA-CB-OG1 | -6.11 | 96.17 | 109.00 |
| 1 | C | 104 | GLY | N-CA-C | 6.11 | 128.38 | 113.10 |
| 1 | E | 157 | GLU | CG-CD-OE1 | -6.11 | 106.08 | 118.30 |
| 1 | F | 172 | TRP | CA-CB-CG | -6.11 | 102.09 | 113.70 |
| 1 | B | 169 | ASP | CA-C-N | -6.11 | 103.76 | 117.20 |
| 1 | C | 108 | TRP | CB-CA-C | -6.11 | 98.19 | 110.40 |
| 1 | D | 80 | SER | CB-CA-C | -6.11 | 98.50 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 102 | ILE | CG1-CB-CG2 | -6.11 | 97.97 | 111.40 |
| 1 | C | 62 | LEU | CD1-CG-CD2 | -6.11 | 92.19 | 110.50 |
| 1 | E | 14 | PRO | CA-CB-CG | -6.11 | 92.40 | 104.00 |
| 1 | C | 136 | ASN | CA-C-N | -6.10 | 103.78 | 117.20 |
| 1 | C | 184 | ARG | CB-CA-C | -6.10 | 98.19 | 110.40 |
| 1 | D | 78 | ARG | C-N-CA | -6.10 | 106.45 | 121.70 |
| 1 | A | 188 | GLN | O-C-N | -6.10 | 109.52 | 121.10 |
| 1 | B | 123 | ASN | CA-C-O | 6.10 | 132.90 | 120.10 |
| 1 | F | 9 | HIS | CA-C-O | 6.10 | 132.90 | 120.10 |
| 1 | A | 24 | GLU | CB-CA-C | -6.09 | 98.21 | 110.40 |
| 1 | D | 7 | LEU | CB-CA-C | -6.09 | 98.62 | 110.20 |
| 1 | F | 83 | THR | OG1-CB-CG2 | -6.09 | 95.98 | 110.00 |
| 1 | B | 28 | PHE | N-CA-C | 6.09 | 127.45 | 111.00 |
| 1 | B | 174 | THR | O-C-N | -6.09 | 112.95 | 122.70 |
| 1 | C | 144 | THR | CA-CB-CG2 | -6.09 | 103.87 | 112.40 |
| 1 | C | 42 | ASP | CB-CG-OD1 | 6.09 | 123.78 | 118.30 |
| 1 | F | 169 | ASP | N-CA-C | -6.08 | 94.57 | 111.00 |
| 1 | C | 130 | SER | N-CA-C | -6.08 | 94.58 | 111.00 |
| 1 | D | 2 | ASN | CA-C-N | 6.08 | 130.58 | 117.20 |
| 1 | D | 26 | SER | CA-CB-OG | -6.08 | 94.78 | 111.20 |
| 1 | D | 187 | LEU | CB-CG-CD2 | -6.08 | 100.67 | 111.00 |
| 1 | E | 17 | LEU | CA-C-N | 6.08 | 130.57 | 117.20 |
| 1 | E | 229 | GLY | N-CA-C | 6.08 | 128.30 | 113.10 |
| 1 | E | 228 | TYR | CZ-CE2-CD2 | 6.08 | 125.27 | 119.80 |
| 1 | B | 139 | GLN | O-C-N | 6.08 | 132.42 | 122.70 |
| 1 | D | 222 | ASP | CA-C-N | 6.08 | 130.56 | 117.20 |
| 1 | E | 147 | LEU | CB-CG-CD1 | -6.08 | 100.67 | 111.00 |
| 1 | A | 136 | ASN | O-C-N | -6.07 | 112.98 | 122.70 |
| 1 | F | 48 | TRP | CB-CA-C | -6.07 | 98.26 | 110.40 |
| 1 | F | 233 | TRP | CD1-NE1-CE2 | -6.07 | 103.54 | 109.00 |
| 1 | B | 98 | ARG | CB-CA-C | 6.07 | 122.54 | 110.40 |
| 1 | B | 197 | THR | N-CA-CB | -6.07 | 98.77 | 110.30 |
| 1 | F | 222 | ASP | CA-C-O | -6.07 | 107.36 | 120.10 |
| 1 | F | 233 | TRP | C-N-CA | 6.07 | 136.87 | 121.70 |
| 1 | D | 201 | ILE | CA-CB-CG1 | -6.07 | 99.48 | 111.00 |
| 1 | D | 211 | SER | C-N-CA | -6.07 | 106.53 | 121.70 |
| 1 | A | 122 | ASN | C-N-CA | 6.06 | 136.86 | 121.70 |
| 1 | F | 35 | ASP | CB-CA-C | -6.06 | 98.27 | 110.40 |
| 1 | F | 147 | LEU | CA-CB-CG | 6.06 | 129.25 | 115.30 |
| 1 | A | 26 | SER | N-CA-C | 6.06 | 127.36 | 111.00 |
| 1 | B | 67 | LEU | CD1-CG-CD2 | 6.06 | 128.68 | 110.50 |
| 1 | E | 42 | ASP | O-C-N | 6.06 | 132.40 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 77 | ILE | N-CA-CB | -6.06 | 96.86 | 110.80 |
| 1 | A | 192 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 1 | B | 105 | PRO | CA-C-N | 6.06 | 128.31 | 116.20 |
| 1 | B | 105 | PRO | CA-CB-CG | -6.06 | 92.49 | 104.00 |
| 1 | B | 202 | ALA | C-N-CA | 6.06 | 136.84 | 121.70 |
| 1 | D | 217 | PHE | N-CA-C | -6.06 | 94.65 | 111.00 |
| 1 | A | 46 | ARG | N-CA-CB | -6.05 | 99.70 | 110.60 |
| 1 | D | 235 | THR | N-CA-CB | -6.05 | 98.80 | 110.30 |
| 1 | E | 30 | PHE | CB-CA-C | -6.05 | 98.29 | 110.40 |
| 1 | E | 234 | THR | O-C-N | 6.05 | 132.39 | 122.70 |
| 1 | B | 30 | PHE | N-CA-CB | -6.05 | 99.71 | 110.60 |
| 1 | B | 215 | TYR | N-CA-CB | 6.05 | 121.49 | 110.60 |
| 1 | E | 231 | ALA | O-C-N | 6.05 | 132.38 | 122.70 |
| 1 | D | 4 | LEU | CB-CG-CD1 | -6.05 | 100.72 | 111.00 |
| 1 | D | 51 | ASN | CA-CB-CG | 6.05 | 126.71 | 113.40 |
| 1 | D | 180 | GLY | CA-C-N | -6.05 | 103.89 | 117.20 |
| 1 | F | 161 | ASN | O-C-N | 6.05 | 132.38 | 122.70 |
| 1 | A | 10 | GLU | N-CA-CB | 6.05 | 121.49 | 110.60 |
| 1 | B | 108 | TRP | CB-CG-CD2 | 6.05 | 134.46 | 126.60 |
| 1 | C | 102 | ILE | CA-C-O | -6.05 | 107.40 | 120.10 |
| 1 | C | 126 | SER | CA-C-O | -6.05 | 107.40 | 120.10 |
| 1 | F | 109 | ASP | N-CA-CB | 6.05 | 121.48 | 110.60 |
| 1 | F | 130 | SER | N-CA-C | 6.04 | 127.32 | 111.00 |
| 1 | A | 167 | ARG | CA-C-O | -6.04 | 107.41 | 120.10 |
| 1 | C | 148 | GLN | CA-C-N | 6.04 | 130.50 | 117.20 |
| 1 | B | 1 | ASN | OD1-CG-ND2 | -6.04 | 108.00 | 121.90 |
| 1 | F | 22 | SER | CA-CB-OG | -6.04 | 94.89 | 111.20 |
| 1 | B | 165 | PHE | O-C-N | 6.04 | 132.36 | 122.70 |
| 1 | E | 165 | PHE | CA-C-O | -6.04 | 107.42 | 120.10 |
| 1 | A | 145 | GLN | O-C-N | -6.04 | 113.04 | 122.70 |
| 1 | E | 177 | ALA | N-CA-CB | 6.04 | 118.55 | 110.10 |
| 1 | B | 162 | LEU | CA-CB-CG | 6.03 | 129.18 | 115.30 |
| 1 | C | 73 | ALA | C-N-CA | 6.03 | 136.78 | 121.70 |
| 1 | C | 210 | ARG | CG-CD-NE | -6.03 | 99.14 | 111.80 |
| 1 | B | 147 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 1 | A | 90 | TYR | CG-CD2-CE2 | 6.03 | 126.12 | 121.30 |
| 1 | A | 136 | ASN | CA-C-N | 6.03 | 130.46 | 117.20 |
| 1 | F | 26 | SER | CA-C-O | 6.03 | 132.75 | 120.10 |
| 1 | C | 87 | ILE | N-CA-CB | 6.02 | 124.65 | 110.80 |
| 1 | F | 201 | ILE | CB-CG1-CD1 | 6.02 | 130.76 | 113.90 |
| 1 | B | 91 | VAL | C-N-CA | 6.02 | 136.75 | 121.70 |
| 1 | C | 159 | ASP | CA-CB-CG | 6.02 | 126.64 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 162 | LEU | N-CA-C | -6.02 | 94.75 | 111.00 |
| 1 | C | 203 | VAL | N-CA-C | -6.02 | 94.75 | 111.00 |
| 1 | E | 189 | PRO | CA-N-CD | -6.01 | 103.08 | 111.50 |
| 1 | F | 153 | ARG | NH1-CZ-NH2 | 6.01 | 126.02 | 119.40 |
| 1 | B | 132 | GLN | CG-CD-OE1 | 6.01 | 133.63 | 121.60 |
| 1 | E | 158 | THR | O-C-N | -6.01 | 113.08 | 122.70 |
| 1 | C | 90 | TYR | CB-CG-CD1 | -6.01 | 117.39 | 121.00 |
| 1 | D | 136 | ASN | O-C-N | -6.01 | 113.08 | 122.70 |
| 1 | B | 102 | ILE | CA-CB-CG1 | 6.01 | 122.42 | 111.00 |
| 1 | A | 227 | ILE | O-C-N | -6.01 | 113.09 | 122.70 |
| 1 | B | 89 | ASN | O-C-N | -6.01 | 113.09 | 122.70 |
| 1 | B | 102 | ILE | O-C-N | -6.01 | 113.09 | 122.70 |
| 1 | E | 214 | ARG | CA-C-O | 6.01 | 132.71 | 120.10 |
| 1 | A | 27 | SER | CA-C-N | 6.00 | 130.41 | 117.20 |
| 1 | A | 31 | THR | OG1-CB-CG2 | -6.00 | 96.19 | 110.00 |
| 1 | A | 130 | SER | CA-C-O | -6.00 | 107.49 | 120.10 |
| 1 | E | 61 | VAL | C-N-CA | 6.00 | 136.71 | 121.70 |
| 1 | A | 74 | GLN | OE1-CD-NE2 | 6.00 | 135.71 | 121.90 |
| 1 | B | 201 | ILE | N-CA-CB | -6.00 | 97.00 | 110.80 |
| 1 | D | 197 | THR | CA-CB-CG2 | 6.00 | 120.80 | 112.40 |
| 1 | F | 10 | GLU | CA-C-O | -6.00 | 107.50 | 120.10 |
| 1 | F | 166 | ASP | O-C-N | -6.00 | 113.10 | 122.70 |
| 1 | B | 143 | ALA | O-C-N | -6.00 | 113.10 | 122.70 |
| 1 | B | 197 | THR | N-CA-C | 6.00 | 127.20 | 111.00 |
| 1 | F | 139 | GLN | N-CA-C | -6.00 | 94.80 | 111.00 |
| 1 | A | 65 | ASP | O-C-N | -6.00 | 113.01 | 123.20 |
| 1 | B | 189 | PRO | O-C-N | 6.00 | 132.29 | 122.70 |
| 1 | A | 11 | GLY | CA-C-N | -6.00 | 104.01 | 117.20 |
| 1 | A | 91 | VAL | N-CA-C | -6.00 | 94.81 | 111.00 |
| 1 | A | 45 | VAL | CA-C-O | 5.99 | 132.69 | 120.10 |
| 1 | E | 234 | THR | CA-C-O | -5.99 | 107.51 | 120.10 |
| 1 | D | 104 | GLY | CA-C-N | -5.99 | 100.32 | 117.10 |
| 1 | B | 79 | TRP | C-N-CA | 5.99 | 136.67 | 121.70 |
| 1 | D | 167 | ARG | N-CA-C | -5.99 | 94.83 | 111.00 |
| 1 | C | 4 | LEU | CA-C-N | 5.99 | 130.37 | 117.20 |
| 1 | C | 207 | GLY | C-N-CA | 5.99 | 136.67 | 121.70 |
| 1 | C | 217 | PHE | O-C-N | 5.99 | 132.28 | 122.70 |
| 1 | D | 157 | GLU | CB-CA-C | -5.99 | 98.43 | 110.40 |
| 1 | D | 214 | ARG | CA-C-N | 5.99 | 130.37 | 117.20 |
| 1 | F | 38 | LEU | N-CA-C | -5.99 | 94.84 | 111.00 |
| 1 | A | 138 | PRO | C-N-CA | -5.98 | 106.74 | 121.70 |
| 1 | B | 226 | ALA | N-CA-C | -5.98 | 94.84 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 146 | SER | CA-CB-OG | -5.98 | 95.04 | 111.20 |
| 1 | A | 192 | ARG | NE-CZ-NH2 | 5.98 | 123.29 | 120.30 |
| 1 | C | 133 | GLY | N-CA-C | -5.98 | 98.14 | 113.10 |
| 1 | E | 197 | THR | CB-CA-C | -5.98 | 95.45 | 111.60 |
| 1 | A | 226 | ALA | C-N-CA | -5.98 | 106.75 | 121.70 |
| 1 | D | 222 | ASP | OD1-CG-OD2 | -5.98 | 111.94 | 123.30 |
| 1 | A | 171 | VAL | CA-C-N | 5.98 | 130.35 | 117.20 |
| 1 | A | 79 | TRP | CE3-CZ3-CH2 | -5.98 | 114.62 | 121.20 |
| 1 | D | 99 | THR | CB-CA-C | 5.98 | 127.74 | 111.60 |
| 1 | E | 102 | ILE | CA-C-O | -5.98 | 107.55 | 120.10 |
| 1 | F | 1 | ASN | CB-CG-OD1 | -5.98 | 109.65 | 121.60 |
| 1 | E | 61 | VAL | O-C-N | -5.98 | 113.14 | 122.70 |
| 1 | D | 33 | GLN | C-N-CA | 5.97 | 136.63 | 121.70 |
| 1 | E | 170 | ARG | CG-CD-NE | 5.97 | 124.33 | 111.80 |
| 1 | B | 74 | GLN | CB-CG-CD | -5.97 | 96.08 | 111.60 |
| 1 | B | 215 | TYR | OH-CZ-CE2 | -5.97 | 103.98 | 120.10 |
| 1 | B | 44 | ASP | N-CA-C | -5.97 | 94.89 | 111.00 |
| 1 | C | 214 | ARG | CA-C-O | 5.97 | 132.63 | 120.10 |
| 1 | E | 102 | ILE | CA-C-N | -5.97 | 104.07 | 117.20 |
| 1 | A | 178 | GLY | CA-C-N | 5.96 | 130.32 | 117.20 |
| 1 | A | 223 | ARG | NE-CZ-NH2 | 5.96 | 123.28 | 120.30 |
| 1 | C | 172 | TRP | CA-C-O | -5.96 | 107.57 | 120.10 |
| 1 | D | 179 | LYS | CA-C-O | -5.96 | 107.58 | 120.10 |
| 1 | A | 38 | LEU | CB-CG-CD1 | 5.96 | 121.14 | 111.00 |
| 1 | B | 224 | ASN | CB-CG-OD1 | 5.96 | 133.52 | 121.60 |
| 1 | C | 47 | VAL | CA-CB-CG1 | 5.96 | 119.84 | 110.90 |
| 1 | F | 67 | LEU | C-N-CA | -5.96 | 106.80 | 121.70 |
| 1 | F | 126 | SER | O-C-N | -5.96 | 113.16 | 122.70 |
| 1 | F | 168 | ASP | O-C-N | -5.96 | 113.16 | 122.70 |
| 1 | A | 68 | LEU | O-C-N | -5.96 | 113.17 | 122.70 |
| 1 | C | 105 | PRO | C-N-CA | -5.96 | 109.79 | 122.30 |
| 1 | A | 40 | LEU | CB-CG-CD2 | -5.96 | 100.88 | 111.00 |
| 1 | C | 165 | PHE | CA-CB-CG | 5.96 | 128.19 | 113.90 |
| 1 | F | 164 | LEU | CB-CG-CD2 | 5.96 | 121.12 | 111.00 |
| 1 | B | 37 | ASN | CA-CB-CG | -5.95 | 100.30 | 113.40 |
| 1 | B | 8 | SER | N-CA-C | -5.95 | 94.93 | 111.00 |
| 1 | A | 111 | GLY | O-C-N | -5.95 | 113.18 | 122.70 |
| 1 | D | 203 | VAL | CA-C-O | -5.95 | 107.60 | 120.10 |
| 1 | F | 170 | ARG | N-CA-C | 5.95 | 127.07 | 111.00 |
| 1 | B | 45 | VAL | N-CA-C | -5.95 | 94.94 | 111.00 |
| 1 | D | 127 | ILE | CG1-CB-CG2 | 5.95 | 124.48 | 111.40 |
| 1 | E | 107 | LEU | N-CA-CB | -5.95 | 98.50 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 182 | GLY | N-CA-C | 5.95 | 127.97 | 113.10 |
| 1 | E | 16 | THR | N-CA-CB | -5.95 | 99.00 | 110.30 |
| 1 | E | 196 | LEU | O-C-N | 5.95 | 132.22 | 122.70 |
| 1 | C | 72 | THR | CA-C-N | -5.94 | 104.13 | 117.20 |
| 1 | E | 36 | CYS | CA-C-N | 5.94 | 130.26 | 117.20 |
| 1 | E | 109 | ASP | CB-CG-OD2 | -5.94 | 112.96 | 118.30 |
| 1 | C | 9 | HIS | CB-CG-ND1 | -5.93 | 108.36 | 123.20 |
| 1 | A | 22 | SER | C-N-CA | 5.93 | 136.53 | 121.70 |
| 1 | A | 165 | PHE | CB-CG-CD1 | 5.93 | 124.95 | 120.80 |
| 1 | B | 180 | GLY | CA-C-O | -5.93 | 109.92 | 120.60 |
| 1 | C | 217 | PHE | CA-C-O | -5.93 | 107.64 | 120.10 |
| 1 | D | 23 | LEU | CB-CG-CD2 | -5.93 | 100.92 | 111.00 |
| 1 | B | 74 | GLN | CA-C-O | 5.93 | 132.55 | 120.10 |
| 1 | A | 233 | TRP | CB-CG-CD1 | -5.93 | 119.29 | 127.00 |
| 1 | F | 17 | LEU | N-CA-CB | 5.93 | 122.26 | 110.40 |
| 1 | D | 169 | ASP | C-N-CA | 5.93 | 136.52 | 121.70 |
| 1 | E | 144 | THR | O-C-N | 5.93 | 132.18 | 122.70 |
| 1 | B | 74 | GLN | CA-C-N | -5.92 | 104.17 | 117.20 |
| 1 | C | 51 | ASN | CA-C-N | 5.92 | 130.24 | 117.20 |
| 1 | E | 44 | ASP | CA-CB-CG | 5.92 | 126.43 | 113.40 |
| 1 | E | 78 | ARG | CA-C-O | -5.92 | 107.66 | 120.10 |
| 1 | B | 23 | LEU | N-CA-C | -5.92 | 95.02 | 111.00 |
| 1 | A | 15 | GLN | C-N-CA | 5.92 | 136.50 | 121.70 |
| 1 | C | 26 | SER | O-C-N | -5.92 | 113.23 | 122.70 |
| 1 | E | 152 | TYR | CA-C-N | -5.92 | 104.18 | 117.20 |
| 1 | C | 225 | LEU | CA-C-O | -5.92 | 107.68 | 120.10 |
| 1 | D | 14 | PRO | CB-CA-C | -5.92 | 97.21 | 112.00 |
| 1 | B | 184 | ARG | NE-CZ-NH1 | -5.92 | 117.34 | 120.30 |
| 1 | A | 25 | LEU | N-CA-C | -5.91 | 95.05 | 111.00 |
| 1 | B | 126 | SER | CA-CB-OG | -5.91 | 95.25 | 111.20 |
| 1 | D | 205 | THR | CA-C-O | 5.91 | 132.51 | 120.10 |
| 1 | B | 26 | SER | CA-C-O | 5.91 | 132.50 | 120.10 |
| 1 | E | 29 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 1 | B | 41 | PHE | O-C-N | -5.90 | 113.25 | 122.70 |
| 1 | C | 2 | ASN | CB-CA-C | 5.90 | 122.20 | 110.40 |
| 1 | F | 181 | THR | N-CA-C | 5.90 | 126.93 | 111.00 |
| 1 | E | 210 | ARG | O-C-N | -5.90 | 113.26 | 122.70 |
| 1 | F | 56 | THR | N-CA-CB | 5.90 | 121.51 | 110.30 |
| 1 | C | 51 | ASN | CA-C-O | -5.90 | 107.72 | 120.10 |
| 1 | A | 37 | ASN | CB-CA-C | 5.90 | 122.19 | 110.40 |
| 1 | A | 58 | CYS | O-C-N | -5.90 | 113.27 | 122.70 |
| 1 | D | 159 | ASP | O-C-N | -5.90 | 113.27 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 12 | SER | CA-C-O | -5.89 | 107.72 | 120.10 |
| 1 | C | 37 | ASN | N-CA-CB | -5.89 | 99.99 | 110.60 |
| 1 | E | 90 | TYR | CG-CD1-CE1 | 5.89 | 126.02 | 121.30 |
| 1 | E | 143 | ALA | CB-CA-C | 5.89 | 118.94 | 110.10 |
| 1 | F | 40 | LEU | CA-C-N | -5.89 | 104.23 | 117.20 |
| 1 | C | 21 | GLN | CB-CA-C | 5.89 | 122.18 | 110.40 |
| 1 | C | 108 | TRP | CB-CG-CD1 | 5.89 | 134.66 | 127.00 |
| 1 | A | 151 | PRO | C-N-CA | 5.89 | 136.43 | 121.70 |
| 1 | B | 83 | THR | C-N-CA | 5.89 | 136.42 | 121.70 |
| 1 | B | 112 | THR | N-CA-C | 5.89 | 126.90 | 111.00 |
| 1 | D | 230 | GLY | C-N-CA | 5.89 | 136.42 | 121.70 |
| 1 | B | 35 | ASP | O-C-N | -5.89 | 113.28 | 122.70 |
| 1 | C | 58 | CYS | O-C-N | -5.89 | 113.28 | 122.70 |
| 1 | D | 233 | TRP | CG-CD2-CE3 | -5.89 | 128.60 | 133.90 |
| 1 | E | 156 | MET | CB-CG-SD | 5.89 | 130.06 | 112.40 |
| 1 | B | 85 | GLY | O-C-N | -5.88 | 113.28 | 122.70 |
| 1 | B | 164 | LEU | CD1-CG-CD2 | -5.88 | 92.85 | 110.50 |
| 1 | C | 72 | THR | CA-CB-CG2 | -5.88 | 104.16 | 112.40 |
| 1 | E | 4 | LEU | CA-C-O | -5.88 | 107.74 | 120.10 |
| 1 | E | 126 | SER | C-N-CA | 5.88 | 136.41 | 121.70 |
| 1 | E | 165 | PHE | N-CA-C | 5.88 | 126.89 | 111.00 |
| 1 | B | 1 | ASN | CB-CA-C | 5.88 | 122.17 | 110.40 |
| 1 | B | 57 | GLY | C-N-CA | 5.88 | 136.41 | 121.70 |
| 1 | D | 161 | ASN | O-C-N | 5.88 | 132.11 | 122.70 |
| 1 | F | 11 | GLY | N-CA-C | -5.88 | 98.39 | 113.10 |
| 1 | A | 9 | HIS | ND1-CG-CD2 | -5.88 | 97.77 | 106.00 |
| 1 | F | 233 | TRP | N-CA-C | -5.88 | 95.13 | 111.00 |
| 1 | A | 141 | LEU | CA-C-N | -5.88 | 104.27 | 117.20 |
| 1 | B | 193 | MET | CB-CA-C | 5.88 | 122.15 | 110.40 |
| 1 | E | 117 | SER | N-CA-C | 5.88 | 126.87 | 111.00 |
| 1 | B | 226 | ALA | C-N-CA | -5.88 | 107.01 | 121.70 |
| 1 | E | 141 | LEU | CA-CB-CG | 5.88 | 128.81 | 115.30 |
| 1 | A | 168 | ASP | CA-CB-CG | -5.87 | 100.48 | 113.40 |
| 1 | A | 173 | SER | O-C-N | -5.87 | 113.30 | 122.70 |
| 1 | B | 63 | GLN | C-N-CA | -5.87 | 107.02 | 121.70 |
| 1 | E | 9 | HIS | O-C-N | 5.87 | 132.09 | 122.70 |
| 1 | A | 204 | TRP | O-C-N | -5.87 | 113.31 | 122.70 |
| 1 | D | 164 | LEU | CA-CB-CG | -5.87 | 101.81 | 115.30 |
| 1 | E | 184 | ARG | CB-CG-CD | 5.87 | 126.85 | 111.60 |
| 1 | F | 212 | ALA | N-CA-CB | -5.87 | 101.89 | 110.10 |
| 1 | D | 215 | TYR | CE1-CZ-OH | 5.86 | 135.93 | 120.10 |
| 1 | F | 32 | MET | N-CA-CB | -5.86 | 100.05 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 69 | VAL | C-N-CA | 5.86 | 136.36 | 121.70 |
| 1 | A | 203 | VAL | CG1-CB-CG2 | -5.86 | 101.52 | 110.90 |
| 1 | C | 120 | VAL | CB-CA-C | -5.86 | 100.26 | 111.40 |
| 1 | C | 166 | ASP | CA-C-O | -5.86 | 107.79 | 120.10 |
| 1 | F | 97 | ASP | CA-CB-CG | 5.86 | 126.29 | 113.40 |
| 1 | E | 62 | LEU | N-CA-CB | 5.86 | 122.12 | 110.40 |
| 1 | A | 36 | CYS | CA-C-O | -5.86 | 107.80 | 120.10 |
| 1 | D | 32 | MET | N-CA-C | -5.86 | 95.18 | 111.00 |
| 1 | D | 179 | LYS | N-CA-CB | 5.86 | 121.14 | 110.60 |
| 1 | A | 192 | ARG | O-C-N | -5.86 | 113.33 | 122.70 |
| 1 | D | 233 | TRP | CB-CA-C | -5.86 | 98.69 | 110.40 |
| 1 | F | 141 | LEU | CA-C-O | -5.86 | 107.80 | 120.10 |
| 1 | B | 78 | ARG | CB-CA-C | 5.85 | 122.11 | 110.40 |
| 1 | E | 172 | TRP | CB-CG-CD2 | 5.85 | 134.21 | 126.60 |
| 1 | A | 188 | GLN | CA-CB-CG | -5.85 | 100.53 | 113.40 |
| 1 | B | 87 | ILE | CA-C-O | 5.85 | 132.39 | 120.10 |
| 1 | B | 198 | ASN | N-CA-C | 5.85 | 126.80 | 111.00 |
| 1 | F | 48 | TRP | CG-CD1-NE1 | -5.85 | 104.25 | 110.10 |
| 1 | A | 201 | ILE | CA-CB-CG1 | 5.85 | 122.11 | 111.00 |
| 1 | D | 9 | HIS | N-CA-CB | -5.85 | 100.07 | 110.60 |
| 1 | D | 63 | GLN | N-CA-C | 5.85 | 126.79 | 111.00 |
| 1 | C | 202 | ALA | C-N-CA | 5.84 | 136.31 | 121.70 |
| 1 | E | 16 | THR | C-N-CA | -5.84 | 107.09 | 121.70 |
| 1 | B | 95 | GLN | O-C-N | -5.84 | 110.00 | 121.10 |
| 1 | B | 153 | ARG | NH1-CZ-NH2 | 5.84 | 125.83 | 119.40 |
| 1 | F | 159 | ASP | O-C-N | -5.84 | 113.35 | 122.70 |
| 1 | B | 90 | TYR | CA-CB-CG | 5.84 | 124.50 | 113.40 |
| 1 | F | 56 | THR | OG1-CB-CG2 | -5.84 | 96.56 | 110.00 |
| 1 | F | 110 | SER | O-C-N | 5.84 | 133.13 | 123.20 |
| 1 | C | 40 | LEU | CB-CG-CD2 | 5.84 | 120.93 | 111.00 |
| 1 | C | 112 | THR | CA-CB-OG1 | -5.84 | 96.74 | 109.00 |
| 1 | B | 166 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | F | 41 | PHE | CZ-CE2-CD2 | 5.84 | 127.11 | 120.10 |
| 1 | A | 7 | LEU | CB-CG-CD2 | 5.84 | 120.92 | 111.00 |
| 1 | A | 97 | ASP | CB-CG-OD1 | 5.84 | 123.55 | 118.30 |
| 1 | D | 126 | SER | N-CA-CB | -5.84 | 101.75 | 110.50 |
| 1 | B | 25 | LEU | CA-C-N | -5.83 | 104.36 | 117.20 |
| 1 | D | 7 | LEU | CA-CB-CG | -5.83 | 101.89 | 115.30 |
| 1 | B | 10 | GLU | CG-CD-OE1 | -5.83 | 106.64 | 118.30 |
| 1 | D | 174 | THR | CB-CA-C | -5.83 | 95.85 | 111.60 |
| 1 | D | 201 | ILE | CA-C-O | -5.83 | 107.86 | 120.10 |
| 1 | D | 5 | PHE | CA-C-N | 5.83 | 127.86 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 17 | LEU | CA-C-O | -5.83 | 107.86 | 120.10 |
| 1 | E | 51 | ASN | O-C-N | 5.83 | 132.03 | 122.70 |
| 1 | A | 119 | VAL | N-CA-CB | -5.83 | 98.68 | 111.50 |
| 1 | E | 121 | ALA | CA-C-O | 5.83 | 132.34 | 120.10 |
| 1 | B | 128 | LEU | C-N-CA | 5.83 | 136.26 | 121.70 |
| 1 | B | 146 | SER | CA-C-O | -5.83 | 107.87 | 120.10 |
| 1 | C | 192 | ARG | NE-CZ-NH1 | -5.83 | 117.39 | 120.30 |
| 1 | D | 149 | LEU | CA-CB-CG | -5.83 | 101.90 | 115.30 |
| 1 | F | 185 | ALA | C-N-CA | -5.82 | 107.14 | 121.70 |
| 1 | C | 233 | TRP | CD1-NE1-CE2 | -5.82 | 103.76 | 109.00 |
| 1 | F | 76 | THR | O-C-N | -5.82 | 113.38 | 122.70 |
| 1 | E | 90 | TYR | CD1-CG-CD2 | -5.82 | 111.50 | 117.90 |
| 1 | F | 47 | VAL | CA-C-N | 5.82 | 130.00 | 117.20 |
| 1 | B | 22 | SER | CA-C-O | 5.82 | 132.32 | 120.10 |
| 1 | B | 37 | ASN | C-N-CA | -5.82 | 107.16 | 121.70 |
| 1 | D | 46 | ARG | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | B | 92 | LEU | CB-CG-CD2 | 5.82 | 120.89 | 111.00 |
| 1 | C | 120 | VAL | CA-C-N | 5.81 | 129.99 | 117.20 |
| 1 | E | 119 | VAL | N-CA-CB | -5.81 | 98.71 | 111.50 |
| 1 | B | 205 | THR | OG1-CB-CG2 | -5.81 | 96.64 | 110.00 |
| 1 | F | 194 | ASP | CB-CA-C | -5.81 | 98.78 | 110.40 |
| 1 | C | 26 | SER | CA-C-O | -5.81 | 107.90 | 120.10 |
| 1 | C | 140 | THR | CA-C-O | 5.81 | 132.29 | 120.10 |
| 1 | F | 79 | TRP | CZ3-CH2-CZ2 | 5.81 | 128.57 | 121.60 |
| 1 | B | 36 | CYS | C-N-CA | -5.80 | 107.19 | 121.70 |
| 1 | B | 203 | VAL | O-C-N | -5.80 | 113.42 | 122.70 |
| 1 | C | 224 | ASN | CB-CG-ND2 | -5.80 | 102.77 | 116.70 |
| 1 | C | 62 | LEU | CA-C-N | -5.80 | 104.44 | 117.20 |
| 1 | D | 110 | SER | CB-CA-C | 5.80 | 121.12 | 110.10 |
| 1 | F | 175 | ASN | CB-CA-C | -5.80 | 98.80 | 110.40 |
| 1 | A | 134 | ASN | C-N-CA | 5.80 | 136.20 | 121.70 |
| 1 | B | 136 | ASN | CA-C-O | -5.80 | 107.92 | 120.10 |
| 1 | C | 200 | ASN | C-N-CA | 5.80 | 136.20 | 121.70 |
| 1 | F | 105 | PRO | CB-CA-C | -5.80 | 97.50 | 112.00 |
| 1 | A | 24 | GLU | OE1-CD-OE2 | -5.79 | 116.35 | 123.30 |
| 1 | A | 232 | LEU | CA-C-N | 5.79 | 129.95 | 117.20 |
| 1 | F | 29 | ARG | CA-C-N | -5.79 | 104.45 | 117.20 |
| 1 | F | 169 | ASP | C-N-CA | 5.79 | 136.19 | 121.70 |
| 1 | B | 163 | VAL | CA-CB-CG2 | -5.79 | 102.21 | 110.90 |
| 1 | E | 77 | ILE | O-C-N | -5.79 | 113.43 | 122.70 |
| 1 | E | 26 | SER | CA-C-O | -5.79 | 107.94 | 120.10 |
| 1 | E | 192 | ARG | CG-CD-NE | 5.79 | 123.96 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 25 | LEU | CA-CB-CG | 5.79 | 128.62 | 115.30 |
| 1 | C | 139 | GLN | CA-C-O | 5.79 | 132.25 | 120.10 |
| 1 | F | 64 | SER | N-CA-C | 5.79 | 126.63 | 111.00 |
| 1 | A | 51 | ASN | CB-CG-OD1 | -5.79 | 110.03 | 121.60 |
| 1 | A | 193 | MET | N-CA-C | -5.79 | 95.38 | 111.00 |
| 1 | F | 100 | VAL | O-C-N | -5.79 | 113.44 | 122.70 |
| 1 | B | 12 | SER | CA-C-N | -5.78 | 104.48 | 117.20 |
| 1 | F | 6 | GLY | C-N-CA | 5.78 | 136.15 | 121.70 |
| 1 | F | 84 | LYS | O-C-N | -5.78 | 113.37 | 123.20 |
| 1 | B | 72 | THR | N-CA-CB | -5.78 | 99.32 | 110.30 |
| 1 | E | 144 | THR | OG1-CB-CG2 | 5.78 | 123.29 | 110.00 |
| 1 | B | 78 | ARG | CD-NE-CZ | 5.78 | 131.69 | 123.60 |
| 1 | F | 52 | THR | CA-CB-CG2 | -5.78 | 104.31 | 112.40 |
| 1 | A | 201 | ILE | CG1-CB-CG2 | -5.77 | 98.70 | 111.40 |
| 1 | E | 48 | TRP | CA-CB-CG | -5.77 | 102.73 | 113.70 |
| 1 | E | 61 | VAL | CA-CB-CG1 | 5.77 | 119.56 | 110.90 |
| 1 | A | 5 | PHE | C-N-CA | -5.77 | 110.18 | 122.30 |
| 1 | C | 223 | ARG | O-C-N | -5.77 | 113.47 | 122.70 |
| 1 | A | 30 | PHE | N-CA-CB | 5.77 | 120.98 | 110.60 |
| 1 | B | 101 | THR | CB-CA-C | -5.77 | 96.03 | 111.60 |
| 1 | B | 123 | ASN | CB-CA-C | 5.77 | 121.94 | 110.40 |
| 1 | C | 177 | ALA | C-N-CA | 5.77 | 134.41 | 122.30 |
| 1 | D | 89 | ASN | CB-CG-ND2 | 5.77 | 130.54 | 116.70 |
| 1 | E | 83 | THR | C-N-CA | 5.77 | 136.12 | 121.70 |
| 1 | F | 16 | THR | C-N-CA | -5.77 | 107.28 | 121.70 |
| 1 | A | 90 | TYR | N-CA-CB | 5.77 | 120.98 | 110.60 |
| 1 | B | 24 | GLU | CG-CD-OE2 | -5.76 | 106.77 | 118.30 |
| 1 | C | 176 | THR | CA-CB-CG2 | -5.76 | 104.33 | 112.40 |
| 1 | D | 184 | ARG | CB-CA-C | -5.76 | 98.87 | 110.40 |
| 1 | A | 233 | TRP | N-CA-CB | -5.76 | 100.23 | 110.60 |
| 1 | F | 107 | LEU | O-C-N | -5.76 | 113.48 | 122.70 |
| 1 | A | 69 | VAL | N-CA-CB | 5.76 | 124.17 | 111.50 |
| 1 | A | 102 | ILE | CB-CA-C | 5.76 | 123.11 | 111.60 |
| 1 | E | 46 | ARG | O-C-N | -5.76 | 113.49 | 122.70 |
| 1 | F | 75 | ASN | CB-CG-OD1 | -5.76 | 110.09 | 121.60 |
| 1 | F | 165 | PHE | CB-CG-CD2 | -5.76 | 116.77 | 120.80 |
| 1 | A | 102 | ILE | CA-C-O | -5.75 | 108.02 | 120.10 |
| 1 | E | 102 | ILE | CG1-CB-CG2 | -5.75 | 98.74 | 111.40 |
| 1 | C | 46 | ARG | CA-C-O | -5.75 | 108.02 | 120.10 |
| 1 | E | 79 | TRP | CG-CD1-NE1 | 5.75 | 115.85 | 110.10 |
| 1 | B | 166 | ASP | N-CA-CB | 5.75 | 120.95 | 110.60 |
| 1 | B | 233 | TRP | NE1-CE2-CZ2 | -5.75 | 124.08 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 172 | TRP | CE2-CD2-CE3 | -5.75 | 111.80 | 118.70 |
| 1 | A | 84 | LYS | N-CA-CB | -5.75 | 100.26 | 110.60 |
| 1 | C | 33 | GLN | CG-CD-NE2 | -5.75 | 102.91 | 116.70 |
| 1 | C | 41 | PHE | CA-C-O | -5.75 | 108.03 | 120.10 |
| 1 | B | 233 | TRP | C-N-CA | 5.74 | 136.06 | 121.70 |
| 1 | D | 88 | GLY | N-CA-C | 5.74 | 127.46 | 113.10 |
| 1 | E | 169 | ASP | CB-CG-OD1 | -5.74 | 113.13 | 118.30 |
| 1 | F | 155 | SER | N-CA-CB | 5.74 | 119.12 | 110.50 |
| 1 | A | 129 | TYR | CA-CB-CG | -5.74 | 102.50 | 113.40 |
| 1 | B | 91 | VAL | CA-C-N | 5.74 | 129.82 | 117.20 |
| 1 | C | 164 | LEU | CD1-CG-CD2 | 5.74 | 127.71 | 110.50 |
| 1 | A | 147 | LEU | N-CA-CB | 5.74 | 121.87 | 110.40 |
| 1 | B | 163 | VAL | N-CA-CB | -5.74 | 98.88 | 111.50 |
| 1 | D | 79 | TRP | CG-CD1-NE1 | -5.74 | 104.36 | 110.10 |
| 1 | A | 6 | GLY | N-CA-C | -5.73 | 98.77 | 113.10 |
| 1 | B | 26 | SER | CA-C-N | -5.73 | 104.58 | 117.20 |
| 1 | A | 41 | PHE | CE1-CZ-CE2 | 5.73 | 130.31 | 120.00 |
| 1 | B | 41 | PHE | N-CA-C | 5.73 | 126.47 | 111.00 |
| 1 | C | 45 | VAL | C-N-CA | 5.73 | 136.02 | 121.70 |
| 1 | D | 87 | ILE | O-C-N | 5.73 | 132.94 | 123.20 |
| 1 | C | 99 | THR | CA-C-N | 5.73 | 129.80 | 117.20 |
| 1 | E | 183 | CYS | O-C-N | 5.73 | 131.86 | 122.70 |
| 1 | A | 233 | TRP | CD2-CE3-CZ3 | -5.72 | 111.36 | 118.80 |
| 1 | F | 233 | TRP | CB-CG-CD2 | -5.72 | 119.16 | 126.60 |
| 1 | A | 70 | ILE | CA-CB-CG1 | -5.72 | 100.13 | 111.00 |
| 1 | F | 223 | ARG | O-C-N | -5.72 | 113.55 | 122.70 |
| 1 | D | 93 | VAL | CA-CB-CG1 | 5.72 | 119.48 | 110.90 |
| 1 | C | 15 | GLN | CG-CD-NE2 | -5.72 | 102.98 | 116.70 |
| 1 | A | 147 | LEU | O-C-N | -5.71 | 113.56 | 122.70 |
| 1 | B | 9 | HIS | CA-C-N | -5.71 | 104.63 | 117.20 |
| 1 | B | 221 | PRO | N-CA-CB | -5.71 | 96.31 | 102.60 |
| 1 | C | 36 | CYS | CA-C-O | -5.71 | 108.10 | 120.10 |
| 1 | E | 198 | ASN | CB-CA-C | -5.71 | 98.97 | 110.40 |
| 1 | A | 5 | PHE | CG-CD2-CE2 | 5.71 | 127.08 | 120.80 |
| 1 | C | 226 | ALA | N-CA-CB | 5.71 | 118.10 | 110.10 |
| 1 | B | 10 | GLU | CB-CG-CD | -5.71 | 98.78 | 114.20 |
| 1 | D | 157 | GLU | CG-CD-OE1 | 5.71 | 129.72 | 118.30 |
| 1 | E | 47 | VAL | N-CA-CB | 5.71 | 124.06 | 111.50 |
| 1 | D | 1 | ASN | CB-CA-C | 5.71 | 121.82 | 110.40 |
| 1 | D | 45 | VAL | CA-C-O | 5.71 | 132.09 | 120.10 |
| 1 | D | 29 | ARG | CB-CG-CD | 5.71 | 126.43 | 111.60 |
| 1 | D | 108 | TRP | CG-CD2-CE3 | 5.71 | 139.03 | 133.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 18 | HIS | O-C-N | 5.71 | 131.83 | 122.70 |
| 1 | B | 141 | LEU | CA-C-N | 5.70 | 129.75 | 117.20 |
| 1 | B | 145 | GLN | OE1-CD-NE2 | -5.70 | 108.78 | 121.90 |
| 1 | A | 215 | TYR | CB-CA-C | -5.70 | 99.00 | 110.40 |
| 1 | D | 127 | ILE | CA-CB-CG2 | -5.70 | 99.50 | 110.90 |
| 1 | F | 216 | VAL | CA-CB-CG2 | 5.70 | 119.45 | 110.90 |
| 1 | A | 138 | PRO | CB-CA-C | -5.70 | 97.76 | 112.00 |
| 1 | B | 99 | THR | CA-CB-CG2 | 5.70 | 120.38 | 112.40 |
| 1 | E | 54 | GLY | CA-C-O | -5.70 | 110.35 | 120.60 |
| 1 | F | 110 | SER | CA-C-N | 5.70 | 127.59 | 116.20 |
| 1 | A | 224 | ASN | CA-CB-CG | -5.69 | 100.87 | 113.40 |
| 1 | D | 129 | TYR | O-C-N | -5.69 | 113.59 | 122.70 |
| 1 | F | 95 | GLN | CG-CD-OE1 | -5.69 | 110.22 | 121.60 |
| 1 | A | 197 | THR | CA-CB-CG2 | 5.69 | 120.37 | 112.40 |
| 1 | E | 30 | PHE | CA-C-O | -5.69 | 108.15 | 120.10 |
| 1 | E | 79 | TRP | CD1-CG-CD2 | -5.69 | 101.75 | 106.30 |
| 1 | A | 217 | PHE | CG-CD1-CE1 | 5.69 | 127.06 | 120.80 |
| 1 | E | 65 | ASP | CA-C-O | 5.69 | 132.05 | 120.10 |
| 1 | A | 215 | TYR | CD1-CG-CD2 | -5.69 | 111.64 | 117.90 |
| 1 | B | 26 | SER | C-N-CA | 5.69 | 135.92 | 121.70 |
| 1 | C | 29 | ARG | CB-CA-C | -5.69 | 99.02 | 110.40 |
| 1 | D | 102 | ILE | CA-CB-CG2 | 5.69 | 122.27 | 110.90 |
| 1 | A | 151 | PRO | N-CA-CB | -5.69 | 96.35 | 102.60 |
| 1 | C | 89 | ASN | CA-C-O | -5.69 | 108.16 | 120.10 |
| 1 | B | 59 | ARG | CA-C-O | 5.68 | 132.04 | 120.10 |
| 1 | E | 137 | HIS | CE1-NE2-CD2 | -5.68 | 92.39 | 106.60 |
| 1 | F | 152 | TYR | CG-CD1-CE1 | -5.68 | 116.75 | 121.30 |
| 1 | E | 59 | ARG | CA-C-N | -5.68 | 104.70 | 117.20 |
| 1 | E | 41 | PHE | CA-CB-CG | 5.68 | 127.53 | 113.90 |
| 1 | A | 42 | ASP | CB-CG-OD2 | 5.68 | 123.41 | 118.30 |
| 1 | D | 37 | ASN | CB-CA-C | 5.68 | 121.75 | 110.40 |
| 1 | B | 91 | VAL | CB-CA-C | 5.68 | 122.18 | 111.40 |
| 1 | C | 226 | ALA | CB-CA-C | -5.68 | 101.59 | 110.10 |
| 1 | E | 105 | PRO | N-CA-C | -5.68 | 97.34 | 112.10 |
| 1 | D | 109 | ASP | CA-CB-CG | -5.67 | 100.91 | 113.40 |
| 1 | C | 40 | LEU | CA-C-N | 5.67 | 129.68 | 117.20 |
| 1 | D | 153 | ARG | CA-C-N | -5.67 | 104.72 | 117.20 |
| 1 | B | 89 | ASN | N-CA-C | 5.67 | 126.31 | 111.00 |
| 1 | B | 181 | THR | CA-C-N | 5.67 | 127.54 | 116.20 |
| 1 | E | 24 | GLU | C-N-CA | 5.67 | 135.88 | 121.70 |
| 1 | E | 141 | LEU | CB-CA-C | 5.67 | 120.97 | 110.20 |
| 1 | E | 112 | THR | CA-C-O | -5.67 | 108.19 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 136 | ASN | CA-CB-CG | 5.67 | 125.87 | 113.40 |
| 1 | A | 109 | ASP | CB-CG-OD2 | 5.67 | 123.40 | 118.30 |
| 1 | F | 99 | THR | N-CA-CB | 5.67 | 121.06 | 110.30 |
| 1 | C | 16 | THR | CA-CB-CG2 | -5.66 | 104.47 | 112.40 |
| 1 | F | 203 | VAL | CA-C-N | 5.66 | 129.66 | 117.20 |
| 1 | C | 5 | PHE | CA-C-N | -5.66 | 104.88 | 116.20 |
| 1 | F | 16 | THR | CB-CA-C | -5.66 | 96.33 | 111.60 |
| 1 | B | 200 | ASN | CB-CA-C | -5.66 | 99.09 | 110.40 |
| 1 | A | 192 | ARG | NH1-CZ-NH2 | -5.65 | 113.18 | 119.40 |
| 1 | A | 210 | ARG | CA-C-O | 5.65 | 131.97 | 120.10 |
| 1 | C | 91 | VAL | CG1-CB-CG2 | -5.65 | 101.86 | 110.90 |
| 1 | D | 20 | ALA | N-CA-C | -5.65 | 95.74 | 111.00 |
| 1 | E | 52 | THR | N-CA-C | -5.65 | 95.74 | 111.00 |
| 1 | B | 208 | ASN | CB-CA-C | -5.65 | 99.10 | 110.40 |
| 1 | E | 166 | ASP | O-C-N | -5.65 | 113.66 | 122.70 |
| 1 | B | 35 | ASP | CA-C-O | 5.65 | 131.96 | 120.10 |
| 1 | D | 16 | THR | CA-CB-OG1 | 5.65 | 120.86 | 109.00 |
| 1 | E | 127 | ILE | N-CA-C | 5.65 | 126.25 | 111.00 |
| 1 | E | 127 | ILE | N-CA-CB | -5.65 | 97.81 | 110.80 |
| 1 | C | 156 | MET | C-N-CA | -5.65 | 107.58 | 121.70 |
| 1 | C | 215 | TYR | CB-CA-C | -5.64 | 99.11 | 110.40 |
| 1 | D | 10 | GLU | OE1-CD-OE2 | 5.64 | 130.07 | 123.30 |
| 1 | E | 105 | PRO | CB-CA-C | -5.64 | 97.89 | 112.00 |
| 1 | C | 37 | ASN | CB-CG-ND2 | 5.64 | 130.24 | 116.70 |
| 1 | D | 87 | ILE | CA-CB-CG2 | 5.64 | 122.18 | 110.90 |
| 1 | D | 156 | MET | O-C-N | -5.64 | 113.67 | 122.70 |
| 1 | D | 168 | ASP | CA-C-N | -5.64 | 104.79 | 117.20 |
| 1 | D | 62 | LEU | O-C-N | -5.64 | 113.68 | 122.70 |
| 1 | D | 191 | GLY | N-CA-C | 5.64 | 127.20 | 113.10 |
| 1 | F | 108 | TRP | N-CA-CB | -5.64 | 100.45 | 110.60 |
| 1 | A | 161 | ASN | CA-CB-CG | 5.64 | 125.80 | 113.40 |
| 1 | E | 206 | SER | CB-CA-C | 5.64 | 120.81 | 110.10 |
| 1 | A | 203 | VAL | N-CA-CB | -5.63 | 99.11 | 111.50 |
| 1 | C | 120 | VAL | CA-C-O | -5.63 | 108.27 | 120.10 |
| 1 | D | 129 | TYR | CG-CD2-CE2 | 5.63 | 125.81 | 121.30 |
| 1 | B | 20 | ALA | N-CA-C | -5.63 | 95.80 | 111.00 |
| 1 | B | 79 | TRP | CE2-CD2-CG | 5.63 | 111.81 | 107.30 |
| 1 | B | 148 | GLN | CG-CD-NE2 | -5.63 | 103.18 | 116.70 |
| 1 | F | 29 | ARG | CB-CA-C | 5.63 | 121.66 | 110.40 |
| 1 | E | 62 | LEU | C-N-CA | -5.63 | 107.63 | 121.70 |
| 1 | E | 73 | ALA | N-CA-CB | -5.63 | 102.22 | 110.10 |
| 1 | E | 189 | PRO | N-CD-CG | -5.63 | 94.76 | 103.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 137 | HIS | CA-CB-CG | -5.63 | 104.03 | 113.60 |
| 1 | B | 104 | GLY | CA-C-O | 5.63 | 130.73 | 120.60 |
| 1 | C | 76 | THR | CA-C-N | 5.62 | 129.57 | 117.20 |
| 1 | C | 162 | LEU | C-N-CA | -5.62 | 107.64 | 121.70 |
| 1 | A | 110 | SER | N-CA-CB | -5.62 | 102.07 | 110.50 |
| 1 | E | 103 | TYR | CA-C-N | 5.62 | 127.44 | 116.20 |
| 1 | A | 23 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |
| 1 | D | 209 | SER | CB-CA-C | -5.62 | 99.42 | 110.10 |
| 1 | E | 56 | THR | CA-CB-OG1 | 5.62 | 120.80 | 109.00 |
| 1 | D | 195 | VAL | C-N-CA | 5.62 | 135.74 | 121.70 |
| 1 | D | 185 | ALA | CB-CA-C | -5.62 | 101.68 | 110.10 |
| 1 | D | 190 | ASN | CB-CA-C | 5.62 | 121.63 | 110.40 |
| 1 | A | 205 | THR | CA-C-O | 5.61 | 131.89 | 120.10 |
| 1 | F | 40 | LEU | CB-CG-CD1 | -5.61 | 101.46 | 111.00 |
| 1 | A | 230 | GLY | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | A | 5 | PHE | CB-CG-CD1 | -5.61 | 116.88 | 120.80 |
| 1 | A | 129 | TYR | OH-CZ-CE2 | 5.61 | 135.24 | 120.10 |
| 1 | B | 160 | CYS | CA-C-O | -5.61 | 108.33 | 120.10 |
| 1 | D | 58 | CYS | CB-CA-C | 5.61 | 121.61 | 110.40 |
| 1 | F | 24 | GLU | C-N-CA | 5.61 | 135.71 | 121.70 |
| 1 | B | 70 | ILE | O-C-N | -5.60 | 113.73 | 122.70 |
| 1 | A | 180 | GLY | C-N-CA | -5.60 | 107.69 | 121.70 |
| 1 | A | 205 | THR | C-N-CA | 5.60 | 135.71 | 121.70 |
| 1 | B | 161 | ASN | N-CA-CB | -5.60 | 100.52 | 110.60 |
| 1 | D | 218 | VAL | CA-C-O | -5.60 | 108.34 | 120.10 |
| 1 | E | 188 | GLN | CG-CD-OE1 | -5.60 | 110.40 | 121.60 |
| 1 | C | 172 | TRP | CB-CG-CD1 | 5.60 | 134.28 | 127.00 |
| 1 | C | 188 | GLN | CG-CD-NE2 | -5.60 | 103.27 | 116.70 |
| 1 | D | 153 | ARG | O-C-N | 5.60 | 131.65 | 122.70 |
| 1 | C | 13 | HIS | ND1-CG-CD2 | -5.59 | 98.17 | 106.00 |
| 1 | E | 5 | PHE | CD1-CG-CD2 | -5.59 | 111.03 | 118.30 |
| 1 | E | 6 | GLY | CA-C-O | -5.59 | 110.53 | 120.60 |
| 1 | B | 47 | VAL | CB-CA-C | -5.59 | 100.78 | 111.40 |
| 1 | B | 68 | LEU | CA-C-N | -5.59 | 104.90 | 117.20 |
| 1 | B | 145 | GLN | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 1 | F | 89 | ASN | CA-CB-CG | 5.59 | 125.69 | 113.40 |
| 1 | A | 9 | HIS | O-C-N | -5.59 | 113.76 | 122.70 |
| 1 | B | 106 | GLY | N-CA-C | -5.58 | 99.14 | 113.10 |
| 1 | A | 105 | PRO | CA-C-O | -5.58 | 106.80 | 120.20 |
| 1 | D | 113 | SER | N-CA-C | 5.58 | 126.08 | 111.00 |
| 1 | E | 210 | ARG | CA-CB-CG | 5.58 | 125.68 | 113.40 |
| 1 | F | 158 | THR | CA-C-N | 5.58 | 129.48 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 167 | ARG | O-C-N | 5.58 | 131.63 | 122.70 |
| 1 | E | 157 | GLU | N-CA-CB | -5.58 | 100.56 | 110.60 |
| 1 | A | 90 | TYR | CD1-CE1-CZ | -5.57 | 114.78 | 119.80 |
| 1 | A | 196 | LEU | CB-CA-C | -5.57 | 99.61 | 110.20 |
| 1 | D | 8 | SER | O-C-N | 5.57 | 131.62 | 122.70 |
| 1 | F | 62 | LEU | CB-CA-C | -5.57 | 99.61 | 110.20 |
| 1 | E | 146 | SER | N-CA-CB | -5.57 | 102.14 | 110.50 |
| 1 | A | 66 | GLY | C-N-CA | -5.57 | 107.77 | 121.70 |
| 1 | B | 103 | TYR | CE1-CZ-CE2 | 5.57 | 128.71 | 119.80 |
| 1 | B | 169 | ASP | CB-CA-C | 5.57 | 121.53 | 110.40 |
| 1 | F | 34 | SER | CA-C-O | -5.57 | 108.41 | 120.10 |
| 1 | A | 102 | ILE | CG1-CB-CG2 | -5.57 | 99.15 | 111.40 |
| 1 | C | 39 | VAL | CB-CA-C | -5.57 | 100.83 | 111.40 |
| 1 | D | 105 | PRO | O-C-N | 5.56 | 132.66 | 123.20 |
| 1 | D | 50 | SER | CB-CA-C | 5.56 | 120.67 | 110.10 |
| 1 | E | 91 | VAL | O-C-N | -5.56 | 113.80 | 122.70 |
| 1 | E | 24 | GLU | CA-C-N | 5.56 | 129.43 | 117.20 |
| 1 | E | 155 | SER | N-CA-C | 5.56 | 126.01 | 111.00 |
| 1 | E | 180 | GLY | O-C-N | 5.56 | 131.60 | 122.70 |
| 1 | C | 81 | SER | CB-CA-C | 5.56 | 120.66 | 110.10 |
| 1 | F | 79 | TRP | NE1-CE2-CZ2 | -5.56 | 124.29 | 130.40 |
| 1 | D | 153 | ARG | NH1-CZ-NH2 | 5.55 | 125.51 | 119.40 |
| 1 | B | 234 | THR | OG1-CB-CG2 | -5.55 | 97.23 | 110.00 |
| 1 | A | 134 | ASN | CB-CG-ND2 | 5.55 | 130.02 | 116.70 |
| 1 | D | 197 | THR | CB-CA-C | -5.55 | 96.62 | 111.60 |
| 1 | E | 91 | VAL | CA-C-N | 5.55 | 129.41 | 117.20 |
| 1 | F | 46 | ARG | N-CA-C | -5.55 | 96.02 | 111.00 |
| 1 | C | 14 | PRO | CA-N-CD | -5.55 | 103.74 | 111.50 |
| 1 | E | 151 | PRO | O-C-N | -5.55 | 113.83 | 122.70 |
| 1 | A | 192 | ARG | CB-CA-C | 5.54 | 121.49 | 110.40 |
| 1 | B | 20 | ALA | N-CA-CB | -5.54 | 102.34 | 110.10 |
| 1 | B | 172 | TRP | CB-CG-CD2 | 5.54 | 133.81 | 126.60 |
| 1 | E | 109 | ASP | OD1-CG-OD2 | -5.54 | 112.77 | 123.30 |
| 1 | D | 79 | TRP | CA-C-N | 5.54 | 129.39 | 117.20 |
| 1 | E | 78 | ARG | CA-C-N | 5.54 | 129.39 | 117.20 |
| 1 | A | 79 | TRP | CH2-CZ2-CE2 | 5.54 | 122.94 | 117.40 |
| 1 | E | 29 | ARG | CB-CA-C | 5.54 | 121.47 | 110.40 |
| 1 | E | 74 | GLN | OE1-CD-NE2 | -5.54 | 109.17 | 121.90 |
| 1 | C | 46 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 1 | E | 48 | TRP | CZ3-CH2-CZ2 | -5.53 | 114.97 | 121.60 |
| 1 | B | 177 | ALA | N-CA-CB | -5.53 | 102.36 | 110.10 |
| 1 | D | 92 | LEU | CB-CG-CD2 | 5.53 | 120.40 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 157 | GLU | N-CA-C | 5.53 | 125.92 | 111.00 |
| 1 | E | 144 | THR | CA-C-O | -5.53 | 108.49 | 120.10 |
| 1 | A | 119 | VAL | CA-C-N | 5.53 | 129.35 | 117.20 |
| 1 | B | 15 | GLN | CA-C-O | -5.53 | 108.50 | 120.10 |
| 1 | B | 38 | LEU | N-CA-C | -5.53 | 96.08 | 111.00 |
| 1 | B | 136 | ASN | N-CA-C | 5.53 | 125.92 | 111.00 |
| 1 | C | 231 | ALA | N-CA-C | 5.53 | 125.92 | 111.00 |
| 1 | A | 4 | LEU | CB-CG-CD2 | 5.52 | 120.39 | 111.00 |
| 1 | B | 195 | VAL | N-CA-CB | 5.52 | 123.65 | 111.50 |
| 1 | D | 91 | VAL | CA-CB-CG2 | -5.52 | 102.61 | 110.90 |
| 1 | E | 155 | SER | O-C-N | -5.52 | 113.86 | 122.70 |
| 1 | E | 176 | THR | CA-CB-OG1 | 5.52 | 120.60 | 109.00 |
| 1 | F | 110 | SER | N-CA-C | -5.52 | 96.09 | 111.00 |
| 1 | A | 115 | LYS | CB-CA-C | 5.52 | 121.44 | 110.40 |
| 1 | C | 72 | THR | N-CA-CB | -5.52 | 99.81 | 110.30 |
| 1 | E | 161 | ASN | OD1-CG-ND2 | 5.52 | 134.60 | 121.90 |
| 1 | A | 166 | ASP | N-CA-C | -5.52 | 96.10 | 111.00 |
| 1 | E | 78 | ARG | N-CA-CB | 5.52 | 120.53 | 110.60 |
| 1 | A | 24 | GLU | CA-CB-CG | 5.52 | 125.54 | 113.40 |
| 1 | A | 70 | ILE | CB-CA-C | -5.52 | 100.57 | 111.60 |
| 1 | C | 207 | GLY | O-C-N | -5.51 | 113.88 | 122.70 |
| 1 | E | 225 | LEU | CA-CB-CG | 5.51 | 127.98 | 115.30 |
| 1 | E | 103 | TYR | CA-C-O | -5.51 | 108.52 | 120.10 |
| 1 | C | 108 | TRP | CA-C-O | -5.51 | 108.53 | 120.10 |
| 1 | C | 172 | TRP | CA-C-N | 5.51 | 129.32 | 117.20 |
| 1 | D | 209 | SER | CA-CB-OG | -5.51 | 96.32 | 111.20 |
| 1 | F | 233 | TRP | CB-CG-CD1 | 5.51 | 134.16 | 127.00 |
| 1 | E | 197 | THR | N-CA-CB | -5.51 | 99.83 | 110.30 |
| 1 | D | 141 | LEU | CA-C-N | 5.51 | 129.32 | 117.20 |
| 1 | D | 164 | LEU | CA-C-N | 5.51 | 129.32 | 117.20 |
| 1 | F | 79 | TRP | CB-CG-CD1 | -5.51 | 119.84 | 127.00 |
| 1 | F | 91 | VAL | O-C-N | -5.50 | 113.89 | 122.70 |
| 1 | A | 41 | PHE | CD1-CG-CD2 | 5.50 | 125.45 | 118.30 |
| 1 | B | 99 | THR | CA-CB-OG1 | 5.50 | 120.55 | 109.00 |
| 1 | B | 43 | SER | CA-CB-OG | 5.50 | 126.05 | 111.20 |
| 1 | F | 158 | THR | OG1-CB-CG2 | 5.50 | 122.65 | 110.00 |
| 1 | C | 124 | GLY | CA-C-N | 5.50 | 129.29 | 117.20 |
| 1 | C | 187 | LEU | CA-C-O | 5.50 | 131.64 | 120.10 |
| 1 | B | 35 | ASP | N-CA-C | -5.49 | 96.17 | 111.00 |
| 1 | E | 90 | TYR | OH-CZ-CE2 | 5.49 | 134.92 | 120.10 |
| 1 | E | 96 | PRO | N-CA-CB | -5.49 | 96.56 | 102.60 |
| 1 | C | 222 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 62 | LEU | CA-CB-CG | 5.49 | 127.92 | 115.30 |
| 1 | D | 139 | GLN | CG-CD-NE2 | -5.49 | 103.53 | 116.70 |
| 1 | D | 48 | TRP | CA-C-O | -5.49 | 108.58 | 120.10 |
| 1 | A | 187 | LEU | C-N-CA | -5.48 | 107.99 | 121.70 |
| 1 | A | 78 | ARG | C-N-CA | 5.48 | 135.41 | 121.70 |
| 1 | E | 41 | PHE | O-C-N | 5.48 | 131.47 | 122.70 |
| 1 | F | 197 | THR | OG1-CB-CG2 | 5.48 | 122.61 | 110.00 |
| 1 | A | 11 | GLY | C-N-CA | -5.48 | 108.00 | 121.70 |
| 1 | B | 99 | THR | C-N-CA | -5.48 | 108.00 | 121.70 |
| 1 | D | 186 | VAL | CA-CB-CG2 | 5.48 | 119.12 | 110.90 |
| 1 | E | 137 | HIS | CG-CD2-NE2 | 5.48 | 119.61 | 109.20 |
| 1 | C | 30 | PHE | N-CA-CB | 5.48 | 120.46 | 110.60 |
| 1 | C | 106 | GLY | O-C-N | -5.48 | 113.93 | 122.70 |
| 1 | F | 109 | ASP | N-CA-C | -5.48 | 96.21 | 111.00 |
| 1 | F | 215 | TYR | CB-CA-C | -5.48 | 99.44 | 110.40 |
| 1 | E | 152 | TYR | N-CA-C | -5.48 | 96.22 | 111.00 |
| 1 | B | 190 | ASN | CA-CB-CG | 5.47 | 125.44 | 113.40 |
| 1 | D | 177 | ALA | CB-CA-C | -5.47 | 101.89 | 110.10 |
| 1 | F | 168 | ASP | OD1-CG-OD2 | -5.47 | 112.90 | 123.30 |
| 1 | A | 185 | ALA | CA-C-O | 5.47 | 131.59 | 120.10 |
| 1 | C | 83 | THR | CA-C-O | -5.47 | 108.61 | 120.10 |
| 1 | F | 59 | ARG | CA-C-O | 5.47 | 131.59 | 120.10 |
| 1 | C | 8 | SER | CA-CB-OG | -5.47 | 96.43 | 111.20 |
| 1 | C | 76 | THR | O-C-N | -5.47 | 113.95 | 122.70 |
| 1 | E | 10 | GLU | N-CA-C | -5.47 | 96.23 | 111.00 |
| 1 | E | 109 | ASP | N-CA-CB | 5.47 | 120.45 | 110.60 |
| 1 | E | 196 | LEU | CB-CA-C | -5.47 | 99.81 | 110.20 |
| 1 | E | 89 | ASN | CB-CA-C | 5.47 | 121.33 | 110.40 |
| 1 | B | 8 | SER | CB-CA-C | -5.47 | 99.71 | 110.10 |
| 1 | D | 16 | THR | N-CA-CB | 5.47 | 120.69 | 110.30 |
| 1 | D | 227 | ILE | CA-C-N | 5.47 | 129.23 | 117.20 |
| 1 | F | 65 | ASP | CA-C-N | 5.46 | 127.13 | 116.20 |
| 1 | A | 85 | GLY | O-C-N | 5.46 | 131.44 | 122.70 |
| 1 | D | 90 | TYR | CB-CG-CD2 | -5.46 | 117.72 | 121.00 |
| 1 | F | 167 | ARG | N-CA-CB | -5.46 | 100.77 | 110.60 |
| 1 | D | 86 | SER | CA-C-O | -5.46 | 108.63 | 120.10 |
| 1 | F | 210 | ARG | CB-CA-C | 5.46 | 121.32 | 110.40 |
| 1 | C | 187 | LEU | CB-CA-C | -5.46 | 99.83 | 110.20 |
| 1 | D | 14 | PRO | N-CA-CB | 5.46 | 109.85 | 103.30 |
| 1 | F | 202 | ALA | CA-C-O | 5.46 | 131.56 | 120.10 |
| 1 | B | 227 | ILE | O-C-N | -5.45 | 113.97 | 122.70 |
| 1 | E | 27 | SER | CA-C-O | 5.45 | 131.55 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 179 | LYS | CG-CD-CE | -5.45 | 95.55 | 111.90 |
| 1 | A | 103 | TYR | CD1-CE1-CZ | -5.45 | 114.90 | 119.80 |
| 1 | B | 167 | ARG | N-CA-C | -5.45 | 96.29 | 111.00 |
| 1 | C | 30 | PHE | O-C-N | 5.45 | 131.42 | 122.70 |
| 1 | C | 175 | ASN | CB-CG-OD1 | 5.45 | 132.50 | 121.60 |
| 1 | A | 18 | HIS | N-CA-C | -5.44 | 96.31 | 111.00 |
| 1 | A | 120 | VAL | CA-C-O | -5.44 | 108.68 | 120.10 |
| 1 | A | 228 | TYR | CA-C-O | 5.44 | 131.52 | 120.10 |
| 1 | C | 162 | LEU | CB-CA-C | 5.44 | 120.53 | 110.20 |
| 1 | C | 194 | ASP | O-C-N | -5.44 | 114.00 | 122.70 |
| 1 | D | 201 | ILE | CB-CA-C | -5.44 | 100.72 | 111.60 |
| 1 | E | 137 | HIS | ND1-CE1-NE2 | 5.44 | 121.87 | 109.90 |
| 1 | A | 35 | ASP | OD1-CG-OD2 | -5.44 | 112.97 | 123.30 |
| 1 | B | 232 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | D | 22 | SER | N-CA-CB | -5.44 | 102.34 | 110.50 |
| 1 | B | 23 | LEU | O-C-N | 5.44 | 131.40 | 122.70 |
| 1 | E | 192 | ARG | CB-CG-CD | 5.44 | 125.74 | 111.60 |
| 1 | F | 164 | LEU | O-C-N | 5.44 | 131.40 | 122.70 |
| 1 | A | 98 | ARG | CD-NE-CZ | -5.43 | 115.99 | 123.60 |
| 1 | A | 222 | ASP | O-C-N | 5.43 | 131.40 | 122.70 |
| 1 | C | 50 | SER | CA-CB-OG | 5.43 | 125.87 | 111.20 |
| 1 | F | 10 | GLU | CA-CB-CG | -5.43 | 101.44 | 113.40 |
| 1 | F | 102 | ILE | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | A | 226 | ALA | CA-C-O | -5.43 | 108.69 | 120.10 |
| 1 | C | 39 | VAL | C-N-CA | 5.43 | 135.28 | 121.70 |
| 1 | E | 105 | PRO | C-N-CA | -5.43 | 110.89 | 122.30 |
| 1 | C | 5 | PHE | CE1-CZ-CE2 | -5.43 | 110.22 | 120.00 |
| 1 | C | 68 | LEU | CA-CB-CG | 5.43 | 127.79 | 115.30 |
| 1 | E | 139 | GLN | N-CA-CB | -5.43 | 100.82 | 110.60 |
| 1 | B | 210 | ARG | CA-CB-CG | 5.43 | 125.35 | 113.40 |
| 1 | C | 24 | GLU | C-N-CA | 5.43 | 135.27 | 121.70 |
| 1 | B | 158 | THR | CA-C-O | -5.43 | 108.70 | 120.10 |
| 1 | E | 39 | VAL | CB-CA-C | -5.43 | 101.09 | 111.40 |
| 1 | B | 129 | TYR | CE1-CZ-OH | 5.42 | 134.75 | 120.10 |
| 1 | B | 32 | MET | CG-SD-CE | 5.42 | 108.88 | 100.20 |
| 1 | D | 5 | PHE | CA-C-O | -5.42 | 108.71 | 120.10 |
| 1 | E | 217 | PHE | CZ-CE2-CD2 | 5.42 | 126.61 | 120.10 |
| 1 | A | 59 | ARG | N-CA-C | -5.42 | 96.36 | 111.00 |
| 1 | B | 207 | GLY | O-C-N | -5.42 | 114.03 | 122.70 |
| 1 | C | 71 | LEU | CA-C-O | 5.42 | 131.49 | 120.10 |
| 1 | C | 111 | GLY | CA-C-O | -5.42 | 110.84 | 120.60 |
| 1 | E | 64 | SER | CA-C-O | 5.42 | 131.48 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 96 | PRO | CB-CA-C | 5.42 | 125.55 | 112.00 |
| 1 | F | 142 | HIS | CB-CA-C | -5.42 | 99.56 | 110.40 |
| 1 | A | 221 | PRO | CA-C-O | 5.42 | 133.20 | 120.20 |
| 1 | B | 62 | LEU | CD1-CG-CD2 | -5.42 | 94.25 | 110.50 |
| 1 | B | 216 | VAL | CA-C-O | 5.42 | 131.47 | 120.10 |
| 1 | A | 100 | VAL | CA-C-N | 5.42 | 129.11 | 117.20 |
| 1 | D | 158 | THR | CA-CB-OG1 | -5.41 | 97.63 | 109.00 |
| 1 | E | 216 | VAL | CA-C-N | 5.41 | 129.11 | 117.20 |
| 1 | F | 74 | GLN | O-C-N | -5.41 | 114.04 | 122.70 |
| 1 | A | 131 | THR | CA-CB-CG2 | -5.41 | 104.83 | 112.40 |
| 1 | B | 59 | ARG | CA-C-N | -5.41 | 105.30 | 117.20 |
| 1 | D | 141 | LEU | CB-CA-C | -5.41 | 99.92 | 110.20 |
| 1 | E | 42 | ASP | CA-C-O | -5.41 | 108.74 | 120.10 |
| 1 | A | 168 | ASP | O-C-N | -5.41 | 114.05 | 122.70 |
| 1 | E | 48 | TRP | CG-CD1-NE1 | -5.41 | 104.69 | 110.10 |
| 1 | A | 183 | CYS | CA-CB-SG | 5.40 | 123.73 | 114.00 |
| 1 | A | 45 | VAL | CG1-CB-CG2 | -5.40 | 102.26 | 110.90 |
| 1 | A | 184 | ARG | CA-C-N | -5.40 | 105.32 | 117.20 |
| 1 | C | 203 | VAL | N-CA-CB | -5.40 | 99.62 | 111.50 |
| 1 | C | 27 | SER | C-N-CA | -5.40 | 108.21 | 121.70 |
| 1 | C | 82 | GLY | O-C-N | -5.40 | 114.06 | 122.70 |
| 1 | D | 5 | PHE | CD1-CG-CD2 | -5.40 | 111.28 | 118.30 |
| 1 | D | 180 | GLY | CA-C-O | 5.40 | 130.32 | 120.60 |
| 1 | D | 207 | GLY | CA-C-N | -5.40 | 105.32 | 117.20 |
| 1 | E | 192 | ARG | N-CA-CB | -5.40 | 100.89 | 110.60 |
| 1 | C | 174 | THR | CA-CB-CG2 | 5.39 | 119.95 | 112.40 |
| 1 | F | 139 | GLN | CA-CB-CG | -5.39 | 101.53 | 113.40 |
| 1 | B | 187 | LEU | CB-CG-CD2 | 5.39 | 120.17 | 111.00 |
| 1 | E | 92 | LEU | CB-CG-CD1 | 5.39 | 120.17 | 111.00 |
| 1 | A | 79 | TRP | N-CA-CB | -5.39 | 100.90 | 110.60 |
| 1 | E | 129 | TYR | C-N-CA | 5.39 | 135.17 | 121.70 |
| 1 | F | 7 | LEU | N-CA-C | 5.39 | 125.55 | 111.00 |
| 1 | C | 69 | VAL | CB-CA-C | -5.39 | 101.16 | 111.40 |
| 1 | E | 143 | ALA | N-CA-C | -5.39 | 96.45 | 111.00 |
| 1 | A | 228 | TYR | C-N-CA | 5.39 | 133.61 | 122.30 |
| 1 | B | 198 | ASN | O-C-N | -5.39 | 114.08 | 122.70 |
| 1 | C | 2 | ASN | CA-C-O | 5.39 | 131.41 | 120.10 |
| 1 | C | 125 | ASN | C-N-CA | 5.39 | 135.17 | 121.70 |
| 1 | F | 159 | ASP | CB-CA-C | 5.39 | 121.17 | 110.40 |
| 1 | F | 228 | TYR | CA-C-N | 5.39 | 126.97 | 116.20 |
| 1 | B | 164 | LEU | CA-C-O | -5.38 | 108.79 | 120.10 |
| 1 | C | 165 | PHE | O-C-N | 5.38 | 131.31 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 19 | ALA | CA-C-N | 5.38 | 129.04 | 117.20 |
| 1 | F | 219 | LEU | C-N-CA | -5.38 | 108.24 | 121.70 |
| 1 | B | 125 | ASN | CA-CB-CG | 5.38 | 125.24 | 113.40 |
| 1 | E | 210 | ARG | C-N-CA | 5.38 | 135.15 | 121.70 |
| 1 | F | 175 | ASN | OD1-CG-ND2 | 5.38 | 134.28 | 121.90 |
| 1 | F | 191 | GLY | O-C-N | 5.38 | 131.31 | 122.70 |
| 1 | E | 71 | LEU | C-N-CA | -5.38 | 108.25 | 121.70 |
| 1 | D | 87 | ILE | CA-CB-CG1 | -5.38 | 100.78 | 111.00 |
| 1 | D | 157 | GLU | CB-CG-CD | 5.38 | 128.72 | 114.20 |
| 1 | F | 45 | VAL | CB-CA-C | 5.38 | 121.62 | 111.40 |
| 1 | F | 80 | SER | CA-C-N | -5.38 | 105.37 | 117.20 |
| 1 | D | 103 | TYR | CZ-CE2-CD2 | -5.38 | 114.96 | 119.80 |
| 1 | F | 96 | PRO | O-C-N | -5.38 | 114.10 | 122.70 |
| 1 | E | 113 | SER | CA-C-O | 5.38 | 131.39 | 120.10 |
| 1 | E | 221 | PRO | CA-C-O | -5.38 | 107.30 | 120.20 |
| 1 | A | 12 | SER | O-C-N | 5.37 | 131.30 | 122.70 |
| 1 | C | 64 | SER | CB-CA-C | -5.37 | 99.89 | 110.10 |
| 1 | D | 140 | THR | C-N-CA | 5.37 | 135.13 | 121.70 |
| 1 | A | 234 | THR | CA-C-O | -5.37 | 108.82 | 120.10 |
| 1 | B | 52 | THR | OG1-CB-CG2 | -5.37 | 97.65 | 110.00 |
| 1 | E | 148 | GLN | CB-CG-CD | 5.37 | 125.56 | 111.60 |
| 1 | A | 214 | ARG | NH1-CZ-NH2 | -5.37 | 113.50 | 119.40 |
| 1 | B | 163 | VAL | C-N-CA | 5.37 | 135.12 | 121.70 |
| 1 | F | 41 | PHE | CG-CD1-CE1 | 5.37 | 126.70 | 120.80 |
| 1 | D | 78 | ARG | N-CA-CB | -5.36 | 100.95 | 110.60 |
| 1 | D | 114 | ASN | CB-CG-OD1 | 5.36 | 132.33 | 121.60 |
| 1 | D | 184 | ARG | N-CA-CB | 5.36 | 120.25 | 110.60 |
| 1 | B | 77 | ILE | N-CA-CB | -5.36 | 98.47 | 110.80 |
| 1 | E | 75 | ASN | C-N-CA | -5.36 | 108.30 | 121.70 |
| 1 | F | 57 | GLY | C-N-CA | 5.36 | 135.10 | 121.70 |
| 1 | F | 139 | GLN | CG-CD-NE2 | -5.36 | 103.83 | 116.70 |
| 1 | C | 204 | TRP | C-N-CA | 5.36 | 135.10 | 121.70 |
| 1 | F | 233 | TRP | N-CA-CB | -5.36 | 100.95 | 110.60 |
| 1 | A | 14 | PRO | N-CA-CB | 5.36 | 109.73 | 103.30 |
| 1 | C | 204 | TRP | CE3-CZ3-CH2 | 5.36 | 127.09 | 121.20 |
| 1 | F | 164 | LEU | C-N-CA | -5.36 | 108.31 | 121.70 |
| 1 | A | 79 | TRP | CD2-CE3-CZ3 | 5.35 | 125.76 | 118.80 |
| 1 | E | 12 | SER | N-CA-CB | 5.35 | 118.53 | 110.50 |
| 1 | E | 117 | SER | C-N-CA | 5.35 | 135.07 | 121.70 |
| 1 | F | 19 | ALA | CA-C-N | 5.35 | 128.97 | 117.20 |
| 1 | F | 196 | LEU | CD1-CG-CD2 | -5.35 | 94.45 | 110.50 |
| 1 | A | 208 | ASN | CB-CG-ND2 | 5.35 | 129.53 | 116.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 74 | GLN | CA-CB-CG | -5.35 | 101.64 | 113.40 |
| 1 | B | 103 | TYR | CB-CG-CD1 | -5.35 | 117.79 | 121.00 |
| 1 | B | 175 | ASN | CA-C-N | 5.35 | 128.97 | 117.20 |
| 1 | C | 116 | GLY | CA-C-N | 5.35 | 128.97 | 117.20 |
| 1 | E | 139 | GLN | N-CA-C | -5.35 | 96.56 | 111.00 |
| 1 | F | 193 | MET | N-CA-C | -5.35 | 96.57 | 111.00 |
| 1 | A | 34 | SER | C-N-CA | 5.34 | 135.06 | 121.70 |
| 1 | E | 35 | ASP | CA-C-O | 5.34 | 131.32 | 120.10 |
| 1 | E | 71 | LEU | CB-CA-C | -5.34 | 100.05 | 110.20 |
| 1 | B | 221 | PRO | O-C-N | -5.34 | 114.16 | 122.70 |
| 1 | D | 41 | PHE | CA-C-O | 5.34 | 131.31 | 120.10 |
| 1 | E | 35 | ASP | CB-CA-C | -5.34 | 99.73 | 110.40 |
| 1 | F | 70 | ILE | CA-C-N | -5.34 | 105.46 | 117.20 |
| 1 | F | 86 | SER | CA-CB-OG | 5.34 | 125.61 | 111.20 |
| 1 | C | 17 | LEU | CB-CG-CD1 | -5.33 | 101.93 | 111.00 |
| 1 | C | 74 | GLN | CG-CD-OE1 | -5.33 | 110.93 | 121.60 |
| 1 | A | 12 | SER | CA-C-N | -5.33 | 105.47 | 117.20 |
| 1 | C | 4 | LEU | O-C-N | 5.33 | 131.23 | 122.70 |
| 1 | D | 55 | ALA | O-C-N | -5.33 | 114.17 | 122.70 |
| 1 | F | 189 | PRO | CA-N-CD | -5.33 | 104.04 | 111.50 |
| 1 | B | 2 | ASN | O-C-N | -5.33 | 114.17 | 122.70 |
| 1 | D | 75 | ASN | C-N-CA | -5.33 | 108.38 | 121.70 |
| 1 | D | 146 | SER | CA-CB-OG | -5.33 | 96.81 | 111.20 |
| 1 | B | 201 | ILE | CA-CB-CG2 | 5.33 | 121.55 | 110.90 |
| 1 | C | 179 | LYS | CA-CB-CG | -5.33 | 101.68 | 113.40 |
| 1 | D | 28 | PHE | N-CA-C | -5.33 | 96.62 | 111.00 |
| 1 | D | 42 | ASP | CB-CG-OD1 | -5.33 | 113.51 | 118.30 |
| 1 | F | 152 | TYR | CA-C-N | 5.33 | 128.92 | 117.20 |
| 1 | E | 231 | ALA | CA-C-O | -5.32 | 108.92 | 120.10 |
| 1 | B | 208 | ASN | CA-C-O | 5.32 | 131.27 | 120.10 |
| 1 | C | 37 | ASN | O-C-N | 5.32 | 131.21 | 122.70 |
| 1 | F | 189 | PRO | N-CD-CG | 5.32 | 111.18 | 103.20 |
| 1 | A | 97 | ASP | OD1-CG-OD2 | 5.32 | 133.40 | 123.30 |
| 1 | E | 111 | GLY | CA-C-N | -5.32 | 105.50 | 117.20 |
| 1 | E | 231 | ALA | N-CA-C | -5.32 | 96.64 | 111.00 |
| 1 | C | 114 | ASN | CA-CB-CG | 5.32 | 125.09 | 113.40 |
| 1 | D | 200 | ASN | N-CA-C | 5.32 | 125.35 | 111.00 |
| 1 | A | 94 | LEU | CA-C-O | 5.31 | 131.26 | 120.10 |
| 1 | C | 163 | VAL | CB-CA-C | 5.31 | 121.49 | 111.40 |
| 1 | C | 225 | LEU | CA-C-N | 5.31 | 128.89 | 117.20 |
| 1 | D | 234 | THR | N-CA-CB | -5.31 | 100.21 | 110.30 |
| 1 | C | 87 | ILE | CA-CB-CG1 | -5.31 | 100.91 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 158 | THR | N-CA-CB | 5.31 | 120.39 | 110.30 |
| 1 | C | 30 | PHE | CE1-CZ-CE2 | -5.31 | 110.44 | 120.00 |
| 1 | E | 18 | HIS | CG-ND1-CE1 | 5.31 | 115.63 | 108.20 |
| 1 | F | 170 | ARG | CD-NE-CZ | 5.31 | 131.03 | 123.60 |
| 1 | F | 225 | LEU | CB-CG-CD1 | -5.31 | 101.97 | 111.00 |
| 1 | E | 37 | ASN | CA-C-O | -5.31 | 108.95 | 120.10 |
| 1 | A | 28 | PHE | CA-C-N | -5.30 | 105.53 | 117.20 |
| 1 | B | 142 | HIS | CA-C-O | -5.30 | 108.96 | 120.10 |
| 1 | D | 90 | TYR | O-C-N | 5.30 | 131.19 | 122.70 |
| 1 | F | 213 | GLY | CA-C-N | 5.30 | 128.87 | 117.20 |
| 1 | C | 132 | GLN | CA-C-N | 5.30 | 126.81 | 116.20 |
| 1 | D | 170 | ARG | CG-CD-NE | 5.30 | 122.94 | 111.80 |
| 1 | F | 62 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | D | 70 | ILE | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | E | 79 | TRP | CA-C-O | -5.30 | 108.97 | 120.10 |
| 1 | A | 157 | GLU | N-CA-C | 5.30 | 125.31 | 111.00 |
| 1 | B | 21 | GLN | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | B | 162 | LEU | CB-CG-CD2 | -5.30 | 101.99 | 111.00 |
| 1 | C | 93 | VAL | CA-CB-CG1 | 5.30 | 118.85 | 110.90 |
| 1 | C | 148 | GLN | CA-C-O | -5.30 | 108.97 | 120.10 |
| 1 | C | 204 | TRP | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | C | 154 | LEU | C-N-CA | -5.29 | 108.46 | 121.70 |
| 1 | C | 102 | ILE | CG1-CB-CG2 | -5.29 | 99.75 | 111.40 |
| 1 | E | 104 | GLY | N-CA-C | 5.29 | 126.34 | 113.10 |
| 1 | B | 211 | SER | CA-C-N | 5.29 | 128.84 | 117.20 |
| 1 | C | 199 | GLN | C-N-CA | 5.29 | 134.93 | 121.70 |
| 1 | D | 153 | ARG | CB-CG-CD | -5.29 | 97.84 | 111.60 |
| 1 | A | 40 | LEU | N-CA-CB | 5.29 | 120.98 | 110.40 |
| 1 | A | 73 | ALA | CB-CA-C | -5.29 | 102.17 | 110.10 |
| 1 | B | 144 | THR | N-CA-CB | 5.29 | 120.35 | 110.30 |
| 1 | A | 49 | ALA | CA-C-N | 5.29 | 128.83 | 117.20 |
| 1 | B | 200 | ASN | CB-CG-ND2 | -5.29 | 104.01 | 116.70 |
| 1 | C | 5 | PHE | N-CA-CB | 5.29 | 120.12 | 110.60 |
| 1 | C | 199 | GLN | CG-CD-OE1 | 5.29 | 132.18 | 121.60 |
| 1 | E | 21 | GLN | OE1-CD-NE2 | 5.29 | 134.06 | 121.90 |
| 1 | F | 103 | TYR | CZ-CE2-CD2 | -5.29 | 115.04 | 119.80 |
| 1 | E | 9 | HIS | N-CA-C | 5.29 | 125.27 | 111.00 |
| 1 | F | 218 | VAL | CA-C-O | -5.29 | 109.00 | 120.10 |
| 1 | C | 25 | LEU | CA-C-N | 5.29 | 128.83 | 117.20 |
| 1 | C | 148 | GLN | N-CA-C | 5.29 | 125.27 | 111.00 |
| 1 | F | 23 | LEU | C-N-CA | -5.29 | 108.49 | 121.70 |
| 1 | A | 3 | ILE | CA-C-O | 5.28 | 131.19 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 214 | ARG | CA-CB-CG | -5.28 | 101.77 | 113.40 |
| 1 | E | 143 | ALA | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | A | 101 | THR | CA-C-O | -5.28 | 109.01 | 120.10 |
| 1 | A | 56 | THR | C-N-CA | 5.28 | 133.39 | 122.30 |
| 1 | D | 153 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | A | 38 | LEU | CB-CA-C | -5.28 | 100.17 | 110.20 |
| 1 | C | 91 | VAL | O-C-N | -5.28 | 114.26 | 122.70 |
| 1 | B | 139 | GLN | CA-C-O | -5.28 | 109.02 | 120.10 |
| 1 | B | 158 | THR | CB-CA-C | -5.28 | 97.35 | 111.60 |
| 1 | C | 103 | TYR | O-C-N | -5.28 | 114.23 | 123.20 |
| 1 | E | 86 | SER | CA-C-O | -5.28 | 109.02 | 120.10 |
| 1 | C | 149 | LEU | CB-CG-CD2 | 5.27 | 119.97 | 111.00 |
| 1 | B | 196 | LEU | N-CA-C | 5.27 | 125.23 | 111.00 |
| 1 | B | 148 | GLN | CA-C-O | -5.27 | 109.03 | 120.10 |
| 1 | D | 16 | THR | N-CA-C | 5.27 | 125.23 | 111.00 |
| 1 | D | 215 | TYR | CB-CA-C | -5.27 | 99.86 | 110.40 |
| 1 | E | 103 | TYR | CD1-CG-CD2 | -5.27 | 112.10 | 117.90 |
| 1 | E | 108 | TRP | CD1-NE1-CE2 | -5.27 | 104.26 | 109.00 |
| 1 | C | 169 | ASP | C-N-CA | 5.27 | 134.87 | 121.70 |
| 1 | F | 145 | GLN | N-CA-C | 5.27 | 125.22 | 111.00 |
| 1 | A | 4 | LEU | N-CA-CB | -5.27 | 99.87 | 110.40 |
| 1 | E | 111 | GLY | CA-C-O | -5.26 | 111.12 | 120.60 |
| 1 | F | 33 | GLN | CG-CD-NE2 | -5.26 | 104.06 | 116.70 |
| 1 | B | 189 | PRO | N-CA-CB | 5.26 | 109.62 | 103.30 |
| 1 | B | 83 | THR | CA-C-N | 5.26 | 128.78 | 117.20 |
| 1 | E | 73 | ALA | CA-C-O | 5.26 | 131.15 | 120.10 |
| 1 | F | 163 | VAL | CB-CA-C | 5.26 | 121.40 | 111.40 |
| 1 | C | 198 | ASN | CA-CB-CG | -5.26 | 101.83 | 113.40 |
| 1 | E | 43 | SER | N-CA-CB | -5.26 | 102.61 | 110.50 |
| 1 | F | 45 | VAL | C-N-CA | -5.26 | 108.55 | 121.70 |
| 1 | A | 123 | ASN | CB-CA-C | -5.26 | 99.88 | 110.40 |
| 1 | A | 201 | ILE | CA-C-O | 5.26 | 131.14 | 120.10 |
| 1 | D | 175 | ASN | C-N-CA | 5.25 | 134.84 | 121.70 |
| 1 | F | 170 | ARG | O-C-N | -5.25 | 114.29 | 122.70 |
| 1 | C | 49 | ALA | N-CA-C | 5.25 | 125.18 | 111.00 |
| 1 | C | 77 | ILE | N-CA-C | 5.25 | 125.18 | 111.00 |
| 1 | D | 100 | VAL | C-N-CA | 5.25 | 134.83 | 121.70 |
| 1 | F | 87 | ILE | CA-C-O | -5.25 | 109.07 | 120.10 |
| 1 | C | 193 | MET | N-CA-C | -5.25 | 96.83 | 111.00 |
| 1 | B | 206 | SER | CA-C-N | 5.25 | 126.69 | 116.20 |
| 1 | F | 78 | ARG | CD-NE-CZ | -5.25 | 116.25 | 123.60 |
| 1 | A | 181 | THR | CA-C-O | -5.25 | 109.09 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 215 | TYR | N-CA-CB | 5.25 | 120.04 | 110.60 |
| 1 | E | 214 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | E | 107 | LEU | CA-CB-CG | 5.24 | 127.36 | 115.30 |
| 1 | E | 223 | ARG | O-C-N | -5.24 | 114.31 | 122.70 |
| 1 | B | 128 | LEU | CD1-CG-CD2 | -5.24 | 94.77 | 110.50 |
| 1 | E | 57 | GLY | CA-C-O | 5.24 | 130.04 | 120.60 |
| 1 | A | 89 | ASN | CA-C-N | 5.24 | 128.73 | 117.20 |
| 1 | B | 14 | PRO | CA-N-CD | -5.24 | 104.16 | 111.50 |
| 1 | B | 153 | ARG | CB-CA-C | -5.24 | 99.92 | 110.40 |
| 1 | B | 5 | PHE | C-N-CA | 5.24 | 133.30 | 122.30 |
| 1 | F | 217 | PHE | CZ-CE2-CD2 | -5.24 | 113.81 | 120.10 |
| 1 | C | 154 | LEU | CB-CG-CD1 | 5.24 | 119.90 | 111.00 |
| 1 | F | 69 | VAL | CB-CA-C | 5.24 | 121.35 | 111.40 |
| 1 | D | 219 | LEU | CB-CG-CD1 | 5.24 | 119.90 | 111.00 |
| 1 | E | 70 | ILE | N-CA-CB | -5.24 | 98.76 | 110.80 |
| 1 | E | 82 | GLY | CA-C-O | -5.24 | 111.17 | 120.60 |
| 1 | F | 139 | GLN | O-C-N | 5.24 | 131.08 | 122.70 |
| 1 | A | 163 | VAL | O-C-N | 5.23 | 131.07 | 122.70 |
| 1 | C | 23 | LEU | O-C-N | 5.23 | 131.07 | 122.70 |
| 1 | F | 10 | GLU | OE1-CD-OE2 | -5.23 | 117.02 | 123.30 |
| 1 | D | 167 | ARG | N-CA-CB | 5.23 | 120.02 | 110.60 |
| 1 | E | 127 | ILE | CA-CB-CG2 | -5.23 | 100.44 | 110.90 |
| 1 | E | 157 | GLU | N-CA-C | 5.23 | 125.12 | 111.00 |
| 1 | F | 21 | GLN | CA-CB-CG | 5.22 | 124.89 | 113.40 |
| 1 | A | 217 | PHE | O-C-N | 5.22 | 131.05 | 122.70 |
| 1 | F | 125 | ASN | N-CA-C | 5.22 | 125.10 | 111.00 |
| 1 | B | 208 | ASN | OD1-CG-ND2 | 5.22 | 133.90 | 121.90 |
| 1 | C | 175 | ASN | CA-C-O | -5.22 | 109.14 | 120.10 |
| 1 | E | 64 | SER | CA-CB-OG | 5.22 | 125.29 | 111.20 |
| 1 | E | 172 | TRP | CE2-CD2-CG | 5.22 | 111.47 | 107.30 |
| 1 | A | 157 | GLU | CB-CG-CD | 5.21 | 128.28 | 114.20 |
| 1 | D | 59 | ARG | CD-NE-CZ | 5.21 | 130.90 | 123.60 |
| 1 | E | 89 | ASN | OD1-CG-ND2 | 5.21 | 133.89 | 121.90 |
| 1 | E | 153 | ARG | CG-CD-NE | -5.21 | 100.85 | 111.80 |
| 1 | F | 37 | ASN | C-N-CA | -5.21 | 108.66 | 121.70 |
| 1 | F | 144 | THR | N-CA-C | -5.21 | 96.92 | 111.00 |
| 1 | B | 105 | PRO | O-C-N | 5.21 | 132.06 | 123.20 |
| 1 | C | 63 | GLN | OE1-CD-NE2 | -5.21 | 109.92 | 121.90 |
| 1 | D | 145 | GLN | CA-C-O | 5.21 | 131.04 | 120.10 |
| 1 | F | 44 | ASP | OD1-CG-OD2 | 5.21 | 133.20 | 123.30 |
| 1 | B | 197 | THR | CA-C-O | 5.21 | 131.04 | 120.10 |
| 1 | C | 139 | GLN | CG-CD-OE1 | -5.21 | 111.18 | 121.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 169 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | F | 182 | GLY | CA-C-N | -5.21 | 105.74 | 117.20 |
| 1 | C | 199 | GLN | CB-CG-CD | -5.21 | 98.06 | 111.60 |
| 1 | D | 127 | ILE | CA-CB-CG1 | 5.21 | 120.89 | 111.00 |
| 1 | E | 232 | LEU | CA-C-N | 5.21 | 128.65 | 117.20 |
| 1 | A | 118 | VAL | CG1-CB-CG2 | -5.20 | 102.57 | 110.90 |
| 1 | A | 172 | TRP | CD1-CG-CD2 | -5.20 | 102.14 | 106.30 |
| 1 | B | 224 | ASN | C-N-CA | 5.20 | 134.70 | 121.70 |
| 1 | C | 116 | GLY | O-C-N | -5.20 | 114.38 | 122.70 |
| 1 | C | 140 | THR | CB-CA-C | -5.20 | 97.56 | 111.60 |
| 1 | D | 66 | GLY | O-C-N | -5.20 | 114.38 | 122.70 |
| 1 | D | 90 | TYR | CG-CD2-CE2 | 5.20 | 125.46 | 121.30 |
| 1 | E | 129 | TYR | N-CA-CB | -5.20 | 101.24 | 110.60 |
| 1 | A | 141 | LEU | CB-CA-C | -5.20 | 100.32 | 110.20 |
| 1 | B | 100 | VAL | CG1-CB-CG2 | -5.20 | 102.58 | 110.90 |
| 1 | C | 129 | TYR | CA-C-N | 5.20 | 128.64 | 117.20 |
| 1 | E | 108 | TRP | CA-C-O | -5.20 | 109.19 | 120.10 |
| 1 | A | 217 | PHE | CA-C-N | 5.20 | 128.63 | 117.20 |
| 1 | E | 226 | ALA | CA-C-O | -5.20 | 109.19 | 120.10 |
| 1 | F | 103 | TYR | CD1-CG-CD2 | -5.20 | 112.19 | 117.90 |
| 1 | F | 215 | TYR | CZ-CE2-CD2 | 5.20 | 124.47 | 119.80 |
| 1 | B | 175 | ASN | CA-C-O | -5.19 | 109.19 | 120.10 |
| 1 | E | 189 | PRO | CB-CG-CD | -5.19 | 86.25 | 106.50 |
| 1 | C | 72 | THR | N-CA-C | 5.19 | 125.02 | 111.00 |
| 1 | F | 30 | PHE | CB-CA-C | -5.19 | 100.02 | 110.40 |
| 1 | A | 39 | VAL | N-CA-C | 5.19 | 125.02 | 111.00 |
| 1 | D | 108 | TRP | CB-CG-CD2 | 5.19 | 133.35 | 126.60 |
| 1 | E | 118 | VAL | CA-CB-CG1 | 5.19 | 118.68 | 110.90 |
| 1 | A | 53 | ALA | O-C-N | -5.19 | 114.38 | 123.20 |
| 1 | C | 19 | ALA | O-C-N | -5.19 | 114.40 | 122.70 |
| 1 | D | 107 | LEU | N-CA-C | -5.19 | 96.99 | 111.00 |
| 1 | C | 19 | ALA | N-CA-C | 5.18 | 125.00 | 111.00 |
| 1 | E | 48 | TRP | CA-C-O | -5.18 | 109.21 | 120.10 |
| 1 | A | 79 | TRP | CB-CG-CD2 | 5.18 | 133.34 | 126.60 |
| 1 | C | 136 | ASN | CB-CG-OD1 | -5.18 | 111.23 | 121.60 |
| 1 | F | 36 | CYS | CA-C-N | 5.18 | 128.60 | 117.20 |
| 1 | F | 159 | ASP | CA-CB-CG | 5.18 | 124.80 | 113.40 |
| 1 | A | 114 | ASN | OD1-CG-ND2 | 5.18 | 133.81 | 121.90 |
| 1 | B | 63 | GLN | OE1-CD-NE2 | -5.18 | 109.99 | 121.90 |
| 1 | C | 118 | VAL | CA-CB-CG1 | 5.18 | 118.67 | 110.90 |
| 1 | E | 145 | GLN | C-N-CA | 5.18 | 134.65 | 121.70 |
| 1 | F | 207 | GLY | O-C-N | -5.18 | 114.41 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 202 | ALA | CB-CA-C | 5.18 | 117.87 | 110.10 |
| 1 | F | 85 | GLY | C-N-CA | 5.18 | 134.65 | 121.70 |
| 1 | C | 13 | HIS | CG-CD2-NE2 | 5.17 | 119.03 | 109.20 |
| 1 | C | 21 | GLN | CA-CB-CG | -5.17 | 102.01 | 113.40 |
| 1 | E | 121 | ALA | C-N-CA | 5.17 | 134.63 | 121.70 |
| 1 | A | 115 | LYS | C-N-CA | 5.17 | 133.16 | 122.30 |
| 1 | C | 137 | HIS | ND1-CE1-NE2 | 5.17 | 121.28 | 109.90 |
| 1 | C | 193 | MET | CA-CB-CG | -5.17 | 104.51 | 113.30 |
| 1 | D | 69 | VAL | CA-C-O | -5.17 | 109.24 | 120.10 |
| 1 | A | 59 | ARG | CG-CD-NE | 5.17 | 122.65 | 111.80 |
| 1 | B | 39 | VAL | O-C-N | -5.17 | 114.43 | 122.70 |
| 1 | E | 233 | TRP | C-N-CA | -5.17 | 108.78 | 121.70 |
| 1 | A | 128 | LEU | CB-CG-CD2 | 5.17 | 119.78 | 111.00 |
| 1 | C | 180 | GLY | CA-C-O | -5.17 | 111.30 | 120.60 |
| 1 | C | 156 | MET | CA-C-N | -5.17 | 105.84 | 117.20 |
| 1 | C | 3 | ILE | CB-CG1-CD1 | -5.16 | 99.44 | 113.90 |
| 1 | E | 137 | HIS | C-N-CA | 5.16 | 143.69 | 122.00 |
| 1 | F | 95 | GLN | CA-C-O | -5.16 | 109.25 | 120.10 |
| 1 | A | 173 | SER | CB-CA-C | 5.16 | 119.91 | 110.10 |
| 1 | D | 213 | GLY | C-N-CA | -5.16 | 108.80 | 121.70 |
| 1 | F | 30 | PHE | CA-C-O | 5.16 | 130.94 | 120.10 |
| 1 | C | 153 | ARG | C-N-CA | -5.16 | 108.80 | 121.70 |
| 1 | A | 33 | GLN | O-C-N | -5.16 | 114.45 | 122.70 |
| 1 | B | 97 | ASP | CB-CA-C | 5.16 | 120.71 | 110.40 |
| 1 | E | 164 | LEU | C-N-CA | -5.16 | 108.81 | 121.70 |
| 1 | E | 28 | PHE | CB-CG-CD1 | 5.16 | 124.41 | 120.80 |
| 1 | C | 30 | PHE | CG-CD1-CE1 | -5.15 | 115.13 | 120.80 |
| 1 | E | 32 | MET | CA-CB-CG | 5.15 | 122.06 | 113.30 |
| 1 | B | 204 | TRP | CB-CG-CD1 | 5.15 | 133.70 | 127.00 |
| 1 | F | 159 | ASP | OD1-CG-OD2 | 5.15 | 133.09 | 123.30 |
| 1 | D | 3 | ILE | CA-CB-CG1 | -5.15 | 101.22 | 111.00 |
| 1 | E | 31 | THR | CA-CB-CG2 | -5.15 | 105.19 | 112.40 |
| 1 | D | 217 | PHE | CE1-CZ-CE2 | 5.15 | 129.26 | 120.00 |
| 1 | A | 192 | ARG | N-CA-C | 5.15 | 124.89 | 111.00 |
| 1 | A | 198 | ASN | O-C-N | -5.15 | 114.47 | 122.70 |
| 1 | B | 109 | ASP | CA-C-N | -5.15 | 105.88 | 117.20 |
| 1 | D | 85 | GLY | O-C-N | -5.14 | 114.47 | 122.70 |
| 1 | D | 103 | TYR | CD1-CG-CD2 | -5.14 | 112.24 | 117.90 |
| 1 | F | 78 | ARG | NE-CZ-NH1 | -5.14 | 117.73 | 120.30 |
| 1 | F | 232 | LEU | O-C-N | 5.14 | 130.93 | 122.70 |
| 1 | B | 30 | PHE | CG-CD1-CE1 | 5.14 | 126.45 | 120.80 |
| 1 | C | 66 | GLY | CA-C-O | 5.14 | 129.85 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 89 | ASN | CA-C-O | -5.14 | 109.31 | 120.10 |
| 1 | B | 193 | MET | CB-CG-SD | -5.14 | 96.99 | 112.40 |
| 1 | D | 130 | SER | CA-C-N | -5.14 | 105.90 | 117.20 |
| 1 | E | 47 | VAL | CA-C-N | 5.14 | 128.50 | 117.20 |
| 1 | B | 138 | PRO | CB-CA-C | -5.13 | 99.16 | 112.00 |
| 1 | C | 45 | VAL | CA-C-O | 5.13 | 130.88 | 120.10 |
| 1 | D | 196 | LEU | CD1-CG-CD2 | -5.13 | 95.10 | 110.50 |
| 1 | F | 81 | SER | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | F | 183 | CYS | CA-C-O | 5.13 | 130.87 | 120.10 |
| 1 | D | 11 | GLY | N-CA-C | -5.13 | 100.28 | 113.10 |
| 1 | D | 84 | LYS | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | E | 63 | GLN | CG-CD-OE1 | 5.12 | 131.85 | 121.60 |
| 1 | E | 155 | SER | CA-C-N | 5.12 | 128.47 | 117.20 |
| 1 | F | 21 | GLN | CB-CA-C | 5.12 | 120.65 | 110.40 |
| 1 | C | 3 | ILE | CA-C-O | -5.12 | 109.34 | 120.10 |
| 1 | D | 212 | ALA | CA-C-N | 5.12 | 126.44 | 116.20 |
| 1 | A | 152 | TYR | CA-C-O | -5.12 | 109.35 | 120.10 |
| 1 | A | 190 | ASN | CB-CA-C | 5.12 | 120.64 | 110.40 |
| 1 | B | 48 | TRP | C-N-CA | -5.12 | 108.91 | 121.70 |
| 1 | E | 97 | ASP | CA-C-O | -5.12 | 109.36 | 120.10 |
| 1 | B | 157 | GLU | O-C-N | 5.11 | 130.88 | 122.70 |
| 1 | A | 96 | PRO | CA-N-CD | -5.11 | 104.34 | 111.50 |
| 1 | C | 40 | LEU | CA-C-O | 5.11 | 130.83 | 120.10 |
| 1 | F | 49 | ALA | CA-C-O | -5.11 | 109.36 | 120.10 |
| 1 | A | 50 | SER | N-CA-C | -5.11 | 97.20 | 111.00 |
| 1 | C | 65 | ASP | CB-CA-C | 5.11 | 120.62 | 110.40 |
| 1 | F | 161 | ASN | CA-C-N | -5.11 | 105.96 | 117.20 |
| 1 | C | 7 | LEU | CB-CA-C | 5.11 | 119.91 | 110.20 |
| 1 | C | 49 | ALA | O-C-N | -5.11 | 114.53 | 122.70 |
| 1 | D | 2 | ASN | C-N-CA | 5.11 | 134.47 | 121.70 |
| 1 | E | 172 | TRP | O-C-N | 5.11 | 130.87 | 122.70 |
| 1 | F | 15 | GLN | N-CA-C | -5.10 | 97.22 | 111.00 |
| 1 | A | 164 | LEU | CD1-CG-CD2 | -5.10 | 95.19 | 110.50 |
| 1 | C | 145 | GLN | N-CA-C | -5.10 | 97.22 | 111.00 |
| 1 | D | 156 | MET | N-CA-CB | -5.10 | 101.42 | 110.60 |
| 1 | A | 164 | LEU | CB-CG-CD2 | -5.10 | 102.33 | 111.00 |
| 1 | B | 166 | ASP | N-CA-C | -5.10 | 97.23 | 111.00 |
| 1 | E | 98 | ARG | C-N-CA | 5.10 | 134.45 | 121.70 |
| 1 | A | 221 | PRO | N-CA-C | -5.10 | 98.85 | 112.10 |
| 1 | E | 4 | LEU | CB-CA-C | 5.10 | 119.89 | 110.20 |
| 1 | F | 18 | HIS | N-CA-CB | -5.10 | 101.43 | 110.60 |
| 1 | D | 233 | TRP | CB-CG-CD2 | 5.10 | 133.22 | 126.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 30 | PHE | CZ-CE2-CD2 | -5.10 | 113.98 | 120.10 |
| 1 | B | 69 | VAL | CA-C-O | -5.09 | 109.40 | 120.10 |
| 1 | D | 52 | THR | CA-C-O | -5.09 | 109.40 | 120.10 |
| 1 | C | 14 | PRO | C-N-CA | -5.09 | 108.97 | 121.70 |
| 1 | E | 145 | GLN | N-CA-CB | 5.09 | 119.77 | 110.60 |
| 1 | C | 78 | ARG | CB-CG-CD | -5.09 | 98.38 | 111.60 |
| 1 | C | 201 | ILE | CA-C-O | 5.09 | 130.78 | 120.10 |
| 1 | A | 114 | ASN | CB-CG-ND2 | 5.08 | 128.91 | 116.70 |
| 1 | B | 175 | ASN | CB-CG-OD1 | -5.08 | 111.43 | 121.60 |
| 1 | B | 231 | ALA | N-CA-C | -5.08 | 97.27 | 111.00 |
| 1 | C | 36 | CYS | N-CA-CB | -5.08 | 101.45 | 110.60 |
| 1 | A | 76 | THR | CA-CB-OG1 | 5.08 | 119.67 | 109.00 |
| 1 | D | 77 | ILE | O-C-N | -5.08 | 114.57 | 122.70 |
| 1 | E | 159 | ASP | CA-C-O | 5.08 | 130.77 | 120.10 |
| 1 | C | 28 | PHE | C-N-CA | 5.08 | 134.39 | 121.70 |
| 1 | C | 208 | ASN | N-CA-C | -5.08 | 97.29 | 111.00 |
| 1 | E | 48 | TRP | CE3-CZ3-CH2 | 5.08 | 126.79 | 121.20 |
| 1 | E | 89 | ASN | CA-C-N | 5.08 | 128.37 | 117.20 |
| 1 | F | 153 | ARG | N-CA-C | 5.08 | 124.71 | 111.00 |
| 1 | B | 161 | ASN | O-C-N | 5.08 | 130.82 | 122.70 |
| 1 | A | 2 | ASN | CA-C-N | 5.08 | 128.36 | 117.20 |
| 1 | B | 81 | SER | O-C-N | -5.07 | 114.58 | 123.20 |
| 1 | B | 234 | THR | CA-C-N | 5.07 | 128.36 | 117.20 |
| 1 | D | 156 | MET | CA-C-N | 5.07 | 128.36 | 117.20 |
| 1 | F | 76 | THR | OG1-CB-CG2 | -5.07 | 98.33 | 110.00 |
| 1 | E | 88 | GLY | C-N-CA | -5.07 | 109.02 | 121.70 |
| 1 | A | 13 | HIS | CB-CA-C | 5.07 | 120.54 | 110.40 |
| 1 | B | 127 | ILE | CG1-CB-CG2 | 5.07 | 122.56 | 111.40 |
| 1 | B | 208 | ASN | C-N-CA | -5.07 | 109.03 | 121.70 |
| 1 | C | 59 | ARG | N-CA-CB | -5.07 | 101.47 | 110.60 |
| 1 | C | 79 | TRP | C-N-CA | 5.07 | 134.38 | 121.70 |
| 1 | C | 93 | VAL | C-N-CA | 5.07 | 134.38 | 121.70 |
| 1 | B | 31 | THR | CA-C-N | -5.07 | 106.05 | 117.20 |
| 1 | C | 225 | LEU | N-CA-CB | -5.07 | 100.27 | 110.40 |
| 1 | F | 161 | ASN | CB-CG-OD1 | -5.07 | 111.47 | 121.60 |
| 1 | B | 51 | ASN | CA-CB-CG | 5.07 | 124.54 | 113.40 |
| 1 | D | 74 | GLN | CG-CD-NE2 | 5.07 | 128.85 | 116.70 |
| 1 | F | 53 | ALA | CA-C-O | -5.07 | 109.46 | 120.10 |
| 1 | A | 196 | LEU | CA-C-N | -5.06 | 106.06 | 117.20 |
| 1 | E | 82 | GLY | O-C-N | 5.06 | 130.80 | 122.70 |
| 1 | A | 71 | LEU | C-N-CA | -5.06 | 109.04 | 121.70 |
| 1 | A | 192 | ARG | CD-NE-CZ | 5.06 | 130.69 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 113 | SER | CA-C-O | 5.06 | 130.73 | 120.10 |
| 1 | A | 99 | THR | CA-C-N | 5.06 | 128.34 | 117.20 |
| 1 | B | 152 | TYR | CZ-CE2-CD2 | -5.06 | 115.25 | 119.80 |
| 1 | C | 212 | ALA | N-CA-C | 5.06 | 124.67 | 111.00 |
| 1 | F | 50 | SER | CA-CB-OG | -5.06 | 97.54 | 111.20 |
| 1 | B | 210 | ARG | CB-CG-CD | 5.06 | 124.75 | 111.60 |
| 1 | E | 206 | SER | CA-C-N | 5.06 | 126.32 | 116.20 |
| 1 | D | 39 | VAL | N-CA-CB | 5.06 | 122.62 | 111.50 |
| 1 | D | 190 | ASN | C-N-CA | 5.06 | 132.92 | 122.30 |
| 1 | F | 99 | THR | OG1-CB-CG2 | 5.06 | 121.63 | 110.00 |
| 1 | A | 143 | ALA | CA-C-O | -5.06 | 109.48 | 120.10 |
| 1 | C | 144 | THR | CA-CB-OG1 | 5.05 | 119.61 | 109.00 |
| 1 | B | 170 | ARG | CA-C-O | 5.05 | 130.71 | 120.10 |
| 1 | B | 10 | GLU | N-CA-CB | -5.05 | 101.51 | 110.60 |
| 1 | B | 125 | ASN | C-N-CA | 5.05 | 134.33 | 121.70 |
| 1 | E | 177 | ALA | CA-C-O | 5.05 | 130.71 | 120.10 |
| 1 | C | 62 | LEU | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | D | 24 | GLU | N-CA-C | 5.05 | 124.63 | 111.00 |
| 1 | F | 192 | ARG | CA-C-O | 5.05 | 130.70 | 120.10 |
| 1 | C | 180 | GLY | O-C-N | 5.05 | 130.77 | 122.70 |
| 1 | D | 191 | GLY | O-C-N | 5.05 | 130.77 | 122.70 |
| 1 | B | 111 | GLY | N-CA-C | 5.04 | 125.71 | 113.10 |
| 1 | A | 77 | ILE | CB-CG1-CD1 | 5.04 | 128.02 | 113.90 |
| 1 | D | 32 | MET | CA-C-N | -5.04 | 106.11 | 117.20 |
| 1 | D | 141 | LEU | CA-CB-CG | -5.04 | 103.70 | 115.30 |
| 1 | E | 128 | LEU | N-CA-CB | -5.04 | 100.31 | 110.40 |
| 1 | F | 181 | THR | C-N-CA | -5.04 | 111.71 | 122.30 |
| 1 | C | 9 | HIS | CB-CG-CD2 | 5.04 | 146.43 | 130.80 |
| 1 | E | 227 | ILE | CA-CB-CG2 | 5.04 | 120.98 | 110.90 |
| 1 | A | 25 | LEU | CA-C-O | -5.04 | 109.52 | 120.10 |
| 1 | F | 30 | PHE | O-C-N | -5.04 | 114.64 | 122.70 |
| 1 | E | 20 | ALA | N-CA-CB | 5.04 | 117.15 | 110.10 |
| 1 | B | 28 | PHE | CD1-CE1-CZ | 5.04 | 126.14 | 120.10 |
| 1 | B | 30 | PHE | CD1-CG-CD2 | 5.04 | 124.85 | 118.30 |
| 1 | C | 48 | TRP | NE1-CE2-CZ2 | -5.04 | 124.86 | 130.40 |
| 1 | D | 69 | VAL | C-N-CA | 5.04 | 134.29 | 121.70 |
| 1 | D | 230 | GLY | CA-C-O | -5.04 | 111.54 | 120.60 |
| 1 | E | 164 | LEU | N-CA-CB | -5.04 | 100.33 | 110.40 |
| 1 | D | 62 | LEU | CB-CA-C | -5.03 | 100.64 | 110.20 |
| 1 | D | 68 | LEU | CD1-CG-CD2 | -5.03 | 95.40 | 110.50 |
| 1 | F | 49 | ALA | C-N-CA | 5.03 | 134.28 | 121.70 |
| 1 | A | 217 | PHE | CD1-CE1-CZ | -5.03 | 114.06 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 101 | THR | CA-C-N | 5.03 | 128.27 | 117.20 |
| 1 | D | 67 | LEU | CB-CA-C | 5.03 | 119.76 | 110.20 |
| 1 | A | 10 | GLU | CG-CD-OE1 | 5.03 | 128.36 | 118.30 |
| 1 | E | 6 | GLY | C-N-CA | -5.03 | 109.13 | 121.70 |
| 1 | A | 69 | VAL | C-N-CA | 5.03 | 134.27 | 121.70 |
| 1 | A | 172 | TRP | CA-C-O | -5.03 | 109.54 | 120.10 |
| 1 | C | 14 | PRO | CB-CA-C | -5.03 | 99.43 | 112.00 |
| 1 | C | 185 | ALA | C-N-CA | 5.03 | 134.26 | 121.70 |
| 1 | D | 114 | ASN | N-CA-CB | -5.03 | 101.56 | 110.60 |
| 1 | D | 202 | ALA | CA-C-O | -5.03 | 109.55 | 120.10 |
| 1 | F | 75 | ASN | C-N-CA | -5.03 | 109.14 | 121.70 |
| 1 | F | 107 | LEU | CB-CG-CD1 | -5.03 | 102.45 | 111.00 |
| 1 | D | 41 | PHE | CG-CD2-CE2 | 5.02 | 126.33 | 120.80 |
| 1 | B | 34 | SER | CA-C-O | -5.02 | 109.55 | 120.10 |
| 1 | D | 105 | PRO | CB-CA-C | -5.02 | 99.44 | 112.00 |
| 1 | E | 94 | LEU | C-N-CA | 5.02 | 134.26 | 121.70 |
| 1 | E | 225 | LEU | N-CA-C | -5.02 | 97.44 | 111.00 |
| 1 | F | 9 | HIS | CG-ND1-CE1 | 5.02 | 115.23 | 108.20 |
| 1 | F | 99 | THR | CA-CB-OG1 | 5.02 | 119.55 | 109.00 |
| 1 | C | 109 | ASP | C-N-CA | 5.02 | 134.25 | 121.70 |
| 1 | F | 231 | ALA | N-CA-C | -5.02 | 97.45 | 111.00 |
| 1 | C | 236 | GLY | CA-C-O | 5.02 | 129.63 | 120.60 |
| 1 | D | 17 | LEU | CB-CG-CD2 | 5.01 | 119.53 | 111.00 |
| 1 | D | 55 | ALA | CB-CA-C | -5.01 | 102.58 | 110.10 |
| 1 | D | 63 | GLN | O-C-N | 5.01 | 130.72 | 122.70 |
| 1 | B | 94 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 1 | E | 8 | SER | CA-CB-OG | -5.01 | 97.67 | 111.20 |
| 1 | C | 235 | THR | CA-C-N | 5.01 | 126.22 | 116.20 |
| 1 | E | 187 | LEU | CB-CG-CD2 | -5.01 | 102.48 | 111.00 |
| 1 | E | 192 | ARG | CA-CB-CG | 5.00 | 124.41 | 113.40 |
| 1 | E | 210 | ARG | NE-CZ-NH2 | 5.00 | 122.80 | 120.30 |
| 1 | F | 42 | ASP | CA-CB-CG | 5.00 | 124.41 | 113.40 |
| 1 | F | 224 | ASN | CA-C-O | -5.00 | 109.59 | 120.10 |
| 1 | D | 79 | TRP | NE1-CE2-CD2 | -5.00 | 102.30 | 107.30 |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | A | 9 | HIS | CA |
| 1 | A | 87 | ILE | CA |
| 1 | B | 60 | ALA | CA |
| 1 | B | 168 | ASP | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | F | 60 | ALA | CA |
| 1 | F | 195 | VAL | CA |

All (342) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 103 | TYR | Mainchain |
| 1 | A | 104 | GLY | Peptide,Mainchain |
| 1 | A | 108 | TRP | Mainchain |
| 1 | A | 111 | GLY | Mainchain |
| 1 | A | 119 | VAL | Mainchain |
| 1 | A | 128 | LEU | Mainchain |
| 1 | A | 13 | HIS | Mainchain |
| 1 | A | 136 | ASN | Mainchain |
| 1 | A | 137 | HIS | Peptide,Mainchain |
| 1 | A | 138 | PRO | Mainchain |
| 1 | A | 139 | GLN | Mainchain |
| 1 | A | 146 | SER | Mainchain |
| 1 | A | 157 | GLU | Mainchain |
| 1 | A | 158 | THR | Mainchain |
| 1 | A | 166 | ASP | Mainchain |
| 1 | A | 170 | ARG | Mainchain |
| 1 | A | 171 | VAL | Mainchain |
| 1 | A | 173 | SER | Mainchain |
| 1 | A | 181 | THR | Mainchain |
| 1 | A | 185 | ALA | Mainchain |
| 1 | A | 188 | GLN | Mainchain |
| 1 | A | 189 | PRO | Mainchain |
| 1 | A | 19 | ALA | Mainchain |
| 1 | A | 192 | ARG | Mainchain |
| 1 | A | 199 | GLN | Mainchain |
| 1 | A | 2 | ASN | Peptide |
| 1 | A | 214 | ARG | Mainchain |
| 1 | A | 215 | TYR | Mainchain |
| 1 | A | 219 | LEU | Mainchain |
| 1 | A | 220 | GLN | Mainchain |
| 1 | A | 221 | PRO | Mainchain |
| 1 | A | 222 | ASP | Mainchain |
| 1 | A | 228 | TYR | Mainchain |
| 1 | A | 231 | ALA | Mainchain |
| 1 | A | 25 | LEU | Mainchain |
| 1 | A | 30 | PHE | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 34 | SER | Mainchain |
| 1 | A | 37 | ASN | Mainchain |
| 1 | A | 38 | LEU | Mainchain |
| 1 | A | 44 | ASP | Mainchain |
| 1 | A | 49 | ALA | Mainchain |
| 1 | A | 5 | PHE | Mainchain |
| 1 | A | 53 | ALA | Mainchain |
| 1 | A | 55 | ALA | Mainchain |
| 1 | A | 60 | ALA | Mainchain |
| 1 | A | 62 | LEU | Mainchain |
| 1 | A | 63 | GLN | Mainchain |
| 1 | A | 68 | LEU | Mainchain |
| 1 | A | 72 | THR | Peptide,Mainchain |
| 1 | A | 75 | ASN | Mainchain |
| 1 | A | 76 | THR | Mainchain |
| 1 | A | 78 | ARG | Mainchain |
| 1 | A | 81 | SER | Mainchain |
| 1 | A | 87 | ILE | Mainchain |
| 1 | A | 89 | ASN | Mainchain |
| 1 | A | 90 | TYR | Mainchain |
| 1 | A | 98 | ARG | Mainchain |
| 1 | B | 104 | GLY | Peptide |
| 1 | B | 105 | PRO | Mainchain |
| 1 | B | 107 | LEU | Peptide,Mainchain |
| 1 | B | 108 | TRP | Peptide,Mainchain |
| 1 | B | 11 | GLY | Peptide,Mainchain |
| 1 | B | 12 | SER | Mainchain |
| 1 | B | 127 | ILE | Mainchain |
| 1 | B | 129 | TYR | Mainchain |
| 1 | B | 13 | HIS | Peptide,Mainchain |
| 1 | B | 130 | SER | Mainchain |
| 1 | B | 131 | THR | Mainchain |
| 1 | B | 136 | ASN | Mainchain |
| 1 | B | 137 | HIS | Peptide,Mainchain |
| 1 | B | 143 | ALA | Mainchain |
| 1 | B | 150 | SER | Mainchain |
| 1 | B | 151 | PRO | Mainchain |
| 1 | B | 156 | MET | Mainchain |
| 1 | B | 158 | THR | Mainchain |
| 1 | B | 159 | ASP | Mainchain |
| 1 | B | 162 | LEU | Mainchain |
| 1 | B | 164 | LEU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 175 | ASN | Mainchain |
| 1 | B | 18 | HIS | Peptide |
| 1 | B | 189 | PRO | Mainchain |
| 1 | B | 194 | ASP | Mainchain |
| 1 | B | 195 | VAL | Mainchain |
| 1 | B | 198 | ASN | Mainchain |
| 1 | B | 20 | ALA | Mainchain |
| 1 | B | 209 | SER | Mainchain |
| 1 | B | 21 | GLN | Peptide |
| 1 | B | 210 | ARG | Mainchain |
| 1 | B | 214 | ARG | Mainchain |
| 1 | B | 222 | ASP | Mainchain |
| 1 | B | 225 | LEU | Mainchain |
| 1 | B | 226 | ALA | Mainchain |
| 1 | B | 228 | TYR | Peptide |
| 1 | B | 229 | GLY | Mainchain |
| 1 | B | 234 | THR | Mainchain |
| 1 | B | 24 | GLU | Mainchain |
| 1 | B | 27 | SER | Mainchain |
| 1 | B | 30 | PHE | Mainchain |
| 1 | B | 31 | THR | Mainchain |
| 1 | B | 32 | MET | Mainchain |
| 1 | B | 41 | PHE | Mainchain |
| 1 | B | 42 | ASP | Mainchain |
| 1 | B | 46 | ARG | Mainchain |
| 1 | B | 48 | TRP | Mainchain |
| 1 | B | 53 | ALA | Peptide |
| 1 | B | 55 | ALA | Mainchain |
| 1 | B | 56 | THR | Mainchain |
| 1 | B | 57 | GLY | Mainchain |
| 1 | B | 6 | GLY | Peptide |
| 1 | B | 60 | ALA | Mainchain |
| 1 | B | 62 | LEU | Mainchain |
| 1 | B | 7 | LEU | Mainchain |
| 1 | B | 70 | ILE | Peptide |
| 1 | B | 72 | THR | Mainchain |
| 1 | B | 73 | ALA | Mainchain |
| 1 | B | 76 | THR | Peptide |
| 1 | B | 86 | SER | Mainchain |
| 1 | B | 88 | GLY | Mainchain |
| 1 | B | 90 | TYR | Sidechain,Mainchain |
| 1 | B | 91 | VAL | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 92 | LEU | Mainchain |
| 1 | B | 94 | LEU | Mainchain |
| 1 | B | 95 | GLN | Mainchain |
| 1 | B | 97 | ASP | Mainchain |
| 1 | C | 102 | ILE | Mainchain |
| 1 | C | 104 | GLY | Peptide,Mainchain |
| 1 | C | 111 | GLY | Mainchain |
| 1 | C | 117 | SER | Peptide |
| 1 | C | 12 | SER | Mainchain |
| 1 | C | 124 | GLY | Peptide,Mainchain |
| 1 | C | 126 | SER | Mainchain |
| 1 | C | 128 | LEU | Mainchain |
| 1 | C | 13 | HIS | Peptide,Mainchain |
| 1 | C | 132 | GLN | Mainchain |
| 1 | C | 137 | HIS | Peptide,Mainchain |
| 1 | C | 138 | PRO | Mainchain |
| 1 | C | 142 | HIS | Mainchain |
| 1 | C | 145 | GLN | Mainchain |
| 1 | C | 154 | LEU | Mainchain |
| 1 | C | 155 | SER | Mainchain |
| 1 | C | 156 | MET | Mainchain |
| 1 | C | 157 | GLU | Mainchain |
| 1 | C | 16 | THR | Mainchain |
| 1 | C | 166 | ASP | Mainchain |
| 1 | C | 167 | ARG | Mainchain |
| 1 | C | 168 | ASP | Sidechain,Mainchain |
| 1 | C | 175 | ASN | Peptide |
| 1 | C | 180 | GLY | Mainchain |
| 1 | C | 189 | PRO | Mainchain |
| 1 | C | 193 | MET | Mainchain |
| 1 | C | 195 | VAL | Mainchain |
| 1 | C | 199 | GLN | Mainchain |
| 1 | C | 2 | ASN | Mainchain |
| 1 | C | 200 | ASN | Mainchain |
| 1 | C | 201 | ILE | Mainchain |
| 1 | C | 206 | SER | Peptide |
| 1 | C | 207 | GLY | Mainchain |
| 1 | C | 21 | GLN | Mainchain |
| 1 | C | 215 | TYR | Mainchain |
| 1 | C | 216 | VAL | Mainchain |
| 1 | C | 22 | SER | Mainchain |
| 1 | C | 227 | ILE | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | C | 229 | GLY | Mainchain |
| 1 | C | 230 | GLY | Peptide,Mainchain |
| 1 | C | 231 | ALA | Mainchain |
| 1 | C | 233 | TRP | Mainchain |
| 1 | C | 234 | THR | Mainchain |
| 1 | C | 24 | GLU | Mainchain |
| 1 | C | 26 | SER | Mainchain |
| 1 | C | 30 | PHE | Sidechain |
| 1 | C | 38 | LEU | Mainchain |
| 1 | C | 46 | ARG | Mainchain |
| 1 | C | 48 | TRP | Mainchain |
| 1 | C | 49 | ALA | Mainchain |
| 1 | C | 51 | ASN | Mainchain |
| 1 | C | 60 | ALA | Mainchain |
| 1 | C | 65 | ASP | Mainchain |
| 1 | C | 7 | LEU | Mainchain |
| 1 | C | 73 | ALA | Mainchain |
| 1 | C | 74 | GLN | Mainchain |
| 1 | C | 76 | THR | Mainchain |
| 1 | C | 8 | SER | Peptide,Mainchain |
| 1 | C | 90 | TYR | Mainchain |
| 1 | D | 100 | VAL | Mainchain |
| 1 | D | 104 | GLY | Peptide |
| 1 | D | 105 | PRO | Mainchain |
| 1 | D | 124 | GLY | Mainchain |
| 1 | D | 129 | TYR | Mainchain |
| 1 | D | 13 | HIS | Peptide,Mainchain |
| 1 | D | 130 | SER | Mainchain |
| 1 | D | 137 | HIS | Peptide,Mainchain |
| 1 | D | 141 | LEU | Mainchain |
| 1 | D | 143 | ALA | Mainchain |
| 1 | D | 146 | SER | Mainchain |
| 1 | D | 148 | GLN | Mainchain |
| 1 | D | 150 | SER | Peptide |
| 1 | D | 158 | THR | Mainchain |
| 1 | D | 16 | THR | Mainchain |
| 1 | D | 167 | ARG | Sidechain,Mainchain |
| 1 | D | 187 | LEU | Mainchain |
| 1 | D | 192 | ARG | Mainchain |
| 1 | D | 193 | MET | Mainchain |
| 1 | D | 20 | ALA | Mainchain |
| 1 | D | 206 | SER | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | D | 209 | SER | Mainchain |
| 1 | D | 21 | GLN | Mainchain |
| 1 | D | 210 | ARG | Mainchain |
| 1 | D | 215 | TYR | Mainchain |
| 1 | D | 217 | PHE | Mainchain |
| 1 | D | 227 | ILE | Mainchain |
| 1 | D | 228 | TYR | Mainchain |
| 1 | D | 229 | GLY | Peptide,Mainchain |
| 1 | D | 230 | GLY | Mainchain |
| 1 | D | 24 | GLU | Mainchain |
| 1 | D | 33 | GLN | Mainchain |
| 1 | D | 34 | SER | Mainchain |
| 1 | D | 35 | ASP | Mainchain |
| 1 | D | 45 | VAL | Mainchain |
| 1 | D | 5 | PHE | Mainchain |
| 1 | D | 56 | THR | Mainchain |
| 1 | D | 6 | GLY | Peptide,Mainchain |
| 1 | D | 60 | ALA | Peptide,Mainchain |
| 1 | D | 61 | VAL | Mainchain |
| 1 | D | 64 | SER | Mainchain |
| 1 | D | 69 | VAL | Mainchain |
| 1 | D | 81 | SER | Mainchain |
| 1 | D | 86 | SER | Mainchain |
| 1 | D | 89 | ASN | Mainchain |
| 1 | E | 104 | GLY | Peptide,Mainchain |
| 1 | E | 11 | GLY | Mainchain |
| 1 | E | 110 | SER | Mainchain |
| 1 | E | 128 | LEU | Peptide,Mainchain |
| 1 | E | 13 | HIS | Peptide,Mainchain |
| 1 | E | 130 | SER | Mainchain |
| 1 | E | 136 | ASN | Mainchain |
| 1 | E | 137 | HIS | Peptide,Mainchain |
| 1 | E | 138 | PRO | Mainchain |
| 1 | E | 147 | LEU | Mainchain |
| 1 | E | 151 | PRO | Mainchain |
| 1 | E | 158 | THR | Mainchain |
| 1 | E | 162 | LEU | Mainchain |
| 1 | E | 165 | PHE | Mainchain |
| 1 | E | 173 | SER | Mainchain |
| 1 | E | 177 | ALA | Mainchain |
| 1 | E | 188 | GLN | Mainchain |
| 1 | E | 206 | SER | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | E | 22 | SER | Mainchain |
| 1 | E | 227 | ILE | Mainchain |
| 1 | E | 231 | ALA | Mainchain |
| 1 | E | 25 | LEU | Mainchain |
| 1 | E | 30 | PHE | Mainchain |
| 1 | E | 33 | GLN | Mainchain |
| 1 | E | 34 | SER | Mainchain |
| 1 | E | 38 | LEU | Mainchain |
| 1 | E | 63 | GLN | Mainchain |
| 1 | E | 66 | GLY | Mainchain |
| 1 | E | 70 | ILE | Mainchain |
| 1 | E | 78 | ARG | Mainchain |
| 1 | E | 86 | SER | Mainchain |
| 1 | E | 9 | HIS | Peptide |
| 1 | E | 90 | TYR | Mainchain |
| 1 | E | 91 | VAL | Mainchain |
| 1 | E | 97 | ASP | Mainchain |
| 1 | F | 103 | TYR | Mainchain |
| 1 | F | 105 | PRO | Mainchain |
| 1 | F | 107 | LEU | Mainchain |
| 1 | F | 124 | GLY | Peptide |
| 1 | F | 128 | LEU | Mainchain |
| 1 | F | 13 | HIS | Peptide,Mainchain |
| 1 | F | 130 | SER | Peptide |
| 1 | F | 137 | HIS | Peptide,Mainchain |
| 1 | F | 14 | PRO | Mainchain |
| 1 | F | 140 | THR | Mainchain |
| 1 | F | 141 | LEU | Mainchain |
| 1 | F | 146 | SER | Mainchain |
| 1 | F | 149 | LEU | Mainchain |
| 1 | F | 15 | GLN | Mainchain |
| 1 | F | 150 | SER | Mainchain |
| 1 | F | 152 | TYR | Mainchain |
| 1 | F | 158 | THR | Mainchain |
| 1 | F | 184 | ARG | Mainchain |
| 1 | F | 185 | ALA | Mainchain |
| 1 | F | 189 | PRO | Mainchain |
| 1 | F | 193 | MET | Peptide,Mainchain |
| 1 | F | 195 | VAL | Mainchain |
| 1 | F | 197 | THR | Mainchain |
| 1 | F | 205 | THR | Mainchain |
| 1 | F | 208 | ASN | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | F | 210 | ARG | Mainchain |
| 1 | F | 214 | ARG | Mainchain |
| 1 | F | 219 | LEU | Mainchain |
| 1 | F | 222 | ASP | Mainchain |
| 1 | F | 23 | LEU | Mainchain |
| 1 | F | 230 | GLY | Mainchain |
| 1 | F | 231 | ALA | Peptide |
| 1 | F | 45 | VAL | Mainchain |
| 1 | F | 52 | THR | Mainchain |
| 1 | F | 54 | GLY | Mainchain |
| 1 | F | 55 | ALA | Mainchain |
| 1 | F | 56 | THR | Mainchain |
| 1 | F | 60 | ALA | Mainchain |
| 1 | F | 63 | GLN | Mainchain |
| 1 | F | 76 | THR | Peptide,Mainchain |
| 1 | F | 78 | ARG | Sidechain |
| 1 | F | 83 | THR | Mainchain |
| 1 | F | 85 | GLY | Peptide |
| 1 | F | 86 | SER | Mainchain |
| 1 | F | 89 | ASN | Mainchain |
| 1 | F | 9 | HIS | Peptide,Mainchain |
| 1 | F | 91 | VAL | Mainchain |
| 1 | F | 95 | GLN | Mainchain |

## 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 | 1778 | 0 | 1700 | 282 | 0 |
| 1 | B | 1694 | 0 | 1600 | 265 | 0 |
| 1 | C | 1772 | 0 | 1695 | 270 | 0 |
| 1 | D | 1702 | 0 | 1613 | 321 | 0 |
| 1 | E | 1759 | 0 | 1684 | 310 | 0 |
| 1 | F | 1659 | 0 | 1579 | 305 | 0 |
| 2 | A | 19 | 0 | 0 | 1 | 0 |
| 2 | B | 15 | 0 | 0 | 0 | 0 |
| 2 | C | 6 | 0 | 0 | 0 | 0 |
| 2 | D | 8 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | E | 8 | 0 | 0 | 0 | 0 |
| 2 | F | 11 | 0 | 0 | 0 | 0 |
| All | All | 10431 | 0 | 9871 | 1677 | 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 84.

All (1677) 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:D:77:ILE:CD1 | 1:D:77:ILE:CG1 | 1.80 | 1.57 |
| 1:E:131:THR:C | 1:E:131:THR:CA | 1.75 | 1.50 |
| 1:E:136:ASN:CB | 1:E:136:ASN:CA | 1.88 | 1.49 |
| 1:A:131:THR:OG1 | 1:A:131:THR:CB | 1.64 | 1.46 |
| 1:D:64:SER:CB | 1:D:64:SER:OG | 1.67 | 1.43 |
| 1:E:158:THR:CB | 1:F:151:PRO:HG2 | 1.55 | 1.32 |
| 1:C:72:THR:CG2 | 1:C:76:THR:H | 1.49 | 1.25 |
| 1:C:73:ALA:CA | 1:F:189:PRO:HG2 | 1.70 | 1.21 |
| 1:E:158:THR:CB | 1:F:151:PRO:CG | 2.22 | 1.16 |
| 1:B:37:ASN:HB2 | 1:B:53:ALA:HB2 | 1.23 | 1.16 |
| 1:F:159:ASP:O | 1:F:160:CYS:HB3 | 1.41 | 1.16 |
| 1:B:151:PRO:CD | 1:D:34:SER:HB2 | 1.76 | 1.16 |
| 1:D:7:LEU:O | 1:D:9:HIS:N | 1.80 | 1.15 |
| 1:B:72:THR:HG22 | 1:B:74:GLN:HB2 | 1.17 | 1.14 |
| 1:C:73:ALA:C | 1:F:189:PRO:HG2 | 1.68 | 1.13 |
| 1:E:87:ILE:HG23 | 1:E:88:GLY:H | 1.03 | 1.12 |
| 1:B:3:ILE:HG22 | 1:B:93:VAL:HB | 1.30 | 1.11 |
| 1:E:6:GLY:HA2 | 1:E:62:LEU:HD23 | 1.27 | 1.11 |
| 1:E:26:SER:O | 1:E:27:SER:HB2 | 1.46 | 1.10 |
| 1:A:72:THR:HG22 | 1:A:76:THR:H | 0.99 | 1.10 |
| 1:D:217:PHE:CE2 | 1:D:225:LEU:HD22 | 1.86 | 1.10 |
| 1:C:7:LEU:HD11 | 1:C:61:VAL:HG11 | 1.29 | 1.09 |
| 1:D:16:THR:HG22 | 1:D:61:VAL:H | 1.07 | 1.09 |
| 1:A:131:THR:O | 1:A:131:THR:HG22 | 1.42 | 1.08 |
| 1:C:72:THR:HG21 | 1:C:76:THR:H | 1.09 | 1.07 |
| 1:F:7:LEU:O | 1:F:9:HIS:N | 1.88 | 1.07 |
| 1:C:26:SER:O | 1:C:27:SER:HB3 | 1.43 | 1.06 |
| 1:E:131:THR:C | 1:E:131:THR:CB | 2.24 | 1.06 |
| 1:B:197:THR:HG21 | 1:B:201:ILE:HB | 1.08 | 1.06 |
| 1:E:32:MET:HE2 | 1:E:60:ALA:HB2 | 1.31 | 1.06 |
| 1:C:74:GLN:N | 1:F:189:PRO:HG2 | 1.71 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:26:SER:OG | 1:F:33:GLN:HG3 | 1.54 | 1.05 |
| 1:E:158:THR:N | 1:F:151:PRO:HG3 | 1.72 | 1.04 |
| 1:F:126:SER:O | 1:F:147:LEU:HD11 | 1.54 | 1.04 |
| 1:C:146:SER:OG | 1:C:147:LEU:N | 1.84 | 1.04 |
| 1:E:4:LEU:HD12 | 1:E:5:PHE:N | 1.69 | 1.04 |
| 1:E:64:SER:O | 1:E:65:ASP:HB3 | 1.55 | 1.04 |
| 1:D:77:ILE:O | 1:D:77:ILE:HG22 | 1.56 | 1.03 |
| 1:F:161:ASN:ND2 | 1:F:176:THR:H | 1.54 | 1.03 |
| 1:C:74:GLN:HG3 | 1:F:189:PRO:HB2 | 1.40 | 1.03 |
| 1:B:151:PRO:HD2 | 1:D:34:SER:HB2 | 1.04 | 1.02 |
| 1:B:217:PHE:CE1 | 1:B:225:LEU:HB3 | 1.94 | 1.02 |
| 1:E:158:THR:CA | 1:F:151:PRO:HG3 | 1.89 | 1.02 |
| 1:E:158:THR:HB | 1:F:151:PRO:HG2 | 1.38 | 1.01 |
| 1:A:12:SER:HB3 | 1:A:221:PRO:HD2 | 1.41 | 1.01 |
| 1:B:154:LEU:HG | 1:B:225:LEU:HD11 | 1.40 | 1.01 |
| 1:B:222:ASP:HB2 | 1:B:224:ASN:OD1 | 1.61 | 1.01 |
| 1:D:170:ARG:HG2 | 1:D:170:ARG:HH11 | 1.25 | 1.01 |
| 1:E:97:ASP:OD1 | 1:E:99:THR:HB | 1.59 | 1.00 |
| 1:A:12:SER:HB3 | 1:A:221:PRO:CD | 1.89 | 1.00 |
| 1:E:9:HIS:HB2 | 1:E:10:GLU:HG3 | 1.43 | 1.00 |
| 1:B:68:LEU:HD13 | 1:B:92:LEU:HD13 | 1.44 | 1.00 |
| 1:B:197:THR:HG21 | 1:B:201:ILE:CB | 1.91 | 0.99 |
| 1:D:127:ILE:HG22 | 1:D:147:LEU:HD21 | 1.44 | 0.99 |
| 1:B:217:PHE:HE1 | 1:B:225:LEU:HB3 | 1.22 | 0.98 |
| 1:A:72:THR:HG22 | 1:A:76:THR:N | 1.78 | 0.98 |
| 1:E:6:GLY:CA | 1:E:62:LEU:HD23 | 1.94 | 0.98 |
| 1:C:97:ASP:HB3 | 1:C:136:ASN:HD22 | 1.27 | 0.97 |
| 1:E:127:ILE:HG23 | 1:E:127:ILE:O | 1.64 | 0.97 |
| 1:D:64:SER:OG | 1:D:64:SER:CA | 2.10 | 0.97 |
| 1:C:4:LEU:HD22 | 1:C:17:LEU:HD23 | 1.45 | 0.96 |
| 1:D:83:THR:O | 1:D:84:LYS:HB3 | 1.62 | 0.96 |
| 1:B:146:SER:O | 1:B:147:LEU:HB2 | 1.63 | 0.96 |
| 1:A:72:THR:HG23 | 1:A:74:GLN:H | 1.24 | 0.96 |
| 1:D:220:GLN:NE2 | 1:D:228:TYR:OH | 1.98 | 0.95 |
| 1:A:62:LEU:HD21 | 1:A:90:TYR:HB2 | 1.47 | 0.95 |
| 1:B:151:PRO:HD2 | 1:D:34:SER:CB | 1.95 | 0.95 |
| 1:C:73:ALA:O | 1:C:75:ASN:N | 2.00 | 0.95 |
| 1:E:158:THR:O | 1:E:160:CYS:N | 1.99 | 0.95 |
| 1:C:73:ALA:CA | 1:F:189:PRO:CG | 2.46 | 0.94 |
| 1:E:87:ILE:HG23 | 1:E:88:GLY:N | 1.68 | 0.94 |
| 1:F:230:GLY:O | 1:F:231:ALA:HB2 | 1.66 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:5:PHE:CZ | 1:D:220:GLN:HG2 | 2.03 | 0.94 |
| 1:A:151:PRO:HD2 | 1:A:152:TYR:H | 1.30 | 0.93 |
| 1:B:28:PHE:CE2 | 1:B:98:ARG:HG3 | 2.03 | 0.93 |
| 1:C:72:THR:O | 1:C:73:ALA:HB3 | 1.67 | 0.93 |
| 1:D:184:ARG:HH22 | 1:D:200:ASN:HD21 | 0.94 | 0.93 |
| 1:B:154:LEU:CG | 1:B:225:LEU:HD11 | 1.97 | 0.93 |
| 1:F:100:VAL:HG23 | 1:F:235:THR:HG21 | 1.50 | 0.93 |
| 1:D:178:GLY:O | 1:D:180:GLY:N | 2.00 | 0.92 |
| 1:F:131:THR:O | 1:F:131:THR:HG22 | 1.70 | 0.92 |
| 1:A:110:SER:HB2 | 1:A:112:THR:HG23 | 1.50 | 0.92 |
| 1:E:22:SER:HB3 | 1:E:31:THR:HG22 | 1.51 | 0.92 |
| 1:A:77:ILE:O | 1:A:77:ILE:HG22 | 1.65 | 0.92 |
| 1:C:72:THR:CG2 | 1:C:76:THR:N | 2.32 | 0.92 |
| 1:D:16:THR:CG2 | 1:D:61:VAL:H | 1.82 | 0.92 |
| 1:F:224:ASN:O | 1:F:225:LEU:HD12 | 1.68 | 0.92 |
| 1:A:179:LYS:NZ | 1:A:179:LYS:HB3 | 1.83 | 0.92 |
| 1:D:217:PHE:HE2 | 1:D:225:LEU:HD22 | 1.29 | 0.92 |
| 1:A:200:ASN:H | 1:A:200:ASN:HD22 | 1.10 | 0.92 |
| 1:E:158:THR:CA | 1:F:151:PRO:CG | 2.47 | 0.92 |
| 1:F:25:LEU:HB2 | 1:F:94:LEU:HD21 | 1.52 | 0.91 |
| 1:C:18:HIS:HB2 | 1:C:21:GLN:NE2 | 1.83 | 0.91 |
| 1:C:72:THR:HG21 | 1:C:76:THR:N | 1.84 | 0.91 |
| 1:E:105:PRO:HD2 | 1:E:210:ARG:NH2 | 1.86 | 0.90 |
| 1:A:86:SER:O | 1:A:87:ILE:HG13 | 1.71 | 0.90 |
| 1:A:32:MET:HE2 | 1:A:60:ALA:HB2 | 1.51 | 0.90 |
| 1:A:108:TRP:HB2 | 1:A:208:ASN:ND2 | 1.86 | 0.90 |
| 1:D:131:THR:HG21 | 1:D:214:ARG:CZ | 2.01 | 0.90 |
| 1:C:176:THR:O | 1:C:177:ALA:HB3 | 1.70 | 0.90 |
| 1:F:2:ASN:HA | 1:F:23:LEU:HD22 | 1.54 | 0.90 |
| 1:A:127:ILE:HG23 | 1:A:127:ILE:O | 1.69 | 0.90 |
| 1:A:22:SER:HB3 | 1:A:31:THR:HG22 | 1.55 | 0.89 |
| 1:B:47:VAL:HG12 | 1:B:47:VAL:O | 1.70 | 0.89 |
| 1:C:7:LEU:HD11 | 1:C:61:VAL:CG1 | 2.01 | 0.89 |
| 1:C:29:ARG:HH21 | 1:C:31:THR:CG2 | 1.86 | 0.89 |
| 1:E:22:SER:CB | 1:E:31:THR:HG22 | 2.03 | 0.89 |
| 1:D:217:PHE:HD2 | 1:D:217:PHE:O | 1.55 | 0.89 |
| 1:A:56:THR:O | 1:A:73:ALA:HB2 | 1.72 | 0.89 |
| 1:F:129:TYR:HD1 | 1:F:130:SER:N | 1.68 | 0.89 |
| 1:A:131:THR:OG1 | 1:A:131:THR:CG2 | 2.21 | 0.89 |
| 1:B:188:GLN:HG3 | 1:B:189:PRO:HD3 | 1.53 | 0.88 |
| 1:D:37:ASN:HD22 | 1:D:38:LEU:H | 1.21 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:3:ILE:HG22 | 1:D:93:VAL:HB | 1.54 | 0.88 |
| 1:E:26:SER:O | 1:E:27:SER:CB | 2.13 | 0.88 |
| 1:E:101:THR:OG1 | 1:E:234:THR:HB | 1.72 | 0.88 |
| 1:D:184:ARG:HH22 | 1:D:200:ASN:ND2 | 1.70 | 0.88 |
| 1:D:176:THR:O | 1:D:177:ALA:HB2 | 1.74 | 0.88 |
| 1:D:100:VAL:HB | 1:D:235:THR:OG1 | 1.74 | 0.87 |
| 1:C:73:ALA:HA | 1:F:189:PRO:CG | 2.02 | 0.87 |
| 1:D:161:ASN:HA | 1:D:176:THR:CG2 | 2.04 | 0.87 |
| 1:C:97:ASP:HB3 | 1:C:136:ASN:ND2 | 1.88 | 0.87 |
| 1:C:217:PHE:HA | 1:C:227:ILE:CG2 | 2.03 | 0.87 |
| 1:D:161:ASN:HA | 1:D:176:THR:HG22 | 1.57 | 0.87 |
| 1:D:150:SER:HB3 | 1:D:151:PRO:CD | 2.05 | 0.86 |
| 1:B:197:THR:OG1 | 1:B:201:ILE:HD12 | 1.73 | 0.86 |
| 1:C:140:THR:OG1 | 1:C:141:LEU:N | 2.05 | 0.86 |
| 1:D:25:LEU:O | 1:D:28:PHE:HB2 | 1.75 | 0.86 |
| 1:F:87:ILE:HG23 | 1:F:88:GLY:N | 1.87 | 0.86 |
| 1:F:159:ASP:O | 1:F:160:CYS:CB | 2.19 | 0.86 |
| 1:E:12:SER:HB3 | 1:E:221:PRO:HD2 | 1.57 | 0.86 |
| 1:A:215:TYR:N | 1:A:215:TYR:HD2 | 1.74 | 0.86 |
| 1:B:217:PHE:HZ | 1:B:225:LEU:HD13 | 1.39 | 0.86 |
| 1:E:4:LEU:HD12 | 1:E:5:PHE:H | 1.37 | 0.86 |
| 1:B:143:ALA:O | 1:B:145:GLN:N | 2.09 | 0.86 |
| 1:D:176:THR:O | 1:D:177:ALA:CB | 2.09 | 0.86 |
| 1:E:129:TYR:O | 1:E:130:SER:HB2 | 1.74 | 0.86 |
| 1:E:87:ILE:CG2 | 1:E:88:GLY:H | 1.88 | 0.85 |
| 1:C:72:THR:HG22 | 1:C:76:THR:H | 1.41 | 0.85 |
| 1:E:101:THR:HG22 | 1:E:103:TYR:CE1 | 2.10 | 0.85 |
| 1:B:22:SER:HA | 1:B:31:THR:HA | 1.59 | 0.85 |
| 1:B:37:ASN:ND2 | 1:B:52:THR:H | 1.74 | 0.85 |
| 1:B:90:TYR:CD2 | 1:B:104:GLY:HA3 | 2.12 | 0.85 |
| 1:C:56:THR:HG22 | 1:C:57:GLY:H | 1.42 | 0.85 |
| 1:D:208:ASN:OD1 | 1:D:208:ASN:N | 2.09 | 0.85 |
| 1:C:49:ALA:O | 1:C:50:SER:C | 2.13 | 0.84 |
| 1:C:74:GLN:CG | 1:F:189:PRO:HB2 | 2.05 | 0.84 |
| 1:C:90:TYR:CD2 | 1:C:104:GLY:HA3 | 2.12 | 0.84 |
| 1:C:110:SER:OG | 1:C:225:LEU:HB2 | 1.77 | 0.84 |
| 1:C:205:THR:HG23 | 1:C:205:THR:O | 1.74 | 0.84 |
| 1:F:16:THR:HG22 | 1:F:17:LEU:N | 1.91 | 0.84 |
| 1:D:39:VAL:HG12 | 1:D:40:LEU:N | 1.92 | 0.84 |
| 1:B:3:ILE:HG22 | 1:B:93:VAL:CB | 2.08 | 0.84 |
| 1:C:73:ALA:HA | 1:F:189:PRO:HG2 | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:119:VAL:O | 1:A:120:VAL:HB | 1.77 | 0.84 |
| 1:B:18:HIS:HB2 | 1:B:21:GLN:OE1 | 1.77 | 0.84 |
| 1:E:92:LEU:HG | 1:E:100:VAL:CG1 | 2.07 | 0.84 |
| 1:E:72:THR:HG22 | 1:E:76:THR:H | 1.42 | 0.84 |
| 1:F:30:PHE:HZ | 1:F:38:LEU:HD21 | 1.43 | 0.84 |
| 1:A:129:TYR:HD2 | 1:A:130:SER:N | 1.76 | 0.84 |
| 1:B:197:THR:HG23 | 1:B:197:THR:O | 1.78 | 0.83 |
| 1:E:127:ILE:CG2 | 1:E:217:PHE:HB3 | 2.07 | 0.83 |
| 1:B:35:ASP:O | 1:B:36:CYS:HB2 | 1.77 | 0.83 |
| 1:A:129:TYR:CD2 | 1:A:130:SER:N | 2.46 | 0.83 |
| 1:D:7:LEU:O | 1:D:8:SER:C | 2.14 | 0.83 |
| 1:B:189:PRO:HG3 | 1:E:74:GLN:HG2 | 1.60 | 0.83 |
| 1:A:195:VAL:CG1 | 1:A:204:TRP:HB3 | 2.08 | 0.83 |
| 1:A:161:ASN:ND2 | 1:A:176:THR:H | 1.77 | 0.83 |
| 1:B:157:GLU:HG3 | 1:B:161:ASN:HB3 | 1.58 | 0.83 |
| 1:C:67:LEU:HD21 | 1:C:82:GLY:HA2 | 1.60 | 0.83 |
| 1:D:150:SER:HB3 | 1:D:151:PRO:HD3 | 1.59 | 0.83 |
| 1:C:2:ASN:OD1 | 1:C:3:ILE:HG22 | 1.76 | 0.83 |
| 1:D:166:ASP:O | 1:D:167:ARG:O | 1.97 | 0.82 |
| 1:B:188:GLN:CG | 1:B:189:PRO:HD3 | 2.10 | 0.82 |
| 1:B:163:VAL:HG21 | 1:B:165:PHE:CE1 | 2.13 | 0.82 |
| 1:F:74:GLN:O | 1:F:76:THR:HG22 | 1.79 | 0.82 |
| 1:A:56:THR:HG22 | 1:A:57:GLY:H | 1.44 | 0.82 |
| 1:D:184:ARG:NH2 | 1:D:200:ASN:HD21 | 1.77 | 0.82 |
| 1:D:217:PHE:CZ | 1:D:225:LEU:HD13 | 2.15 | 0.82 |
| 1:D:63:GLN:NE2 | 1:D:69:VAL:HG22 | 1.95 | 0.81 |
| 1:F:195:VAL:HG13 | 1:F:204:TRP:HB3 | 1.61 | 0.81 |
| 1:A:105:PRO:HB2 | 1:A:210:ARG:HH22 | 1.45 | 0.81 |
| 1:E:72:THR:HB | 1:E:76:THR:HG22 | 1.62 | 0.81 |
| 1:A:22:SER:HB3 | 1:A:31:THR:CG2 | 2.09 | 0.81 |
| 1:B:67:LEU:HD11 | 1:B:84:LYS:HG3 | 1.60 | 0.81 |
| 1:C:18:HIS:HB2 | 1:C:21:GLN:HE21 | 1.43 | 0.81 |
| 1:D:63:GLN:HE22 | 1:D:69:VAL:CG2 | 1.92 | 0.81 |
| 1:C:74:GLN:N | 1:F:189:PRO:CG | 2.43 | 0.81 |
| 1:E:32:MET:CE | 1:E:60:ALA:HB2 | 2.08 | 0.81 |
| 1:D:127:ILE:CG2 | 1:D:147:LEU:HD21 | 2.10 | 0.81 |
| 1:E:150:SER:HB3 | 1:E:151:PRO:HD3 | 1.63 | 0.81 |
| 1:E:17:LEU:HB2 | 1:E:60:ALA:HB3 | 1.59 | 0.81 |
| 1:E:72:THR:CB | 1:E:76:THR:HG22 | 2.11 | 0.81 |
| 1:D:16:THR:HG22 | 1:D:61:VAL:N | 1.92 | 0.80 |
| 1:F:41:PHE:CE2 | 1:F:46:ARG:HG2 | 2.16 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:77:ILE:O | 1:F:77:ILE:HG22 | 1.78 | 0.80 |
| 1:D:63:GLN:HB2 | 1:D:67:LEU:O | 1.81 | 0.80 |
| 1:D:142:HIS:O | 1:D:143:ALA:CB | 2.26 | 0.80 |
| 1:D:16:THR:HG21 | 1:D:61:VAL:HG22 | 1.63 | 0.80 |
| 1:A:131:THR:O | 1:A:131:THR:CG2 | 2.28 | 0.80 |
| 1:B:129:TYR:O | 1:B:130:SER:HB2 | 1.81 | 0.80 |
| 1:E:61:VAL:HG22 | 1:E:62:LEU:N | 1.96 | 0.80 |
| 1:E:129:TYR:O | 1:E:130:SER:CB | 2.28 | 0.80 |
| 1:A:22:SER:HA | 1:A:31:THR:HA | 1.61 | 0.80 |
| 1:C:61:VAL:HG12 | 1:C:62:LEU:N | 1.96 | 0.80 |
| 1:C:152:TYR:CE2 | 1:C:223:ARG:HG3 | 2.16 | 0.80 |
| 1:B:217:PHE:CZ | 1:B:225:LEU:HD13 | 2.17 | 0.80 |
| 1:D:142:HIS:O | 1:D:143:ALA:HB3 | 1.81 | 0.80 |
| 1:D:158:THR:O | 1:D:160:CYS:N | 2.14 | 0.80 |
| 1:E:115:LYS:H | 1:E:115:LYS:HD2 | 1.46 | 0.80 |
| 1:A:200:ASN:HD22 | 1:A:200:ASN:N | 1.75 | 0.79 |
| 1:C:127:ILE:CG2 | 1:C:217:PHE:HB3 | 2.11 | 0.79 |
| 1:A:157:GLU:HG3 | 1:C:26:SER:OG | 1.81 | 0.79 |
| 1:C:89:ASN:H | 1:C:89:ASN:ND2 | 1.80 | 0.79 |
| 1:C:29:ARG:HH21 | 1:C:31:THR:HG21 | 1.47 | 0.79 |
| 1:A:37:ASN:HD21 | 1:A:51:ASN:H | 1.30 | 0.79 |
| 1:E:158:THR:H | 1:F:151:PRO:HG3 | 1.47 | 0.79 |
| 1:B:197:THR:CG2 | 1:B:201:ILE:HB | 2.03 | 0.78 |
| 1:D:70:ILE:O | 1:D:70:ILE:HG22 | 1.82 | 0.78 |
| 1:E:72:THR:HB | 1:E:76:THR:O | 1.84 | 0.78 |
| 1:A:75:ASN:ND2 | 1:D:196:LEU:HD11 | 1.98 | 0.78 |
| 1:B:109:ASP:HB2 | 1:B:111:GLY:H | 1.49 | 0.78 |
| 1:A:129:TYR:HD2 | 1:A:129:TYR:C | 1.87 | 0.78 |
| 1:D:140:THR:OG1 | 1:D:141:LEU:N | 2.16 | 0.78 |
| 1:D:217:PHE:HZ | 1:D:225:LEU:HD13 | 1.47 | 0.78 |
| 1:E:69:VAL:HG21 | 1:E:71:LEU:HG | 1.65 | 0.78 |
| 1:D:39:VAL:HG12 | 1:D:40:LEU:H | 1.49 | 0.78 |
| 1:E:158:THR:N | 1:F:151:PRO:CG | 2.47 | 0.78 |
| 1:B:55:ALA:HB1 | 1:B:56:THR:HG23 | 1.64 | 0.78 |
| 1:E:192:ARG:NH2 | 1:E:194:ASP:OD2 | 2.17 | 0.78 |
| 1:B:151:PRO:CD | 1:D:34:SER:CB | 2.58 | 0.77 |
| 1:C:97:ASP:CB | 1:C:136:ASN:HD22 | 1.97 | 0.77 |
| 1:C:176:THR:O | 1:C:177:ALA:CB | 2.31 | 0.77 |
| 1:F:197:THR:HG21 | 1:F:201:ILE:HD12 | 1.64 | 0.77 |
| 1:D:170:ARG:HG2 | 1:D:170:ARG:NH1 | 1.98 | 0.77 |
| 1:D:77:ILE:O | 1:D:77:ILE:CG2 | 2.32 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:146:SER:HG | 1:C:147:LEU:H | 1.33 | 0.77 |
| 1:F:176:THR:HG21 | 1:F:203:VAL:HG13 | 1.65 | 0.77 |
| 1:F:197:THR:HB | 1:F:201:ILE:HB | 1.66 | 0.77 |
| 1:A:112:THR:O | 1:A:223:ARG:NH1 | 2.18 | 0.77 |
| 1:C:74:GLN:HA | 1:F:189:PRO:HD2 | 1.67 | 0.77 |
| 1:C:167:ARG:O | 1:C:169:ASP:N | 2.17 | 0.77 |
| 1:A:47:VAL:HG12 | 1:A:47:VAL:O | 1.83 | 0.77 |
| 1:D:56:THR:HG22 | 1:D:57:GLY:N | 2.00 | 0.77 |
| 1:A:223:ARG:HH11 | 1:A:223:ARG:HB3 | 1.50 | 0.76 |
| 1:C:73:ALA:HB1 | 1:F:189:PRO:CG | 2.15 | 0.76 |
| 1:D:229:GLY:C | 1:D:230:GLY:O | 2.22 | 0.76 |
| 1:A:5:PHE:HE2 | 1:A:220:GLN:HE21 | 1.31 | 0.76 |
| 1:E:70:ILE:HG13 | 1:E:79:TRP:CE3 | 2.21 | 0.76 |
| 1:E:177:ALA:O | 1:E:179:LYS:HG3 | 1.85 | 0.76 |
| 1:F:217:PHE:C | 1:F:217:PHE:CD2 | 2.56 | 0.76 |
| 1:B:63:GLN:CG | 1:B:64:SER:H | 1.98 | 0.76 |
| 1:A:129:TYR:CD2 | 1:A:129:TYR:C | 2.57 | 0.76 |
| 1:E:12:SER:HB3 | 1:E:221:PRO:CD | 2.15 | 0.76 |
| 1:A:37:ASN:ND2 | 1:A:52:THR:H | 1.83 | 0.76 |
| 1:B:35:ASP:O | 1:B:36:CYS:CB | 2.32 | 0.76 |
| 1:C:83:THR:HG22 | 1:C:84:LYS:H | 1.50 | 0.76 |
| 1:C:92:LEU:HD21 | 1:C:100:VAL:HG13 | 1.68 | 0.76 |
| 1:F:29:ARG:O | 1:F:40:LEU:HD12 | 1.86 | 0.76 |
| 1:B:94:LEU:HB2 | 1:B:100:VAL:HG12 | 1.66 | 0.76 |
| 1:F:42:ASP:O | 1:F:43:SER:HB2 | 1.86 | 0.76 |
| 1:B:72:THR:CG2 | 1:B:74:GLN:HB2 | 2.10 | 0.76 |
| 1:A:39:VAL:HG22 | 1:A:49:ALA:HB1 | 1.68 | 0.75 |
| 1:F:41:PHE:HE2 | 1:F:46:ARG:HG2 | 1.51 | 0.75 |
| 1:A:161:ASN:HD22 | 1:A:176:THR:H | 1.34 | 0.75 |
| 1:E:72:THR:HG21 | 1:E:76:THR:HG22 | 1.67 | 0.75 |
| 1:B:21:GLN:O | 1:B:32:MET:N | 2.14 | 0.75 |
| 1:D:217:PHE:O | 1:D:217:PHE:CD2 | 2.38 | 0.75 |
| 1:D:43:SER:O | 1:D:44:ASP:HB3 | 1.86 | 0.75 |
| 1:E:56:THR:HG22 | 1:E:57:GLY:H | 1.51 | 0.75 |
| 1:B:63:GLN:HG3 | 1:B:64:SER:H | 1.51 | 0.75 |
| 1:F:87:ILE:CG2 | 1:F:88:GLY:N | 2.50 | 0.75 |
| 1:D:150:SER:H | 1:D:152:TYR:H | 1.35 | 0.75 |
| 1:F:101:THR:HG23 | 1:F:102:ILE:N | 2.02 | 0.74 |
| 1:A:119:VAL:HG23 | 1:A:151:PRO:HD3 | 1.69 | 0.74 |
| 1:A:10:GLU:O | 1:A:12:SER:N | 2.19 | 0.74 |
| 1:E:18:HIS:H | 1:E:21:GLN:CG | 2.00 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:61:VAL:HG22 | 1:E:62:LEU:H | 1.50 | 0.74 |
| 1:E:136:ASN:CB | 1:E:136:ASN:HA | 2.14 | 0.74 |
| 1:F:67:LEU:N | 1:F:67:LEU:HD13 | 2.01 | 0.74 |
| 1:E:150:SER:HB3 | 1:E:151:PRO:CD | 2.16 | 0.74 |
| 1:F:161:ASN:HD21 | 1:F:175:ASN:N | 1.86 | 0.74 |
| 1:C:146:SER:O | 1:C:154:LEU:O | 2.05 | 0.74 |
| 1:E:110:SER:OG | 1:E:225:LEU:HB3 | 1.87 | 0.74 |
| 1:E:161:ASN:HB2 | 1:E:176:THR:O | 1.87 | 0.74 |
| 1:E:220:GLN:HB3 | 1:E:222:ASP:OD1 | 1.88 | 0.74 |
| 1:E:170:ARG:HH11 | 1:E:170:ARG:CG | 1.99 | 0.74 |
| 1:A:32:MET:CE | 1:A:60:ALA:HB2 | 2.17 | 0.74 |
| 1:D:63:GLN:HE22 | 1:D:69:VAL:HG22 | 1.49 | 0.74 |
| 1:A:151:PRO:CD | 1:A:152:TYR:H | 2.00 | 0.74 |
| 1:B:37:ASN:HD21 | 1:B:51:ASN:N | 1.86 | 0.74 |
| 1:B:44:ASP:OD1 | 1:B:45:VAL:N | 2.21 | 0.74 |
| 1:B:63:GLN:CG | 1:B:64:SER:N | 2.51 | 0.74 |
| 1:E:143:ALA:HA | 1:E:156:MET:O | 1.88 | 0.73 |
| 1:F:28:PHE:HB3 | 1:F:94:LEU:HD11 | 1.70 | 0.73 |
| 1:A:18:HIS:O | 1:A:20:ALA:N | 2.21 | 0.73 |
| 1:B:25:LEU:O | 1:B:28:PHE:N | 2.21 | 0.73 |
| 1:C:217:PHE:HA | 1:C:227:ILE:HG22 | 1.69 | 0.73 |
| 1:D:217:PHE:HD2 | 1:D:217:PHE:C | 1.90 | 0.73 |
| 1:E:129:TYR:HD1 | 1:E:130:SER:N | 1.86 | 0.73 |
| 1:A:154:LEU:HD22 | 1:A:162:LEU:HD22 | 1.69 | 0.73 |
| 1:C:166:ASP:OD1 | 1:C:166:ASP:O | 2.07 | 0.73 |
| 1:E:19:ALA:O | 1:E:20:ALA:HB2 | 1.89 | 0.73 |
| 1:E:72:THR:CG2 | 1:E:76:THR:HG22 | 2.19 | 0.73 |
| 1:E:87:ILE:CG2 | 1:E:88:GLY:N | 2.50 | 0.73 |
| 1:F:67:LEU:HD13 | 1:F:67:LEU:H | 1.53 | 0.73 |
| 1:C:97:ASP:CB | 1:C:136:ASN:ND2 | 2.52 | 0.73 |
| 1:D:77:ILE:CD1 | 1:D:77:ILE:CB | 2.66 | 0.73 |
| 1:A:196:LEU:CD1 | 1:A:202:ALA:HB2 | 2.18 | 0.73 |
| 1:E:142:HIS:O | 1:E:143:ALA:CB | 2.37 | 0.73 |
| 1:F:129:TYR:CD1 | 1:F:130:SER:N | 2.55 | 0.73 |
| 1:A:127:ILE:CG2 | 1:A:217:PHE:HB3 | 2.19 | 0.72 |
| 1:C:73:ALA:HA | 1:F:189:PRO:HG3 | 1.71 | 0.72 |
| 1:F:204:TRP:CE3 | 1:F:205:THR:N | 2.57 | 0.72 |
| 1:A:210:ARG:HB3 | 1:A:215:TYR:OH | 1.90 | 0.72 |
| 1:D:37:ASN:ND2 | 1:D:38:LEU:H | 1.86 | 0.72 |
| 1:B:30:PHE:HE1 | 1:B:38:LEU:HG | 1.54 | 0.72 |
| 1:E:72:THR:HG23 | 1:E:73:ALA:N | 2.03 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:215:TYR:N | 1:A:215:TYR:CD2 | 2.41 | 0.72 |
| 1:B:78:ARG:HA | 1:B:78:ARG:NE | 1.91 | 0.72 |
| 1:B:220:GLN:CB | 1:B:221:PRO:CD | 2.66 | 0.72 |
| 1:B:199:GLN:O | 1:B:200:ASN:HB2 | 1.89 | 0.72 |
| 1:C:48:TRP:O | 1:C:49:ALA:HB2 | 1.90 | 0.72 |
| 1:F:67:LEU:N | 1:F:67:LEU:CD1 | 2.52 | 0.72 |
| 1:F:90:TYR:CD2 | 1:F:104:GLY:HA3 | 2.24 | 0.72 |
| 1:A:179:LYS:HB3 | 1:A:179:LYS:HZ1 | 1.53 | 0.72 |
| 1:B:30:PHE:CE1 | 1:B:38:LEU:HG | 2.25 | 0.72 |
| 1:D:197:THR:HG21 | 1:D:201:ILE:HB | 1.71 | 0.72 |
| 1:A:18:HIS:O | 1:A:21:GLN:HB2 | 1.90 | 0.72 |
| 1:A:22:SER:HB3 | 1:A:31:THR:CB | 2.20 | 0.71 |
| 1:B:90:TYR:HD2 | 1:B:104:GLY:HA3 | 1.54 | 0.71 |
| 1:C:48:TRP:O | 1:C:49:ALA:CB | 2.38 | 0.71 |
| 1:D:131:THR:HG21 | 1:D:214:ARG:NE | 2.05 | 0.71 |
| 1:E:111:GLY:H | 1:E:224:ASN:HD21 | 1.36 | 0.71 |
| 1:B:77:ILE:HG22 | 1:B:77:ILE:O | 1.90 | 0.71 |
| 1:E:163:VAL:HG21 | 1:E:170:ARG:HG2 | 1.71 | 0.71 |
| 1:F:31:THR:HG23 | 1:F:31:THR:O | 1.90 | 0.71 |
| 1:C:182:GLY:H | 1:C:198:ASN:HB2 | 1.55 | 0.71 |
| 1:F:127:ILE:HG22 | 1:F:147:LEU:HD11 | 1.73 | 0.71 |
| 1:D:64:SER:OG | 1:D:64:SER:HA | 1.90 | 0.71 |
| 1:B:95:GLN:HB3 | 1:B:96:PRO:CD | 2.20 | 0.71 |
| 1:B:189:PRO:CG | 1:E:74:GLN:HG2 | 2.21 | 0.71 |
| 1:F:197:THR:CB | 1:F:201:ILE:HB | 2.20 | 0.71 |
| 1:A:26:SER:OG | 1:C:157:GLU:OE1 | 2.08 | 0.71 |
| 1:E:154:LEU:HD12 | 1:E:154:LEU:O | 1.91 | 0.71 |
| 1:A:63:GLN:HE22 | 1:A:67:LEU:HD13 | 1.56 | 0.70 |
| 1:D:217:PHE:CD2 | 1:D:217:PHE:C | 2.58 | 0.70 |
| 1:A:157:GLU:HG3 | 1:C:26:SER:HG | 1.54 | 0.70 |
| 1:D:8:SER:HA | 1:D:9:HIS:ND1 | 2.06 | 0.70 |
| 1:D:168:ASP:O | 1:D:169:ASP:HB3 | 1.89 | 0.70 |
| 1:E:129:TYR:CD1 | 1:E:130:SER:N | 2.59 | 0.70 |
| 1:C:72:THR:O | 1:C:73:ALA:CB | 2.34 | 0.70 |
| 1:A:69:VAL:HG23 | 1:A:69:VAL:O | 1.91 | 0.70 |
| 1:C:26:SER:O | 1:C:27:SER:CB | 2.25 | 0.70 |
| 1:D:109:ASP:HB2 | 1:D:225:LEU:O | 1.91 | 0.70 |
| 1:E:117:SER:O | 1:E:119:VAL:HG13 | 1.91 | 0.70 |
| 1:A:37:ASN:HD21 | 1:A:51:ASN:N | 1.89 | 0.70 |
| 1:C:77:ILE:HG22 | 1:C:77:ILE:O | 1.92 | 0.70 |
| 1:E:220:GLN:OE1 | 1:E:224:ASN:HB3 | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:149:LEU:HD11 | 1:A:221:PRO:HB3 | 1.72 | 0.70 |
| 1:A:223:ARG:HH11 | 1:A:223:ARG:CG | 2.03 | 0.70 |
| 1:C:89:ASN:ND2 | 1:C:89:ASN:N | 2.40 | 0.70 |
| 1:E:97:ASP:OD1 | 1:E:99:THR:CB | 2.39 | 0.70 |
| 1:A:95:GLN:OE1 | 1:A:103:TYR:OH | 2.08 | 0.69 |
| 1:A:146:SER:O | 1:A:147:LEU:HB2 | 1.92 | 0.69 |
| 1:F:141:LEU:HD12 | 1:F:145:GLN:HB3 | 1.73 | 0.69 |
| 1:E:72:THR:HG21 | 1:E:76:THR:CG2 | 2.22 | 0.69 |
| 1:F:7:LEU:O | 1:F:9:HIS:CA | 2.41 | 0.69 |
| 1:A:10:GLU:O | 1:A:11:GLY:C | 2.28 | 0.69 |
| 1:B:78:ARG:HA | 1:B:78:ARG:HE | 1.56 | 0.69 |
| 1:F:155:SER:O | 1:F:162:LEU:HD23 | 1.92 | 0.69 |
| 1:B:48:TRP:O | 1:B:49:ALA:HB2 | 1.93 | 0.69 |
| 1:D:170:ARG:HH11 | 1:D:170:ARG:CG | 1.97 | 0.69 |
| 1:A:222:ASP:OD1 | 1:A:222:ASP:N | 2.21 | 0.69 |
| 1:B:185:ALA:HA | 1:B:194:ASP:O | 1.93 | 0.69 |
| 1:E:195:VAL:HG12 | 1:E:204:TRP:O | 1.92 | 0.69 |
| 1:C:75:ASN:ND2 | 1:F:188:GLN:HE22 | 1.91 | 0.69 |
| 1:D:77:ILE:CD1 | 1:D:77:ILE:HB | 2.21 | 0.69 |
| 1:A:9:HIS:O | 1:A:11:GLY:N | 2.26 | 0.69 |
| 1:D:93:VAL:HG23 | 1:D:94:LEU:N | 2.07 | 0.69 |
| 1:E:131:THR:C | 1:E:131:THR:CG2 | 2.60 | 0.69 |
| 1:E:18:HIS:H | 1:E:21:GLN:HG2 | 1.58 | 0.68 |
| 1:F:211:SER:OG | 1:F:212:ALA:N | 2.22 | 0.68 |
| 1:B:85:GLY:O | 1:B:86:SER:O | 2.10 | 0.68 |
| 1:D:5:PHE:CE2 | 1:D:220:GLN:HG2 | 2.29 | 0.68 |
| 1:E:26:SER:HG | 1:F:33:GLN:HG3 | 1.57 | 0.68 |
| 1:E:101:THR:CG2 | 1:E:103:TYR:CE1 | 2.76 | 0.68 |
| 1:B:203:VAL:O | 1:B:204:TRP:HB2 | 1.94 | 0.68 |
| 1:C:73:ALA:CB | 1:F:189:PRO:CG | 2.71 | 0.68 |
| 1:D:152:TYR:CB | 1:D:219:LEU:HD21 | 2.24 | 0.68 |
| 1:A:142:HIS:N | 1:A:145:GLN:OE1 | 2.20 | 0.68 |
| 1:C:52:THR:CG2 | 1:C:79:TRP:HB2 | 2.23 | 0.68 |
| 1:C:193:MET:H | 1:C:206:SER:HB3 | 1.57 | 0.68 |
| 1:E:158:THR:H | 1:F:151:PRO:CG | 2.04 | 0.68 |
| 1:E:158:THR:OG1 | 1:F:151:PRO:CD | 2.41 | 0.68 |
| 1:F:30:PHE:CZ | 1:F:38:LEU:HD21 | 2.28 | 0.68 |
| 1:C:53:ALA:O | 1:C:78:ARG:NH2 | 2.25 | 0.68 |
| 1:F:137:HIS:HB3 | 1:F:138:PRO:HA | 1.75 | 0.68 |
| 1:B:107:LEU:O | 1:B:107:LEU:HD12 | 1.94 | 0.68 |
| 1:C:30:PHE:HB2 | 1:C:40:LEU:HB2 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:129:TYR:CE1 | 1:D:131:THR:HB | 2.28 | 0.68 |
| 1:D:137:HIS:HB2 | 1:D:138:PRO:CA | 2.23 | 0.68 |
| 1:E:131:THR:C | 1:E:131:THR:HG22 | 2.15 | 0.68 |
| 1:B:158:THR:OG1 | 1:B:159:ASP:N | 2.22 | 0.68 |
| 1:A:113:SER:HB2 | 1:A:222:ASP:HB2 | 1.75 | 0.68 |
| 1:B:95:GLN:HB3 | 1:B:96:PRO:HD3 | 1.75 | 0.68 |
| 1:D:105:PRO:C | 1:D:106:GLY:O | 2.32 | 0.68 |
| 1:D:52:THR:CG2 | 1:D:79:TRP:HB2 | 2.25 | 0.67 |
| 1:E:106:GLY:HA2 | 1:E:228:TYR:HA | 1.74 | 0.67 |
| 1:A:62:LEU:HD21 | 1:A:90:TYR:CB | 2.24 | 0.67 |
| 1:A:223:ARG:HH11 | 1:A:223:ARG:CB | 2.08 | 0.67 |
| 1:A:229:GLY:HA2 | 1:A:230:GLY:O | 1.93 | 0.67 |
| 1:D:37:ASN:HD22 | 1:D:38:LEU:N | 1.90 | 0.67 |
| 1:D:224:ASN:N | 1:D:224:ASN:HD22 | 1.90 | 0.67 |
| 1:F:94:LEU:O | 1:F:94:LEU:HG | 1.94 | 0.67 |
| 1:B:195:VAL:HG12 | 1:B:195:VAL:O | 1.94 | 0.67 |
| 1:E:115:LYS:H | 1:E:115:LYS:CD | 2.07 | 0.67 |
| 1:F:184:ARG:O | 1:F:185:ALA:HB2 | 1.95 | 0.67 |
| 1:B:71:LEU:HD22 | 1:B:77:ILE:H | 1.59 | 0.67 |
| 1:B:109:ASP:OD1 | 1:B:224:ASN:ND2 | 2.28 | 0.67 |
| 1:C:16:THR:HG22 | 1:C:17:LEU:N | 2.10 | 0.67 |
| 1:D:169:ASP:O | 1:D:169:ASP:OD2 | 2.13 | 0.67 |
| 1:E:25:LEU:O | 1:E:26:SER:C | 2.30 | 0.67 |
| 1:A:72:THR:OG1 | 1:A:73:ALA:N | 2.27 | 0.67 |
| 1:B:129:TYR:HD1 | 1:B:131:THR:H | 1.42 | 0.67 |
| 1:F:176:THR:HG21 | 1:F:203:VAL:CG1 | 2.25 | 0.67 |
| 1:F:215:TYR:CD1 | 1:F:227:ILE:HD11 | 2.30 | 0.67 |
| 1:A:18:HIS:HB2 | 1:A:21:GLN:OE1 | 1.94 | 0.67 |
| 1:B:70:ILE:O | 1:B:70:ILE:HG22 | 1.92 | 0.67 |
| 1:C:72:THR:HG21 | 1:C:76:THR:OG1 | 1.95 | 0.67 |
| 1:D:37:ASN:HD21 | 1:D:51:ASN:H | 1.43 | 0.67 |
| 1:D:197:THR:HG22 | 1:D:199:GLN:H | 1.60 | 0.67 |
| 1:F:161:ASN:HD21 | 1:F:175:ASN:H | 1.42 | 0.67 |
| 1:A:75:ASN:HD21 | 1:D:196:LEU:HD21 | 1.60 | 0.67 |
| 1:B:195:VAL:O | 1:B:195:VAL:CG1 | 2.42 | 0.67 |
| 1:C:56:THR:CG2 | 1:C:57:GLY:H | 2.04 | 0.67 |
| 1:F:28:PHE:O | 1:F:29:ARG:HB2 | 1.95 | 0.67 |
| 1:B:146:SER:OG | 1:B:155:SER:HB2 | 1.95 | 0.66 |
| 1:B:222:ASP:CB | 1:B:224:ASN:OD1 | 2.41 | 0.66 |
| 1:C:137:HIS:N | 1:C:137:HIS:CD2 | 2.59 | 0.66 |
| 1:A:32:MET:HE2 | 1:A:60:ALA:CB | 2.23 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:70:ILE:O | 1:D:70:ILE:CG2 | 2.43 | 0.66 |
| 1:D:72:THR:HG22 | 1:D:74:GLN:HB2 | 1.77 | 0.66 |
| 1:F:23:LEU:HB2 | 1:F:30:PHE:O | 1.96 | 0.66 |
| 1:B:154:LEU:HG | 1:B:225:LEU:CD1 | 2.24 | 0.66 |
| 1:D:141:LEU:O | 1:D:185:ALA:HB3 | 1.94 | 0.66 |
| 1:E:39:VAL:HG12 | 1:E:40:LEU:N | 2.08 | 0.66 |
| 1:A:179:LYS:NZ | 1:A:179:LYS:CB | 2.56 | 0.66 |
| 1:F:158:THR:O | 1:F:159:ASP:C | 2.34 | 0.66 |
| 1:A:7:LEU:HD11 | 1:A:61:VAL:HG13 | 1.78 | 0.66 |
| 1:E:58:CYS:HA | 1:E:71:LEU:O | 1.95 | 0.66 |
| 1:A:72:THR:O | 1:A:75:ASN:N | 2.23 | 0.66 |
| 1:B:9:HIS:CD2 | 1:B:10:GLU:HB2 | 2.31 | 0.66 |
| 1:D:201:ILE:HG22 | 1:D:201:ILE:O | 1.94 | 0.66 |
| 1:E:26:SER:OG | 1:F:33:GLN:CG | 2.37 | 0.66 |
| 1:C:155:SER:N | 1:C:163:VAL:O | 2.25 | 0.66 |
| 1:E:100:VAL:O | 1:E:235:THR:HG22 | 1.96 | 0.66 |
| 1:C:2:ASN:HD21 | 1:C:125:ASN:ND2 | 1.93 | 0.66 |
| 1:C:220:GLN:OE1 | 1:C:224:ASN:HB3 | 1.95 | 0.66 |
| 1:D:42:ASP:O | 1:D:43:SER:HB2 | 1.95 | 0.66 |
| 1:D:162:LEU:HB2 | 1:D:174:THR:OG1 | 1.96 | 0.66 |
| 1:E:72:THR:CG2 | 1:E:76:THR:H | 2.09 | 0.66 |
| 1:A:22:SER:HB3 | 1:A:31:THR:HB | 1.78 | 0.66 |
| 1:A:63:GLN:NE2 | 1:A:67:LEU:HD13 | 2.10 | 0.66 |
| 1:B:216:VAL:HG22 | 1:B:217:PHE:H | 1.61 | 0.66 |
| 1:F:143:ALA:HA | 1:F:156:MET:O | 1.95 | 0.66 |
| 1:C:72:THR:HG23 | 1:C:73:ALA:C | 2.17 | 0.65 |
| 1:C:130:SER:HA | 1:C:139:GLN:HG3 | 1.79 | 0.65 |
| 1:F:149:LEU:O | 1:F:150:SER:CB | 2.43 | 0.65 |
| 1:B:202:ALA:O | 1:B:203:VAL:HB | 1.96 | 0.65 |
| 1:F:129:TYR:HE1 | 1:F:131:THR:N | 1.94 | 0.65 |
| 1:E:158:THR:C | 1:F:151:PRO:HG3 | 2.15 | 0.65 |
| 1:E:194:ASP:HB3 | 1:E:196:LEU:HD13 | 1.78 | 0.65 |
| 1:D:150:SER:CB | 1:D:151:PRO:CD | 2.74 | 0.65 |
| 1:D:165:PHE:HB3 | 1:D:169:ASP:H | 1.62 | 0.65 |
| 1:A:62:LEU:CD2 | 1:A:90:TYR:HB2 | 2.25 | 0.65 |
| 1:A:86:SER:O | 1:A:87:ILE:CG1 | 2.45 | 0.65 |
| 1:B:95:GLN:CB | 1:B:96:PRO:CD | 2.73 | 0.65 |
| 1:C:110:SER:HB2 | 1:C:112:THR:HG23 | 1.78 | 0.65 |
| 1:D:137:HIS:ND1 | 1:D:137:HIS:N | 2.42 | 0.65 |
| 1:E:219:LEU:HD13 | 1:E:225:LEU:CD2 | 2.27 | 0.65 |
| 1:F:129:TYR:HD1 | 1:F:129:TYR:C | 1.94 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:161:ASN:HD21 | 1:F:176:THR:H | 1.42 | 0.65 |
| 1:C:72:THR:HG22 | 1:C:76:THR:N | 2.05 | 0.65 |
| 1:E:22:SER:HA | 1:E:31:THR:HA | 1.78 | 0.65 |
| 1:E:61:VAL:HG12 | 1:E:69:VAL:HG22 | 1.78 | 0.65 |
| 1:B:92:LEU:HB2 | 1:B:102:ILE:HG13 | 1.78 | 0.65 |
| 1:C:65:ASP:C | 1:C:65:ASP:OD1 | 2.33 | 0.65 |
| 1:C:197:THR:HG21 | 1:C:199:GLN:OE1 | 1.97 | 0.65 |
| 1:E:100:VAL:H | 1:E:235:THR:HG21 | 1.61 | 0.65 |
| 1:B:100:VAL:O | 1:B:101:THR:OG1 | 2.12 | 0.65 |
| 1:B:142:HIS:O | 1:B:143:ALA:CB | 2.43 | 0.65 |
| 1:C:52:THR:O | 1:C:78:ARG:NH1 | 2.29 | 0.65 |
| 1:E:219:LEU:HD13 | 1:E:225:LEU:HD23 | 1.79 | 0.65 |
| 1:F:129:TYR:OH | 1:F:131:THR:CB | 2.44 | 0.65 |
| 1:A:12:SER:CB | 1:A:221:PRO:HD2 | 2.22 | 0.65 |
| 1:D:44:ASP:O | 1:D:45:VAL:CB | 2.43 | 0.65 |
| 1:D:97:ASP:OD1 | 1:D:97:ASP:N | 2.30 | 0.65 |
| 1:A:37:ASN:HB2 | 1:A:53:ALA:HB2 | 1.78 | 0.64 |
| 1:B:217:PHE:CG | 1:B:217:PHE:O | 2.45 | 0.64 |
| 1:D:42:ASP:O | 1:D:44:ASP:N | 2.30 | 0.64 |
| 1:E:165:PHE:HE2 | 1:E:170:ARG:HG3 | 1.62 | 0.64 |
| 1:F:154:LEU:CD2 | 1:F:225:LEU:HD21 | 2.27 | 0.64 |
| 1:A:195:VAL:HG11 | 1:A:204:TRP:HB3 | 1.78 | 0.64 |
| 1:C:210:ARG:HB2 | 1:C:215:TYR:OH | 1.96 | 0.64 |
| 1:E:181:THR:O | 1:E:182:GLY:C | 2.34 | 0.64 |
| 1:E:72:THR:HG23 | 1:E:73:ALA:HB3 | 1.79 | 0.64 |
| 1:F:185:ALA:HA | 1:F:194:ASP:O | 1.96 | 0.64 |
| 1:A:26:SER:O | 1:A:27:SER:CB | 2.41 | 0.64 |
| 1:B:82:GLY:O | 1:B:83:THR:C | 2.36 | 0.64 |
| 1:B:148:GLN:HA | 1:B:153:ARG:HA | 1.79 | 0.64 |
| 1:B:228:TYR:N | 1:B:228:TYR:CD2 | 2.66 | 0.64 |
| 1:F:204:TRP:CD2 | 1:F:205:THR:N | 2.66 | 0.64 |
| 1:B:154:LEU:CD2 | 1:B:225:LEU:HD11 | 2.28 | 0.64 |
| 1:C:59:ARG:HH12 | 1:F:184:ARG:NH2 | 1.95 | 0.64 |
| 1:D:32:MET:HE2 | 1:D:38:LEU:HB2 | 1.78 | 0.64 |
| 1:F:190:ASN:OD1 | 1:F:190:ASN:O | 2.15 | 0.64 |
| 1:B:163:VAL:HG21 | 1:B:165:PHE:CZ | 2.32 | 0.64 |
| 1:C:127:ILE:HG22 | 1:C:217:PHE:HB3 | 1.80 | 0.64 |
| 1:C:152:TYR:CD2 | 1:C:223:ARG:HG3 | 2.32 | 0.64 |
| 1:D:150:SER:CB | 1:D:151:PRO:HD3 | 2.28 | 0.64 |
| 1:E:127:ILE:HG21 | 1:E:217:PHE:HB3 | 1.79 | 0.64 |
| 1:F:193:MET:HB3 | 1:F:206:SER:HB3 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:39:VAL:HG12 | 1:A:41:PHE:CE1 | 2.31 | 0.64 |
| 1:A:110:SER:OG | 1:A:225:LEU:HB2 | 1.97 | 0.64 |
| 1:B:26:SER:O | 1:B:27:SER:CB | 2.46 | 0.64 |
| 1:C:162:LEU:O | 1:C:173:SER:OG | 2.16 | 0.64 |
| 1:D:9:HIS:HA | 1:D:15:GLN:HE22 | 1.62 | 0.64 |
| 1:D:153:ARG:HG3 | 1:D:153:ARG:O | 1.95 | 0.64 |
| 1:E:119:VAL:HG21 | 1:E:151:PRO:HD3 | 1.78 | 0.64 |
| 1:E:142:HIS:O | 1:E:143:ALA:HB3 | 1.97 | 0.64 |
| 1:C:4:LEU:CD1 | 1:C:14:PRO:HB2 | 2.28 | 0.64 |
| 1:E:77:ILE:HG22 | 1:E:77:ILE:O | 1.97 | 0.64 |
| 1:F:40:LEU:HB3 | 1:F:48:TRP:H | 1.61 | 0.64 |
| 1:A:17:LEU:O | 1:A:59:ARG:HB2 | 1.98 | 0.64 |
| 1:A:26:SER:O | 1:A:27:SER:HB3 | 1.96 | 0.64 |
| 1:C:7:LEU:CD1 | 1:C:61:VAL:CG1 | 2.76 | 0.64 |
| 1:C:222:ASP:N | 1:C:222:ASP:OD1 | 2.29 | 0.64 |
| 1:D:101:THR:OG1 | 1:D:234:THR:HA | 1.98 | 0.64 |
| 1:D:217:PHE:CZ | 1:D:225:LEU:HD22 | 2.33 | 0.64 |
| 1:F:7:LEU:HA | 1:F:15:GLN:HG2 | 1.79 | 0.64 |
| 1:F:58:CYS:HA | 1:F:71:LEU:O | 1.97 | 0.64 |
| 1:C:4:LEU:CD2 | 1:C:17:LEU:HD23 | 2.24 | 0.63 |
| 1:D:6:GLY:HA3 | 1:D:62:LEU:HD23 | 1.80 | 0.63 |
| 1:D:233:TRP:CH2 | 1:D:235:THR:HG23 | 2.33 | 0.63 |
| 1:E:32:MET:HG2 | 1:E:60:ALA:CB | 2.28 | 0.63 |
| 1:E:195:VAL:HG11 | 1:E:204:TRP:HB3 | 1.79 | 0.63 |
| 1:E:195:VAL:HG13 | 1:E:195:VAL:O | 1.97 | 0.63 |
| 1:C:188:GLN:O | 1:C:191:GLY:N | 2.31 | 0.63 |
| 1:E:4:LEU:HD12 | 1:E:4:LEU:C | 2.15 | 0.63 |
| 1:F:30:PHE:HA | 1:F:39:VAL:O | 1.98 | 0.63 |
| 1:F:31:THR:HG22 | 1:F:39:VAL:O | 1.99 | 0.63 |
| 1:A:44:ASP:O | 1:A:45:VAL:O | 2.17 | 0.63 |
| 1:A:191:GLY:HA3 | 1:A:215:TYR:CD1 | 2.33 | 0.63 |
| 1:B:109:ASP:CB | 1:B:111:GLY:H | 2.10 | 0.63 |
| 1:B:143:ALA:O | 1:B:144:THR:C | 2.36 | 0.63 |
| 1:D:157:GLU:HB2 | 1:D:161:ASN:O | 1.99 | 0.63 |
| 1:E:150:SER:CB | 1:E:151:PRO:CD | 2.73 | 0.63 |
| 1:F:188:GLN:HE21 | 1:F:189:PRO:HD2 | 1.62 | 0.63 |
| 1:F:229:GLY:C | 1:F:230:GLY:O | 2.31 | 0.63 |
| 1:C:97:ASP:CG | 1:C:136:ASN:ND2 | 2.52 | 0.63 |
| 1:D:143:ALA:C | 1:D:145:GLN:H | 2.02 | 0.63 |
| 1:B:217:PHE:CD1 | 1:B:217:PHE:C | 2.67 | 0.63 |
| 1:C:47:VAL:HG12 | 1:C:47:VAL:O | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:169:ASP:OD2 | 1:F:169:ASP:C | 2.37 | 0.63 |
| 1:F:215:TYR:CE1 | 1:F:229:GLY:HA3 | 2.34 | 0.63 |
| 1:F:223:ARG:HH11 | 1:F:223:ARG:HB3 | 1.63 | 0.63 |
| 1:B:30:PHE:CD1 | 1:B:30:PHE:C | 2.65 | 0.63 |
| 1:F:223:ARG:HH11 | 1:F:223:ARG:CB | 2.12 | 0.63 |
| 1:A:74:GLN:HE21 | 1:D:189:PRO:HG3 | 1.64 | 0.62 |
| 1:C:156:MET:O | 1:C:157:GLU:O | 2.17 | 0.62 |
| 1:E:69:VAL:HG23 | 1:E:71:LEU:N | 2.14 | 0.62 |
| 1:D:152:TYR:HB3 | 1:D:219:LEU:HD21 | 1.79 | 0.62 |
| 1:F:137:HIS:HB3 | 1:F:138:PRO:CA | 2.28 | 0.62 |
| 1:C:162:LEU:HB3 | 1:C:174:THR:HG23 | 1.80 | 0.62 |
| 1:D:27:SER:HB2 | 1:D:28:PHE:CD2 | 2.34 | 0.62 |
| 1:F:127:ILE:HG22 | 1:F:147:LEU:CD1 | 2.29 | 0.62 |
| 1:A:29:ARG:HE | 1:A:31:THR:CG2 | 2.13 | 0.62 |
| 1:B:28:PHE:HE2 | 1:B:98:ARG:HG3 | 1.63 | 0.62 |
| 1:B:34:SER:OG | 1:D:151:PRO:CD | 2.48 | 0.62 |
| 1:E:37:ASN:OD1 | 1:E:51:ASN:N | 2.30 | 0.62 |
| 1:E:188:GLN:HG3 | 1:E:189:PRO:HD2 | 1.82 | 0.62 |
| 1:A:127:ILE:HG21 | 1:A:217:PHE:HB3 | 1.81 | 0.62 |
| 1:A:157:GLU:CG | 1:C:26:SER:OG | 2.47 | 0.62 |
| 1:B:12:SER:OG | 1:B:222:ASP:OD1 | 2.08 | 0.62 |
| 1:B:146:SER:O | 1:B:147:LEU:CB | 2.29 | 0.62 |
| 1:F:217:PHE:HZ | 1:F:225:LEU:CD2 | 2.13 | 0.62 |
| 1:B:37:ASN:OD1 | 1:B:49:ALA:HB1 | 2.00 | 0.62 |
| 1:C:7:LEU:CD1 | 1:C:61:VAL:HG11 | 2.19 | 0.62 |
| 1:D:70:ILE:HG21 | 1:D:79:TRP:HB3 | 1.82 | 0.62 |
| 1:D:226:ALA:HB3 | 1:D:228:TYR:CE2 | 2.35 | 0.62 |
| 1:E:101:THR:HG22 | 1:E:103:TYR:CD1 | 2.34 | 0.62 |
| 1:D:38:LEU:O | 1:D:49:ALA:HA | 2.00 | 0.62 |
| 1:B:18:HIS:O | 1:B:32:MET:HB3 | 1.99 | 0.62 |
| 1:C:157:GLU:HB3 | 1:C:159:ASP:OD1 | 2.00 | 0.62 |
| 1:F:91:VAL:O | 1:F:102:ILE:HG23 | 2.00 | 0.62 |
| 1:F:102:ILE:HG22 | 1:F:103:TYR:N | 2.16 | 0.61 |
| 1:D:128:LEU:O | 1:D:129:TYR:CB | 2.47 | 0.61 |
| 1:C:90:TYR:CE2 | 1:C:104:GLY:HA3 | 2.35 | 0.61 |
| 1:C:216:VAL:O | 1:C:227:ILE:HG22 | 2.01 | 0.61 |
| 1:D:129:TYR:HD1 | 1:D:130:SER:N | 1.98 | 0.61 |
| 1:E:112:THR:OG1 | 1:E:223:ARG:O | 2.13 | 0.61 |
| 1:E:195:VAL:CG1 | 1:E:204:TRP:HB3 | 2.30 | 0.61 |
| 1:F:156:MET:SD | 1:F:185:ALA:HB2 | 2.41 | 0.61 |
| 1:D:130:SER:O | 1:D:131:THR:OG1 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:16:THR:CG2 | 1:D:61:VAL:N | 2.57 | 0.61 |
| 1:D:63:GLN:HE22 | 1:D:69:VAL:HG21 | 1.66 | 0.61 |
| 1:D:161:ASN:HA | 1:D:176:THR:HG21 | 1.79 | 0.61 |
| 1:E:92:LEU:CG | 1:E:100:VAL:HG11 | 2.31 | 0.61 |
| 1:A:56:THR:CG2 | 1:A:57:GLY:H | 2.12 | 0.61 |
| 1:A:75:ASN:HD22 | 1:D:196:LEU:HD11 | 1.64 | 0.61 |
| 1:E:234:THR:OG1 | 1:E:235:THR:N | 2.33 | 0.61 |
| 1:F:154:LEU:HD23 | 1:F:225:LEU:HD21 | 1.81 | 0.61 |
| 1:A:4:LEU:C | 1:A:4:LEU:CD2 | 2.68 | 0.61 |
| 1:A:131:THR:CB | 1:A:131:THR:HG1 | 2.07 | 0.61 |
| 1:B:30:PHE:C | 1:B:30:PHE:HD1 | 2.02 | 0.61 |
| 1:C:127:ILE:O | 1:C:127:ILE:HG23 | 2.00 | 0.61 |
| 1:E:158:THR:H | 1:F:151:PRO:HD3 | 1.65 | 0.61 |
| 1:B:129:TYR:O | 1:B:130:SER:CB | 2.49 | 0.61 |
| 1:C:193:MET:H | 1:C:206:SER:CB | 2.14 | 0.61 |
| 1:E:162:LEU:HB3 | 1:E:174:THR:CG2 | 2.31 | 0.61 |
| 1:F:142:HIS:O | 1:F:156:MET:HB3 | 2.00 | 0.61 |
| 1:B:35:ASP:OD2 | 1:B:53:ALA:HB1 | 2.00 | 0.60 |
| 1:B:217:PHE:HZ | 1:B:225:LEU:CD1 | 2.10 | 0.60 |
| 1:D:92:LEU:HA | 1:D:102:ILE:HG13 | 1.82 | 0.60 |
| 1:A:163:VAL:HG23 | 1:A:164:LEU:N | 2.16 | 0.60 |
| 1:B:186:VAL:O | 1:B:194:ASP:HB2 | 2.01 | 0.60 |
| 1:E:109:ASP:HA | 1:E:225:LEU:O | 2.00 | 0.60 |
| 1:B:109:ASP:OD2 | 1:B:109:ASP:N | 2.33 | 0.60 |
| 1:D:32:MET:CE | 1:D:38:LEU:HB2 | 2.32 | 0.60 |
| 1:D:101:THR:HG23 | 1:D:102:ILE:N | 2.16 | 0.60 |
| 1:E:215:TYR:CE1 | 1:E:229:GLY:HA2 | 2.36 | 0.60 |
| 1:F:67:LEU:HD11 | 1:F:84:LYS:HB3 | 1.82 | 0.60 |
| 1:F:220:GLN:NE2 | 1:F:228:TYR:OH | 2.33 | 0.60 |
| 1:D:100:VAL:O | 1:D:101:THR:OG1 | 2.15 | 0.60 |
| 1:D:147:LEU:O | 1:D:153:ARG:HA | 2.00 | 0.60 |
| 1:A:110:SER:HG | 1:A:225:LEU:HB2 | 1.66 | 0.60 |
| 1:D:107:LEU:HD11 | 1:D:209:SER:HA | 1.84 | 0.60 |
| 1:D:159:ASP:O | 1:D:177:ALA:HA | 2.02 | 0.60 |
| 1:F:166:ASP:O | 1:F:167:ARG:C | 2.35 | 0.60 |
| 1:A:154:LEU:HD23 | 1:A:163:VAL:O | 2.01 | 0.60 |
| 1:D:36:CYS:SG | 1:D:55:ALA:HB3 | 2.42 | 0.60 |
| 1:D:42:ASP:O | 1:D:43:SER:CB | 2.49 | 0.60 |
| 1:D:153:ARG:NH2 | 1:D:165:PHE:CE1 | 2.70 | 0.60 |
| 1:A:156:MET:HE3 | 1:A:156:MET:HA | 1.82 | 0.60 |
| 1:D:187:LEU:HD13 | 1:D:227:ILE:HD12 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:193:MET:H | 1:E:206:SER:HB3 | 1.66 | 0.60 |
| 1:C:33:GLN:NE2 | 1:C:35:ASP:OD1 | 2.34 | 0.60 |
| 1:D:64:SER:CB | 1:D:64:SER:HG | 2.10 | 0.60 |
| 1:E:27:SER:HB2 | 1:F:34:SER:OG | 2.01 | 0.60 |
| 1:E:119:VAL:CG2 | 1:E:151:PRO:HD3 | 2.32 | 0.60 |
| 1:B:192:ARG:HA | 1:B:206:SER:OG | 2.02 | 0.60 |
| 1:F:63:GLN:HE21 | 1:F:69:VAL:HG21 | 1.65 | 0.60 |
| 1:F:129:TYR:HE1 | 1:F:131:THR:H | 1.48 | 0.60 |
| 1:A:200:ASN:N | 1:A:200:ASN:ND2 | 2.48 | 0.60 |
| 1:C:195:VAL:HG13 | 1:C:204:TRP:HB3 | 1.83 | 0.60 |
| 1:D:167:ARG:O | 1:D:168:ASP:C | 2.38 | 0.60 |
| 1:D:197:THR:HB | 1:D:201:ILE:HB | 1.83 | 0.60 |
| 1:E:72:THR:CG2 | 1:E:73:ALA:N | 2.64 | 0.60 |
| 1:E:116:GLY:O | 1:E:118:VAL:HG23 | 2.02 | 0.60 |
| 1:F:141:LEU:CD1 | 1:F:145:GLN:HB3 | 2.31 | 0.60 |
| 1:F:188:GLN:HB3 | 1:F:192:ARG:H | 1.66 | 0.60 |
| 1:B:9:HIS:HD2 | 1:B:10:GLU:HB2 | 1.65 | 0.59 |
| 1:B:148:GLN:HB3 | 1:B:153:ARG:HB3 | 1.85 | 0.59 |
| 1:E:162:LEU:HB3 | 1:E:174:THR:HG21 | 1.84 | 0.59 |
| 1:B:183:CYS:HA | 1:B:196:LEU:O | 2.02 | 0.59 |
| 1:C:72:THR:HG23 | 1:C:73:ALA:O | 2.02 | 0.59 |
| 1:D:128:LEU:O | 1:D:129:TYR:CG | 2.55 | 0.59 |
| 1:E:158:THR:H | 1:F:151:PRO:CD | 2.15 | 0.59 |
| 1:D:44:ASP:O | 1:D:45:VAL:HB | 2.02 | 0.59 |
| 1:D:112:THR:O | 1:D:223:ARG:NH1 | 2.30 | 0.59 |
| 1:F:187:LEU:HD11 | 1:F:227:ILE:HD12 | 1.82 | 0.59 |
| 1:A:104:GLY:C | 1:A:105:PRO:O | 2.39 | 0.59 |
| 1:B:60:ALA:HB2 | 1:B:70:ILE:CD1 | 2.32 | 0.59 |
| 1:C:56:THR:HG22 | 1:C:57:GLY:N | 2.17 | 0.59 |
| 1:E:63:GLN:HB2 | 1:E:67:LEU:H | 1.66 | 0.59 |
| 1:D:153:ARG:NH2 | 1:D:165:PHE:HE1 | 2.00 | 0.59 |
| 1:D:137:HIS:HB2 | 1:D:138:PRO:HA | 1.82 | 0.59 |
| 1:D:197:THR:HG22 | 1:D:199:GLN:O | 2.03 | 0.59 |
| 1:F:59:ARG:O | 1:F:70:ILE:HA | 2.01 | 0.59 |
| 1:F:63:GLN:HB2 | 1:F:67:LEU:O | 2.03 | 0.59 |
| 1:B:70:ILE:O | 1:B:78:ARG:N | 2.35 | 0.59 |
| 1:D:71:LEU:HD21 | 1:D:77:ILE:HG13 | 1.83 | 0.59 |
| 1:E:9:HIS:HB2 | 1:E:10:GLU:CG | 2.26 | 0.59 |
| 1:F:217:PHE:CZ | 1:F:225:LEU:HD23 | 2.37 | 0.59 |
| 1:A:161:ASN:HD21 | 1:A:175:ASN:H | 1.50 | 0.59 |
| 1:B:37:ASN:HD21 | 1:B:51:ASN:H | 1.48 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:215:TYR:CD1 | 1:C:229:GLY:HA2 | 2.38 | 0.59 |
| 1:D:84:LYS:O | 1:D:84:LYS:HG3 | 2.02 | 0.59 |
| 1:D:95:GLN:HB2 | 1:D:99:THR:O | 2.03 | 0.59 |
| 1:D:174:THR:HG22 | 1:D:174:THR:O | 2.02 | 0.59 |
| 1:F:2:ASN:O | 1:F:93:VAL:HG23 | 2.03 | 0.59 |
| 1:A:90:TYR:N | 1:A:90:TYR:CD1 | 2.69 | 0.59 |
| 1:B:168:ASP:O | 1:B:169:ASP:HB3 | 2.03 | 0.59 |
| 1:C:188:GLN:O | 1:C:190:ASN:N | 2.36 | 0.59 |
| 1:D:165:PHE:HD2 | 1:D:170:ARG:HA | 1.66 | 0.59 |
| 1:D:182:GLY:HA3 | 1:D:198:ASN:H | 1.67 | 0.59 |
| 1:A:52:THR:HG21 | 1:A:79:TRP:HB2 | 1.83 | 0.59 |
| 1:A:120:VAL:HG22 | 1:A:122:ASN:O | 2.03 | 0.59 |
| 1:E:92:LEU:CG | 1:E:100:VAL:CG1 | 2.81 | 0.59 |
| 1:B:3:ILE:HG22 | 1:B:93:VAL:CG1 | 2.32 | 0.58 |
| 1:F:2:ASN:HA | 1:F:23:LEU:CD2 | 2.32 | 0.58 |
| 1:E:39:VAL:CG1 | 1:E:40:LEU:N | 2.66 | 0.58 |
| 1:F:126:SER:O | 1:F:147:LEU:CD1 | 2.42 | 0.58 |
| 1:A:101:THR:HG22 | 1:A:103:TYR:CZ | 2.39 | 0.58 |
| 1:A:210:ARG:O | 1:A:211:SER:C | 2.40 | 0.58 |
| 1:B:106:GLY:O | 1:B:107:LEU:HB3 | 2.02 | 0.58 |
| 1:B:171:VAL:HB | 1:B:223:ARG:HH12 | 1.69 | 0.58 |
| 1:D:32:MET:HE1 | 1:D:70:ILE:HD11 | 1.85 | 0.58 |
| 1:E:92:LEU:HG | 1:E:100:VAL:HG11 | 1.83 | 0.58 |
| 1:E:70:ILE:HG13 | 1:E:79:TRP:HE3 | 1.64 | 0.58 |
| 1:F:25:LEU:O | 1:F:28:PHE:HB2 | 2.04 | 0.58 |
| 1:B:48:TRP:CG | 1:B:49:ALA:N | 2.69 | 0.58 |
| 1:A:58:CYS:HA | 1:A:71:LEU:O | 2.03 | 0.58 |
| 1:A:104:GLY:HA2 | 1:A:105:PRO:O | 2.04 | 0.58 |
| 1:C:30:PHE:HB2 | 1:C:40:LEU:HA | 1.85 | 0.58 |
| 1:D:16:THR:HG22 | 1:D:17:LEU:N | 2.17 | 0.58 |
| 1:E:92:LEU:HD11 | 1:E:100:VAL:HG11 | 1.84 | 0.58 |
| 1:A:108:TRP:HB2 | 1:A:208:ASN:HD21 | 1.63 | 0.58 |
| 1:B:183:CYS:HB3 | 1:B:196:LEU:O | 2.04 | 0.58 |
| 1:C:64:SER:O | 1:C:87:ILE:O | 2.21 | 0.58 |
| 1:D:129:TYR:HD2 | 1:D:215:TYR:O | 1.86 | 0.58 |
| 1:E:163:VAL:CG2 | 1:E:170:ARG:HG2 | 2.33 | 0.58 |
| 1:A:64:SER:O | 1:A:87:ILE:O | 2.22 | 0.58 |
| 1:B:42:ASP:O | 1:B:43:SER:HB2 | 2.03 | 0.58 |
| 1:E:170:ARG:HH11 | 1:E:170:ARG:CB | 2.17 | 0.58 |
| 1:A:220:GLN:HG2 | 1:A:221:PRO:HD3 | 1.86 | 0.58 |
| 1:C:4:LEU:HD12 | 1:C:5:PHE:N | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:32:MET:HG2 | 1:E:60:ALA:HB3 | 1.85 | 0.58 |
| 1:E:219:LEU:CD1 | 1:E:225:LEU:HD23 | 2.34 | 0.58 |
| 1:F:142:HIS:CD2 | 1:F:145:GLN:OE1 | 2.56 | 0.58 |
| 1:F:162:LEU:HD11 | 1:F:193:MET:CE | 2.34 | 0.58 |
| 1:D:5:PHE:HZ | 1:D:220:GLN:HG2 | 1.63 | 0.58 |
| 1:E:59:ARG:O | 1:E:71:LEU:N | 2.36 | 0.58 |
| 1:E:69:VAL:O | 1:E:69:VAL:CG2 | 2.52 | 0.58 |
| 1:B:192:ARG:C | 1:B:193:MET:O | 2.41 | 0.57 |
| 1:D:204:TRP:CG | 1:D:205:THR:N | 2.70 | 0.57 |
| 1:A:161:ASN:HD21 | 1:A:175:ASN:N | 2.02 | 0.57 |
| 1:D:37:ASN:ND2 | 1:D:38:LEU:N | 2.51 | 0.57 |
| 1:D:204:TRP:CE3 | 1:D:205:THR:HA | 2.39 | 0.57 |
| 1:E:119:VAL:O | 1:E:120:VAL:HB | 2.03 | 0.57 |
| 1:E:157:GLU:HG2 | 1:F:150:SER:OG | 2.04 | 0.57 |
| 1:F:128:LEU:HB3 | 1:F:129:TYR:CD2 | 2.39 | 0.57 |
| 1:A:167:ARG:O | 1:A:169:ASP:N | 2.37 | 0.57 |
| 1:F:197:THR:O | 1:F:199:GLN:N | 2.38 | 0.57 |
| 1:C:4:LEU:HD22 | 1:C:17:LEU:CD2 | 2.27 | 0.57 |
| 1:D:3:ILE:CG2 | 1:D:93:VAL:HB | 2.31 | 0.57 |
| 1:E:92:LEU:CD1 | 1:E:100:VAL:HG11 | 2.34 | 0.57 |
| 1:E:161:ASN:ND2 | 1:E:176:THR:H | 2.01 | 0.57 |
| 1:C:41:PHE:HA | 1:C:45:VAL:O | 2.05 | 0.57 |
| 1:D:154:LEU:CG | 1:D:225:LEU:HD11 | 2.35 | 0.57 |
| 1:D:156:MET:O | 1:D:157:GLU:O | 2.22 | 0.57 |
| 1:E:128:LEU:O | 1:E:129:TYR:C | 2.38 | 0.57 |
| 1:A:127:ILE:O | 1:A:127:ILE:CG2 | 2.47 | 0.57 |
| 1:A:220:GLN:HB2 | 1:A:224:ASN:HB3 | 1.86 | 0.57 |
| 1:C:80:SER:OG | 1:C:81:SER:N | 2.37 | 0.57 |
| 1:C:89:ASN:H | 1:C:89:ASN:HD22 | 1.51 | 0.57 |
| 1:D:137:HIS:CB | 1:D:138:PRO:CA | 2.83 | 0.57 |
| 1:A:152:TYR:CD2 | 1:A:223:ARG:HG3 | 2.40 | 0.57 |
| 1:C:67:LEU:HD21 | 1:C:82:GLY:CA | 2.31 | 0.57 |
| 1:A:4:LEU:C | 1:A:4:LEU:HD23 | 2.25 | 0.57 |
| 1:C:120:VAL:HG13 | 1:C:122:ASN:O | 2.05 | 0.57 |
| 1:E:64:SER:O | 1:E:65:ASP:CB | 2.30 | 0.57 |
| 1:E:152:TYR:O | 1:E:153:ARG:HB3 | 2.04 | 0.57 |
| 1:F:142:HIS:CD2 | 1:F:142:HIS:N | 2.70 | 0.57 |
| 1:A:160:CYS:O | 1:A:176:THR:HG23 | 2.05 | 0.57 |
| 1:E:188:GLN:HG3 | 1:E:189:PRO:CD | 2.34 | 0.57 |
| 1:A:22:SER:CB | 1:A:31:THR:HG22 | 2.33 | 0.57 |
| 1:D:62:LEU:HA | 1:D:68:LEU:HA | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:160:CYS:SG | 1:D:180:GLY:HA3 | 2.44 | 0.57 |
| 1:E:148:GLN:HA | 1:E:153:ARG:HA | 1.87 | 0.57 |
| 1:F:30:PHE:HA | 1:F:31:THR:HG22 | 1.87 | 0.57 |
| 1:A:119:VAL:CG2 | 1:A:151:PRO:HD3 | 2.35 | 0.56 |
| 1:D:39:VAL:CG1 | 1:D:40:LEU:N | 2.67 | 0.56 |
| 1:D:156:MET:O | 1:D:157:GLU:C | 2.41 | 0.56 |
| 1:A:13:HIS:HA | 1:A:14:PRO:O | 2.04 | 0.56 |
| 1:B:35:ASP:OD1 | 1:B:35:ASP:N | 2.33 | 0.56 |
| 1:C:74:GLN:HG3 | 1:F:189:PRO:CB | 2.26 | 0.56 |
| 1:C:74:GLN:H | 1:F:189:PRO:CG | 2.17 | 0.56 |
| 1:E:29:ARG:NH2 | 1:E:41:PHE:CE1 | 2.73 | 0.56 |
| 1:E:149:LEU:HD13 | 1:E:221:PRO:HA | 1.87 | 0.56 |
| 1:B:29:ARG:O | 1:B:41:PHE:N | 2.38 | 0.56 |
| 1:C:211:SER:O | 1:C:212:ALA:C | 2.44 | 0.56 |
| 1:D:166:ASP:C | 1:D:167:ARG:O | 2.43 | 0.56 |
| 1:E:158:THR:CG2 | 1:F:151:PRO:HG2 | 2.32 | 0.56 |
| 1:E:159:ASP:OD1 | 1:E:159:ASP:N | 2.36 | 0.56 |
| 1:F:146:SER:OG | 1:F:155:SER:HB3 | 2.05 | 0.56 |
| 1:F:167:ARG:O | 1:F:168:ASP:C | 2.43 | 0.56 |
| 1:C:114:ASN:ND2 | 1:C:223:ARG:HD3 | 2.21 | 0.56 |
| 1:E:177:ALA:O | 1:E:179:LYS:N | 2.39 | 0.56 |
| 1:F:72:THR:HG22 | 1:F:74:GLN:HB2 | 1.87 | 0.56 |
| 1:C:69:VAL:HG23 | 1:C:69:VAL:O | 2.06 | 0.56 |
| 1:C:87:ILE:O | 1:C:88:GLY:O | 2.24 | 0.56 |
| 1:C:163:VAL:HG23 | 1:C:164:LEU:N | 2.20 | 0.56 |
| 1:D:215:TYR:O | 1:D:216:VAL:HB | 2.04 | 0.56 |
| 1:F:227:ILE:O | 1:F:227:ILE:HG12 | 2.04 | 0.56 |
| 1:B:100:VAL:O | 1:B:234:THR:HA | 2.05 | 0.56 |
| 1:D:137:HIS:HB3 | 1:D:138:PRO:C | 2.26 | 0.56 |
| 1:E:159:ASP:O | 1:E:160:CYS:HB3 | 2.05 | 0.56 |
| 1:F:215:TYR:HD1 | 1:F:227:ILE:HD11 | 1.70 | 0.56 |
| 1:A:52:THR:O | 1:A:78:ARG:NH1 | 2.38 | 0.56 |
| 1:A:69:VAL:O | 1:A:69:VAL:CG2 | 2.51 | 0.56 |
| 1:D:104:GLY:HA2 | 1:D:105:PRO:O | 2.06 | 0.56 |
| 1:E:80:SER:OG | 1:E:81:SER:N | 2.35 | 0.56 |
| 1:E:111:GLY:H | 1:E:224:ASN:ND2 | 2.03 | 0.56 |
| 1:A:54:GLY:O | 1:A:55:ALA:HB2 | 2.05 | 0.56 |
| 1:A:74:GLN:HE21 | 1:D:189:PRO:CG | 2.18 | 0.56 |
| 1:B:132:GLN:HG2 | 1:B:214:ARG:HH12 | 1.71 | 0.56 |
| 1:D:31:THR:N | 1:D:39:VAL:O | 2.32 | 0.56 |
| 1:A:75:ASN:ND2 | 1:D:196:LEU:HD21 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:154:LEU:O | 1:A:155:SER:CB | 2.46 | 0.56 |
| 1:B:17:LEU:H | 1:B:61:VAL:H | 1.53 | 0.56 |
| 1:C:129:TYR:CB | 1:C:131:THR:HG22 | 2.36 | 0.56 |
| 1:F:90:TYR:CD1 | 1:F:90:TYR:N | 2.72 | 0.56 |
| 1:A:134:ASN:N | 1:A:214:ARG:HH22 | 2.03 | 0.56 |
| 1:B:37:ASN:HD21 | 1:B:52:THR:H | 1.52 | 0.56 |
| 1:B:188:GLN:CG | 1:B:189:PRO:CD | 2.83 | 0.56 |
| 1:D:103:TYR:HB3 | 1:D:228:TYR:O | 2.06 | 0.56 |
| 1:B:37:ASN:HD22 | 1:B:52:THR:H | 1.49 | 0.55 |
| 1:B:146:SER:O | 1:B:147:LEU:O | 2.23 | 0.55 |
| 1:C:113:SER:HA | 1:C:222:ASP:O | 2.06 | 0.55 |
| 1:A:131:THR:OG1 | 1:A:131:THR:HG21 | 2.03 | 0.55 |
| 1:E:141:LEU:CD2 | 1:E:185:ALA:HB3 | 2.36 | 0.55 |
| 1:A:5:PHE:HE2 | 1:A:220:GLN:NE2 | 2.03 | 0.55 |
| 1:A:72:THR:HG21 | 1:A:76:THR:OG1 | 2.07 | 0.55 |
| 1:C:166:ASP:HB2 | 1:C:171:VAL:HG11 | 1.87 | 0.55 |
| 1:A:152:TYR:CE2 | 1:A:223:ARG:HG3 | 2.41 | 0.55 |
| 1:D:152:TYR:HB2 | 1:D:219:LEU:HD21 | 1.88 | 0.55 |
| 1:E:176:THR:HG23 | 1:E:179:LYS:HD3 | 1.87 | 0.55 |
| 1:F:71:LEU:CD2 | 1:F:77:ILE:H | 2.19 | 0.55 |
| 1:A:232:LEU:O | 1:A:232:LEU:HG | 2.05 | 0.55 |
| 1:B:59:ARG:NH2 | 1:B:71:LEU:HD12 | 2.21 | 0.55 |
| 1:D:163:VAL:HG21 | 1:D:165:PHE:CZ | 2.42 | 0.55 |
| 1:F:76:THR:HA | 1:F:77:ILE:HG13 | 1.89 | 0.55 |
| 1:F:211:SER:OG | 1:F:212:ALA:O | 2.24 | 0.55 |
| 1:A:37:ASN:HD22 | 1:A:52:THR:H | 1.52 | 0.55 |
| 1:A:225:LEU:O | 1:A:226:ALA:HB2 | 2.06 | 0.55 |
| 1:F:67:LEU:CD1 | 1:F:84:LYS:HB3 | 2.36 | 0.55 |
| 1:C:161:ASN:HD21 | 1:C:175:ASN:CA | 2.20 | 0.55 |
| 1:C:217:PHE:HA | 1:C:227:ILE:HG23 | 1.88 | 0.55 |
| 1:F:77:ILE:O | 1:F:77:ILE:CG2 | 2.49 | 0.55 |
| 1:D:18:HIS:H | 1:D:21:GLN:HG3 | 1.72 | 0.55 |
| 1:E:56:THR:HG22 | 1:E:57:GLY:N | 2.20 | 0.55 |
| 1:F:16:THR:HG23 | 1:F:61:VAL:H | 1.72 | 0.55 |
| 1:A:43:SER:C | 1:A:44:ASP:O | 2.43 | 0.55 |
| 1:C:95:GLN:HE21 | 1:C:99:THR:HG22 | 1.72 | 0.55 |
| 1:F:87:ILE:CG2 | 1:F:88:GLY:H | 2.18 | 0.55 |
| 1:A:110:SER:OG | 1:A:225:LEU:N | 2.39 | 0.54 |
| 1:D:101:THR:HG21 | 1:D:103:TYR:OH | 2.08 | 0.54 |
| 1:F:110:SER:OG | 1:F:225:LEU:HD13 | 2.07 | 0.54 |
| 1:A:166:ASP:O | 1:A:167:ARG:O | 2.25 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:167:ARG:O | 1:C:168:ASP:C | 2.44 | 0.54 |
| 1:F:193:MET:O | 1:F:204:TRP:HZ3 | 1.90 | 0.54 |
| 1:A:4:LEU:HD12 | 1:A:17:LEU:HD21 | 1.89 | 0.54 |
| 1:A:174:THR:O | 1:A:175:ASN:OD1 | 2.26 | 0.54 |
| 1:C:163:VAL:HG23 | 1:C:164:LEU:H | 1.73 | 0.54 |
| 1:A:77:ILE:O | 1:A:77:ILE:CG2 | 2.40 | 0.54 |
| 1:A:150:SER:OG | 1:A:151:PRO:N | 2.40 | 0.54 |
| 1:C:93:VAL:CG2 | 1:C:95:GLN:HG3 | 2.37 | 0.54 |
| 1:D:223:ARG:HH11 | 1:D:223:ARG:CB | 2.21 | 0.54 |
| 1:E:152:TYR:HA | 1:E:165:PHE:O | 2.07 | 0.54 |
| 1:F:75:ASN:O | 1:F:76:THR:HB | 2.06 | 0.54 |
| 1:A:222:ASP:O | 1:A:223:ARG:C | 2.44 | 0.54 |
| 1:B:220:GLN:HB2 | 1:B:221:PRO:CD | 2.38 | 0.54 |
| 1:C:95:GLN:NE2 | 1:C:99:THR:CG2 | 2.71 | 0.54 |
| 1:C:163:VAL:CG2 | 1:C:164:LEU:N | 2.69 | 0.54 |
| 1:F:142:HIS:H | 1:F:145:GLN:HB2 | 1.73 | 0.54 |
| 1:B:214:ARG:O | 1:B:215:TYR:HD2 | 1.91 | 0.54 |
| 1:C:52:THR:HG21 | 1:C:79:TRP:HB2 | 1.89 | 0.54 |
| 1:B:28:PHE:CE2 | 1:B:98:ARG:CG | 2.87 | 0.54 |
| 1:B:228:TYR:N | 1:B:228:TYR:HD2 | 2.06 | 0.54 |
| 1:F:95:GLN:HE21 | 1:F:99:THR:CG2 | 2.20 | 0.54 |
| 1:D:95:GLN:HG2 | 1:D:128:LEU:CD2 | 2.37 | 0.54 |
| 1:D:161:ASN:ND2 | 1:D:175:ASN:H | 2.06 | 0.54 |
| 1:D:197:THR:CG2 | 1:D:201:ILE:HB | 2.36 | 0.54 |
| 1:A:151:PRO:HD2 | 1:A:152:TYR:N | 2.13 | 0.54 |
| 1:B:65:ASP:OD1 | 1:B:65:ASP:N | 2.40 | 0.54 |
| 1:B:176:THR:HG22 | 1:B:176:THR:O | 2.06 | 0.54 |
| 1:C:74:GLN:H | 1:F:189:PRO:CB | 2.20 | 0.54 |
| 1:E:110:SER:N | 1:E:225:LEU:O | 2.40 | 0.54 |
| 1:F:63:GLN:NE2 | 1:F:69:VAL:CG2 | 2.71 | 0.54 |
| 1:A:101:THR:HA | 1:A:233:TRP:O | 2.08 | 0.54 |
| 1:C:119:VAL:O | 1:C:120:VAL:HG23 | 2.08 | 0.54 |
| 1:D:101:THR:CG2 | 1:D:102:ILE:N | 2.70 | 0.54 |
| 1:E:37:ASN:OD1 | 1:E:51:ASN:HA | 2.08 | 0.54 |
| 1:F:70:ILE:HG22 | 1:F:70:ILE:O | 2.08 | 0.54 |
| 1:A:143:ALA:O | 1:A:144:THR:CB | 2.51 | 0.53 |
| 1:A:220:GLN:HB2 | 1:A:224:ASN:CB | 2.38 | 0.53 |
| 1:C:2:ASN:OD1 | 1:C:2:ASN:C | 2.45 | 0.53 |
| 1:E:5:PHE:O | 1:E:6:GLY:C | 2.44 | 0.53 |
| 1:E:62:LEU:O | 1:E:62:LEU:HG | 2.04 | 0.53 |
| 1:B:189:PRO:CD | 1:B:190:ASN:N | 2.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:6:GLY:HA2 | 1:E:62:LEU:CD2 | 2.18 | 0.53 |
| 1:B:197:THR:O | 1:B:199:GLN:N | 2.41 | 0.53 |
| 1:C:63:GLN:OE1 | 1:F:200:ASN:ND2 | 2.41 | 0.53 |
| 1:C:220:GLN:O | 1:C:221:PRO:C | 2.46 | 0.53 |
| 1:E:166:ASP:O | 1:E:168:ASP:N | 2.41 | 0.53 |
| 1:A:63:GLN:HG2 | 1:D:199:GLN:HA | 1.90 | 0.53 |
| 1:A:185:ALA:HA | 1:A:194:ASP:O | 2.07 | 0.53 |
| 1:B:90:TYR:CD2 | 1:B:104:GLY:CA | 2.89 | 0.53 |
| 1:C:101:THR:CG2 | 1:C:103:TYR:CE1 | 2.92 | 0.53 |
| 1:D:197:THR:CB | 1:D:201:ILE:HB | 2.39 | 0.53 |
| 1:C:73:ALA:HB1 | 1:F:189:PRO:HG3 | 1.88 | 0.53 |
| 1:C:235:THR:O | 1:C:236:GLY:C | 2.47 | 0.53 |
| 1:D:44:ASP:OD1 | 1:D:44:ASP:C | 2.47 | 0.53 |
| 1:E:83:THR:HG22 | 1:E:84:LYS:N | 2.24 | 0.53 |
| 1:E:101:THR:HG1 | 1:E:234:THR:HB | 1.73 | 0.53 |
| 1:F:2:ASN:OD1 | 1:F:3:ILE:N | 2.41 | 0.53 |
| 1:F:142:HIS:HD2 | 1:F:145:GLN:OE1 | 1.92 | 0.53 |
| 1:F:146:SER:HG | 1:F:155:SER:HB3 | 1.74 | 0.53 |
| 1:F:148:GLN:HG3 | 1:F:153:ARG:HB3 | 1.90 | 0.53 |
| 1:A:56:THR:HG22 | 1:A:57:GLY:N | 2.18 | 0.53 |
| 1:B:220:GLN:NE2 | 1:B:228:TYR:OH | 2.41 | 0.53 |
| 1:D:16:THR:CG2 | 1:D:61:VAL:HG22 | 2.38 | 0.53 |
| 1:B:67:LEU:O | 1:B:68:LEU:C | 2.45 | 0.53 |
| 1:D:152:TYR:N | 1:D:152:TYR:CD2 | 2.76 | 0.53 |
| 1:D:166:ASP:O | 1:D:167:ARG:C | 2.46 | 0.53 |
| 1:E:63:GLN:HB2 | 1:E:67:LEU:N | 2.24 | 0.53 |
| 1:F:156:MET:SD | 1:F:184:ARG:O | 2.66 | 0.53 |
| 1:A:7:LEU:CD1 | 1:A:61:VAL:HG13 | 2.39 | 0.53 |
| 1:A:157:GLU:CD | 1:C:26:SER:OG | 2.48 | 0.53 |
| 1:A:193:MET:CG | 1:A:204:TRP:HZ3 | 2.21 | 0.53 |
| 1:B:67:LEU:CD1 | 1:B:84:LYS:HG3 | 2.34 | 0.53 |
| 1:C:33:GLN:HG3 | 1:C:37:ASN:O | 2.08 | 0.53 |
| 1:F:220:GLN:CB | 1:F:221:PRO:CD | 2.86 | 0.53 |
| 1:F:230:GLY:O | 1:F:231:ALA:CB | 2.29 | 0.53 |
| 1:B:199:GLN:O | 1:B:200:ASN:CB | 2.56 | 0.52 |
| 1:D:187:LEU:CD2 | 1:D:217:PHE:HB2 | 2.39 | 0.52 |
| 1:D:197:THR:O | 1:D:198:ASN:C | 2.46 | 0.52 |
| 1:E:29:ARG:HH21 | 1:E:31:THR:CG2 | 2.22 | 0.52 |
| 1:F:71:LEU:HD23 | 1:F:77:ILE:H | 1.73 | 0.52 |
| 1:A:72:THR:O | 1:A:74:GLN:N | 2.42 | 0.52 |
| 1:A:127:ILE:HG22 | 1:A:217:PHE:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:12:SER:HB3 | 1:C:221:PRO:HB2 | 1.92 | 0.52 |
| 1:C:32:MET:HE3 | 1:C:59:ARG:HA | 1.91 | 0.52 |
| 1:C:112:THR:O | 1:C:113:SER:C | 2.42 | 0.52 |
| 1:E:162:LEU:HD12 | 1:E:174:THR:HG21 | 1.91 | 0.52 |
| 1:F:140:THR:OG1 | 1:F:141:LEU:N | 2.40 | 0.52 |
| 1:A:18:HIS:O | 1:A:19:ALA:C | 2.47 | 0.52 |
| 1:C:197:THR:CG2 | 1:C:199:GLN:OE1 | 2.56 | 0.52 |
| 1:E:38:LEU:N | 1:E:50:SER:OG | 2.37 | 0.52 |
| 1:E:72:THR:HG22 | 1:E:75:ASN:N | 2.24 | 0.52 |
| 1:D:109:ASP:CB | 1:D:225:LEU:O | 2.57 | 0.52 |
| 1:B:110:SER:HB3 | 1:B:112:THR:HG22 | 1.91 | 0.52 |
| 1:C:92:LEU:HD21 | 1:C:100:VAL:CG1 | 2.37 | 0.52 |
| 1:C:162:LEU:CB | 1:C:174:THR:HG23 | 2.40 | 0.52 |
| 1:F:18:HIS:HB2 | 1:F:21:GLN:CD | 2.30 | 0.52 |
| 1:A:134:ASN:N | 1:A:214:ARG:NH2 | 2.58 | 0.52 |
| 1:A:142:HIS:O | 1:A:156:MET:HB3 | 2.10 | 0.52 |
| 1:C:147:LEU:O | 1:C:154:LEU:N | 2.25 | 0.52 |
| 1:D:37:ASN:HD21 | 1:D:51:ASN:N | 2.08 | 0.52 |
| 1:F:167:ARG:O | 1:F:169:ASP:N | 2.43 | 0.52 |
| 1:F:220:GLN:HB3 | 1:F:221:PRO:CD | 2.40 | 0.52 |
| 1:B:61:VAL:HG22 | 1:B:62:LEU:N | 2.25 | 0.52 |
| 1:C:18:HIS:CB | 1:C:21:GLN:NE2 | 2.66 | 0.52 |
| 1:D:63:GLN:NE2 | 1:D:69:VAL:CG2 | 2.61 | 0.52 |
| 1:D:93:VAL:CG2 | 1:D:94:LEU:N | 2.69 | 0.52 |
| 1:D:101:THR:HG23 | 1:D:102:ILE:H | 1.75 | 0.52 |
| 1:D:108:TRP:O | 1:D:109:ASP:HB3 | 2.10 | 0.52 |
| 1:E:27:SER:HB3 | 1:E:28:PHE:CD2 | 2.43 | 0.52 |
| 1:E:69:VAL:CG2 | 1:E:71:LEU:HG | 2.39 | 0.52 |
| 1:B:224:ASN:O | 1:B:225:LEU:HD23 | 2.10 | 0.52 |
| 1:C:36:CYS:HB3 | 1:C:78:ARG:NH1 | 2.25 | 0.52 |
| 1:C:58:CYS:HA | 1:C:71:LEU:O | 2.10 | 0.52 |
| 1:C:58:CYS:HB2 | 1:C:71:LEU:O | 2.09 | 0.52 |
| 1:F:67:LEU:N | 1:F:67:LEU:HD12 | 2.23 | 0.52 |
| 1:F:129:TYR:HH | 1:F:131:THR:CB | 2.23 | 0.52 |
| 1:A:48:TRP:CD1 | 1:A:235:THR:HG22 | 2.45 | 0.52 |
| 1:B:143:ALA:HA | 1:B:156:MET:O | 2.09 | 0.52 |
| 1:B:157:GLU:CG | 1:B:161:ASN:HB3 | 2.34 | 0.52 |
| 1:E:141:LEU:HD22 | 1:E:185:ALA:HB3 | 1.91 | 0.52 |
| 1:B:188:GLN:CB | 1:B:189:PRO:CD | 2.88 | 0.52 |
| 1:C:130:SER:C | 1:C:131:THR:O | 2.43 | 0.52 |
| 1:C:195:VAL:CG2 | 1:C:203:VAL:HG12 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:129:TYR:CE1 | 1:D:131:THR:CB | 2.92 | 0.52 |
| 1:D:161:ASN:ND2 | 1:D:176:THR:H | 2.08 | 0.52 |
| 1:D:161:ASN:HD21 | 1:D:175:ASN:H | 1.58 | 0.52 |
| 1:D:161:ASN:HD22 | 1:D:176:THR:HB | 1.75 | 0.52 |
| 1:E:210:ARG:HG3 | 1:E:211:SER:H | 1.74 | 0.52 |
| 1:A:12:SER:HB3 | 1:A:221:PRO:CG | 2.39 | 0.51 |
| 1:C:4:LEU:HD12 | 1:C:4:LEU:C | 2.29 | 0.51 |
| 1:C:72:THR:HG21 | 1:C:76:THR:CA | 2.39 | 0.51 |
| 1:D:224:ASN:O | 1:D:225:LEU:HD23 | 2.10 | 0.51 |
| 1:E:127:ILE:HG12 | 1:E:138:PRO:O | 2.09 | 0.51 |
| 1:B:216:VAL:HG22 | 1:B:217:PHE:N | 2.22 | 0.51 |
| 1:B:220:GLN:HB3 | 1:B:221:PRO:CD | 2.40 | 0.51 |
| 1:D:28:PHE:CZ | 1:D:98:ARG:HG3 | 2.45 | 0.51 |
| 1:F:128:LEU:HA | 1:F:129:TYR:HB3 | 1.91 | 0.51 |
| 1:A:39:VAL:CG1 | 1:A:41:PHE:CE1 | 2.92 | 0.51 |
| 1:B:44:ASP:O | 1:B:45:VAL:HB | 2.10 | 0.51 |
| 1:B:142:HIS:O | 1:B:143:ALA:HB2 | 2.11 | 0.51 |
| 1:C:137:HIS:HB3 | 1:C:138:PRO:CA | 2.40 | 0.51 |
| 1:D:178:GLY:O | 1:D:179:LYS:C | 2.48 | 0.51 |
| 1:D:211:SER:O | 1:D:212:ALA:C | 2.46 | 0.51 |
| 1:E:93:VAL:HG23 | 1:E:94:LEU:N | 2.25 | 0.51 |
| 1:F:201:ILE:HG22 | 1:F:202:ALA:N | 2.24 | 0.51 |
| 1:A:90:TYR:CD2 | 1:A:104:GLY:HA3 | 2.46 | 0.51 |
| 1:A:161:ASN:ND2 | 1:A:176:THR:N | 2.54 | 0.51 |
| 1:A:179:LYS:HB3 | 1:A:179:LYS:HZ2 | 1.68 | 0.51 |
| 1:A:179:LYS:HZ1 | 1:A:179:LYS:CB | 2.22 | 0.51 |
| 1:E:109:ASP:HA | 1:E:226:ALA:HA | 1.92 | 0.51 |
| 1:E:185:ALA:HA | 1:E:194:ASP:O | 2.10 | 0.51 |
| 1:A:104:GLY:CA | 1:A:105:PRO:O | 2.59 | 0.51 |
| 1:A:119:VAL:HG21 | 1:A:151:PRO:CG | 2.40 | 0.51 |
| 1:A:156:MET:HA | 1:A:156:MET:CE | 2.40 | 0.51 |
| 1:B:188:GLN:HG3 | 1:E:74:GLN:HA | 1.92 | 0.51 |
| 1:C:34:SER:O | 1:C:56:THR:HG23 | 2.09 | 0.51 |
| 1:C:44:ASP:O | 1:C:45:VAL:CG2 | 2.58 | 0.51 |
| 1:C:155:SER:O | 1:C:162:LEU:HD23 | 2.11 | 0.51 |
| 1:D:23:LEU:H | 1:D:30:PHE:HB3 | 1.76 | 0.51 |
| 1:D:87:ILE:O | 1:D:88:GLY:O | 2.28 | 0.51 |
| 1:E:125:ASN:HA | 1:E:147:LEU:CD1 | 2.40 | 0.51 |
| 1:F:161:ASN:ND2 | 1:F:176:THR:N | 2.39 | 0.51 |
| 1:F:220:GLN:HB3 | 1:F:221:PRO:HD2 | 1.92 | 0.51 |
| 1:A:30:PHE:CD1 | 1:A:100:VAL:HG21 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:42:ASP:O | 1:A:43:SER:CB | 2.58 | 0.51 |
| 1:B:94:LEU:CB | 1:B:100:VAL:HG12 | 2.40 | 0.51 |
| 1:B:225:LEU:O | 1:B:226:ALA:HB2 | 2.10 | 0.51 |
| 1:C:161:ASN:HD21 | 1:C:175:ASN:HA | 1.75 | 0.51 |
| 1:D:39:VAL:CG1 | 1:D:40:LEU:H | 2.20 | 0.51 |
| 1:D:154:LEU:CD2 | 1:D:225:LEU:HD11 | 2.40 | 0.51 |
| 1:E:117:SER:O | 1:E:119:VAL:HG22 | 2.10 | 0.51 |
| 1:E:159:ASP:H | 1:F:151:PRO:HB3 | 1.75 | 0.51 |
| 1:A:159:ASP:HB2 | 1:A:177:ALA:HB1 | 1.92 | 0.51 |
| 1:B:101:THR:HG21 | 1:B:103:TYR:CZ | 2.45 | 0.51 |
| 1:B:71:LEU:HD22 | 1:B:77:ILE:N | 2.25 | 0.51 |
| 1:B:94:LEU:HA | 1:B:100:VAL:HG12 | 1.93 | 0.51 |
| 1:B:142:HIS:H | 1:B:145:GLN:HB3 | 1.76 | 0.51 |
| 1:D:89:ASN:O | 1:D:90:TYR:CD1 | 2.64 | 0.51 |
| 1:E:26:SER:CB | 1:F:33:GLN:HG3 | 2.39 | 0.51 |
| 1:E:48:TRP:CD2 | 1:E:49:ALA:N | 2.78 | 0.51 |
| 1:E:107:LEU:HD12 | 1:E:208:ASN:HB2 | 1.91 | 0.51 |
| 1:F:30:PHE:CZ | 1:F:38:LEU:HD11 | 2.46 | 0.51 |
| 1:A:97:ASP:O | 1:A:98:ARG:C | 2.48 | 0.51 |
| 1:C:101:THR:HG22 | 1:C:103:TYR:CE1 | 2.46 | 0.51 |
| 1:C:143:ALA:O | 1:C:144:THR:CB | 2.58 | 0.51 |
| 1:C:159:ASP:HB2 | 1:C:177:ALA:HA | 1.93 | 0.51 |
| 1:D:56:THR:CG2 | 1:D:57:GLY:N | 2.65 | 0.51 |
| 1:D:100:VAL:HB | 1:D:235:THR:HG1 | 1.73 | 0.51 |
| 1:F:50:SER:O | 1:F:52:THR:N | 2.44 | 0.51 |
| 1:B:71:LEU:CD2 | 1:B:77:ILE:H | 2.22 | 0.51 |
| 1:B:103:TYR:CD1 | 1:B:216:VAL:HB | 2.46 | 0.51 |
| 1:D:189:PRO:CD | 1:D:190:ASN:H | 2.19 | 0.51 |
| 1:E:4:LEU:CD1 | 1:E:5:PHE:H | 2.15 | 0.51 |
| 1:E:105:PRO:HD2 | 1:E:210:ARG:HH22 | 1.70 | 0.51 |
| 1:A:150:SER:OG | 1:A:151:PRO:CD | 2.59 | 0.50 |
| 1:C:112:THR:OG1 | 1:C:223:ARG:O | 2.27 | 0.50 |
| 1:E:18:HIS:HB2 | 1:E:21:GLN:NE2 | 2.26 | 0.50 |
| 1:C:42:ASP:O | 1:C:43:SER:C | 2.50 | 0.50 |
| 1:C:141:LEU:HD11 | 1:C:147:LEU:HD13 | 1.92 | 0.50 |
| 1:E:12:SER:HB3 | 1:E:221:PRO:CG | 2.40 | 0.50 |
| 1:E:19:ALA:O | 1:E:20:ALA:CB | 2.50 | 0.50 |
| 1:A:28:PHE:CZ | 1:A:98:ARG:HG3 | 2.46 | 0.50 |
| 1:A:117:SER:O | 1:A:119:VAL:HG13 | 2.11 | 0.50 |
| 1:B:217:PHE:O | 1:B:217:PHE:CD1 | 2.64 | 0.50 |
| 1:C:97:ASP:OD1 | 1:C:99:THR:HB | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:166:ASP:C | 1:C:167:ARG:O | 2.42 | 0.50 |
| 1:D:9:HIS:HA | 1:D:15:GLN:NE2 | 2.26 | 0.50 |
| 1:D:142:HIS:HB2 | 1:D:145:GLN:HB2 | 1.93 | 0.50 |
| 1:F:153:ARG:HE | 1:F:165:PHE:HD1 | 1.56 | 0.50 |
| 1:D:4:LEU:HD22 | 1:D:17:LEU:CD2 | 2.41 | 0.50 |
| 1:B:216:VAL:O | 1:B:217:PHE:HB2 | 2.12 | 0.50 |
| 1:C:74:GLN:H | 1:F:189:PRO:HB2 | 1.76 | 0.50 |
| 1:C:97:ASP:OD1 | 1:C:97:ASP:C | 2.49 | 0.50 |
| 1:D:168:ASP:O | 1:D:169:ASP:CB | 2.54 | 0.50 |
| 1:E:30:PHE:CE1 | 1:E:100:VAL:HG21 | 2.46 | 0.50 |
| 1:B:63:GLN:O | 1:B:64:SER:C | 2.47 | 0.50 |
| 1:B:107:LEU:HD12 | 1:B:107:LEU:C | 2.32 | 0.50 |
| 1:B:163:VAL:CG2 | 1:B:165:PHE:CE1 | 2.92 | 0.50 |
| 1:B:215:TYR:CD2 | 1:B:229:GLY:HA2 | 2.47 | 0.50 |
| 1:C:2:ASN:HD21 | 1:C:125:ASN:HD22 | 1.60 | 0.50 |
| 1:D:25:LEU:O | 1:D:26:SER:C | 2.50 | 0.50 |
| 1:D:108:TRP:C | 1:D:108:TRP:CD2 | 2.83 | 0.50 |
| 1:E:36:CYS:SG | 1:E:55:ALA:HB3 | 2.52 | 0.50 |
| 1:F:16:THR:HG22 | 1:F:17:LEU:H | 1.75 | 0.50 |
| 1:F:101:THR:OG1 | 1:F:234:THR:HA | 2.11 | 0.50 |
| 1:A:159:ASP:HB2 | 1:A:178:GLY:H | 1.75 | 0.50 |
| 1:B:90:TYR:HB3 | 1:B:103:TYR:O | 2.12 | 0.50 |
| 1:C:97:ASP:CG | 1:C:136:ASN:HD21 | 2.14 | 0.50 |
| 1:D:181:THR:O | 1:D:182:GLY:C | 2.50 | 0.50 |
| 1:E:69:VAL:HG22 | 1:E:69:VAL:O | 2.11 | 0.50 |
| 1:B:142:HIS:HB2 | 1:B:145:GLN:OE1 | 2.11 | 0.50 |
| 1:B:156:MET:O | 1:B:157:GLU:C | 2.49 | 0.50 |
| 1:E:9:HIS:CB | 1:E:10:GLU:HG3 | 2.29 | 0.50 |
| 1:E:69:VAL:HG21 | 1:E:71:LEU:CG | 2.39 | 0.50 |
| 1:E:159:ASP:O | 1:E:177:ALA:HA | 2.12 | 0.50 |
| 1:F:220:GLN:HG2 | 1:F:221:PRO:HD3 | 1.94 | 0.50 |
| 1:A:72:THR:HG23 | 1:A:74:GLN:N | 2.08 | 0.50 |
| 1:C:137:HIS:CB | 1:C:138:PRO:CA | 2.86 | 0.50 |
| 1:D:169:ASP:O | 1:D:171:VAL:HG12 | 2.12 | 0.50 |
| 1:A:199:GLN:CG | 1:A:199:GLN:O | 2.59 | 0.49 |
| 1:B:68:LEU:CD1 | 1:B:92:LEU:HD13 | 2.30 | 0.49 |
| 1:C:50:SER:HB2 | 1:C:79:TRP:CD1 | 2.47 | 0.49 |
| 1:C:152:TYR:CZ | 1:C:223:ARG:HG3 | 2.47 | 0.49 |
| 1:F:7:LEU:O | 1:F:9:HIS:HA | 2.09 | 0.49 |
| 1:A:195:VAL:HG12 | 1:A:204:TRP:HE3 | 1.77 | 0.49 |
| 1:C:137:HIS:CD2 | 1:C:137:HIS:H | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:22:SER:OG | 1:E:31:THR:HG22 | 2.12 | 0.49 |
| 1:F:106:GLY:O | 1:F:107:LEU:CB | 2.57 | 0.49 |
| 1:B:34:SER:OG | 1:D:151:PRO:HD3 | 2.12 | 0.49 |
| 1:B:213:GLY:O | 1:B:214:ARG:C | 2.51 | 0.49 |
| 1:D:151:PRO:HB3 | 1:D:167:ARG:HG2 | 1.93 | 0.49 |
| 1:D:161:ASN:CA | 1:D:176:THR:HG22 | 2.36 | 0.49 |
| 1:E:63:GLN:HB2 | 1:E:67:LEU:O | 2.11 | 0.49 |
| 1:F:188:GLN:HE21 | 1:F:189:PRO:CD | 2.25 | 0.49 |
| 1:C:4:LEU:HD13 | 1:C:14:PRO:HB2 | 1.94 | 0.49 |
| 1:E:9:HIS:HD2 | 1:E:10:GLU:HB2 | 1.76 | 0.49 |
| 1:F:217:PHE:HZ | 1:F:225:LEU:HD22 | 1.77 | 0.49 |
| 1:B:110:SER:HB3 | 1:B:112:THR:CG2 | 2.43 | 0.49 |
| 1:C:190:ASN:OD1 | 1:C:209:SER:HB2 | 2.13 | 0.49 |
| 1:D:70:ILE:HG22 | 1:D:79:TRP:N | 2.27 | 0.49 |
| 1:D:197:THR:O | 1:D:199:GLN:O | 2.30 | 0.49 |
| 1:D:204:TRP:CD2 | 1:D:205:THR:N | 2.81 | 0.49 |
| 1:E:136:ASN:CB | 1:E:136:ASN:C | 2.76 | 0.49 |
| 1:F:63:GLN:HE21 | 1:F:69:VAL:CG2 | 2.25 | 0.49 |
| 1:A:4:LEU:HD23 | 1:A:5:PHE:N | 2.27 | 0.49 |
| 1:A:160:CYS:SG | 1:A:203:VAL:HG11 | 2.52 | 0.49 |
| 1:B:132:GLN:HE21 | 1:B:214:ARG:NH1 | 2.09 | 0.49 |
| 1:A:195:VAL:HG13 | 1:A:204:TRP:HB3 | 1.91 | 0.49 |
| 1:D:50:SER:O | 1:D:51:ASN:CB | 2.57 | 0.49 |
| 1:D:63:GLN:CG | 1:D:64:SER:N | 2.75 | 0.49 |
| 1:D:189:PRO:CD | 1:D:190:ASN:N | 2.70 | 0.49 |
| 1:A:90:TYR:HB3 | 1:A:91:VAL:O | 2.12 | 0.49 |
| 1:A:170:ARG:NH1 | 1:A:173:SER:HB3 | 2.28 | 0.49 |
| 1:A:220:GLN:HB3 | 1:A:222:ASP:H | 1.76 | 0.49 |
| 1:B:77:ILE:CG2 | 1:B:78:ARG:N | 2.72 | 0.49 |
| 1:D:29:ARG:O | 1:D:40:LEU:HD12 | 2.11 | 0.49 |
| 1:E:12:SER:HB3 | 1:E:221:PRO:HG2 | 1.92 | 0.49 |
| 1:A:39:VAL:HG22 | 1:A:49:ALA:CB | 2.40 | 0.49 |
| 1:A:164:LEU:HD11 | 1:A:225:LEU:HD21 | 1.93 | 0.49 |
| 1:B:23:LEU:H | 1:B:30:PHE:HB3 | 1.77 | 0.49 |
| 1:C:217:PHE:CA | 1:C:227:ILE:CG2 | 2.85 | 0.49 |
| 1:E:62:LEU:HD21 | 1:E:90:TYR:HB3 | 1.95 | 0.49 |
| 1:E:72:THR:HG23 | 1:E:73:ALA:CB | 2.43 | 0.49 |
| 1:F:142:HIS:N | 1:F:145:GLN:HB2 | 2.28 | 0.49 |
| 1:A:19:ALA:O | 1:A:20:ALA:CB | 2.61 | 0.49 |
| 1:C:47:VAL:O | 1:C:48:TRP:HB2 | 2.12 | 0.49 |
| 1:D:67:LEU:HD22 | 1:D:80:SER:OG | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:87:ILE:HG22 | 1:D:88:GLY:N | 2.27 | 0.49 |
| 1:D:110:SER:HB2 | 1:D:112:THR:OG1 | 2.13 | 0.49 |
| 1:E:8:SER:HB3 | 1:E:9:HIS:ND1 | 2.28 | 0.49 |
| 1:B:194:ASP:OD1 | 1:B:194:ASP:C | 2.50 | 0.48 |
| 1:C:185:ALA:HA | 1:C:195:VAL:HA | 1.93 | 0.48 |
| 1:E:92:LEU:HG | 1:E:100:VAL:HG13 | 1.93 | 0.48 |
| 1:E:161:ASN:HD21 | 1:E:175:ASN:H | 1.61 | 0.48 |
| 1:E:232:LEU:O | 1:E:233:TRP:CB | 2.60 | 0.48 |
| 1:F:50:SER:HB3 | 1:F:52:THR:OG1 | 2.11 | 0.48 |
| 1:A:75:ASN:HB2 | 1:D:188:GLN:NE2 | 2.28 | 0.48 |
| 1:A:151:PRO:CD | 1:A:152:TYR:N | 2.73 | 0.48 |
| 1:B:132:GLN:O | 1:B:132:GLN:HG3 | 2.12 | 0.48 |
| 1:B:187:LEU:C | 1:B:188:GLN:O | 2.52 | 0.48 |
| 1:C:30:PHE:CB | 1:C:40:LEU:HB2 | 2.42 | 0.48 |
| 1:C:150:SER:HB3 | 1:C:151:PRO:HD3 | 1.94 | 0.48 |
| 1:D:107:LEU:CD1 | 1:D:209:SER:HA | 2.43 | 0.48 |
| 1:E:102:ILE:HD12 | 1:E:233:TRP:CE3 | 2.47 | 0.48 |
| 1:E:161:ASN:HD22 | 1:E:176:THR:H | 1.60 | 0.48 |
| 1:A:18:HIS:HB3 | 1:A:19:ALA:HB3 | 1.95 | 0.48 |
| 1:A:52:THR:CG2 | 1:A:79:TRP:HB2 | 2.43 | 0.48 |
| 1:B:94:LEU:HB2 | 1:B:100:VAL:CG1 | 2.41 | 0.48 |
| 1:F:225:LEU:HD12 | 1:F:225:LEU:N | 2.28 | 0.48 |
| 1:A:142:HIS:O | 1:A:156:MET:HG3 | 2.13 | 0.48 |
| 1:A:190:ASN:HB2 | 1:A:210:ARG:O | 2.13 | 0.48 |
| 1:A:217:PHE:HD1 | 1:A:227:ILE:HG22 | 1.78 | 0.48 |
| 1:B:3:ILE:HG21 | 1:B:3:ILE:HD12 | 1.57 | 0.48 |
| 1:C:22:SER:OG | 1:C:31:THR:HB | 2.14 | 0.48 |
| 1:D:197:THR:HG22 | 1:D:199:GLN:N | 2.26 | 0.48 |
| 1:E:32:MET:HG2 | 1:E:60:ALA:HB2 | 1.95 | 0.48 |
| 1:E:107:LEU:CD1 | 1:E:208:ASN:HB2 | 2.43 | 0.48 |
| 1:A:167:ARG:O | 1:A:168:ASP:C | 2.51 | 0.48 |
| 1:B:62:LEU:HG | 1:B:63:GLN:N | 2.25 | 0.48 |
| 1:B:129:TYR:HD2 | 1:B:215:TYR:O | 1.96 | 0.48 |
| 1:F:61:VAL:HG12 | 1:F:62:LEU:N | 2.28 | 0.48 |
| 1:F:87:ILE:O | 1:F:88:GLY:C | 2.51 | 0.48 |
| 1:F:129:TYR:O | 1:F:130:SER:OG | 2.28 | 0.48 |
| 1:B:186:VAL:O | 1:B:194:ASP:CB | 2.61 | 0.48 |
| 1:B:193:MET:HG3 | 1:B:204:TRP:CZ3 | 2.49 | 0.48 |
| 1:B:194:ASP:OD1 | 1:B:195:VAL:N | 2.47 | 0.48 |
| 1:C:29:ARG:NH2 | 1:C:31:THR:HG21 | 2.24 | 0.48 |
| 1:D:165:PHE:HD2 | 1:D:170:ARG:CA | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:81:SER:OG | 1:E:82:GLY:N | 2.46 | 0.48 |
| 1:F:224:ASN:O | 1:F:225:LEU:CD1 | 2.52 | 0.48 |
| 1:A:5:PHE:CE2 | 1:A:220:GLN:NE2 | 2.81 | 0.48 |
| 1:D:215:TYR:CE1 | 1:D:229:GLY:HA3 | 2.49 | 0.48 |
| 1:F:105:PRO:O | 1:F:228:TYR:HA | 2.14 | 0.48 |
| 1:F:162:LEU:HD11 | 1:F:193:MET:HE2 | 1.96 | 0.48 |
| 1:C:102:ILE:HD13 | 1:C:102:ILE:N | 2.28 | 0.48 |
| 1:C:176:THR:HG22 | 1:C:203:VAL:HG13 | 1.95 | 0.48 |
| 1:C:221:PRO:O | 1:C:222:ASP:C | 2.52 | 0.48 |
| 1:E:39:VAL:HG11 | 1:E:41:PHE:CE1 | 2.49 | 0.48 |
| 1:E:163:VAL:HG22 | 1:E:165:PHE:CE2 | 2.48 | 0.48 |
| 1:F:217:PHE:CZ | 1:F:225:LEU:CD2 | 2.94 | 0.48 |
| 1:B:40:LEU:O | 1:B:40:LEU:HG | 2.13 | 0.48 |
| 1:D:82:GLY:O | 1:D:83:THR:O | 2.31 | 0.48 |
| 1:D:187:LEU:HD22 | 1:D:217:PHE:HB2 | 1.95 | 0.48 |
| 1:D:217:PHE:HZ | 1:D:225:LEU:CD1 | 2.20 | 0.48 |
| 1:F:199:GLN:O | 1:F:200:ASN:HB2 | 2.14 | 0.48 |
| 1:A:102:ILE:O | 1:A:231:ALA:HA | 2.13 | 0.48 |
| 1:B:200:ASN:N | 1:B:200:ASN:HD22 | 1.99 | 0.48 |
| 1:F:70:ILE:HG22 | 1:F:78:ARG:HB2 | 1.96 | 0.48 |
| 1:A:176:THR:CG2 | 1:A:176:THR:O | 2.61 | 0.47 |
| 1:B:72:THR:HG21 | 1:B:76:THR:HG23 | 1.94 | 0.47 |
| 1:B:163:VAL:H | 1:B:163:VAL:HG13 | 1.37 | 0.47 |
| 1:B:197:THR:O | 1:B:198:ASN:C | 2.52 | 0.47 |
| 1:D:188:GLN:NE2 | 1:D:194:ASP:OD2 | 2.47 | 0.47 |
| 1:F:193:MET:O | 1:F:204:TRP:CZ3 | 2.66 | 0.47 |
| 1:B:60:ALA:HB2 | 1:B:70:ILE:HD11 | 1.96 | 0.47 |
| 1:C:119:VAL:HG12 | 1:C:120:VAL:H | 1.78 | 0.47 |
| 1:D:162:LEU:CB | 1:D:174:THR:OG1 | 2.62 | 0.47 |
| 1:E:110:SER:OG | 1:E:225:LEU:CB | 2.60 | 0.47 |
| 1:F:188:GLN:HG3 | 1:F:189:PRO:HD2 | 1.96 | 0.47 |
| 1:A:48:TRP:CE2 | 1:A:235:THR:HG22 | 2.50 | 0.47 |
| 1:A:192:ARG:HD2 | 1:A:205:THR:OG1 | 2.13 | 0.47 |
| 1:A:220:GLN:HG2 | 1:A:221:PRO:CD | 2.44 | 0.47 |
| 1:C:8:SER:HB2 | 1:C:9:HIS:HB2 | 1.95 | 0.47 |
| 1:D:2:ASN:N | 1:D:2:ASN:HD22 | 2.12 | 0.47 |
| 1:F:16:THR:CG2 | 1:F:61:VAL:H | 2.27 | 0.47 |
| 1:F:106:GLY:O | 1:F:107:LEU:HB2 | 2.13 | 0.47 |
| 1:F:161:ASN:HD22 | 1:F:161:ASN:HA | 1.35 | 0.47 |
| 1:F:195:VAL:CG1 | 1:F:204:TRP:HB3 | 2.40 | 0.47 |
| 1:A:97:ASP:OD1 | 1:A:99:THR:HB | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:192:ARG:HB3 | 1:B:206:SER:OG | 2.14 | 0.47 |
| 1:B:195:VAL:HG12 | 1:B:203:VAL:CG1 | 2.44 | 0.47 |
| 1:C:203:VAL:HG12 | 1:C:204:TRP:N | 2.29 | 0.47 |
| 1:D:129:TYR:HE1 | 1:D:131:THR:CB | 2.26 | 0.47 |
| 1:F:95:GLN:O | 1:F:97:ASP:N | 2.48 | 0.47 |
| 1:A:193:MET:HG3 | 1:A:204:TRP:HZ3 | 1.79 | 0.47 |
| 1:D:182:GLY:HA3 | 1:D:198:ASN:N | 2.30 | 0.47 |
| 1:E:17:LEU:H | 1:E:61:VAL:H | 1.62 | 0.47 |
| 1:E:37:ASN:OD1 | 1:E:51:ASN:CA | 2.63 | 0.47 |
| 1:A:161:ASN:ND2 | 1:A:175:ASN:N | 2.62 | 0.47 |
| 1:D:55:ALA:HB1 | 1:D:56:THR:H | 1.56 | 0.47 |
| 1:D:70:ILE:HG22 | 1:D:79:TRP:H | 1.79 | 0.47 |
| 1:E:142:HIS:HB2 | 1:E:145:GLN:OE1 | 2.14 | 0.47 |
| 1:E:182:GLY:HA3 | 1:E:198:ASN:CA | 2.45 | 0.47 |
| 1:A:119:VAL:HG21 | 1:A:151:PRO:HG3 | 1.96 | 0.47 |
| 1:A:163:VAL:HB | 1:A:173:SER:OG | 2.14 | 0.47 |
| 1:A:192:ARG:HG3 | 1:A:209:SER:HB3 | 1.97 | 0.47 |
| 1:B:30:PHE:HD1 | 1:B:31:THR:N | 2.12 | 0.47 |
| 1:B:90:TYR:N | 1:B:90:TYR:CD1 | 2.82 | 0.47 |
| 1:C:23:LEU:O | 1:C:30:PHE:N | 2.48 | 0.47 |
| 1:C:157:GLU:HG2 | 1:C:163:VAL:HG13 | 1.97 | 0.47 |
| 1:C:210:ARG:HB3 | 1:C:211:SER:H | 1.37 | 0.47 |
| 1:E:158:THR:HB | 1:F:152:TYR:CZ | 2.49 | 0.47 |
| 1:E:159:ASP:N | 1:F:151:PRO:HG3 | 2.29 | 0.47 |
| 1:F:56:THR:HG23 | 1:F:57:GLY:N | 2.28 | 0.47 |
| 1:F:125:ASN:HA | 1:F:147:LEU:HG | 1.95 | 0.47 |
| 1:F:172:TRP:CH2 | 1:F:174:THR:HG23 | 2.49 | 0.47 |
| 1:F:186:VAL:HG22 | 1:F:194:ASP:CB | 2.45 | 0.47 |
| 1:F:187:LEU:HD22 | 1:F:217:PHE:HB2 | 1.97 | 0.47 |
| 1:A:25:LEU:HD13 | 1:A:25:LEU:HA | 1.81 | 0.47 |
| 1:A:109:ASP:HB3 | 1:A:226:ALA:HB2 | 1.97 | 0.47 |
| 1:A:163:VAL:HG21 | 1:A:165:PHE:CZ | 2.48 | 0.47 |
| 1:B:151:PRO:HD3 | 1:D:34:SER:HB2 | 1.86 | 0.47 |
| 1:B:163:VAL:HG23 | 1:B:164:LEU:N | 2.30 | 0.47 |
| 1:B:220:GLN:HB3 | 1:B:221:PRO:HD3 | 1.97 | 0.47 |
| 1:A:146:SER:HA | 1:A:154:LEU:O | 2.14 | 0.47 |
| 1:C:139:GLN:O | 1:C:140:THR:HB | 2.15 | 0.47 |
| 1:C:217:PHE:CA | 1:C:227:ILE:HG22 | 2.42 | 0.47 |
| 1:D:146:SER:OG | 1:D:155:SER:HB2 | 2.15 | 0.47 |
| 1:E:97:ASP:O | 1:E:98:ARG:CB | 2.63 | 0.47 |
| 1:F:60:ALA:HB2 | 1:F:70:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:86:SER:HB2 | 1:B:90:TYR:OH | 2.15 | 0.47 |
| 1:C:38:LEU:HD22 | 1:C:60:ALA:HB2 | 1.97 | 0.47 |
| 1:C:142:HIS:CD2 | 1:C:145:GLN:OE1 | 2.68 | 0.47 |
| 1:D:80:SER:O | 1:D:81:SER:C | 2.51 | 0.47 |
| 1:E:30:PHE:CE2 | 1:E:92:LEU:HD11 | 2.50 | 0.47 |
| 1:F:25:LEU:N | 1:F:94:LEU:HD21 | 2.30 | 0.47 |
| 1:F:30:PHE:CD1 | 1:F:39:VAL:O | 2.68 | 0.47 |
| 1:F:180:GLY:O | 1:F:181:THR:HB | 2.14 | 0.47 |
| 1:A:60:ALA:O | 1:A:69:VAL:O | 2.33 | 0.46 |
| 1:B:225:LEU:O | 1:B:226:ALA:CB | 2.56 | 0.46 |
| 1:D:72:THR:HG22 | 1:D:74:GLN:CB | 2.45 | 0.46 |
| 1:E:87:ILE:O | 1:E:88:GLY:O | 2.33 | 0.46 |
| 1:E:107:LEU:O | 1:E:208:ASN:ND2 | 2.48 | 0.46 |
| 1:E:216:VAL:O | 1:E:216:VAL:CG1 | 2.59 | 0.46 |
| 1:A:72:THR:HG22 | 1:A:76:THR:CA | 2.44 | 0.46 |
| 1:A:101:THR:CG2 | 1:A:103:TYR:CZ | 2.97 | 0.46 |
| 1:A:119:VAL:CG2 | 1:A:150:SER:OG | 2.63 | 0.46 |
| 1:B:152:TYR:OH | 1:B:221:PRO:O | 2.33 | 0.46 |
| 1:D:64:SER:O | 1:D:87:ILE:O | 2.33 | 0.46 |
| 1:D:102:ILE:HD12 | 1:D:233:TRP:CE3 | 2.50 | 0.46 |
| 1:D:169:ASP:OD2 | 1:D:169:ASP:C | 2.54 | 0.46 |
| 1:D:184:ARG:NH1 | 1:D:184:ARG:HG2 | 2.30 | 0.46 |
| 1:E:32:MET:SD | 1:E:32:MET:O | 2.73 | 0.46 |
| 1:C:8:SER:CB | 1:C:9:HIS:HB2 | 2.44 | 0.46 |
| 1:E:104:GLY:HA2 | 1:E:105:PRO:O | 2.15 | 0.46 |
| 1:E:170:ARG:CG | 1:E:170:ARG:NH1 | 2.66 | 0.46 |
| 1:E:193:MET:CG | 1:E:204:TRP:HZ3 | 2.28 | 0.46 |
| 1:F:63:GLN:O | 1:F:64:SER:C | 2.52 | 0.46 |
| 1:F:63:GLN:O | 1:F:65:ASP:N | 2.48 | 0.46 |
| 1:B:37:ASN:HD22 | 1:B:53:ALA:N | 2.13 | 0.46 |
| 1:B:188:GLN:CB | 1:B:189:PRO:HD3 | 2.43 | 0.46 |
| 1:C:40:LEU:HD22 | 1:C:100:VAL:HG23 | 1.98 | 0.46 |
| 1:C:48:TRP:CD2 | 1:C:49:ALA:N | 2.83 | 0.46 |
| 1:D:195:VAL:HG13 | 1:D:204:TRP:HB3 | 1.97 | 0.46 |
| 1:E:29:ARG:NH2 | 1:E:31:THR:HG21 | 2.30 | 0.46 |
| 1:F:6:GLY:HA2 | 1:F:62:LEU:O | 2.15 | 0.46 |
| 1:A:146:SER:O | 1:A:147:LEU:O | 2.34 | 0.46 |
| 1:B:164:LEU:CD1 | 1:B:171:VAL:HG22 | 2.45 | 0.46 |
| 1:C:36:CYS:HB3 | 1:C:78:ARG:HH11 | 1.80 | 0.46 |
| 1:E:110:SER:HB2 | 1:E:112:THR:HG23 | 1.97 | 0.46 |
| 1:E:171:VAL:HG22 | 1:E:172:TRP:N | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:215:TYR:HE1 | 1:E:229:GLY:HA2 | 1.77 | 0.46 |
| 1:F:128:LEU:HA | 1:F:129:TYR:CG | 2.51 | 0.46 |
| 1:F:204:TRP:CE3 | 1:F:204:TRP:C | 2.89 | 0.46 |
| 1:B:6:GLY:HA2 | 1:B:62:LEU:HD23 | 1.97 | 0.46 |
| 1:D:45:VAL:CA | 1:D:46:ARG:HG3 | 2.46 | 0.46 |
| 1:D:110:SER:CB | 1:D:112:THR:OG1 | 2.64 | 0.46 |
| 1:E:118:VAL:HG13 | 1:E:221:PRO:HB2 | 1.98 | 0.46 |
| 1:F:137:HIS:N | 1:F:137:HIS:CD2 | 2.83 | 0.46 |
| 1:B:17:LEU:H | 1:B:61:VAL:N | 2.13 | 0.46 |
| 1:C:29:ARG:HH21 | 1:C:31:THR:HG23 | 1.74 | 0.46 |
| 1:D:71:LEU:CD2 | 1:D:77:ILE:HG13 | 2.46 | 0.46 |
| 1:D:90:TYR:HE2 | 1:D:232:LEU:HD22 | 1.80 | 0.46 |
| 1:E:4:LEU:CD1 | 1:E:5:PHE:N | 2.61 | 0.46 |
| 1:E:52:THR:HB | 1:E:78:ARG:HD3 | 1.97 | 0.46 |
| 1:E:194:ASP:HB3 | 1:E:196:LEU:CD1 | 2.45 | 0.46 |
| 1:F:90:TYR:CE2 | 1:F:104:GLY:HA3 | 2.51 | 0.46 |
| 1:A:106:GLY:HA2 | 1:A:228:TYR:HA | 1.98 | 0.46 |
| 1:A:119:VAL:HB | 1:A:150:SER:OG | 2.16 | 0.46 |
| 1:C:74:GLN:HG2 | 1:F:189:PRO:HB2 | 1.95 | 0.46 |
| 1:D:161:ASN:HD21 | 1:D:175:ASN:CA | 2.29 | 0.46 |
| 1:E:224:ASN:HD22 | 1:E:224:ASN:HA | 1.41 | 0.46 |
| 1:B:93:VAL:HG23 | 1:B:94:LEU:N | 2.31 | 0.46 |
| 1:C:215:TYR:CD2 | 1:C:215:TYR:N | 2.77 | 0.46 |
| 1:F:28:PHE:HB3 | 1:F:94:LEU:CD1 | 2.43 | 0.46 |
| 1:F:163:VAL:HG21 | 1:F:165:PHE:CZ | 2.51 | 0.46 |
| 1:A:72:THR:CG2 | 1:A:76:THR:OG1 | 2.64 | 0.46 |
| 1:A:95:GLN:HA | 1:A:96:PRO:HD3 | 1.85 | 0.46 |
| 1:F:17:LEU:O | 1:F:60:ALA:N | 2.43 | 0.46 |
| 1:C:33:GLN:HE21 | 1:C:33:GLN:HB2 | 1.17 | 0.45 |
| 1:D:181:THR:O | 1:D:183:CYS:N | 2.49 | 0.45 |
| 1:E:71:LEU:HA | 1:E:71:LEU:HD23 | 1.75 | 0.45 |
| 1:E:113:SER:HB3 | 1:E:114:ASN:H | 1.65 | 0.45 |
| 1:E:193:MET:H | 1:E:206:SER:CB | 2.29 | 0.45 |
| 1:F:23:LEU:HD23 | 1:F:23:LEU:HA | 1.57 | 0.45 |
| 1:F:217:PHE:HZ | 1:F:225:LEU:HD23 | 1.74 | 0.45 |
| 1:B:18:HIS:HB2 | 1:B:21:GLN:HG3 | 1.98 | 0.45 |
| 1:B:103:TYR:CE1 | 1:B:216:VAL:HB | 2.51 | 0.45 |
| 1:D:67:LEU:HD13 | 1:D:69:VAL:HG13 | 1.98 | 0.45 |
| 1:D:68:LEU:HD23 | 1:D:79:TRP:HZ3 | 1.81 | 0.45 |
| 1:F:99:THR:O | 1:F:99:THR:HG23 | 2.16 | 0.45 |
| 1:A:112:THR:H | 1:A:224:ASN:ND2 | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:187:LEU:HD12 | 1:A:191:GLY:HA2 | 1.98 | 0.45 |
| 1:B:193:MET:N | 1:B:206:SER:HB3 | 2.31 | 0.45 |
| 1:D:62:LEU:O | 1:D:63:GLN:O | 2.34 | 0.45 |
| 1:E:172:TRP:CG | 1:E:173:SER:N | 2.84 | 0.45 |
| 1:B:216:VAL:O | 1:B:217:PHE:CB | 2.58 | 0.45 |
| 1:D:4:LEU:HD22 | 1:D:17:LEU:HD21 | 1.98 | 0.45 |
| 1:D:84:LYS:O | 1:D:84:LYS:CG | 2.64 | 0.45 |
| 1:E:23:LEU:O | 1:E:29:ARG:HA | 2.17 | 0.45 |
| 1:F:17:LEU:HA | 1:F:17:LEU:HD23 | 1.74 | 0.45 |
| 1:F:192:ARG:HA | 1:F:206:SER:OG | 2.16 | 0.45 |
| 1:A:150:SER:OG | 1:A:151:PRO:HD3 | 2.17 | 0.45 |
| 1:B:132:GLN:CG | 1:B:214:ARG:HH12 | 2.28 | 0.45 |
| 1:D:129:TYR:CD2 | 1:D:215:TYR:O | 2.68 | 0.45 |
| 1:F:28:PHE:HE2 | 1:F:42:ASP:OD2 | 1.99 | 0.45 |
| 1:F:184:ARG:HB2 | 1:F:185:ALA:H | 1.20 | 0.45 |
| 1:B:60:ALA:HB2 | 1:B:70:ILE:HD12 | 1.98 | 0.45 |
| 1:C:143:ALA:HA | 1:C:156:MET:O | 2.16 | 0.45 |
| 1:D:166:ASP:HB2 | 1:D:171:VAL:HG11 | 1.99 | 0.45 |
| 1:F:217:PHE:C | 1:F:217:PHE:HD2 | 2.13 | 0.45 |
| 1:A:223:ARG:NH1 | 1:A:223:ARG:HB3 | 2.25 | 0.45 |
| 1:C:78:ARG:HH11 | 1:C:78:ARG:HD2 | 1.39 | 0.45 |
| 1:E:149:LEU:CD1 | 1:E:221:PRO:HA | 2.47 | 0.45 |
| 1:F:31:THR:CG2 | 1:F:39:VAL:O | 2.64 | 0.45 |
| 1:B:48:TRP:CE2 | 1:B:235:THR:HG21 | 2.50 | 0.45 |
| 1:C:92:LEU:CD2 | 1:C:100:VAL:HG13 | 2.44 | 0.45 |
| 1:D:23:LEU:HD12 | 1:D:30:PHE:HD2 | 1.81 | 0.45 |
| 1:E:63:GLN:O | 1:E:65:ASP:N | 2.50 | 0.45 |
| 1:E:78:ARG:O | 1:E:79:TRP:HB2 | 2.16 | 0.45 |
| 1:E:95:GLN:HE21 | 1:E:95:GLN:HB2 | 1.45 | 0.45 |
| 1:E:119:VAL:CG2 | 1:E:151:PRO:CD | 2.95 | 0.45 |
| 1:B:161:ASN:HD22 | 1:B:161:ASN:HA | 1.46 | 0.45 |
| 1:C:9:HIS:HB3 | 1:C:10:GLU:H | 1.58 | 0.45 |
| 1:D:201:ILE:HD13 | 1:D:201:ILE:HG23 | 1.73 | 0.45 |
| 1:E:162:LEU:HD12 | 1:E:174:THR:CG2 | 2.47 | 0.45 |
| 1:F:44:ASP:O | 1:F:45:VAL:HG23 | 2.17 | 0.45 |
| 1:F:176:THR:CG2 | 1:F:203:VAL:HG22 | 2.47 | 0.45 |
| 1:B:106:GLY:O | 1:B:107:LEU:CB | 2.61 | 0.44 |
| 1:B:208:ASN:HB2 | 1:B:209:SER:H | 1.40 | 0.44 |
| 1:D:19:ALA:O | 1:D:32:MET:O | 2.35 | 0.44 |
| 1:D:31:THR:O | 1:D:38:LEU:HD12 | 2.16 | 0.44 |
| 1:E:153:ARG:NH2 | 1:E:165:PHE:CE1 | 2.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:18:HIS:O | 1:F:32:MET:CB | 2.65 | 0.44 |
| 1:F:197:THR:HG21 | 1:F:201:ILE:CD1 | 2.42 | 0.44 |
| 1:A:48:TRP:CE3 | 1:A:49:ALA:HA | 2.53 | 0.44 |
| 1:B:5:PHE:HE2 | 1:B:220:GLN:NE2 | 2.15 | 0.44 |
| 1:B:63:GLN:HE22 | 1:B:69:VAL:HG22 | 1.82 | 0.44 |
| 1:D:52:THR:HG21 | 1:D:79:TRP:HB2 | 1.99 | 0.44 |
| 1:D:112:THR:HG21 | 1:D:172:TRP:HB2 | 1.99 | 0.44 |
| 1:F:215:TYR:N | 1:F:215:TYR:CD2 | 2.84 | 0.44 |
| 1:B:9:HIS:HB2 | 1:B:10:GLU:HB2 | 1.99 | 0.44 |
| 1:B:162:LEU:HD23 | 1:B:162:LEU:HA | 1.73 | 0.44 |
| 1:B:220:GLN:O | 1:B:221:PRO:C | 2.54 | 0.44 |
| 1:D:81:SER:OG | 1:D:82:GLY:N | 2.50 | 0.44 |
| 1:E:29:ARG:HH21 | 1:E:31:THR:HG23 | 1.82 | 0.44 |
| 1:E:30:PHE:CD1 | 1:E:100:VAL:HG21 | 2.52 | 0.44 |
| 1:F:42:ASP:OD2 | 1:F:98:ARG:NH1 | 2.43 | 0.44 |
| 1:A:3:ILE:H | 1:A:3:ILE:HG22 | 1.22 | 0.44 |
| 1:A:232:LEU:O | 1:A:233:TRP:HB2 | 2.17 | 0.44 |
| 1:B:65:ASP:O | 1:B:66:GLY:C | 2.56 | 0.44 |
| 1:D:150:SER:HB3 | 1:D:151:PRO:HD2 | 1.97 | 0.44 |
| 1:D:193:MET:HA | 1:D:193:MET:CE | 2.47 | 0.44 |
| 1:D:217:PHE:CZ | 1:D:225:LEU:CD1 | 2.96 | 0.44 |
| 1:F:159:ASP:OD2 | 1:F:161:ASN:HB2 | 2.17 | 0.44 |
| 1:A:116:GLY:O | 1:A:118:VAL:HG23 | 2.18 | 0.44 |
| 1:B:139:GLN:HE21 | 1:B:139:GLN:HB2 | 1.48 | 0.44 |
| 1:C:92:LEU:HA | 1:C:102:ILE:HA | 1.99 | 0.44 |
| 1:C:137:HIS:H | 1:C:137:HIS:HD2 | 1.63 | 0.44 |
| 1:A:96:PRO:HG2 | 1:A:136:ASN:HA | 1.99 | 0.44 |
| 1:A:150:SER:H | 1:A:152:TYR:HB2 | 1.83 | 0.44 |
| 1:B:10:GLU:OE2 | 1:B:222:ASP:OD2 | 2.36 | 0.44 |
| 1:C:25:LEU:O | 1:C:28:PHE:N | 2.47 | 0.44 |
| 1:C:38:LEU:O | 1:C:39:VAL:HG23 | 2.18 | 0.44 |
| 1:C:74:GLN:H | 1:F:189:PRO:HG2 | 1.67 | 0.44 |
| 1:D:2:ASN:HB2 | 1:D:94:LEU:HB3 | 1.99 | 0.44 |
| 1:E:61:VAL:CG2 | 1:E:62:LEU:H | 2.25 | 0.44 |
| 1:F:180:GLY:O | 1:F:181:THR:CB | 2.60 | 0.44 |
| 1:F:208:ASN:OD1 | 1:F:208:ASN:N | 2.50 | 0.44 |
| 1:A:101:THR:HG22 | 1:A:103:TYR:CE1 | 2.52 | 0.44 |
| 1:B:86:SER:HB3 | 1:B:87:ILE:H | 1.06 | 0.44 |
| 1:D:150:SER:N | 1:D:152:TYR:H | 2.10 | 0.44 |
| 1:F:217:PHE:CD2 | 1:F:218:VAL:N | 2.86 | 0.44 |
| 1:C:193:MET:N | 1:C:206:SER:HB3 | 2.28 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:21:GLN:HE21 | 1:E:21:GLN:HB2 | 1.18 | 0.44 |
| 1:E:130:SER:HA | 1:E:139:GLN:OE1 | 2.17 | 0.44 |
| 1:A:112:THR:OG1 | 1:A:223:ARG:O | 2.36 | 0.44 |
| 1:A:176:THR:HG23 | 1:A:176:THR:O | 2.18 | 0.44 |
| 1:A:199:GLN:HG2 | 1:A:201:ILE:HD12 | 1.99 | 0.44 |
| 1:B:63:GLN:HE21 | 1:B:63:GLN:HB2 | 1.26 | 0.44 |
| 1:D:162:LEU:HD23 | 1:D:162:LEU:HA | 1.72 | 0.44 |
| 1:E:200:ASN:N | 1:E:200:ASN:ND2 | 2.64 | 0.44 |
| 1:D:33:GLN:HB2 | 1:D:37:ASN:O | 2.18 | 0.43 |
| 1:E:29:ARG:NH2 | 1:E:41:PHE:CD1 | 2.86 | 0.43 |
| 1:E:37:ASN:HA | 1:E:52:THR:HG1 | 1.83 | 0.43 |
| 1:E:163:VAL:HB | 1:E:173:SER:OG | 2.17 | 0.43 |
| 1:E:172:TRP:CH2 | 1:E:174:THR:HG22 | 2.53 | 0.43 |
| 1:E:179:LYS:NZ | 1:E:203:VAL:HG13 | 2.32 | 0.43 |
| 1:E:223:ARG:CG | 1:E:223:ARG:HH11 | 2.29 | 0.43 |
| 1:F:174:THR:HG22 | 1:F:204:TRP:NE1 | 2.33 | 0.43 |
| 1:A:147:LEU:HA | 1:A:147:LEU:HD12 | 1.79 | 0.43 |
| 1:F:127:ILE:HD13 | 1:F:127:ILE:HG21 | 1.74 | 0.43 |
| 1:F:152:TYR:HD2 | 1:F:166:ASP:HB2 | 1.83 | 0.43 |
| 1:A:65:ASP:N | 1:A:65:ASP:OD1 | 2.51 | 0.43 |
| 1:A:75:ASN:HD22 | 1:D:196:LEU:CD1 | 2.31 | 0.43 |
| 1:A:193:MET:H | 1:A:206:SER:HB3 | 1.83 | 0.43 |
| 1:C:48:TRP:CG | 1:C:49:ALA:N | 2.86 | 0.43 |
| 1:C:83:THR:HG22 | 1:C:84:LYS:N | 2.25 | 0.43 |
| 1:C:140:THR:HG1 | 1:C:141:LEU:H | 1.63 | 0.43 |
| 1:C:155:SER:O | 1:C:163:VAL:N | 2.45 | 0.43 |
| 1:C:188:GLN:HA | 1:C:189:PRO:HD3 | 1.77 | 0.43 |
| 1:C:205:THR:O | 1:C:205:THR:CG2 | 2.53 | 0.43 |
| 1:D:50:SER:O | 1:D:51:ASN:HB3 | 2.18 | 0.43 |
| 1:E:72:THR:CG2 | 1:E:74:GLN:H | 2.31 | 0.43 |
| 1:E:141:LEU:CD1 | 1:E:147:LEU:HD23 | 2.48 | 0.43 |
| 1:F:142:HIS:HD2 | 1:F:145:GLN:CD | 2.22 | 0.43 |
| 1:F:166:ASP:O | 1:F:167:ARG:O | 2.36 | 0.43 |
| 1:A:50:SER:O | 1:A:51:ASN:CB | 2.64 | 0.43 |
| 1:B:153:ARG:HG3 | 1:B:165:PHE:HB2 | 2.01 | 0.43 |
| 1:B:210:ARG:HG3 | 1:B:211:SER:H | 1.84 | 0.43 |
| 1:C:138:PRO:C | 1:C:140:THR:H | 2.20 | 0.43 |
| 1:D:63:GLN:HB3 | 1:D:67:LEU:H | 1.83 | 0.43 |
| 1:D:113:SER:OG | 1:D:114:ASN:N | 2.50 | 0.43 |
| 1:D:161:ASN:HD21 | 1:D:175:ASN:N | 2.17 | 0.43 |
| 1:F:156:MET:CE | 1:F:161:ASN:O | 2.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:185:ALA:O | 1:F:186:VAL:CG1 | 2.66 | 0.43 |
| 1:B:129:TYR:CD1 | 1:B:131:THR:N | 2.87 | 0.43 |
| 1:C:74:GLN:HG3 | 1:C:74:GLN:H | 1.47 | 0.43 |
| 1:C:113:SER:HA | 1:C:222:ASP:HB2 | 2.01 | 0.43 |
| 1:D:164:LEU:HA | 1:D:164:LEU:HD23 | 1.71 | 0.43 |
| 1:E:9:HIS:CD2 | 1:E:10:GLU:HB2 | 2.52 | 0.43 |
| 1:E:166:ASP:O | 1:E:167:ARG:C | 2.57 | 0.43 |
| 1:A:224:ASN:HD22 | 1:A:224:ASN:HA | 1.37 | 0.43 |
| 1:B:35:ASP:O | 1:B:53:ALA:HA | 2.19 | 0.43 |
| 1:B:164:LEU:HD12 | 1:B:172:TRP:HB3 | 2.01 | 0.43 |
| 1:B:193:MET:HG3 | 1:B:204:TRP:HZ3 | 1.83 | 0.43 |
| 1:C:35:ASP:O | 1:C:36:CYS:HB2 | 2.18 | 0.43 |
| 1:C:67:LEU:HD22 | 1:C:80:SER:OG | 2.18 | 0.43 |
| 1:D:187:LEU:CD2 | 1:D:217:PHE:CB | 2.96 | 0.43 |
| 1:E:91:VAL:HG21 | 1:E:228:TYR:CD2 | 2.53 | 0.43 |
| 1:B:157:GLU:HG3 | 1:B:161:ASN:CB | 2.40 | 0.43 |
| 1:B:193:MET:CG | 1:B:204:TRP:CZ3 | 3.02 | 0.43 |
| 1:C:95:GLN:NE2 | 1:C:99:THR:HG22 | 2.33 | 0.43 |
| 1:F:44:ASP:O | 1:F:45:VAL:CB | 2.66 | 0.43 |
| 1:F:186:VAL:HG22 | 1:F:194:ASP:HB3 | 2.00 | 0.43 |
| 1:B:168:ASP:O | 1:B:169:ASP:CB | 2.64 | 0.43 |
| 1:F:190:ASN:OD1 | 1:F:190:ASN:C | 2.57 | 0.43 |
| 1:A:44:ASP:O | 1:A:45:VAL:C | 2.56 | 0.43 |
| 1:D:30:PHE:CD1 | 1:D:30:PHE:C | 2.84 | 0.43 |
| 1:E:87:ILE:HA | 1:E:87:ILE:HD12 | 1.82 | 0.43 |
| 1:E:189:PRO:O | 1:E:213:GLY:O | 2.37 | 0.43 |
| 1:F:77:ILE:HD13 | 1:F:77:ILE:HG21 | 1.73 | 0.43 |
| 1:F:154:LEU:CG | 1:F:225:LEU:HD21 | 2.49 | 0.43 |
| 1:A:19:ALA:O | 1:A:20:ALA:HB2 | 2.19 | 0.43 |
| 1:A:217:PHE:CD1 | 1:A:227:ILE:HG22 | 2.53 | 0.43 |
| 1:B:92:LEU:HA | 1:B:102:ILE:HG13 | 2.01 | 0.43 |
| 1:D:64:SER:OG | 1:D:64:SER:C | 2.56 | 0.43 |
| 1:D:153:ARG:HH21 | 1:D:165:PHE:HE1 | 1.67 | 0.43 |
| 1:E:158:THR:OG1 | 1:F:151:PRO:CG | 2.56 | 0.43 |
| 1:E:159:ASP:HB2 | 1:E:177:ALA:HB1 | 2.01 | 0.43 |
| 1:E:232:LEU:O | 1:E:233:TRP:HB2 | 2.19 | 0.43 |
| 1:B:29:ARG:NH2 | 1:B:41:PHE:CE1 | 2.87 | 0.42 |
| 1:B:201:ILE:O | 1:B:202:ALA:HB2 | 2.19 | 0.42 |
| 1:C:68:LEU:O | 1:C:79:TRP:HZ3 | 2.02 | 0.42 |
| 1:C:107:LEU:HD12 | 1:C:107:LEU:O | 2.19 | 0.42 |
| 1:D:46:ARG:O | 1:D:47:VAL:HG13 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:83:THR:O | 1:D:84:LYS:CB | 2.38 | 0.42 |
| 1:F:18:HIS:O | 1:F:32:MET:HB3 | 2.18 | 0.42 |
| 1:B:110:SER:O | 1:B:112:THR:HG22 | 2.18 | 0.42 |
| 1:E:154:LEU:HD23 | 1:E:225:LEU:HD11 | 2.00 | 0.42 |
| 1:A:128:LEU:O | 1:A:129:TYR:CD2 | 2.72 | 0.42 |
| 1:B:129:TYR:O | 1:B:187:LEU:O | 2.37 | 0.42 |
| 1:B:174:THR:OG1 | 1:B:176:THR:HB | 2.19 | 0.42 |
| 1:B:220:GLN:CB | 1:B:221:PRO:HD2 | 2.49 | 0.42 |
| 1:C:49:ALA:O | 1:C:50:SER:O | 2.38 | 0.42 |
| 1:C:52:THR:HG21 | 1:C:79:TRP:CB | 2.48 | 0.42 |
| 1:C:71:LEU:HA | 1:C:71:LEU:HD23 | 1.71 | 0.42 |
| 1:C:101:THR:HG21 | 1:C:103:TYR:CE1 | 2.54 | 0.42 |
| 1:C:174:THR:HB | 1:C:204:TRP:CG | 2.55 | 0.42 |
| 1:D:217:PHE:CD2 | 1:D:218:VAL:N | 2.88 | 0.42 |
| 1:F:16:THR:CG2 | 1:F:17:LEU:N | 2.70 | 0.42 |
| 1:B:152:TYR:HE1 | 1:B:220:GLN:O | 2.03 | 0.42 |
| 1:B:210:ARG:CG | 1:B:211:SER:H | 2.32 | 0.42 |
| 1:C:61:VAL:HG12 | 1:C:62:LEU:H | 1.78 | 0.42 |
| 1:C:73:ALA:HB1 | 1:F:189:PRO:CB | 2.47 | 0.42 |
| 1:D:94:LEU:C | 1:D:94:LEU:HD12 | 2.31 | 0.42 |
| 1:D:204:TRP:C | 1:D:205:THR:HG22 | 2.40 | 0.42 |
| 1:E:211:SER:O | 1:E:212:ALA:C | 2.57 | 0.42 |
| 1:F:199:GLN:O | 1:F:200:ASN:CB | 2.67 | 0.42 |
| 1:A:50:SER:O | 1:A:51:ASN:HB2 | 2.20 | 0.42 |
| 1:B:163:VAL:HG12 | 1:B:173:SER:OG | 2.19 | 0.42 |
| 1:C:41:PHE:HD2 | 1:C:45:VAL:H | 1.67 | 0.42 |
| 1:C:221:PRO:O | 1:C:223:ARG:N | 2.52 | 0.42 |
| 1:D:137:HIS:CB | 1:D:138:PRO:C | 2.88 | 0.42 |
| 1:E:158:THR:OG1 | 1:F:151:PRO:HD3 | 2.17 | 0.42 |
| 1:F:7:LEU:H | 1:F:7:LEU:HG | 1.37 | 0.42 |
| 1:F:16:THR:HG23 | 1:F:61:VAL:N | 2.34 | 0.42 |
| 1:F:30:PHE:CE1 | 1:F:38:LEU:HG | 2.54 | 0.42 |
| 1:A:151:PRO:HD2 | 1:A:152:TYR:CG | 2.55 | 0.42 |
| 1:B:77:ILE:O | 1:B:78:ARG:HD2 | 2.20 | 0.42 |
| 1:B:172:TRP:CE3 | 1:B:172:TRP:C | 2.93 | 0.42 |
| 1:B:208:ASN:OD1 | 1:B:208:ASN:N | 2.52 | 0.42 |
| 1:C:127:ILE:HA | 1:C:138:PRO:HG2 | 2.00 | 0.42 |
| 1:E:142:HIS:HB2 | 1:E:145:GLN:CG | 2.50 | 0.42 |
| 1:F:68:LEU:C | 1:F:68:LEU:HD23 | 2.38 | 0.42 |
| 1:A:48:TRP:CG | 1:A:235:THR:HG22 | 2.55 | 0.42 |
| 1:D:153:ARG:O | 1:D:164:LEU:HD23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:207:GLY:C | 1:E:208:ASN:O | 2.50 | 0.42 |
| 1:E:217:PHE:HA | 1:E:227:ILE:HB | 2.01 | 0.42 |
| 1:A:70:ILE:O | 1:A:78:ARG:N | 2.48 | 0.42 |
| 1:A:109:ASP:HB2 | 1:A:110:SER:H | 1.66 | 0.42 |
| 1:D:11:GLY:O | 1:D:13:HIS:N | 2.52 | 0.42 |
| 1:D:56:THR:HG22 | 1:D:57:GLY:CA | 2.49 | 0.42 |
| 1:E:100:VAL:N | 1:E:235:THR:HG21 | 2.31 | 0.42 |
| 1:F:32:MET:HE2 | 1:F:38:LEU:HB2 | 2.01 | 0.42 |
| 1:F:143:ALA:CA | 1:F:156:MET:O | 2.65 | 0.42 |
| 1:A:74:GLN:HA | 1:D:189:PRO:HD3 | 2.02 | 0.42 |
| 1:B:154:LEU:HD21 | 1:B:225:LEU:HD11 | 2.02 | 0.42 |
| 1:D:223:ARG:HH11 | 1:D:223:ARG:CG | 2.27 | 0.42 |
| 1:E:199:GLN:HE21 | 1:E:199:GLN:CA | 2.33 | 0.42 |
| 1:E:219:LEU:HA | 1:E:219:LEU:HD12 | 1.65 | 0.42 |
| 1:F:29:ARG:O | 1:F:41:PHE:N | 2.40 | 0.42 |
| 1:A:128:LEU:HD11 | 2:A:244:HOH:O | 2.19 | 0.42 |
| 1:B:190:ASN:OD1 | 1:B:190:ASN:C | 2.58 | 0.42 |
| 1:D:67:LEU:HD13 | 1:D:69:VAL:CG1 | 2.50 | 0.42 |
| 1:D:166:ASP:OD2 | 1:D:223:ARG:HD2 | 2.19 | 0.42 |
| 1:A:160:CYS:O | 1:A:160:CYS:SG | 2.77 | 0.41 |
| 1:B:59:ARG:NH2 | 1:B:71:LEU:CD1 | 2.83 | 0.41 |
| 1:B:220:GLN:HB2 | 1:B:221:PRO:HD2 | 2.02 | 0.41 |
| 1:C:81:SER:O | 1:C:82:GLY:C | 2.58 | 0.41 |
| 1:C:171:VAL:O | 1:C:171:VAL:HG23 | 2.19 | 0.41 |
| 1:C:183:CYS:HB3 | 1:C:196:LEU:O | 2.20 | 0.41 |
| 1:C:195:VAL:HG22 | 1:C:203:VAL:HG12 | 2.02 | 0.41 |
| 1:D:160:CYS:O | 1:D:176:THR:CG2 | 2.67 | 0.41 |
| 1:D:197:THR:O | 1:D:199:GLN:N | 2.53 | 0.41 |
| 1:E:24:GLU:HG2 | 1:E:29:ARG:HB3 | 2.01 | 0.41 |
| 1:E:102:ILE:HD12 | 1:E:233:TRP:HE3 | 1.85 | 0.41 |
| 1:D:85:GLY:O | 1:D:86:SER:O | 2.38 | 0.41 |
| 1:F:97:ASP:N | 1:F:97:ASP:OD1 | 2.52 | 0.41 |
| 1:A:92:LEU:HG | 1:A:100:VAL:HG12 | 2.01 | 0.41 |
| 1:A:101:THR:C | 1:A:102:ILE:HG13 | 2.32 | 0.41 |
| 1:A:161:ASN:HD21 | 1:A:175:ASN:CA | 2.34 | 0.41 |
| 1:C:130:SER:H | 1:C:131:THR:HG23 | 1.85 | 0.41 |
| 1:C:142:HIS:O | 1:C:156:MET:HG3 | 2.20 | 0.41 |
| 1:C:210:ARG:NH1 | 1:C:229:GLY:O | 2.54 | 0.41 |
| 1:D:95:GLN:HG2 | 1:D:128:LEU:HD23 | 2.03 | 0.41 |
| 1:E:158:THR:C | 1:F:151:PRO:CG | 2.82 | 0.41 |
| 1:F:95:GLN:HE21 | 1:F:99:THR:HG21 | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:183:CYS:HA | 1:F:196:LEU:O | 2.20 | 0.41 |
| 1:B:48:TRP:CZ2 | 1:B:235:THR:HG21 | 2.55 | 0.41 |
| 1:D:205:THR:O | 1:D:206:SER:C | 2.59 | 0.41 |
| 1:E:165:PHE:CE2 | 1:E:170:ARG:HG3 | 2.50 | 0.41 |
| 1:F:65:ASP:OD1 | 1:F:67:LEU:HD13 | 2.20 | 0.41 |
| 1:F:76:THR:O | 1:F:76:THR:OG1 | 2.29 | 0.41 |
| 1:F:85:GLY:O | 1:F:86:SER:O | 2.39 | 0.41 |
| 1:F:87:ILE:HG23 | 1:F:88:GLY:H | 1.68 | 0.41 |
| 1:F:95:GLN:HE21 | 1:F:99:THR:HG23 | 1.85 | 0.41 |
| 1:C:23:LEU:HD23 | 1:C:23:LEU:HA | 1.37 | 0.41 |
| 1:C:73:ALA:HB1 | 1:F:189:PRO:HB3 | 2.02 | 0.41 |
| 1:E:35:ASP:O | 1:E:37:ASN:N | 2.54 | 0.41 |
| 1:F:47:VAL:O | 1:F:47:VAL:HG12 | 2.20 | 0.41 |
| 1:F:142:HIS:CD2 | 1:F:142:HIS:H | 2.39 | 0.41 |
| 1:A:25:LEU:N | 1:A:94:LEU:HD23 | 2.35 | 0.41 |
| 1:A:161:ASN:HA | 1:A:176:THR:HG22 | 2.03 | 0.41 |
| 1:B:16:THR:HG22 | 1:B:59:ARG:HG3 | 2.01 | 0.41 |
| 1:B:39:VAL:CG1 | 1:B:40:LEU:N | 2.81 | 0.41 |
| 1:D:142:HIS:HB2 | 1:D:145:GLN:CB | 2.51 | 0.41 |
| 1:D:162:LEU:N | 1:D:174:THR:OG1 | 2.37 | 0.41 |
| 1:D:174:THR:HB | 1:D:176:THR:HB | 2.03 | 0.41 |
| 1:D:189:PRO:HD2 | 1:D:190:ASN:H | 1.86 | 0.41 |
| 1:E:18:HIS:H | 1:E:21:GLN:CB | 2.34 | 0.41 |
| 1:F:40:LEU:HD12 | 1:F:40:LEU:HA | 1.44 | 0.41 |
| 1:F:156:MET:HE3 | 1:F:161:ASN:O | 2.21 | 0.41 |
| 1:F:217:PHE:CE2 | 1:F:225:LEU:HB3 | 2.56 | 0.41 |
| 1:C:25:LEU:HD13 | 1:C:25:LEU:HA | 1.75 | 0.41 |
| 1:C:137:HIS:HB2 | 1:C:138:PRO:HA | 2.03 | 0.41 |
| 1:E:120:VAL:HG22 | 1:E:122:ASN:O | 2.20 | 0.41 |
| 1:E:196:LEU:HD12 | 1:E:202:ALA:HB2 | 2.02 | 0.41 |
| 1:C:195:VAL:HG13 | 1:C:204:TRP:HE3 | 1.85 | 0.41 |
| 1:D:187:LEU:HD11 | 1:D:215:TYR:HB3 | 2.03 | 0.41 |
| 1:E:26:SER:O | 1:E:26:SER:OG | 2.32 | 0.41 |
| 1:E:52:THR:HB | 1:E:78:ARG:HH11 | 1.86 | 0.41 |
| 1:E:119:VAL:HG21 | 1:E:151:PRO:CD | 2.47 | 0.41 |
| 1:E:120:VAL:HG23 | 1:E:149:LEU:CD2 | 2.50 | 0.41 |
| 1:F:204:TRP:CH2 | 1:F:206:SER:N | 2.89 | 0.41 |
| 1:A:102:ILE:HB | 1:A:232:LEU:HB3 | 2.03 | 0.41 |
| 1:A:124:GLY:HA2 | 1:A:125:ASN:HD22 | 1.86 | 0.41 |
| 1:A:124:GLY:HA2 | 1:A:125:ASN:ND2 | 2.35 | 0.41 |
| 1:A:156:MET:CE | 1:A:156:MET:CA | 2.99 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:172:TRP:O | 1:A:173:SER:HB2 | 2.17 | 0.41 |
| 1:A:188:GLN:CG | 1:A:189:PRO:CD | 2.99 | 0.41 |
| 1:B:197:THR:H | 1:B:197:THR:HG22 | 1.66 | 0.41 |
| 1:E:182:GLY:HA3 | 1:E:198:ASN:N | 2.35 | 0.41 |
| 1:F:19:ALA:O | 1:F:32:MET:O | 2.39 | 0.41 |
| 1:F:47:VAL:O | 1:F:47:VAL:CG1 | 2.68 | 0.41 |
| 1:F:76:THR:O | 1:F:77:ILE:HB | 2.08 | 0.41 |
| 1:F:161:ASN:HD21 | 1:F:176:THR:N | 2.14 | 0.41 |
| 1:A:72:THR:CG2 | 1:A:76:THR:H | 1.94 | 0.41 |
| 1:A:179:LYS:HE3 | 1:A:203:VAL:HG22 | 2.03 | 0.41 |
| 1:C:69:VAL:H | 1:C:69:VAL:HG22 | 1.69 | 0.41 |
| 1:C:72:THR:HG22 | 1:C:72:THR:H | 1.51 | 0.41 |
| 1:C:104:GLY:HA2 | 1:C:105:PRO:O | 2.21 | 0.41 |
| 1:C:210:ARG:HH11 | 1:C:210:ARG:HD2 | 1.61 | 0.41 |
| 1:D:215:TYR:O | 1:D:216:VAL:CB | 2.69 | 0.41 |
| 1:E:17:LEU:HA | 1:E:17:LEU:HD23 | 1.66 | 0.41 |
| 1:F:127:ILE:C | 1:F:128:LEU:O | 2.54 | 0.41 |
| 1:A:3:ILE:CD1 | 1:A:218:VAL:HG11 | 2.50 | 0.40 |
| 1:A:166:ASP:OD2 | 1:A:223:ARG:HD2 | 2.20 | 0.40 |
| 1:B:22:SER:CA | 1:B:31:THR:HA | 2.40 | 0.40 |
| 1:C:87:ILE:CG2 | 1:C:88:GLY:N | 2.84 | 0.40 |
| 1:C:127:ILE:HG23 | 1:C:217:PHE:HB3 | 1.96 | 0.40 |
| 1:D:187:LEU:CD1 | 1:D:227:ILE:HD12 | 2.51 | 0.40 |
| 1:E:158:THR:O | 1:E:159:ASP:C | 2.40 | 0.40 |
| 1:A:28:PHE:N | 1:A:28:PHE:CD2 | 2.88 | 0.40 |
| 1:A:196:LEU:CD1 | 1:A:202:ALA:CB | 2.95 | 0.40 |
| 1:C:35:ASP:O | 1:C:36:CYS:CB | 2.69 | 0.40 |
| 1:D:78:ARG:O | 1:D:79:TRP:HB2 | 2.21 | 0.40 |
| 1:D:233:TRP:CG | 1:D:234:THR:N | 2.85 | 0.40 |
| 1:E:32:MET:HE1 | 1:E:70:ILE:HG23 | 2.02 | 0.40 |
| 1:E:129:TYR:HE1 | 1:E:131:THR:N | 2.18 | 0.40 |
| 1:F:44:ASP:OD1 | 1:F:45:VAL:N | 2.54 | 0.40 |
| 1:A:4:LEU:CD1 | 1:A:17:LEU:HD21 | 2.51 | 0.40 |
| 1:A:153:ARG:NH1 | 1:A:165:PHE:CD1 | 2.89 | 0.40 |
| 1:A:214:ARG:C | 1:A:215:TYR:HD2 | 2.21 | 0.40 |
| 1:B:39:VAL:HG12 | 1:B:40:LEU:N | 2.33 | 0.40 |
| 1:B:149:LEU:HD12 | 1:B:219:LEU:HG | 2.04 | 0.40 |
| 1:D:128:LEU:O | 1:D:129:TYR:CD2 | 2.75 | 0.40 |
| 1:B:187:LEU:HD22 | 1:B:217:PHE:HB2 | 2.04 | 0.40 |
| 1:C:137:HIS:HB3 | 1:C:138:PRO:C | 2.42 | 0.40 |
| 1:D:225:LEU:HD23 | 1:D:225:LEU:HA | 1.60 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:129:TYR:CD1 | 1:E:129:TYR:C | 2.95 | 0.40 |
| 1:E:156:MET:CE | 1:E:183:CYS:HB3 | 2.52 | 0.40 |
| 1:F:143:ALA:O | 1:F:144:THR:HG22 | 2.22 | 0.40 |
| 1:B:220:GLN:HA | 1:B:221:PRO:HD3 | 1.76 | 0.40 |
| 1:C:193:MET:O | 1:C:206:SER:N | 2.38 | 0.40 |
| 1:F:191:GLY:HA2 | 1:F:227:ILE:CD1 | 2.51 | 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 | 229/236 (97%) | 158 (69%) | 41 (18%) | 30 (13%) | 0 1 |
| 1 | B | 213/236 (90%) | 132 (62%) | 42 (20%) | 39 (18%) | 0 1 |
| 1 | C | 230/236 (98%) | 150 (65%) | 42 (18%) | 38 (16%) | 0 1 |
| 1 | D | 217/236 (92%) | 148 (68%) | 30 (14%) | 39 (18%) | 0 1 |
| 1 | E | 227/236 (96%) | 150 (66%) | 39 (17%) | 38 (17%) | 0 1 |
| 1 | F | 208/236 (88%) | 138 (66%) | 37 (18%) | 33 (16%) | 0 1 |
| All | All | 1324/1416 (94%) | 876 (66%) | 231 (17%) | 217 (16%) | 0 1 |

All (217) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 10 | GLU |
| 1 | A | 11 | GLY |
| 1 | A | 14 | PRO |
| 1 | A | 19 | ALA |
| 1 | A | 20 | ALA |
| 1 | A | 34 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 45 | VAL |
| 1 | A | 61 | VAL |
| 1 | A | 73 | ALA |
| 1 | A | 77 | ILE |
| 1 | A | 88 | GLY |
| 1 | A | 105 | PRO |
| 1 | A | 119 | VAL |
| 1 | A | 120 | VAL |
| 1 | A | 122 | ASN |
| 1 | A | 138 | PRO |
| 1 | A | 198 | ASN |
| 1 | A | 206 | SER |
| 1 | A | 207 | GLY |
| 1 | A | 231 | ALA |
| 1 | B | 7 | LEU |
| 1 | B | 12 | SER |
| 1 | B | 43 | SER |
| 1 | B | 45 | VAL |
| 1 | B | 56 | THR |
| 1 | B | 77 | ILE |
| 1 | B | 81 | SER |
| 1 | B | 86 | SER |
| 1 | B | 87 | ILE |
| 1 | B | 105 | PRO |
| 1 | B | 130 | SER |
| 1 | B | 143 | ALA |
| 1 | B | 144 | THR |
| 1 | B | 147 | LEU |
| 1 | B | 150 | SER |
| 1 | B | 167 | ARG |
| 1 | B | 189 | PRO |
| 1 | B | 196 | LEU |
| 1 | B | 198 | ASN |
| 1 | B | 200 | ASN |
| 1 | B | 201 | ILE |
| 1 | B | 203 | VAL |
| 1 | C | 9 | HIS |
| 1 | C | 26 | SER |
| 1 | C | 36 | CYS |
| 1 | C | 52 | THR |
| 1 | C | 74 | GLN |
| 1 | C | 77 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 88 | GLY |
| 1 | C | 105 | PRO |
| 1 | C | 117 | SER |
| 1 | C | 119 | VAL |
| 1 | C | 120 | VAL |
| 1 | C | 122 | ASN |
| 1 | C | 130 | SER |
| 1 | C | 146 | SER |
| 1 | C | 150 | SER |
| 1 | C | 157 | GLU |
| 1 | C | 167 | ARG |
| 1 | C | 168 | ASP |
| 1 | C | 176 | THR |
| 1 | C | 200 | ASN |
| 1 | C | 207 | GLY |
| 1 | C | 222 | ASP |
| 1 | D | 7 | LEU |
| 1 | D | 9 | HIS |
| 1 | D | 27 | SER |
| 1 | D | 43 | SER |
| 1 | D | 45 | VAL |
| 1 | D | 61 | VAL |
| 1 | D | 63 | GLN |
| 1 | D | 83 | THR |
| 1 | D | 84 | LYS |
| 1 | D | 88 | GLY |
| 1 | D | 125 | ASN |
| 1 | D | 129 | TYR |
| 1 | D | 130 | SER |
| 1 | D | 143 | ALA |
| 1 | D | 147 | LEU |
| 1 | D | 157 | GLU |
| 1 | D | 159 | ASP |
| 1 | D | 169 | ASP |
| 1 | D | 170 | ARG |
| 1 | D | 177 | ALA |
| 1 | D | 179 | LYS |
| 1 | D | 188 | GLN |
| 1 | D | 230 | GLY |
| 1 | E | 7 | LEU |
| 1 | E | 9 | HIS |
| 1 | E | 10 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 12 | SER |
| 1 | E | 13 | HIS |
| 1 | E | 14 | PRO |
| 1 | E | 33 | GLN |
| 1 | E | 36 | CYS |
| 1 | E | 45 | VAL |
| 1 | E | 65 | ASP |
| 1 | E | 86 | SER |
| 1 | E | 88 | GLY |
| 1 | E | 117 | SER |
| 1 | E | 118 | VAL |
| 1 | E | 120 | VAL |
| 1 | E | 129 | TYR |
| 1 | E | 130 | SER |
| 1 | E | 143 | ALA |
| 1 | E | 159 | ASP |
| 1 | E | 160 | CYS |
| 1 | E | 167 | ARG |
| 1 | E | 168 | ASP |
| 1 | E | 183 | CYS |
| 1 | E | 231 | ALA |
| 1 | F | 8 | SER |
| 1 | F | 9 | HIS |
| 1 | F | 14 | PRO |
| 1 | F | 27 | SER |
| 1 | F | 45 | VAL |
| 1 | F | 87 | ILE |
| 1 | F | 125 | ASN |
| 1 | F | 130 | SER |
| 1 | F | 147 | LEU |
| 1 | F | 160 | CYS |
| 1 | F | 194 | ASP |
| 1 | F | 196 | LEU |
| 1 | F | 198 | ASN |
| 1 | F | 200 | ASN |
| 1 | F | 231 | ALA |
| 1 | A | 26 | SER |
| 1 | A | 191 | GLY |
| 1 | A | 232 | LEU |
| 1 | B | 27 | SER |
| 1 | B | 49 | ALA |
| 1 | B | 61 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 83 | THR |
| 1 | B | 107 | LEU |
| 1 | B | 111 | GLY |
| 1 | B | 159 | ASP |
| 1 | B | 188 | GLN |
| 1 | B | 223 | ARG |
| 1 | B | 231 | ALA |
| 1 | C | 27 | SER |
| 1 | C | 45 | VAL |
| 1 | C | 49 | ALA |
| 1 | C | 50 | SER |
| 1 | C | 61 | VAL |
| 1 | C | 73 | ALA |
| 1 | C | 125 | ASN |
| 1 | D | 8 | SER |
| 1 | D | 13 | HIS |
| 1 | D | 77 | ILE |
| 1 | D | 107 | LEU |
| 1 | D | 167 | ARG |
| 1 | D | 168 | ASP |
| 1 | D | 202 | ALA |
| 1 | E | 27 | SER |
| 1 | E | 61 | VAL |
| 1 | E | 147 | LEU |
| 1 | E | 150 | SER |
| 1 | E | 209 | SER |
| 1 | E | 229 | GLY |
| 1 | E | 232 | LEU |
| 1 | F | 7 | LEU |
| 1 | F | 26 | SER |
| 1 | F | 43 | SER |
| 1 | F | 61 | VAL |
| 1 | F | 75 | ASN |
| 1 | F | 81 | SER |
| 1 | F | 88 | GLY |
| 1 | F | 107 | LEU |
| 1 | F | 150 | SER |
| 1 | F | 168 | ASP |
| 1 | F | 190 | ASN |
| 1 | F | 224 | ASN |
| 1 | A | 129 | TYR |
| 1 | A | 150 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 167 | ARG |
| 1 | B | 168 | ASP |
| 1 | C | 140 | THR |
| 1 | C | 170 | ARG |
| 1 | C | 177 | ALA |
| 1 | C | 221 | PRO |
| 1 | D | 44 | ASP |
| 1 | D | 86 | SER |
| 1 | D | 150 | SER |
| 1 | D | 189 | PRO |
| 1 | E | 107 | LEU |
| 1 | E | 138 | PRO |
| 1 | E | 181 | THR |
| 1 | F | 129 | TYR |
| 1 | F | 225 | LEU |
| 1 | A | 9 | HIS |
| 1 | A | 220 | GLN |
| 1 | B | 11 | GLY |
| 1 | B | 36 | CYS |
| 1 | B | 95 | GLN |
| 1 | B | 229 | GLY |
| 1 | C | 10 | GLU |
| 1 | C | 87 | ILE |
| 1 | C | 147 | LEU |
| 1 | D | 144 | THR |
| 1 | E | 79 | TRP |
| 1 | E | 114 | ASN |
| 1 | F | 189 | PRO |
| 1 | F | 211 | SER |
| 1 | A | 168 | ASP |
| 1 | B | 170 | ARG |
| 1 | B | 191 | GLY |
| 1 | D | 28 | PHE |
| 1 | D | 97 | ASP |
| 1 | D | 182 | GLY |
| 1 | E | 211 | SER |
| 1 | F | 64 | SER |
| 1 | C | 189 | PRO |
| 1 | E | 43 | SER |
| 1 | A | 178 | GLY |
| 1 | D | 14 | PRO |
| 1 | C | 118 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 96 | PRO |

### 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 | 197/198 (100%) | 99 (50%) | 98 (50%) | 0 0 |
| 1 | B | 187/198 (94%) | 96 (51%) | 91 (49%) | 0 0 |
| 1 | C | 195/198 (98%) | 111 (57%) | 84 (43%) | 0 0 |
| 1 | D | 187/198 (94%) | 101 (54%) | 86 (46%) | 0 0 |
| 1 | E | 194/198 (98%) | 112 (58%) | 82 (42%) | 0 0 |
| 1 | F | 183/198 (92%) | 108 (59%) | 75 (41%) | 0 0 |
| All | All | 1143/1188 (96%) | 627 (55%) | 516 (45%) | 0 0 |

All (516) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | LEU |
| 1 | A | 5 | PHE |
| 1 | A | 8 | SER |
| 1 | A | 10 | GLU |
| 1 | A | 12 | SER |
| 1 | A | 14 | PRO |
| 1 | A | 17 | LEU |
| 1 | A | 22 | SER |
| 1 | A | 24 | GLU |
| 1 | A | 25 | LEU |
| 1 | A | 27 | SER |
| 1 | A | 30 | PHE |
| 1 | A | 31 | THR |
| 1 | A | 32 | MET |
| 1 | A | 33 | GLN |
| 1 | A | 34 | SER |
| 1 | A | 37 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 38 | LEU |
| 1 | A | 43 | SER |
| 1 | A | 47 | VAL |
| 1 | A | 50 | SER |
| 1 | A | 52 | THR |
| 1 | A | 56 | THR |
| 1 | A | 58 | CYS |
| 1 | A | 59 | ARG |
| 1 | A | 68 | LEU |
| 1 | A | 71 | LEU |
| 1 | A | 74 | GLN |
| 1 | A | 78 | ARG |
| 1 | A | 84 | LYS |
| 1 | A | 87 | ILE |
| 1 | A | 92 | LEU |
| 1 | A | 93 | VAL |
| 1 | A | 94 | LEU |
| 1 | A | 99 | THR |
| 1 | A | 100 | VAL |
| 1 | A | 103 | TYR |
| 1 | A | 105 | PRO |
| 1 | A | 107 | LEU |
| 1 | A | 108 | TRP |
| 1 | A | 109 | ASP |
| 1 | A | 110 | SER |
| 1 | A | 115 | LYS |
| 1 | A | 119 | VAL |
| 1 | A | 120 | VAL |
| 1 | A | 122 | ASN |
| 1 | A | 125 | ASN |
| 1 | A | 129 | TYR |
| 1 | A | 136 | ASN |
| 1 | A | 138 | PRO |
| 1 | A | 141 | LEU |
| 1 | A | 144 | THR |
| 1 | A | 147 | LEU |
| 1 | A | 154 | LEU |
| 1 | A | 155 | SER |
| 1 | A | 156 | MET |
| 1 | A | 157 | GLU |
| 1 | A | 158 | THR |
| 1 | A | 162 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 163 | VAL |
| 1 | A | 164 | LEU |
| 1 | A | 167 | ARG |
| 1 | A | 168 | ASP |
| 1 | A | 169 | ASP |
| 1 | A | 170 | ARG |
| 1 | A | 171 | VAL |
| 1 | A | 173 | SER |
| 1 | A | 174 | THR |
| 1 | A | 175 | ASN |
| 1 | A | 176 | THR |
| 1 | A | 179 | LYS |
| 1 | A | 181 | THR |
| 1 | A | 183 | CYS |
| 1 | A | 184 | ARG |
| 1 | A | 186 | VAL |
| 1 | A | 187 | LEU |
| 1 | A | 188 | GLN |
| 1 | A | 192 | ARG |
| 1 | A | 195 | VAL |
| 1 | A | 196 | LEU |
| 1 | A | 200 | ASN |
| 1 | A | 201 | ILE |
| 1 | A | 203 | VAL |
| 1 | A | 205 | THR |
| 1 | A | 206 | SER |
| 1 | A | 208 | ASN |
| 1 | A | 210 | ARG |
| 1 | A | 215 | TYR |
| 1 | A | 216 | VAL |
| 1 | A | 217 | PHE |
| 1 | A | 218 | VAL |
| 1 | A | 221 | PRO |
| 1 | A | 222 | ASP |
| 1 | A | 223 | ARG |
| 1 | A | 224 | ASN |
| 1 | A | 227 | ILE |
| 1 | A | 232 | LEU |
| 1 | A | 234 | THR |
| 1 | B | 1 | ASN |
| 1 | B | 2 | ASN |
| 1 | B | 3 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 8 | SER |
| 1 | B | 9 | HIS |
| 1 | B | 10 | GLU |
| 1 | B | 12 | SER |
| 1 | B | 16 | THR |
| 1 | B | 21 | GLN |
| 1 | B | 22 | SER |
| 1 | B | 23 | LEU |
| 1 | B | 29 | ARG |
| 1 | B | 30 | PHE |
| 1 | B | 31 | THR |
| 1 | B | 32 | MET |
| 1 | B | 33 | GLN |
| 1 | B | 36 | CYS |
| 1 | B | 45 | VAL |
| 1 | B | 47 | VAL |
| 1 | B | 56 | THR |
| 1 | B | 58 | CYS |
| 1 | B | 59 | ARG |
| 1 | B | 63 | GLN |
| 1 | B | 64 | SER |
| 1 | B | 67 | LEU |
| 1 | B | 68 | LEU |
| 1 | B | 69 | VAL |
| 1 | B | 71 | LEU |
| 1 | B | 76 | THR |
| 1 | B | 78 | ARG |
| 1 | B | 83 | THR |
| 1 | B | 84 | LYS |
| 1 | B | 86 | SER |
| 1 | B | 87 | ILE |
| 1 | B | 90 | TYR |
| 1 | B | 92 | LEU |
| 1 | B | 93 | VAL |
| 1 | B | 94 | LEU |
| 1 | B | 97 | ASP |
| 1 | B | 98 | ARG |
| 1 | B | 105 | PRO |
| 1 | B | 107 | LEU |
| 1 | B | 112 | THR |
| 1 | B | 125 | ASN |
| 1 | B | 126 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 127 | ILE |
| 1 | B | 129 | TYR |
| 1 | B | 130 | SER |
| 1 | B | 132 | GLN |
| 1 | B | 140 | THR |
| 1 | B | 144 | THR |
| 1 | B | 146 | SER |
| 1 | B | 147 | LEU |
| 1 | B | 148 | GLN |
| 1 | B | 149 | LEU |
| 1 | B | 151 | PRO |
| 1 | B | 153 | ARG |
| 1 | B | 155 | SER |
| 1 | B | 156 | MET |
| 1 | B | 158 | THR |
| 1 | B | 159 | ASP |
| 1 | B | 161 | ASN |
| 1 | B | 162 | LEU |
| 1 | B | 163 | VAL |
| 1 | B | 167 | ARG |
| 1 | B | 169 | ASP |
| 1 | B | 170 | ARG |
| 1 | B | 171 | VAL |
| 1 | B | 172 | TRP |
| 1 | B | 173 | SER |
| 1 | B | 181 | THR |
| 1 | B | 184 | ARG |
| 1 | B | 186 | VAL |
| 1 | B | 187 | LEU |
| 1 | B | 188 | GLN |
| 1 | B | 192 | ARG |
| 1 | B | 194 | ASP |
| 1 | B | 196 | LEU |
| 1 | B | 197 | THR |
| 1 | B | 205 | THR |
| 1 | B | 206 | SER |
| 1 | B | 209 | SER |
| 1 | B | 216 | VAL |
| 1 | B | 220 | GLN |
| 1 | B | 222 | ASP |
| 1 | B | 227 | ILE |
| 1 | B | 228 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 232 | LEU |
| 1 | B | 233 | TRP |
| 1 | B | 234 | THR |
| 1 | B | 235 | THR |
| 1 | C | 3 | ILE |
| 1 | C | 4 | LEU |
| 1 | C | 5 | PHE |
| 1 | C | 8 | SER |
| 1 | C | 9 | HIS |
| 1 | C | 10 | GLU |
| 1 | C | 12 | SER |
| 1 | C | 16 | THR |
| 1 | C | 22 | SER |
| 1 | C | 24 | GLU |
| 1 | C | 25 | LEU |
| 1 | C | 27 | SER |
| 1 | C | 30 | PHE |
| 1 | C | 31 | THR |
| 1 | C | 32 | MET |
| 1 | C | 33 | GLN |
| 1 | C | 40 | LEU |
| 1 | C | 43 | SER |
| 1 | C | 46 | ARG |
| 1 | C | 51 | ASN |
| 1 | C | 56 | THR |
| 1 | C | 59 | ARG |
| 1 | C | 61 | VAL |
| 1 | C | 62 | LEU |
| 1 | C | 63 | GLN |
| 1 | C | 67 | LEU |
| 1 | C | 72 | THR |
| 1 | C | 78 | ARG |
| 1 | C | 79 | TRP |
| 1 | C | 86 | SER |
| 1 | C | 87 | ILE |
| 1 | C | 89 | ASN |
| 1 | C | 92 | LEU |
| 1 | C | 93 | VAL |
| 1 | C | 96 | PRO |
| 1 | C | 110 | SER |
| 1 | C | 112 | THR |
| 1 | C | 113 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 118 | VAL |
| 1 | C | 122 | ASN |
| 1 | C | 127 | ILE |
| 1 | C | 130 | SER |
| 1 | C | 131 | THR |
| 1 | C | 136 | ASN |
| 1 | C | 137 | HIS |
| 1 | C | 139 | GLN |
| 1 | C | 144 | THR |
| 1 | C | 145 | GLN |
| 1 | C | 146 | SER |
| 1 | C | 147 | LEU |
| 1 | C | 149 | LEU |
| 1 | C | 150 | SER |
| 1 | C | 154 | LEU |
| 1 | C | 156 | MET |
| 1 | C | 159 | ASP |
| 1 | C | 160 | CYS |
| 1 | C | 162 | LEU |
| 1 | C | 163 | VAL |
| 1 | C | 164 | LEU |
| 1 | C | 167 | ARG |
| 1 | C | 171 | VAL |
| 1 | C | 173 | SER |
| 1 | C | 175 | ASN |
| 1 | C | 176 | THR |
| 1 | C | 183 | CYS |
| 1 | C | 184 | ARG |
| 1 | C | 192 | ARG |
| 1 | C | 193 | MET |
| 1 | C | 195 | VAL |
| 1 | C | 196 | LEU |
| 1 | C | 199 | GLN |
| 1 | C | 200 | ASN |
| 1 | C | 201 | ILE |
| 1 | C | 203 | VAL |
| 1 | C | 206 | SER |
| 1 | C | 211 | SER |
| 1 | C | 216 | VAL |
| 1 | C | 218 | VAL |
| 1 | C | 219 | LEU |
| 1 | C | 221 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 224 | ASN |
| 1 | C | 227 | ILE |
| 1 | C | 233 | TRP |
| 1 | C | 234 | THR |
| 1 | D | 2 | ASN |
| 1 | D | 3 | ILE |
| 1 | D | 4 | LEU |
| 1 | D | 12 | SER |
| 1 | D | 16 | THR |
| 1 | D | 17 | LEU |
| 1 | D | 25 | LEU |
| 1 | D | 29 | ARG |
| 1 | D | 30 | PHE |
| 1 | D | 32 | MET |
| 1 | D | 37 | ASN |
| 1 | D | 43 | SER |
| 1 | D | 44 | ASP |
| 1 | D | 46 | ARG |
| 1 | D | 47 | VAL |
| 1 | D | 48 | TRP |
| 1 | D | 50 | SER |
| 1 | D | 56 | THR |
| 1 | D | 58 | CYS |
| 1 | D | 59 | ARG |
| 1 | D | 61 | VAL |
| 1 | D | 63 | GLN |
| 1 | D | 65 | ASP |
| 1 | D | 67 | LEU |
| 1 | D | 68 | LEU |
| 1 | D | 70 | ILE |
| 1 | D | 71 | LEU |
| 1 | D | 72 | THR |
| 1 | D | 76 | THR |
| 1 | D | 78 | ARG |
| 1 | D | 81 | SER |
| 1 | D | 83 | THR |
| 1 | D | 84 | LYS |
| 1 | D | 86 | SER |
| 1 | D | 87 | ILE |
| 1 | D | 92 | LEU |
| 1 | D | 93 | VAL |
| 1 | D | 95 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 102 | ILE |
| 1 | D | 105 | PRO |
| 1 | D | 107 | LEU |
| 1 | D | 108 | TRP |
| 1 | D | 109 | ASP |
| 1 | D | 126 | SER |
| 1 | D | 127 | ILE |
| 1 | D | 128 | LEU |
| 1 | D | 129 | TYR |
| 1 | D | 137 | HIS |
| 1 | D | 138 | PRO |
| 1 | D | 147 | LEU |
| 1 | D | 148 | GLN |
| 1 | D | 149 | LEU |
| 1 | D | 153 | ARG |
| 1 | D | 154 | LEU |
| 1 | D | 155 | SER |
| 1 | D | 156 | MET |
| 1 | D | 158 | THR |
| 1 | D | 161 | ASN |
| 1 | D | 162 | LEU |
| 1 | D | 164 | LEU |
| 1 | D | 167 | ARG |
| 1 | D | 169 | ASP |
| 1 | D | 170 | ARG |
| 1 | D | 171 | VAL |
| 1 | D | 176 | THR |
| 1 | D | 181 | THR |
| 1 | D | 186 | VAL |
| 1 | D | 187 | LEU |
| 1 | D | 193 | MET |
| 1 | D | 195 | VAL |
| 1 | D | 196 | LEU |
| 1 | D | 200 | ASN |
| 1 | D | 201 | ILE |
| 1 | D | 204 | TRP |
| 1 | D | 205 | THR |
| 1 | D | 211 | SER |
| 1 | D | 214 | ARG |
| 1 | D | 216 | VAL |
| 1 | D | 217 | PHE |
| 1 | D | 219 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 222 | ASP |
| 1 | D | 223 | ARG |
| 1 | D | 224 | ASN |
| 1 | D | 227 | ILE |
| 1 | D | 233 | TRP |
| 1 | D | 234 | THR |
| 1 | E | 1 | ASN |
| 1 | E | 2 | ASN |
| 1 | E | 3 | ILE |
| 1 | E | 4 | LEU |
| 1 | E | 14 | PRO |
| 1 | E | 21 | GLN |
| 1 | E | 22 | SER |
| 1 | E | 23 | LEU |
| 1 | E | 25 | LEU |
| 1 | E | 27 | SER |
| 1 | E | 29 | ARG |
| 1 | E | 32 | MET |
| 1 | E | 34 | SER |
| 1 | E | 40 | LEU |
| 1 | E | 45 | VAL |
| 1 | E | 51 | ASN |
| 1 | E | 52 | THR |
| 1 | E | 56 | THR |
| 1 | E | 59 | ARG |
| 1 | E | 67 | LEU |
| 1 | E | 70 | ILE |
| 1 | E | 72 | THR |
| 1 | E | 78 | ARG |
| 1 | E | 86 | SER |
| 1 | E | 87 | ILE |
| 1 | E | 89 | ASN |
| 1 | E | 91 | VAL |
| 1 | E | 92 | LEU |
| 1 | E | 96 | PRO |
| 1 | E | 101 | THR |
| 1 | E | 105 | PRO |
| 1 | E | 108 | TRP |
| 1 | E | 110 | SER |
| 1 | E | 115 | LYS |
| 1 | E | 119 | VAL |
| 1 | E | 123 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 125 | ASN |
| 1 | E | 127 | ILE |
| 1 | E | 128 | LEU |
| 1 | E | 129 | TYR |
| 1 | E | 131 | THR |
| 1 | E | 141 | LEU |
| 1 | E | 144 | THR |
| 1 | E | 146 | SER |
| 1 | E | 147 | LEU |
| 1 | E | 148 | GLN |
| 1 | E | 149 | LEU |
| 1 | E | 151 | PRO |
| 1 | E | 154 | LEU |
| 1 | E | 156 | MET |
| 1 | E | 158 | THR |
| 1 | E | 162 | LEU |
| 1 | E | 163 | VAL |
| 1 | E | 164 | LEU |
| 1 | E | 167 | ARG |
| 1 | E | 169 | ASP |
| 1 | E | 170 | ARG |
| 1 | E | 171 | VAL |
| 1 | E | 173 | SER |
| 1 | E | 175 | ASN |
| 1 | E | 189 | PRO |
| 1 | E | 192 | ARG |
| 1 | E | 193 | MET |
| 1 | E | 199 | GLN |
| 1 | E | 200 | ASN |
| 1 | E | 201 | ILE |
| 1 | E | 206 | SER |
| 1 | E | 208 | ASN |
| 1 | E | 210 | ARG |
| 1 | E | 211 | SER |
| 1 | E | 214 | ARG |
| 1 | E | 216 | VAL |
| 1 | E | 217 | PHE |
| 1 | E | 223 | ARG |
| 1 | E | 224 | ASN |
| 1 | E | 225 | LEU |
| 1 | E | 227 | ILE |
| 1 | E | 228 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 232 | LEU |
| 1 | E | 233 | TRP |
| 1 | E | 234 | THR |
| 1 | E | 235 | THR |
| 1 | F | 1 | ASN |
| 1 | F | 3 | ILE |
| 1 | F | 8 | SER |
| 1 | F | 10 | GLU |
| 1 | F | 12 | SER |
| 1 | F | 16 | THR |
| 1 | F | 23 | LEU |
| 1 | F | 25 | LEU |
| 1 | F | 26 | SER |
| 1 | F | 29 | ARG |
| 1 | F | 32 | MET |
| 1 | F | 33 | GLN |
| 1 | F | 37 | ASN |
| 1 | F | 38 | LEU |
| 1 | F | 43 | SER |
| 1 | F | 51 | ASN |
| 1 | F | 52 | THR |
| 1 | F | 61 | VAL |
| 1 | F | 65 | ASP |
| 1 | F | 67 | LEU |
| 1 | F | 68 | LEU |
| 1 | F | 70 | ILE |
| 1 | F | 76 | THR |
| 1 | F | 78 | ARG |
| 1 | F | 81 | SER |
| 1 | F | 84 | LYS |
| 1 | F | 86 | SER |
| 1 | F | 87 | ILE |
| 1 | F | 90 | TYR |
| 1 | F | 92 | LEU |
| 1 | F | 94 | LEU |
| 1 | F | 100 | VAL |
| 1 | F | 101 | THR |
| 1 | F | 109 | ASP |
| 1 | F | 125 | ASN |
| 1 | F | 127 | ILE |
| 1 | F | 128 | LEU |
| 1 | F | 129 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 131 | THR |
| 1 | F | 138 | PRO |
| 1 | F | 140 | THR |
| 1 | F | 142 | HIS |
| 1 | F | 145 | GLN |
| 1 | F | 146 | SER |
| 1 | F | 148 | GLN |
| 1 | F | 150 | SER |
| 1 | F | 152 | TYR |
| 1 | F | 153 | ARG |
| 1 | F | 154 | LEU |
| 1 | F | 155 | SER |
| 1 | F | 157 | GLU |
| 1 | F | 160 | CYS |
| 1 | F | 161 | ASN |
| 1 | F | 162 | LEU |
| 1 | F | 163 | VAL |
| 1 | F | 164 | LEU |
| 1 | F | 166 | ASP |
| 1 | F | 169 | ASP |
| 1 | F | 171 | VAL |
| 1 | F | 174 | THR |
| 1 | F | 181 | THR |
| 1 | F | 183 | CYS |
| 1 | F | 184 | ARG |
| 1 | F | 188 | GLN |
| 1 | F | 192 | ARG |
| 1 | F | 193 | MET |
| 1 | F | 204 | TRP |
| 1 | F | 208 | ASN |
| 1 | F | 210 | ARG |
| 1 | F | 211 | SER |
| 1 | F | 222 | ASP |
| 1 | F | 223 | ARG |
| 1 | F | 224 | ASN |
| 1 | F | 225 | LEU |
| 1 | F | 227 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 33 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 37 | ASN |
| 1 | A | 63 | GLN |
| 1 | A | 74 | GLN |
| 1 | A | 125 | ASN |
| 1 | A | 137 | HIS |
| 1 | A | 161 | ASN |
| 1 | A | 199 | GLN |
| 1 | A | 200 | ASN |
| 1 | A | 208 | ASN |
| 1 | A | 220 | GLN |
| 1 | A | 224 | ASN |
| 1 | B | 2 | ASN |
| 1 | B | 9 | HIS |
| 1 | B | 13 | HIS |
| 1 | B | 37 | ASN |
| 1 | B | 63 | GLN |
| 1 | B | 132 | GLN |
| 1 | B | 139 | GLN |
| 1 | B | 142 | HIS |
| 1 | B | 161 | ASN |
| 1 | B | 188 | GLN |
| 1 | B | 200 | ASN |
| 1 | B | 220 | GLN |
| 1 | C | 21 | GLN |
| 1 | C | 33 | GLN |
| 1 | C | 75 | ASN |
| 1 | C | 89 | ASN |
| 1 | C | 114 | ASN |
| 1 | C | 125 | ASN |
| 1 | C | 136 | ASN |
| 1 | C | 137 | HIS |
| 1 | C | 142 | HIS |
| 1 | C | 161 | ASN |
| 1 | C | 224 | ASN |
| 1 | D | 2 | ASN |
| 1 | D | 18 | HIS |
| 1 | D | 37 | ASN |
| 1 | D | 63 | GLN |
| 1 | D | 161 | ASN |
| 1 | D | 188 | GLN |
| 1 | D | 200 | ASN |
| 1 | D | 220 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 224 | ASN |
| 1 | E | 21 | GLN |
| 1 | E | 63 | GLN |
| 1 | E | 95 | GLN |
| 1 | E | 142 | HIS |
| 1 | E | 161 | ASN |
| 1 | E | 199 | GLN |
| 1 | E | 200 | ASN |
| 1 | E | 208 | ASN |
| 1 | E | 224 | ASN |
| 1 | F | 13 | HIS |
| 1 | F | 21 | GLN |
| 1 | F | 33 | GLN |
| 1 | F | 63 | GLN |
| 1 | F | 95 | GLN |
| 1 | F | 142 | HIS |
| 1 | F | 148 | GLN |
| 1 | F | 161 | ASN |
| 1 | F | 175 | ASN |
| 1 | F | 188 | GLN |
| 1 | F | 200 | ASN |
| 1 | F | 220 | 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)

There are no ligands in this entry.

## 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 | B | 3 |
| 1 | A | 1 |
| 1 | C | 1 |
| 1 | E | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 25:LEU | C | 26:SER | N | 1.19 |
| 1 | B | 8:SER | C | 9:HIS | N | 1.19 |
| 1 | C | 229:GLY | C | 230:GLY | N | 1.19 |
| 1 | E | 85:GLY | C | 86:SER | N | 1.19 |
| 1 | B | 30:PHE | C | 31:THR | N | 1.16 |
| 1 | B | 225:LEU | C | 226:ALA | N | 1.15 |

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.