# Full wwPDB EM Validation Report ⓘ

Apr 29, 2025 – 07:17 pm BST

| | | |
|---|---|---|
| PDB ID | : | 9FWV / pdb_00009fwv |
| EMDB ID | : | EMD-50836 |
| Title | : | Rubisco in native beta-carboxysomes |
| Authors | : | Sheng, Y.; Hardenbrook, N.; Li, K. |
| Deposited on | : | 2024-07-01 |
| Resolution | : | 3.50 Å(reported) |

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

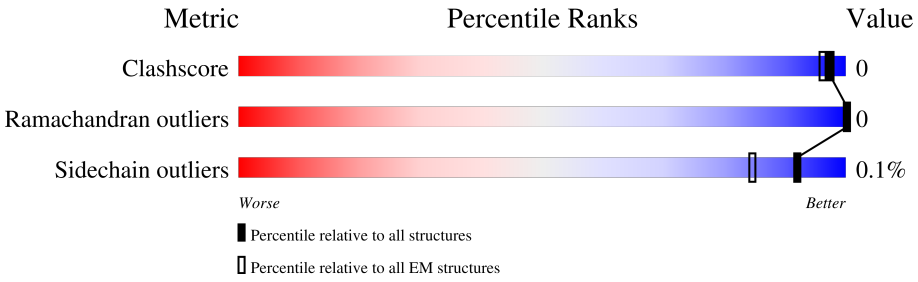
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev118 |
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.43.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 86 | 80% 38% 51% 10% |
| 1 | B | 86 | 84% 48% 45% 7% |
| 1 | F | 86 | 87% 41% 51% 8% |
| 1 | T | 86 | 90% 41% 55% 5% |
| 2 | C | 442 | 38% 52% 6% |
| 2 | G | 442 | 10% 36% 53% 7% |
| 2 | H | 442 | 15% 35% 55% 7% |
| 2 | I | 442 | 9% 35% 54% 7% |

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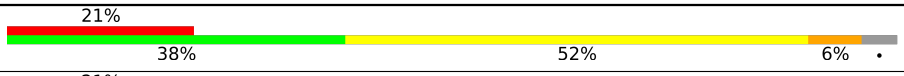
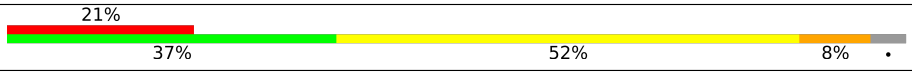
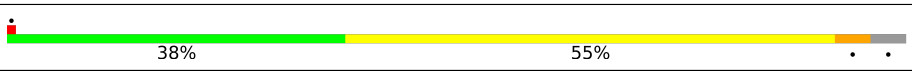
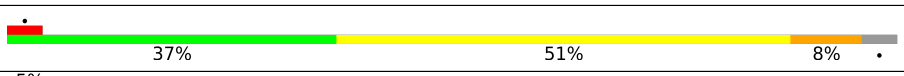
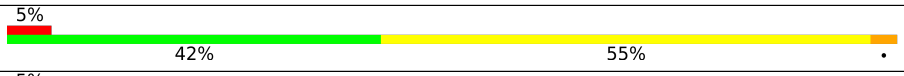
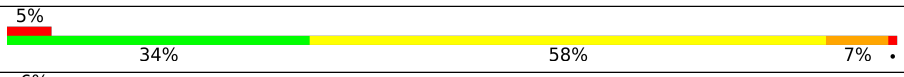
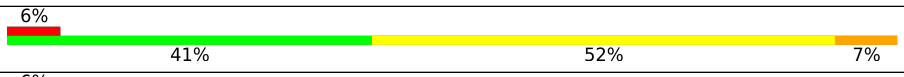
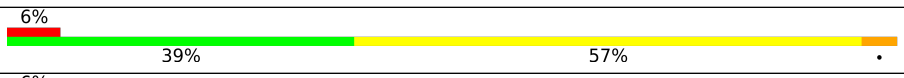
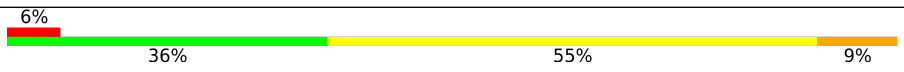
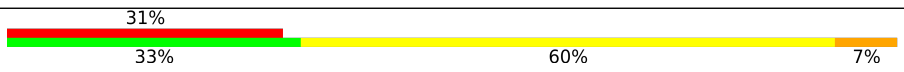
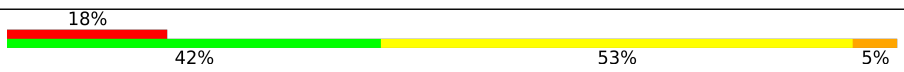
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | J | 442 |   |
| 2 | Q | 442 |   |
| 2 | R | 442 |   |
| 2 | S | 442 |   |
| 3 | D | 101 |   |
| 3 | E | 101 |   |
| 3 | K | 101 |   |
| 3 | L | 101 |   |
| 3 | M | 101 |   |
| 3 | N | 101 |   |
| 3 | O | 101 |   |
| 3 | P | 101 |   |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 36308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Carboxysome assembly protein CcmM.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 697 | 426 | 132 | 137 | 2 | | |
| 1 | B | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 697 | 426 | 132 | 137 | 2 | | |
| 1 | F | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 697 | 426 | 132 | 137 | 2 | | |
| 1 | T | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 697 | 426 | 132 | 137 | 2 | | |

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase large chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | G | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | H | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | I | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | J | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | Q | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | R | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |
| 2 | S | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3333 | 2114 | 587 | 615 | 17 | | |

- Molecule 3 is a protein called Ribulose bisphosphate carboxylase small subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |

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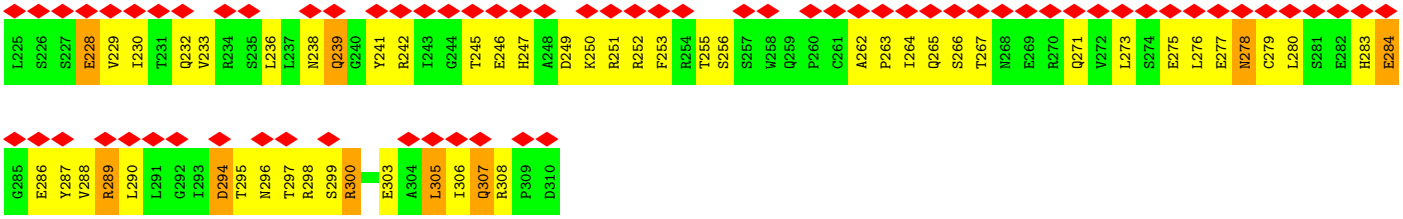
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | E | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | K | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | L | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | M | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | N | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | O | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |
| 3 | P | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 550 | 144 | 157 | 6 | | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

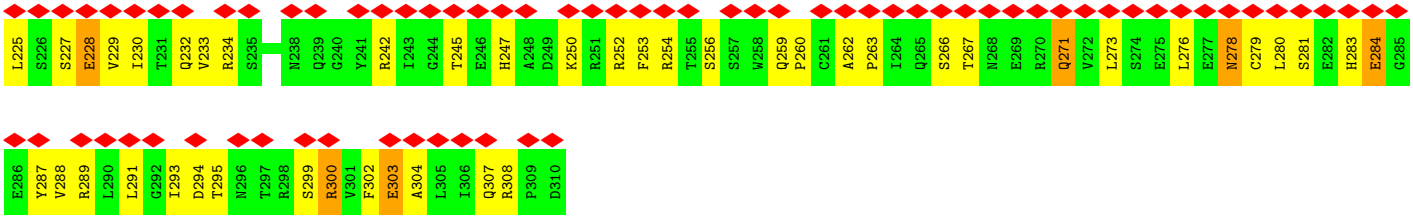
• Molecule 1: Carboxysome assembly protein CcmM

Chain A:

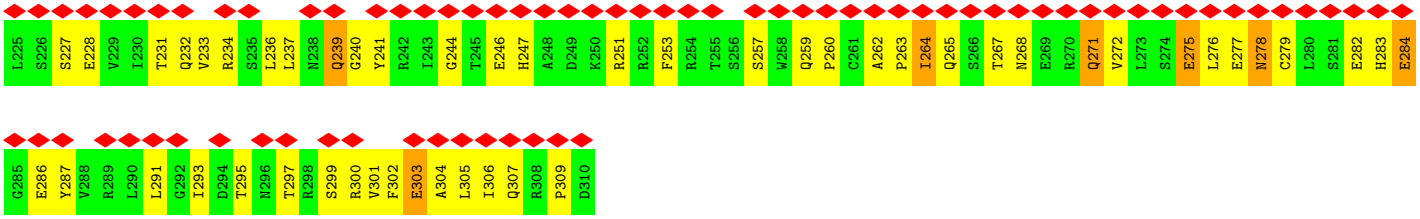

• Molecule 1: Carboxysome assembly protein CcmM

Chain B:

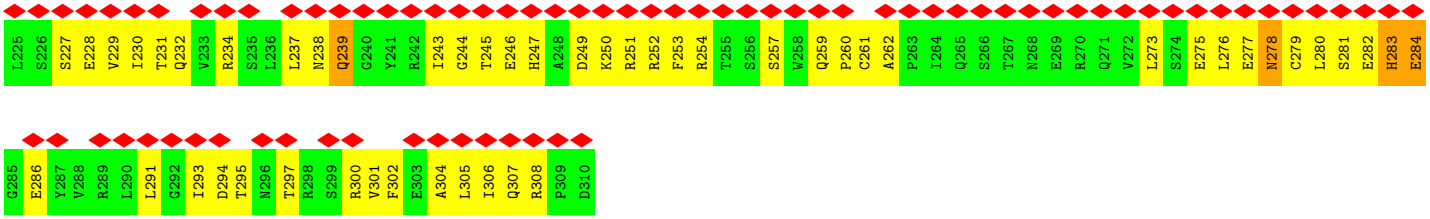

• Molecule 1: Carboxysome assembly protein CcmM

Chain F:

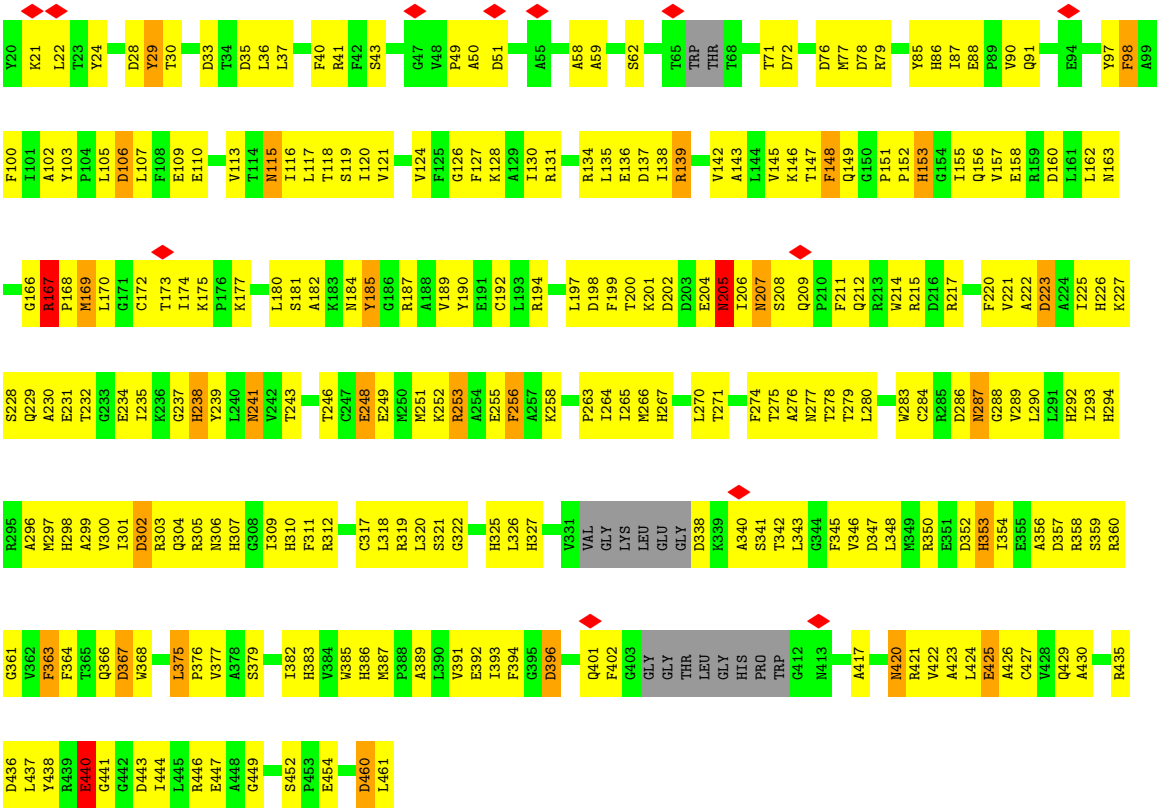




• Molecule 1: Carboxysome assembly protein CcmM

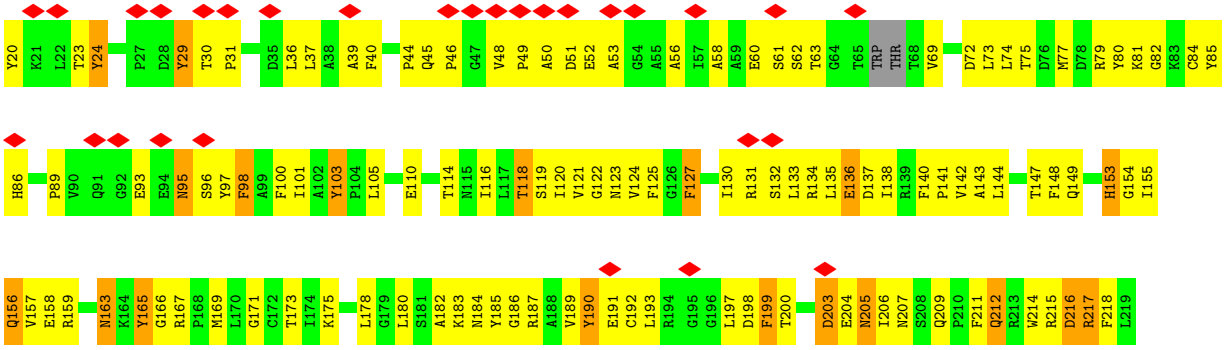
Chain T:

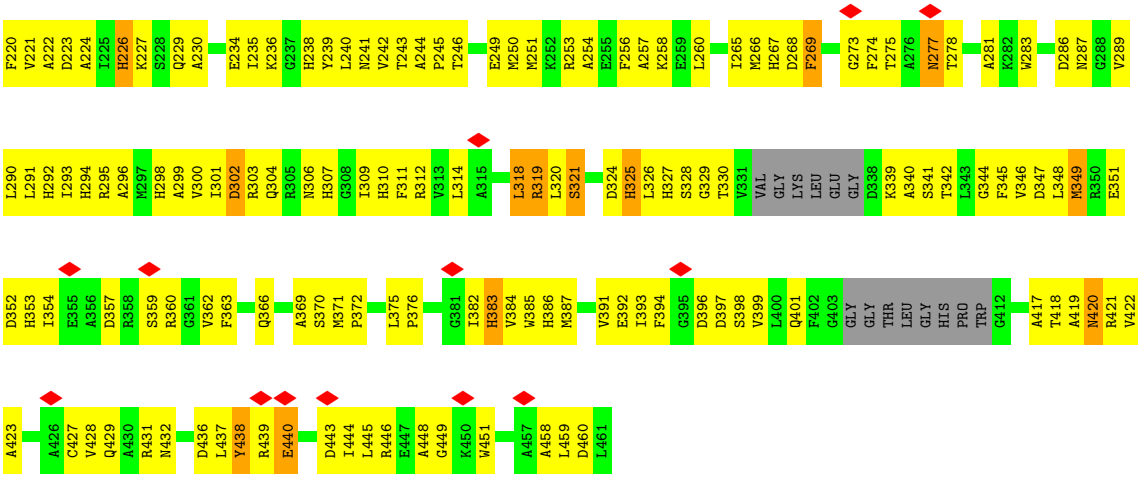



• Molecule 2: Ribulose bisphosphate carboxylase large chain

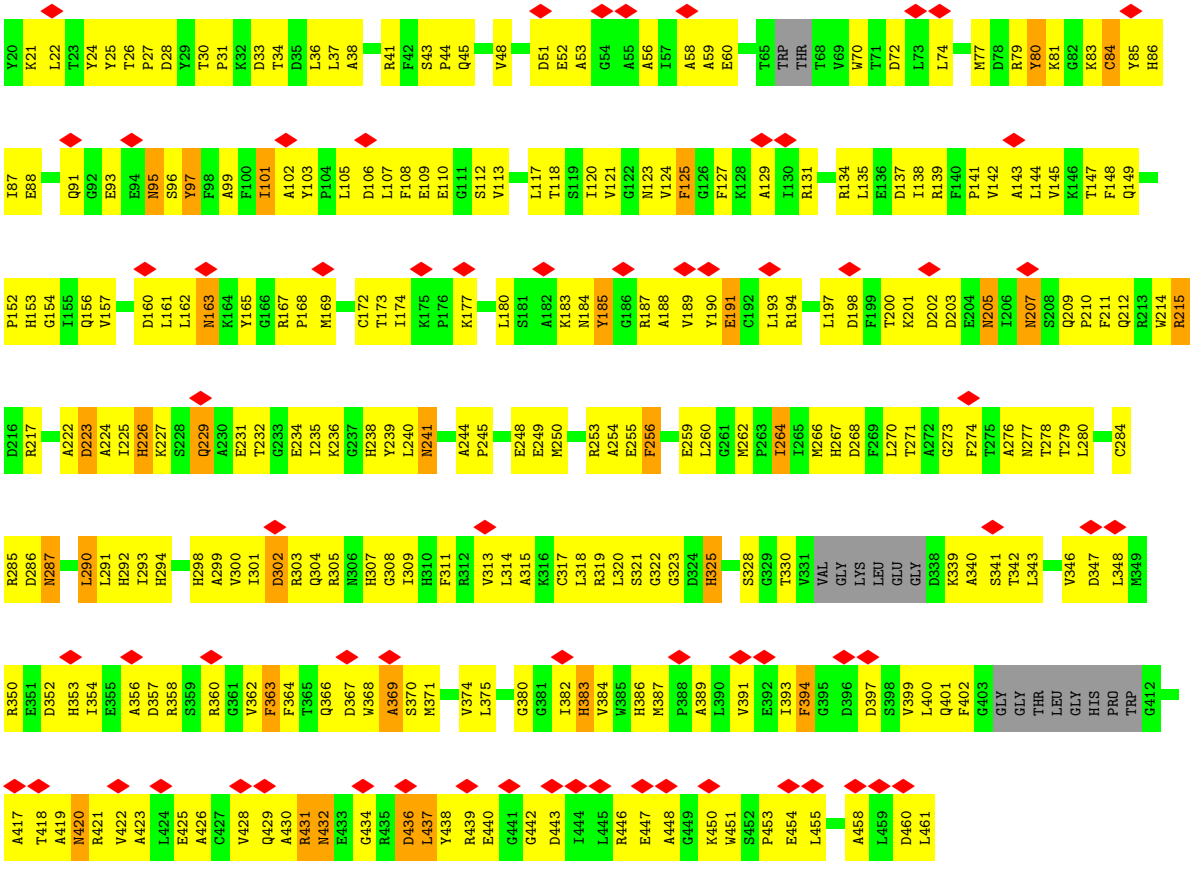

• Molecule 2: Ribulose bisphosphate carboxylase large chain



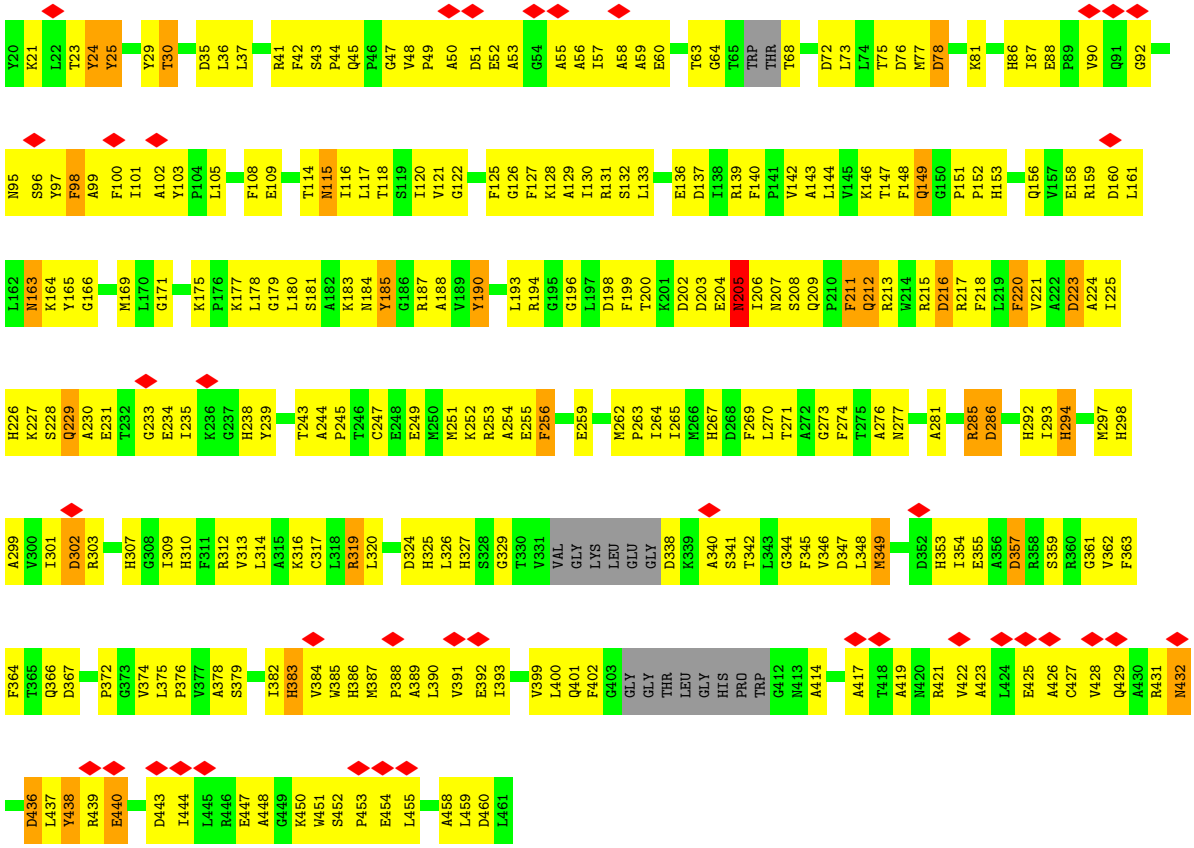
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain H:

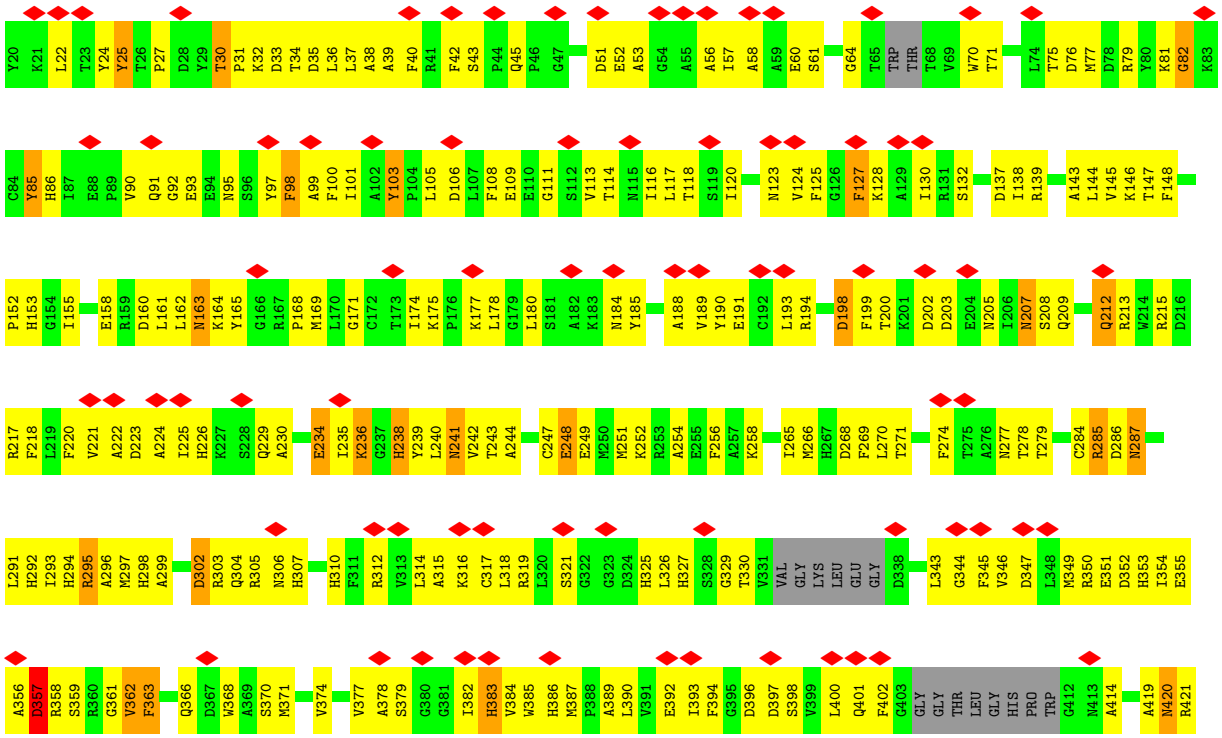
• Molecule 2: Ribulose bisphosphate carboxylase large chain

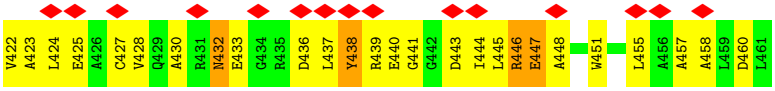
Chain I:



• Molecule 2: Ribulose bisphosphate carboxylase large chain

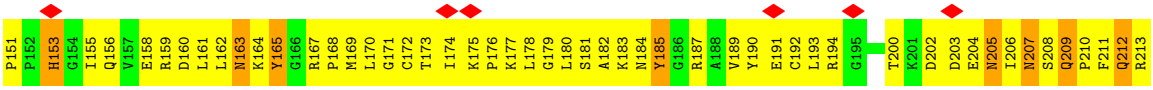
Chain J:

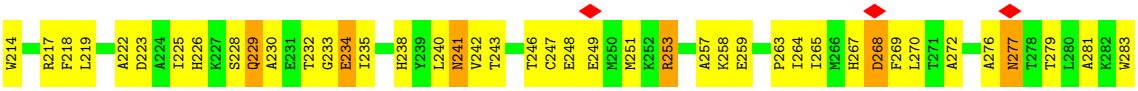





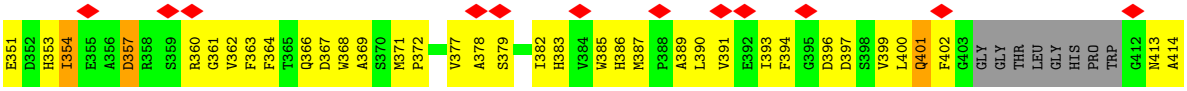

• Molecule 2: Ribulose bisphosphate carboxylase large chain

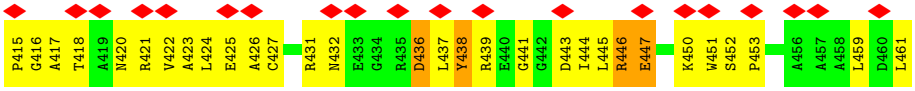


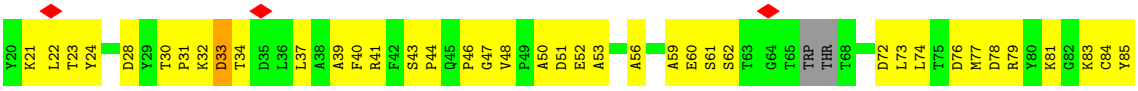



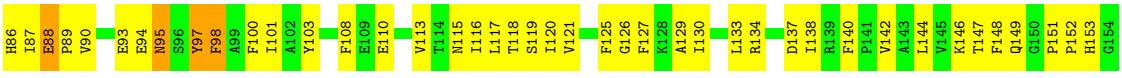




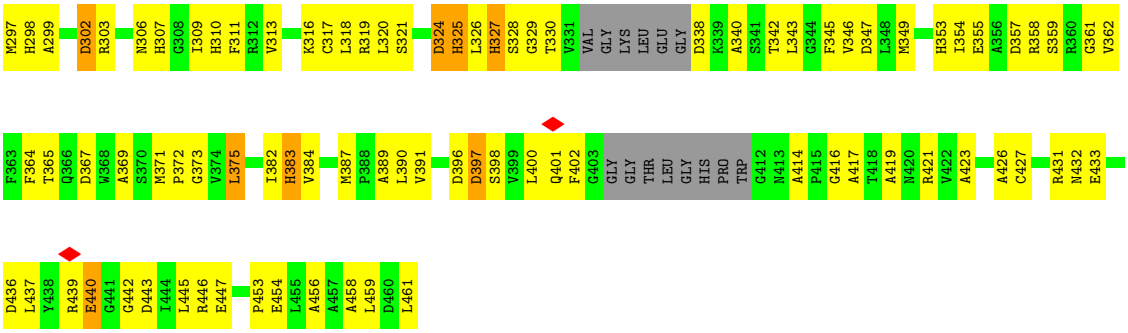



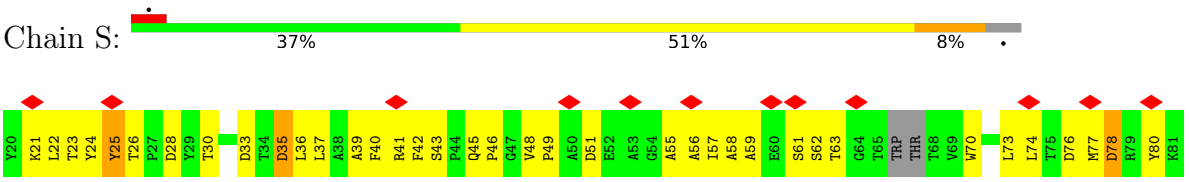

• Molecule 2: Ribulose bisphosphate carboxylase large chain

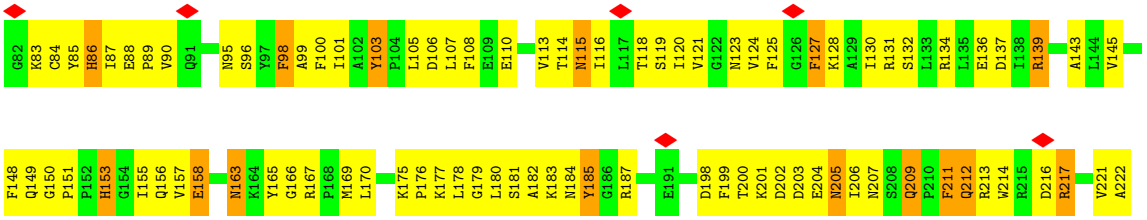



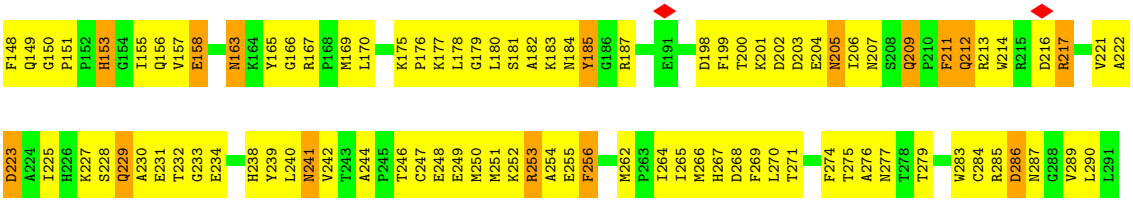



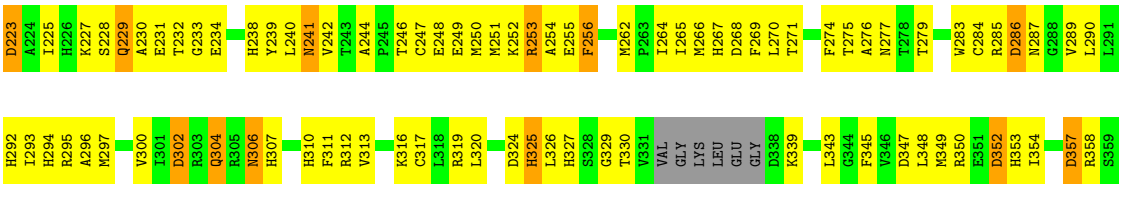




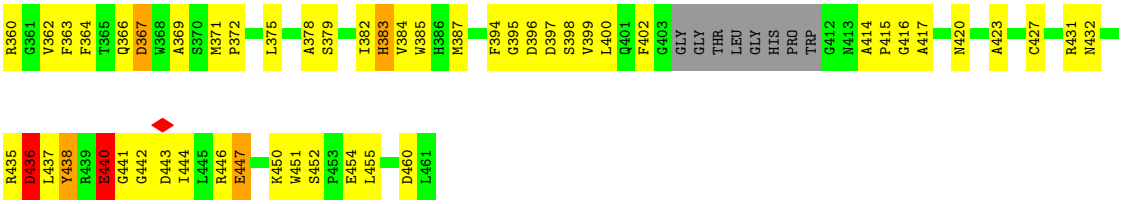


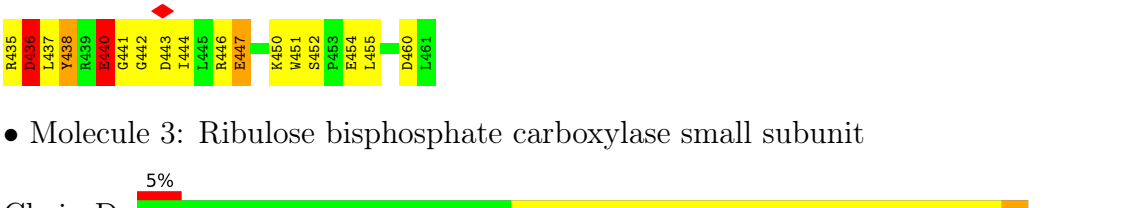


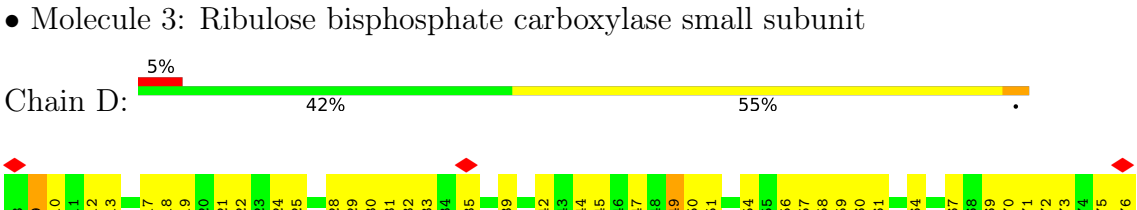


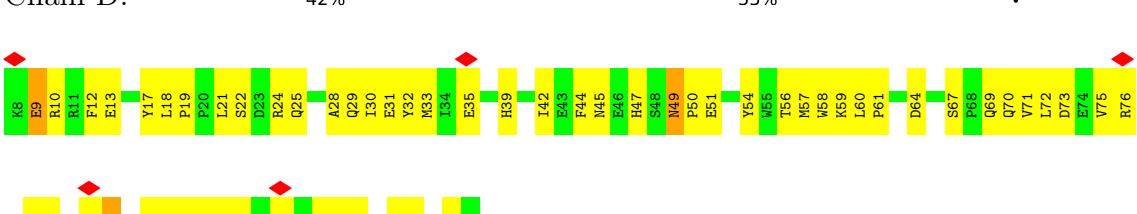


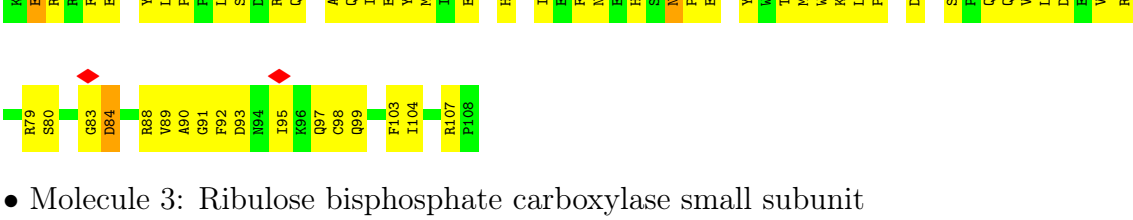


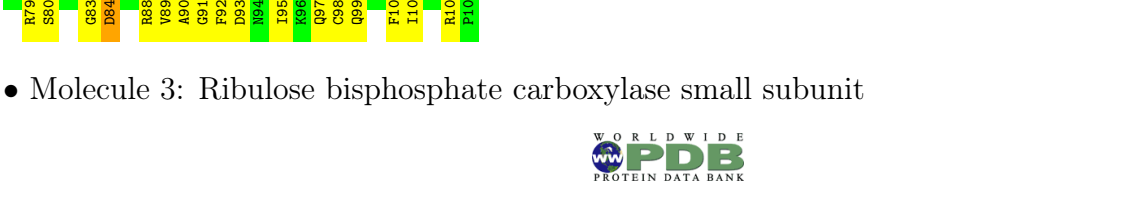




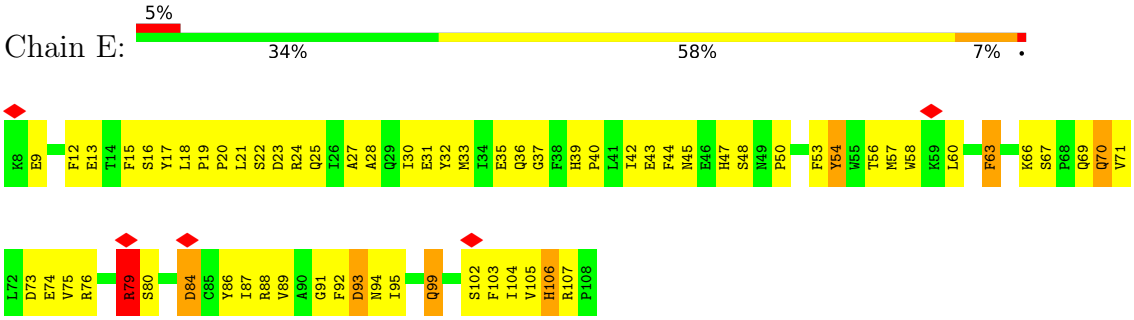






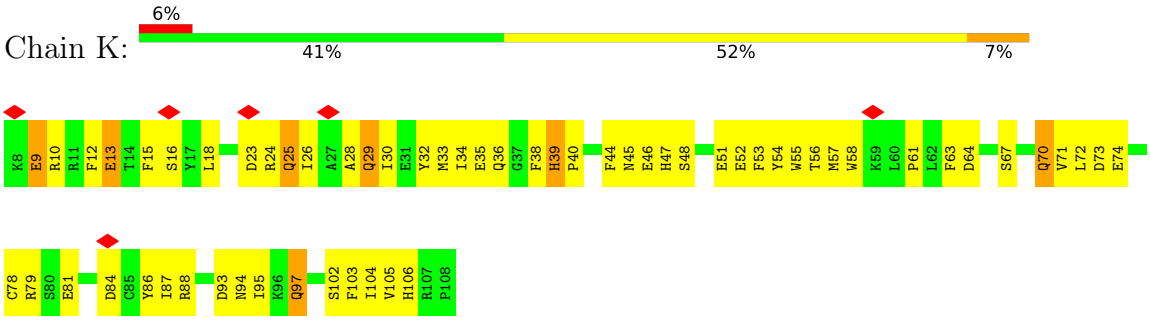


Chain E:



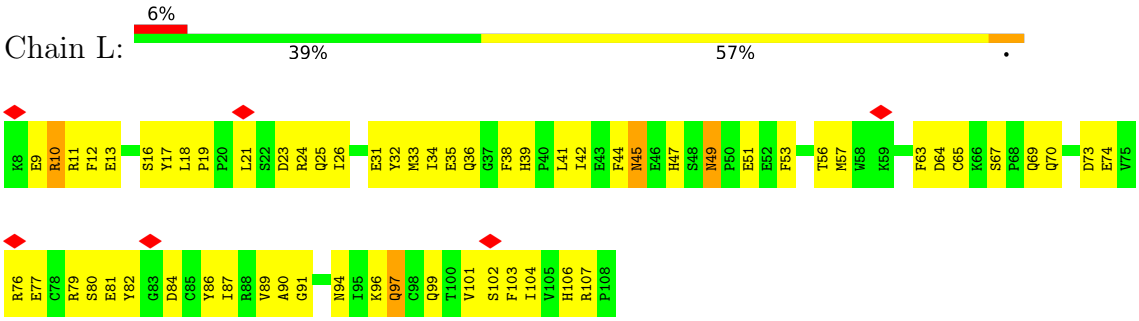

• Molecule 3: Ribulose bisphosphate carboxylase small subunit

Chain K:



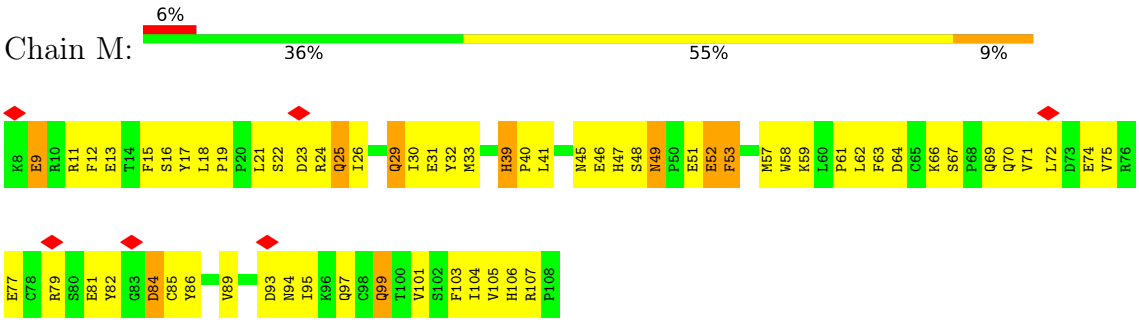

• Molecule 3: Ribulose bisphosphate carboxylase small subunit

Chain L:



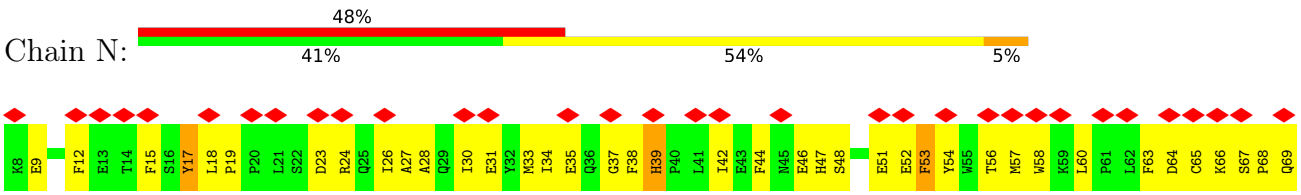

• Molecule 3: Ribulose bisphosphate carboxylase small subunit

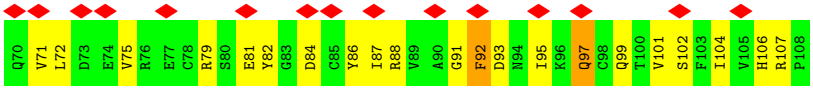
Chain M:




• Molecule 3: Ribulose bisphosphate carboxylase small subunit

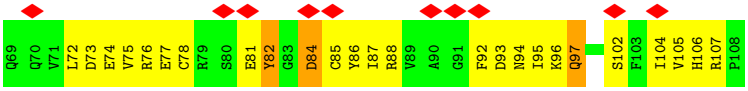
Chain N:



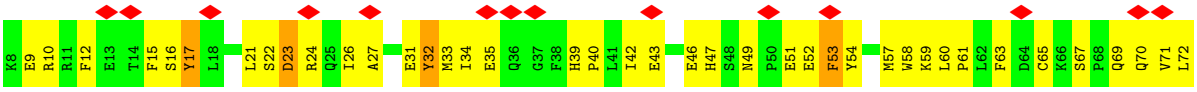


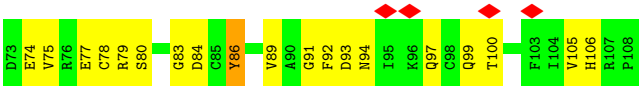

• Molecule 3: Ribulose bisphosphate carboxylase small subunit






• Molecule 3: Ribulose bisphosphate carboxylase small subunit

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, D4 | Depositor |
| Number of subtomograms used | 185 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 123 | Depositor |
| Minimum defocus (nm) | 2500 | Depositor |
| Maximum defocus (nm) | 5500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 4.744 | Depositor |
| Minimum map value | -3.571 | Depositor |
| Average map value | 0.003 | Depositor |
| Map value standard deviation | 0.227 | Depositor |
| Recommended contour level | 0.311 | Depositor |
| Map size (Å) | 275.4, 275.4, 275.4 | wwPDB |
| Map dimensions | 204, 204, 204 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.35, 1.35, 1.35 | Depositor |

# 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 | 2.75 | 48/707 (6.8%) | 2.06 | 33/955 (3.5%) |
| 1 | B | 2.74 | 45/707 (6.4%) | 2.17 | 36/955 (3.8%) |
| 1 | F | 2.71 | 41/707 (5.8%) | 2.10 | 28/955 (2.9%) |
| 1 | T | 2.92 | 57/707 (8.1%) | 2.06 | 35/955 (3.7%) |
| 2 | C | 2.83 | 258/3411 (7.6%) | 2.17 | 178/4617 (3.9%) |
| 2 | G | 2.84 | 265/3411 (7.8%) | 2.15 | 191/4617 (4.1%) |
| 2 | H | 2.84 | 240/3411 (7.0%) | 2.27 | 202/4617 (4.4%) |
| 2 | I | 2.87 | 275/3411 (8.1%) | 2.21 | 193/4617 (4.2%) |
| 2 | J | 2.81 | 233/3411 (6.8%) | 2.26 | 181/4617 (3.9%) |
| 2 | Q | 2.85 | 239/3411 (7.0%) | 2.22 | 205/4617 (4.4%) |
| 2 | R | 2.87 | 257/3411 (7.5%) | 2.19 | 193/4617 (4.2%) |
| 2 | S | 2.88 | 270/3411 (7.9%) | 2.22 | 177/4617 (3.8%) |
| 3 | D | 2.74 | 65/883 (7.4%) | 2.02 | 36/1195 (3.0%) |
| 3 | E | 2.74 | 63/883 (7.1%) | 2.08 | 43/1195 (3.6%) |
| 3 | K | 2.72 | 52/883 (5.9%) | 2.18 | 50/1195 (4.2%) |
| 3 | L | 2.73 | 65/883 (7.4%) | 2.24 | 54/1195 (4.5%) |
| 3 | M | 2.73 | 60/883 (6.8%) | 2.28 | 58/1195 (4.9%) |
| 3 | N | 2.76 | 56/883 (6.3%) | 2.20 | 49/1195 (4.1%) |
| 3 | O | 2.84 | 65/883 (7.4%) | 2.16 | 43/1195 (3.6%) |
| 3 | P | 2.64 | 53/883 (6.0%) | 2.04 | 33/1195 (2.8%) |
| All | All | 2.82 | 2707/37180 (7.3%) | 2.19 | 2018/50316 (4.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 9 |
| 1 | B | 0 | 7 |
| 1 | F | 0 | 7 |
| 1 | T | 0 | 7 |
| 2 | C | 0 | 28 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | G | 0 | 30 |
| 2 | H | 0 | 28 |
| 2 | I | 0 | 34 |
| 2 | J | 0 | 28 |
| 2 | Q | 0 | 35 |
| 2 | R | 0 | 17 |
| 2 | S | 0 | 40 |
| 3 | D | 0 | 6 |
| 3 | E | 0 | 7 |
| 3 | K | 0 | 10 |
| 3 | L | 0 | 3 |
| 3 | M | 0 | 11 |
| 3 | N | 0 | 8 |
| 3 | O | 0 | 9 |
| 3 | P | 0 | 8 |
| All | All | 0 | 332 |

All (2707) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | H | 86 | HIS | CD2-NE2 | 12.07 | 1.51 | 1.37 |
| 2 | R | 383 | HIS | ND1-CE1 | 11.96 | 1.44 | 1.32 |
| 3 | L | 47 | HIS | CD2-NE2 | 10.63 | 1.49 | 1.37 |
| 3 | K | 33 | MET | SD-CE | -10.61 | 1.53 | 1.79 |
| 1 | T | 291 | LEU | C-N | 10.57 | 1.40 | 1.33 |
| 2 | I | 294 | HIS | CD2-NE2 | 10.56 | 1.49 | 1.37 |
| 2 | J | 153 | HIS | CD2-NE2 | 10.54 | 1.49 | 1.37 |
| 2 | Q | 298 | HIS | CD2-NE2 | 10.50 | 1.49 | 1.37 |
| 2 | J | 353 | HIS | CD2-NE2 | 10.40 | 1.49 | 1.37 |
| 2 | I | 226 | HIS | ND1-CE1 | 10.34 | 1.42 | 1.32 |
| 2 | I | 251 | MET | SD-CE | -10.34 | 1.53 | 1.79 |
| 2 | H | 386 | HIS | ND1-CE1 | 10.29 | 1.42 | 1.32 |
| 3 | E | 57 | MET | SD-CE | -10.28 | 1.53 | 1.79 |
| 2 | R | 383 | HIS | CA-C | -10.22 | 1.43 | 1.53 |
| 2 | R | 327 | HIS | CE1-NE2 | -10.17 | 1.22 | 1.32 |
| 2 | I | 294 | HIS | ND1-CE1 | 10.13 | 1.42 | 1.32 |
| 3 | M | 39 | HIS | CE1-NE2 | -10.08 | 1.22 | 1.32 |
| 2 | S | 88 | GLU | CA-C | -10.08 | 1.42 | 1.52 |
| 3 | L | 106 | HIS | CE1-NE2 | -9.94 | 1.22 | 1.32 |
| 2 | S | 251 | MET | SD-CE | -9.94 | 1.54 | 1.79 |
| 3 | N | 47 | HIS | ND1-CE1 | 9.88 | 1.42 | 1.32 |
| 2 | I | 243 | THR | C-N | 9.87 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 292 | HIS | ND1-CE1 | 9.68 | 1.42 | 1.32 |
| 2 | R | 246 | THR | CA-C | 9.68 | 1.64 | 1.52 |
| 3 | K | 48 | SER | CA-C | -9.64 | 1.41 | 1.52 |
| 3 | E | 19 | PRO | C-O | -9.56 | 1.16 | 1.25 |
| 2 | R | 325 | HIS | CE1-NE2 | -9.56 | 1.23 | 1.32 |
| 2 | Q | 394 | PHE | CA-C | -9.52 | 1.42 | 1.52 |
| 2 | G | 120 | ILE | CA-C | -9.49 | 1.41 | 1.52 |
| 2 | I | 364 | PHE | CA-C | 9.44 | 1.63 | 1.52 |
| 2 | R | 306 | ASN | CA-C | 9.34 | 1.64 | 1.52 |
| 2 | Q | 369 | ALA | CA-C | -9.34 | 1.42 | 1.53 |
| 1 | T | 308 | ARG | CA-C | -9.32 | 1.43 | 1.52 |
| 2 | I | 361 | GLY | C-N | -9.31 | 1.24 | 1.33 |
| 3 | N | 64 | ASP | CA-C | 9.22 | 1.64 | 1.53 |
| 2 | Q | 40 | PHE | CA-C | -9.19 | 1.41 | 1.52 |
| 1 | B | 271 | GLN | CA-C | 9.18 | 1.64 | 1.52 |
| 3 | L | 73 | ASP | CA-C | 9.16 | 1.64 | 1.52 |
| 3 | E | 18 | LEU | CA-C | 9.15 | 1.63 | 1.52 |
| 2 | S | 155 | ILE | CA-CB | 9.14 | 1.64 | 1.54 |
| 2 | H | 134 | ARG | CA-C | -9.09 | 1.41 | 1.52 |
| 3 | K | 39 | HIS | CE1-NE2 | -9.06 | 1.23 | 1.32 |
| 2 | C | 292 | HIS | CE1-NE2 | -9.04 | 1.23 | 1.32 |
| 2 | Q | 307 | HIS | CD2-NE2 | 9.04 | 1.47 | 1.37 |
| 3 | M | 57 | MET | SD-CE | -9.03 | 1.56 | 1.79 |
| 2 | S | 169 | MET | SD-CE | -9.03 | 1.56 | 1.79 |
| 3 | N | 39 | HIS | CD2-NE2 | 9.02 | 1.47 | 1.37 |
| 2 | C | 294 | HIS | ND1-CE1 | 8.98 | 1.41 | 1.32 |
| 2 | H | 340 | ALA | CA-C | 8.96 | 1.64 | 1.52 |
| 3 | E | 93 | ASP | CA-C | -8.95 | 1.41 | 1.52 |
| 1 | F | 303 | GLU | CA-C | 8.95 | 1.63 | 1.52 |
| 1 | T | 251 | ARG | CA-C | 8.94 | 1.64 | 1.52 |
| 2 | R | 298 | HIS | CE1-NE2 | -8.92 | 1.23 | 1.32 |
| 1 | A | 249 | ASP | CA-C | -8.88 | 1.41 | 1.53 |
| 2 | G | 387 | MET | SD-CE | -8.87 | 1.57 | 1.79 |
| 3 | O | 106 | HIS | CE1-NE2 | 8.86 | 1.41 | 1.32 |
| 2 | G | 299 | ALA | C-N | 8.84 | 1.43 | 1.33 |
| 2 | G | 310 | HIS | CD2-NE2 | 8.84 | 1.47 | 1.37 |
| 1 | T | 247 | HIS | CE1-NE2 | -8.83 | 1.23 | 1.32 |
| 2 | G | 399 | VAL | CA-C | 8.82 | 1.63 | 1.52 |
| 2 | I | 271 | THR | CA-C | -8.79 | 1.42 | 1.52 |
| 3 | D | 58 | TRP | CA-C | -8.78 | 1.43 | 1.53 |
| 3 | O | 12 | PHE | CA-C | -8.75 | 1.42 | 1.52 |
| 1 | T | 273 | LEU | CA-C | -8.75 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 327 | HIS | ND1-CE1 | -8.73 | 1.23 | 1.32 |
| 2 | H | 112 | SER | CA-C | 8.70 | 1.62 | 1.52 |
| 2 | I | 417 | ALA | CA-C | 8.70 | 1.63 | 1.52 |
| 2 | R | 153 | HIS | ND1-CE1 | -8.69 | 1.23 | 1.32 |
| 2 | R | 446 | ARG | CA-C | -8.69 | 1.42 | 1.52 |
| 2 | S | 414 | ALA | N-CA | -8.68 | 1.38 | 1.46 |
| 2 | Q | 241 | ASN | CA-C | 8.68 | 1.64 | 1.52 |
| 2 | Q | 36 | LEU | CA-C | -8.66 | 1.42 | 1.52 |
| 2 | S | 417 | ALA | CA-C | 8.66 | 1.63 | 1.52 |
| 3 | E | 12 | PHE | CA-C | 8.65 | 1.63 | 1.52 |
| 2 | G | 265 | ILE | CA-C | 8.64 | 1.63 | 1.52 |
| 3 | N | 69 | GLN | CA-C | 8.64 | 1.64 | 1.52 |
| 2 | S | 325 | HIS | CE1-NE2 | -8.64 | 1.24 | 1.32 |
| 2 | Q | 48 | VAL | CA-C | 8.63 | 1.60 | 1.53 |
| 1 | F | 276 | LEU | CA-C | -8.61 | 1.41 | 1.52 |
| 2 | S | 163 | ASN | CA-C | 8.60 | 1.64 | 1.53 |
| 2 | R | 174 | ILE | CA-C | -8.60 | 1.42 | 1.52 |
| 3 | O | 102 | SER | CA-C | 8.59 | 1.62 | 1.52 |
| 3 | P | 39 | HIS | CA-C | 8.59 | 1.62 | 1.52 |
| 2 | S | 264 | ILE | CA-C | -8.58 | 1.41 | 1.52 |
| 3 | N | 58 | TRP | CA-C | -8.58 | 1.43 | 1.53 |
| 2 | C | 79 | ARG | CA-C | 8.57 | 1.64 | 1.52 |
| 2 | G | 93 | GLU | CA-C | -8.56 | 1.42 | 1.52 |
| 2 | G | 325 | HIS | CE1-NE2 | -8.56 | 1.24 | 1.32 |
| 2 | Q | 294 | HIS | CE1-NE2 | 8.54 | 1.41 | 1.32 |
| 2 | C | 267 | HIS | CA-C | 8.54 | 1.62 | 1.52 |
| 2 | Q | 327 | HIS | ND1-CE1 | -8.54 | 1.24 | 1.32 |
| 3 | O | 88 | ARG | CA-C | 8.52 | 1.62 | 1.52 |
| 3 | O | 106 | HIS | CA-C | -8.52 | 1.42 | 1.52 |
| 2 | S | 110 | GLU | CA-C | -8.49 | 1.41 | 1.52 |
| 2 | S | 244 | ALA | CA-C | 8.48 | 1.60 | 1.52 |
| 2 | G | 268 | ASP | CA-C | -8.47 | 1.42 | 1.52 |
| 2 | J | 353 | HIS | CA-C | 8.46 | 1.62 | 1.52 |
| 2 | H | 298 | HIS | CD2-NE2 | 8.45 | 1.47 | 1.37 |
| 1 | A | 289 | ARG | CA-C | 8.40 | 1.62 | 1.52 |
| 2 | S | 37 | LEU | CA-C | -8.39 | 1.42 | 1.52 |
| 2 | Q | 206 | ILE | CA-C | -8.39 | 1.45 | 1.53 |
| 2 | H | 241 | ASN | CA-C | -8.37 | 1.42 | 1.52 |
| 3 | E | 73 | ASP | CA-C | 8.34 | 1.63 | 1.52 |
| 2 | H | 250 | MET | SD-CE | -8.34 | 1.58 | 1.79 |
| 2 | J | 43 | SER | CA-C | 8.33 | 1.62 | 1.52 |
| 2 | H | 153 | HIS | CA-C | 8.33 | 1.64 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | T | 259 | GLN | CA-C | -8.33 | 1.44 | 1.52 |
| 2 | H | 177 | LYS | C-N | 8.33 | 1.43 | 1.33 |
| 2 | I | 349 | MET | C-N | 8.33 | 1.44 | 1.33 |
| 1 | B | 250 | LYS | CA-C | 8.32 | 1.63 | 1.52 |
| 2 | J | 53 | ALA | CA-C | 8.32 | 1.63 | 1.52 |
| 2 | G | 223 | ASP | CA-C | 8.30 | 1.63 | 1.52 |
| 3 | E | 16 | SER | CA-C | -8.30 | 1.42 | 1.52 |
| 2 | H | 193 | LEU | CA-C | -8.28 | 1.42 | 1.52 |
| 2 | R | 130 | ILE | CA-CB | 8.28 | 1.64 | 1.53 |
| 2 | S | 317 | CYS | C-N | -8.27 | 1.24 | 1.33 |
| 2 | Q | 191 | GLU | C-N | -8.27 | 1.24 | 1.33 |
| 3 | N | 81 | GLU | CA-C | 8.24 | 1.63 | 1.52 |
| 2 | R | 353 | HIS | ND1-CE1 | 8.23 | 1.40 | 1.32 |
| 2 | I | 35 | ASP | CA-C | -8.22 | 1.42 | 1.53 |
| 3 | L | 39 | HIS | ND1-CE1 | 8.22 | 1.40 | 1.32 |
| 2 | R | 361 | GLY | C-N | 8.21 | 1.41 | 1.33 |
| 2 | H | 382 | ILE | C-N | 8.21 | 1.44 | 1.33 |
| 2 | I | 140 | PHE | CA-C | 8.21 | 1.61 | 1.52 |
| 2 | Q | 294 | HIS | ND1-CE1 | 8.20 | 1.40 | 1.32 |
| 3 | M | 107 | ARG | CA-C | 8.18 | 1.60 | 1.52 |
| 2 | I | 68 | THR | C-N | -8.16 | 1.26 | 1.33 |
| 3 | D | 47 | HIS | CE1-NE2 | -8.16 | 1.24 | 1.32 |
| 2 | H | 266 | MET | SD-CE | -8.16 | 1.59 | 1.79 |
| 3 | N | 106 | HIS | CA-C | -8.16 | 1.42 | 1.52 |
| 2 | Q | 232 | THR | CA-C | 8.15 | 1.63 | 1.52 |
| 2 | H | 205 | ASN | C-N | 8.14 | 1.43 | 1.33 |
| 2 | Q | 167 | ARG | CA-C | 8.14 | 1.61 | 1.52 |
| 3 | O | 104 | ILE | C-N | -8.13 | 1.25 | 1.33 |
| 2 | C | 88 | GLU | C-O | -8.11 | 1.16 | 1.24 |
| 2 | H | 341 | SER | CA-C | -8.10 | 1.41 | 1.52 |
| 2 | G | 159 | ARG | CA-C | -8.10 | 1.42 | 1.52 |
| 2 | G | 155 | ILE | C-O | -8.09 | 1.15 | 1.24 |
| 2 | C | 386 | HIS | ND1-CE1 | 8.07 | 1.40 | 1.32 |
| 2 | I | 353 | HIS | CD2-NE2 | 8.06 | 1.46 | 1.37 |
| 3 | N | 97 | GLN | C-N | 8.06 | 1.44 | 1.33 |
| 3 | M | 49 | ASN | CA-C | -8.04 | 1.44 | 1.52 |
| 2 | R | 97 | TYR | CA-C | 8.04 | 1.62 | 1.52 |
| 2 | R | 241 | ASN | C-N | -8.03 | 1.24 | 1.33 |
| 2 | I | 100 | PHE | CA-C | 8.03 | 1.61 | 1.52 |
| 2 | J | 224 | ALA | CA-C | -8.02 | 1.42 | 1.52 |
| 2 | R | 251 | MET | SD-CE | -8.02 | 1.59 | 1.79 |
| 3 | L | 19 | PRO | CA-C | 8.02 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 134 | ARG | CA-C | 8.01 | 1.61 | 1.52 |
| 2 | C | 382 | ILE | CA-C | -8.00 | 1.42 | 1.52 |
| 2 | R | 32 | LYS | CA-C | -8.00 | 1.42 | 1.52 |
| 2 | R | 316 | LYS | CA-C | -8.00 | 1.42 | 1.52 |
| 2 | C | 253 | ARG | CA-C | 7.99 | 1.62 | 1.52 |
| 1 | T | 228 | GLU | C-N | 7.99 | 1.44 | 1.33 |
| 2 | H | 124 | VAL | CA-C | 7.98 | 1.62 | 1.52 |
| 2 | H | 226 | HIS | ND1-CE1 | -7.98 | 1.24 | 1.32 |
| 2 | S | 262 | MET | SD-CE | -7.98 | 1.59 | 1.79 |
| 2 | S | 167 | ARG | CA-C | 7.98 | 1.62 | 1.52 |
| 1 | B | 289 | ARG | C-O | -7.97 | 1.14 | 1.24 |
| 2 | G | 187 | ARG | CA-C | -7.96 | 1.42 | 1.52 |
| 2 | Q | 165 | TYR | C-N | 7.96 | 1.43 | 1.33 |
| 2 | J | 387 | MET | SD-CE | -7.96 | 1.59 | 1.79 |
| 2 | C | 358 | ARG | C-N | 7.95 | 1.44 | 1.33 |
| 3 | E | 27 | ALA | CA-C | -7.95 | 1.42 | 1.52 |
| 3 | D | 57 | MET | C-N | 7.93 | 1.44 | 1.33 |
| 3 | D | 103 | PHE | CA-C | -7.92 | 1.43 | 1.52 |
| 2 | G | 63 | THR | CA-CB | -7.92 | 1.43 | 1.54 |
| 1 | A | 295 | THR | CA-C | -7.92 | 1.42 | 1.52 |
| 2 | H | 28 | ASP | CA-C | 7.92 | 1.63 | 1.52 |
| 2 | Q | 310 | HIS | CD2-NE2 | 7.92 | 1.46 | 1.37 |
| 3 | P | 46 | GLU | CA-C | 7.91 | 1.63 | 1.52 |
| 2 | S | 400 | LEU | C-O | -7.91 | 1.15 | 1.24 |
| 2 | S | 214 | TRP | C-O | -7.89 | 1.15 | 1.24 |
| 2 | S | 96 | SER | CA-C | -7.89 | 1.42 | 1.52 |
| 2 | I | 161 | LEU | CA-C | -7.88 | 1.42 | 1.52 |
| 1 | T | 277 | GLU | CA-C | 7.88 | 1.62 | 1.52 |
| 2 | Q | 293 | ILE | C-O | -7.88 | 1.16 | 1.24 |
| 2 | Q | 450 | LYS | CA-C | 7.88 | 1.62 | 1.52 |
| 2 | C | 202 | ASP | CA-C | -7.87 | 1.42 | 1.53 |
| 2 | G | 256 | PHE | C-N | 7.86 | 1.43 | 1.33 |
| 3 | D | 12 | PHE | CA-C | 7.86 | 1.62 | 1.52 |
| 3 | D | 89 | VAL | CA-C | -7.86 | 1.43 | 1.52 |
| 2 | G | 226 | HIS | CE1-NE2 | -7.86 | 1.24 | 1.32 |
| 2 | Q | 204 | GLU | CA-C | 7.85 | 1.62 | 1.52 |
| 2 | C | 425 | GLU | CA-C | -7.85 | 1.42 | 1.52 |
| 2 | H | 420 | ASN | CA-C | 7.85 | 1.62 | 1.52 |
| 2 | Q | 24 | TYR | CA-C | -7.85 | 1.42 | 1.52 |
| 3 | K | 57 | MET | SD-CE | -7.84 | 1.59 | 1.79 |
| 2 | S | 202 | ASP | CA-C | -7.82 | 1.42 | 1.53 |
| 2 | G | 169 | MET | SD-CE | -7.82 | 1.60 | 1.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | L | 64 | ASP | CA-C | 7.81 | 1.62 | 1.53 |
| 2 | C | 446 | ARG | C-N | 7.80 | 1.44 | 1.33 |
| 2 | H | 169 | MET | SD-CE | -7.80 | 1.60 | 1.79 |
| 2 | H | 81 | LYS | CA-C | -7.80 | 1.42 | 1.52 |
| 2 | G | 309 | ILE | C-O | -7.79 | 1.16 | 1.24 |
| 2 | R | 342 | THR | CA-C | -7.79 | 1.43 | 1.52 |
| 2 | H | 439 | ARG | CA-C | 7.79 | 1.63 | 1.52 |
| 3 | D | 70 | GLN | CA-C | 7.79 | 1.62 | 1.52 |
| 2 | C | 214 | TRP | CA-C | 7.78 | 1.62 | 1.52 |
| 2 | Q | 90 | VAL | C-O | -7.77 | 1.14 | 1.24 |
| 3 | P | 57 | MET | C-N | 7.77 | 1.43 | 1.33 |
| 2 | I | 231 | GLU | C-O | -7.76 | 1.15 | 1.24 |
| 1 | A | 294 | ASP | CA-C | -7.75 | 1.43 | 1.52 |
| 2 | J | 297 | MET | SD-CE | -7.75 | 1.60 | 1.79 |
| 2 | Q | 174 | ILE | CA-CB | 7.74 | 1.62 | 1.54 |
| 2 | Q | 48 | VAL | N-CA | -7.73 | 1.39 | 1.46 |
| 3 | N | 28 | ALA | CA-C | -7.73 | 1.42 | 1.52 |
| 2 | H | 180 | LEU | C-N | 7.72 | 1.44 | 1.33 |
| 2 | C | 283 | TRP | C-O | -7.72 | 1.15 | 1.24 |
| 2 | H | 30 | THR | CA-C | 7.72 | 1.61 | 1.52 |
| 2 | Q | 230 | ALA | CA-C | 7.72 | 1.62 | 1.52 |
| 3 | K | 34 | ILE | CA-C | -7.72 | 1.42 | 1.52 |
| 2 | G | 130 | ILE | CA-CB | 7.71 | 1.63 | 1.53 |
| 2 | J | 138 | ILE | CA-C | 7.71 | 1.62 | 1.52 |
| 2 | R | 263 | PRO | C-N | 7.70 | 1.44 | 1.33 |
| 2 | C | 251 | MET | SD-CE | -7.70 | 1.60 | 1.79 |
| 2 | J | 251 | MET | C-N | 7.70 | 1.44 | 1.33 |
| 2 | Q | 52 | GLU | CA-C | 7.70 | 1.62 | 1.52 |
| 1 | T | 253 | PHE | C-O | -7.69 | 1.15 | 1.24 |
| 2 | G | 215 | ARG | C-N | 7.69 | 1.44 | 1.33 |
| 2 | I | 96 | SER | CA-C | 7.68 | 1.62 | 1.52 |
| 2 | Q | 427 | CYS | C-N | -7.68 | 1.24 | 1.33 |
| 2 | H | 248 | GLU | CA-C | 7.67 | 1.62 | 1.52 |
| 1 | T | 281 | SER | C-O | -7.67 | 1.15 | 1.24 |
| 2 | R | 78 | ASP | CA-C | 7.66 | 1.63 | 1.52 |
| 2 | J | 241 | ASN | C-N | 7.66 | 1.42 | 1.33 |
| 2 | Q | 310 | HIS | ND1-CE1 | 7.65 | 1.40 | 1.32 |
| 2 | Q | 444 | ILE | C-O | -7.65 | 1.15 | 1.24 |
| 2 | I | 75 | THR | CA-C | 7.64 | 1.62 | 1.52 |
| 2 | R | 264 | ILE | CA-C | -7.64 | 1.43 | 1.52 |
| 2 | S | 119 | SER | CA-C | 7.64 | 1.62 | 1.52 |
| 2 | Q | 354 | ILE | CA-C | 7.63 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 166 | GLY | C-N | 7.63 | 1.41 | 1.33 |
| 2 | H | 168 | PRO | N-CA | 7.63 | 1.54 | 1.46 |
| 2 | S | 254 | ALA | C-O | -7.62 | 1.15 | 1.24 |
| 2 | G | 142 | VAL | C-N | -7.62 | 1.24 | 1.33 |
| 2 | Q | 160 | ASP | CA-C | 7.62 | 1.62 | 1.52 |
| 2 | G | 401 | GLN | CA-C | 7.62 | 1.61 | 1.52 |
| 2 | G | 40 | PHE | CA-C | -7.61 | 1.43 | 1.52 |
| 2 | S | 349 | MET | C-N | 7.60 | 1.43 | 1.33 |
| 3 | M | 32 | TYR | C-N | -7.60 | 1.24 | 1.33 |
| 2 | S | 40 | PHE | CA-C | 7.60 | 1.61 | 1.52 |
| 3 | N | 53 | PHE | CA-C | 7.59 | 1.62 | 1.52 |
| 3 | D | 72 | LEU | C-O | -7.59 | 1.15 | 1.24 |
| 2 | G | 383 | HIS | ND1-CE1 | -7.58 | 1.25 | 1.32 |
| 2 | R | 226 | HIS | CE1-NE2 | 7.58 | 1.40 | 1.32 |
| 3 | D | 51 | GLU | CA-C | 7.58 | 1.62 | 1.52 |
| 2 | I | 270 | LEU | CA-C | 7.58 | 1.62 | 1.52 |
| 2 | J | 86 | HIS | CA-C | -7.58 | 1.43 | 1.52 |
| 2 | J | 349 | MET | SD-CE | -7.58 | 1.60 | 1.79 |
| 3 | K | 32 | TYR | CA-C | -7.58 | 1.42 | 1.52 |
| 2 | J | 368 | TRP | CA-C | -7.58 | 1.43 | 1.52 |
| 2 | G | 325 | HIS | CA-C | 7.58 | 1.62 | 1.52 |
| 2 | I | 239 | TYR | C-N | 7.58 | 1.44 | 1.33 |
| 3 | O | 18 | LEU | CA-C | 7.58 | 1.62 | 1.52 |
| 2 | C | 49 | PRO | C-O | -7.57 | 1.15 | 1.23 |
| 2 | I | 382 | ILE | C-N | 7.56 | 1.43 | 1.33 |
| 3 | K | 47 | HIS | ND1-CE1 | -7.56 | 1.25 | 1.32 |
| 2 | H | 77 | MET | SD-CE | -7.56 | 1.60 | 1.79 |
| 2 | J | 307 | HIS | CA-C | -7.56 | 1.43 | 1.52 |
| 2 | R | 357 | ASP | CA-C | 7.55 | 1.60 | 1.53 |
| 2 | C | 85 | TYR | C-N | 7.55 | 1.43 | 1.33 |
| 1 | T | 283 | HIS | C-N | 7.55 | 1.43 | 1.33 |
| 2 | C | 37 | LEU | C-O | -7.55 | 1.15 | 1.24 |
| 2 | C | 222 | ALA | CA-C | -7.55 | 1.43 | 1.52 |
| 3 | E | 19 | PRO | C-N | 7.55 | 1.42 | 1.33 |
| 1 | B | 308 | ARG | N-CA | -7.54 | 1.39 | 1.45 |
| 2 | C | 217 | ARG | C-O | -7.54 | 1.15 | 1.24 |
| 2 | S | 379 | SER | C-O | -7.54 | 1.15 | 1.24 |
| 2 | S | 167 | ARG | N-CA | -7.53 | 1.38 | 1.46 |
| 2 | I | 425 | GLU | C-N | -7.53 | 1.24 | 1.33 |
| 1 | A | 251 | ARG | N-CA | -7.52 | 1.37 | 1.46 |
| 1 | T | 301 | VAL | C-N | 7.52 | 1.43 | 1.33 |
| 3 | E | 48 | SER | CA-C | -7.52 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | L | 16 | SER | CA-C | -7.52 | 1.42 | 1.52 |
| 2 | H | 120 | ILE | CA-CB | 7.52 | 1.64 | 1.54 |
| 2 | G | 135 | LEU | CA-C | -7.51 | 1.43 | 1.52 |
| 2 | R | 37 | LEU | C-N | 7.51 | 1.43 | 1.33 |
| 2 | G | 397 | ASP | C-N | -7.50 | 1.23 | 1.33 |
| 2 | S | 182 | ALA | C-N | 7.50 | 1.43 | 1.33 |
| 2 | H | 401 | GLN | CA-C | 7.50 | 1.62 | 1.52 |
| 2 | R | 180 | LEU | CA-C | -7.50 | 1.43 | 1.52 |
| 2 | R | 213 | ARG | CA-C | -7.50 | 1.43 | 1.52 |
| 2 | J | 37 | LEU | C-O | -7.49 | 1.15 | 1.23 |
| 2 | C | 103 | TYR | C-N | 7.49 | 1.43 | 1.33 |
| 2 | R | 215 | ARG | CA-C | 7.49 | 1.62 | 1.52 |
| 2 | I | 327 | HIS | ND1-CE1 | 7.49 | 1.40 | 1.32 |
| 2 | I | 348 | LEU | CA-C | -7.49 | 1.43 | 1.52 |
| 2 | H | 450 | LYS | CA-C | 7.49 | 1.62 | 1.52 |
| 2 | R | 402 | PHE | CA-C | -7.49 | 1.43 | 1.52 |
| 2 | C | 446 | ARG | C-O | -7.48 | 1.15 | 1.24 |
| 2 | I | 114 | THR | N-CA | -7.48 | 1.37 | 1.46 |
| 3 | K | 81 | GLU | C-N | 7.48 | 1.43 | 1.33 |
| 2 | C | 119 | SER | CA-C | -7.48 | 1.43 | 1.52 |
| 2 | J | 379 | SER | CA-C | -7.47 | 1.43 | 1.53 |
| 2 | Q | 100 | PHE | C-N | 7.47 | 1.43 | 1.33 |
| 2 | C | 181 | SER | C-N | -7.47 | 1.24 | 1.33 |
| 2 | I | 215 | ARG | C-N | 7.47 | 1.44 | 1.34 |
| 2 | R | 88 | GLU | N-CA | -7.45 | 1.38 | 1.46 |
| 3 | O | 38 | PHE | CA-C | -7.44 | 1.43 | 1.52 |
| 2 | S | 23 | THR | CA-C | -7.43 | 1.46 | 1.52 |
| 2 | I | 226 | HIS | CA-C | 7.43 | 1.62 | 1.52 |
| 3 | N | 12 | PHE | C-O | -7.42 | 1.15 | 1.23 |
| 2 | H | 386 | HIS | CD2-NE2 | 7.42 | 1.46 | 1.37 |
| 3 | P | 39 | HIS | ND1-CE1 | 7.42 | 1.40 | 1.32 |
| 3 | K | 106 | HIS | CA-C | 7.42 | 1.61 | 1.52 |
| 2 | C | 24 | TYR | CA-C | 7.42 | 1.62 | 1.52 |
| 3 | E | 37 | GLY | C-N | 7.41 | 1.43 | 1.33 |
| 2 | S | 438 | TYR | N-CA | -7.41 | 1.37 | 1.46 |
| 2 | R | 32 | LYS | C-N | 7.40 | 1.43 | 1.34 |
| 2 | J | 378 | ALA | C-N | -7.40 | 1.24 | 1.33 |
| 2 | I | 376 | PRO | C-O | -7.39 | 1.15 | 1.23 |
| 2 | C | 275 | THR | CA-C | -7.39 | 1.43 | 1.52 |
| 2 | Q | 378 | ALA | N-CA | 7.39 | 1.55 | 1.46 |
| 1 | B | 281 | SER | C-N | 7.38 | 1.43 | 1.33 |
| 2 | C | 258 | LYS | CA-C | -7.38 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 402 | PHE | C-O | -7.38 | 1.15 | 1.24 |
| 2 | J | 346 | VAL | CA-CB | 7.38 | 1.63 | 1.54 |
| 2 | R | 242 | VAL | N-CA | 7.38 | 1.53 | 1.46 |
| 2 | R | 307 | HIS | CE1-NE2 | -7.37 | 1.25 | 1.32 |
| 2 | R | 275 | THR | N-CA | -7.37 | 1.37 | 1.46 |
| 2 | I | 42 | PHE | CA-C | -7.37 | 1.43 | 1.52 |
| 2 | R | 197 | LEU | CA-C | -7.37 | 1.43 | 1.52 |
| 2 | S | 268 | ASP | CA-C | -7.37 | 1.43 | 1.52 |
| 2 | H | 80 | TYR | N-CA | 7.36 | 1.54 | 1.46 |
| 2 | J | 347 | ASP | C-N | 7.36 | 1.43 | 1.33 |
| 2 | R | 303 | ARG | CA-C | 7.35 | 1.62 | 1.52 |
| 2 | H | 36 | LEU | C-O | -7.34 | 1.15 | 1.23 |
| 2 | Q | 206 | ILE | CA-CB | 7.34 | 1.61 | 1.53 |
| 2 | C | 227 | LYS | C-N | -7.34 | 1.24 | 1.33 |
| 1 | F | 263 | PRO | C-O | 7.34 | 1.31 | 1.23 |
| 2 | I | 169 | MET | SD-CE | -7.34 | 1.61 | 1.79 |
| 2 | R | 211 | PHE | C-N | 7.33 | 1.43 | 1.33 |
| 2 | Q | 249 | GLU | C-O | -7.33 | 1.15 | 1.24 |
| 2 | Q | 62 | SER | CA-C | -7.32 | 1.45 | 1.52 |
| 2 | Q | 217 | ARG | N-CA | -7.32 | 1.37 | 1.46 |
| 3 | P | 32 | TYR | CA-C | -7.32 | 1.42 | 1.52 |
| 1 | A | 277 | GLU | CA-C | 7.32 | 1.62 | 1.52 |
| 2 | J | 278 | THR | C-N | 7.32 | 1.43 | 1.33 |
| 2 | R | 401 | GLN | CA-C | 7.32 | 1.61 | 1.52 |
| 2 | S | 399 | VAL | C-O | -7.32 | 1.16 | 1.23 |
| 2 | R | 59 | ALA | CA-C | -7.31 | 1.43 | 1.52 |
| 2 | S | 454 | GLU | CA-C | 7.31 | 1.62 | 1.52 |
| 2 | J | 319 | ARG | C-N | -7.31 | 1.25 | 1.33 |
| 2 | S | 420 | ASN | C-N | -7.31 | 1.24 | 1.33 |
| 1 | T | 231 | THR | C-O | -7.30 | 1.15 | 1.24 |
| 3 | P | 72 | LEU | C-N | -7.30 | 1.24 | 1.33 |
| 2 | Q | 140 | PHE | CA-C | 7.30 | 1.61 | 1.52 |
| 2 | R | 78 | ASP | C-O | -7.30 | 1.15 | 1.24 |
| 2 | S | 349 | MET | SD-CE | -7.30 | 1.61 | 1.79 |
| 2 | S | 206 | ILE | C-N | 7.29 | 1.43 | 1.33 |
| 1 | F | 240 | GLY | C-N | 7.29 | 1.43 | 1.33 |
| 2 | C | 182 | ALA | CA-C | -7.29 | 1.43 | 1.52 |
| 1 | B | 230 | ILE | CA-C | 7.29 | 1.62 | 1.52 |
| 2 | S | 347 | ASP | C-N | 7.29 | 1.43 | 1.33 |
| 2 | I | 252 | LYS | C-O | -7.29 | 1.15 | 1.24 |
| 2 | H | 87 | ILE | CA-CB | 7.28 | 1.63 | 1.54 |
| 2 | C | 121 | VAL | CA-C | 7.28 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 85 | TYR | C-N | 7.28 | 1.42 | 1.33 |
| 2 | H | 99 | ALA | C-N | 7.28 | 1.43 | 1.33 |
| 2 | H | 117 | LEU | C-N | -7.27 | 1.24 | 1.33 |
| 2 | J | 354 | ILE | CA-C | -7.27 | 1.43 | 1.52 |
| 2 | I | 226 | HIS | CD2-NE2 | 7.27 | 1.45 | 1.37 |
| 2 | I | 25 | TYR | CA-C | 7.26 | 1.61 | 1.52 |
| 2 | R | 270 | LEU | C-N | -7.26 | 1.24 | 1.33 |
| 2 | C | 231 | GLU | CA-C | 7.25 | 1.62 | 1.53 |
| 2 | Q | 364 | PHE | C-N | 7.25 | 1.43 | 1.33 |
| 1 | F | 305 | LEU | CA-C | 7.25 | 1.62 | 1.52 |
| 2 | H | 319 | ARG | C-N | 7.24 | 1.42 | 1.33 |
| 2 | Q | 315 | ALA | C-N | 7.24 | 1.43 | 1.33 |
| 2 | H | 353 | HIS | CA-C | -7.24 | 1.44 | 1.52 |
| 2 | Q | 362 | VAL | CA-C | 7.24 | 1.61 | 1.52 |
| 2 | I | 52 | GLU | C-N | 7.24 | 1.43 | 1.33 |
| 2 | I | 252 | LYS | CA-C | 7.24 | 1.62 | 1.52 |
| 3 | N | 60 | LEU | CA-C | 7.24 | 1.61 | 1.52 |
| 2 | I | 327 | HIS | CD2-NE2 | 7.23 | 1.45 | 1.37 |
| 2 | S | 300 | VAL | CA-C | 7.22 | 1.62 | 1.52 |
| 2 | R | 138 | ILE | CA-C | 7.22 | 1.61 | 1.52 |
| 3 | E | 104 | ILE | C-N | 7.22 | 1.40 | 1.33 |
| 3 | O | 41 | LEU | CA-C | -7.21 | 1.44 | 1.52 |
| 3 | O | 57 | MET | SD-CE | -7.21 | 1.61 | 1.79 |
| 2 | I | 426 | ALA | CA-C | 7.20 | 1.61 | 1.52 |
| 2 | S | 382 | ILE | C-N | 7.20 | 1.43 | 1.33 |
| 1 | A | 236 | LEU | CA-C | -7.19 | 1.43 | 1.52 |
| 2 | C | 110 | GLU | CA-C | -7.19 | 1.43 | 1.52 |
| 3 | D | 95 | ILE | CA-C | -7.18 | 1.44 | 1.52 |
| 2 | R | 454 | GLU | C-N | 7.18 | 1.43 | 1.33 |
| 2 | Q | 23 | THR | C-N | -7.18 | 1.24 | 1.33 |
| 2 | G | 287 | ASN | CA-CB | -7.17 | 1.43 | 1.53 |
| 2 | Q | 184 | ASN | N-CA | 7.17 | 1.55 | 1.46 |
| 2 | G | 98 | PHE | CA-C | 7.17 | 1.61 | 1.52 |
| 2 | G | 158 | GLU | CA-C | -7.15 | 1.43 | 1.52 |
| 2 | C | 228 | SER | N-CA | 7.15 | 1.54 | 1.46 |
| 2 | R | 167 | ARG | C-N | -7.15 | 1.24 | 1.33 |
| 2 | G | 257 | ALA | CA-C | 7.14 | 1.61 | 1.52 |
| 1 | B | 267 | THR | CA-C | 7.14 | 1.62 | 1.52 |
| 2 | C | 266 | MET | SD-CE | -7.14 | 1.61 | 1.79 |
| 2 | C | 300 | VAL | CA-C | 7.13 | 1.61 | 1.52 |
| 2 | J | 184 | ASN | C-N | 7.13 | 1.43 | 1.33 |
| 3 | K | 45 | ASN | CA-C | -7.13 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 350 | ARG | CA-C | 7.13 | 1.58 | 1.52 |
| 2 | S | 41 | ARG | C-N | 7.12 | 1.42 | 1.33 |
| 2 | S | 266 | MET | CA-C | -7.12 | 1.43 | 1.52 |
| 2 | C | 277 | ASN | C-N | -7.12 | 1.24 | 1.33 |
| 3 | O | 87 | ILE | C-O | -7.12 | 1.16 | 1.24 |
| 2 | S | 312 | ARG | N-CA | 7.12 | 1.55 | 1.46 |
| 2 | G | 265 | ILE | C-O | -7.11 | 1.15 | 1.23 |
| 2 | R | 206 | ILE | CA-CB | 7.11 | 1.61 | 1.53 |
| 2 | C | 134 | ARG | C-O | -7.11 | 1.15 | 1.23 |
| 2 | I | 198 | ASP | N-CA | -7.11 | 1.37 | 1.46 |
| 2 | C | 302 | ASP | CA-C | -7.10 | 1.42 | 1.52 |
| 2 | I | 163 | ASN | CA-C | 7.10 | 1.63 | 1.52 |
| 2 | R | 158 | GLU | CA-C | -7.10 | 1.43 | 1.52 |
| 2 | C | 143 | ALA | C-N | -7.10 | 1.24 | 1.34 |
| 2 | G | 294 | HIS | ND1-CE1 | 7.09 | 1.39 | 1.32 |
| 3 | M | 81 | GLU | CA-C | -7.09 | 1.42 | 1.52 |
| 3 | N | 38 | PHE | CA-C | -7.09 | 1.43 | 1.52 |
| 2 | R | 456 | ALA | CA-C | 7.09 | 1.61 | 1.52 |
| 2 | H | 139 | ARG | CA-CB | 7.09 | 1.62 | 1.53 |
| 2 | S | 36 | LEU | C-O | -7.08 | 1.15 | 1.24 |
| 2 | C | 158 | GLU | CA-C | -7.08 | 1.43 | 1.52 |
| 2 | J | 390 | LEU | C-N | 7.08 | 1.42 | 1.33 |
| 2 | H | 394 | PHE | CA-C | 7.08 | 1.61 | 1.52 |
| 2 | I | 102 | ALA | C-O | -7.08 | 1.15 | 1.23 |
| 2 | I | 262 | MET | SD-CE | -7.08 | 1.61 | 1.79 |
| 2 | I | 384 | VAL | CA-C | 7.08 | 1.62 | 1.52 |
| 2 | J | 75 | THR | C-N | 7.07 | 1.43 | 1.33 |
| 3 | L | 44 | PHE | C-O | -7.07 | 1.15 | 1.23 |
| 2 | S | 292 | HIS | ND1-CE1 | 7.07 | 1.39 | 1.32 |
| 3 | L | 11 | ARG | C-N | -7.07 | 1.24 | 1.33 |
| 3 | O | 63 | PHE | CA-C | 7.07 | 1.62 | 1.52 |
| 3 | M | 48 | SER | CA-C | 7.06 | 1.60 | 1.52 |
| 2 | C | 449 | GLY | C-N | 7.06 | 1.43 | 1.34 |
| 2 | Q | 153 | HIS | CA-C | 7.06 | 1.59 | 1.52 |
| 2 | I | 121 | VAL | C-N | 7.06 | 1.42 | 1.33 |
| 3 | M | 39 | HIS | C-N | 7.06 | 1.42 | 1.33 |
| 2 | J | 457 | ALA | C-N | 7.05 | 1.43 | 1.33 |
| 1 | B | 254 | ARG | CA-C | -7.05 | 1.43 | 1.52 |
| 1 | F | 278 | ASN | C-O | -7.05 | 1.15 | 1.24 |
| 2 | C | 387 | MET | SD-CE | -7.05 | 1.61 | 1.79 |
| 2 | H | 24 | TYR | C-N | -7.05 | 1.24 | 1.33 |
| 2 | J | 274 | PHE | C-N | 7.05 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 267 | HIS | CD2-NE2 | 7.04 | 1.45 | 1.37 |
| 1 | F | 228 | GLU | N-CA | 7.04 | 1.55 | 1.46 |
| 2 | H | 279 | THR | CA-C | -7.04 | 1.43 | 1.52 |
| 2 | Q | 162 | LEU | C-O | -7.04 | 1.14 | 1.24 |
| 2 | C | 271 | THR | CA-C | -7.04 | 1.44 | 1.53 |
| 3 | E | 105 | VAL | C-O | -7.04 | 1.15 | 1.24 |
| 2 | H | 346 | VAL | N-CA | -7.04 | 1.38 | 1.46 |
| 2 | H | 364 | PHE | C-O | -7.04 | 1.15 | 1.23 |
| 2 | S | 148 | PHE | C-N | -7.04 | 1.24 | 1.33 |
| 2 | I | 357 | ASP | CA-C | -7.03 | 1.44 | 1.52 |
| 3 | K | 56 | THR | C-N | -7.03 | 1.24 | 1.33 |
| 2 | I | 45 | GLN | CA-C | -7.03 | 1.46 | 1.53 |
| 2 | Q | 211 | PHE | CA-C | 7.03 | 1.62 | 1.52 |
| 1 | A | 287 | TYR | C-N | 7.03 | 1.42 | 1.33 |
| 2 | I | 76 | ASP | C-N | 7.02 | 1.43 | 1.33 |
| 2 | G | 423 | ALA | C-N | 7.02 | 1.42 | 1.33 |
| 2 | G | 189 | VAL | C-N | -7.02 | 1.24 | 1.33 |
| 3 | K | 12 | PHE | N-CA | 7.02 | 1.54 | 1.45 |
| 2 | J | 345 | PHE | C-O | -7.02 | 1.15 | 1.24 |
| 2 | G | 251 | MET | CA-C | -7.02 | 1.44 | 1.52 |
| 2 | I | 429 | GLN | N-CA | 7.02 | 1.54 | 1.46 |
| 2 | J | 85 | TYR | C-N | 7.01 | 1.42 | 1.33 |
| 2 | R | 313 | VAL | C-N | -7.01 | 1.24 | 1.33 |
| 2 | S | 51 | ASP | C-N | -7.01 | 1.24 | 1.33 |
| 2 | H | 240 | LEU | CA-C | -7.01 | 1.43 | 1.52 |
| 2 | G | 431 | ARG | CA-C | -7.01 | 1.43 | 1.52 |
| 2 | I | 164 | LYS | CA-C | 7.01 | 1.61 | 1.52 |
| 2 | R | 270 | LEU | N-CA | 7.01 | 1.54 | 1.46 |
| 1 | T | 286 | GLU | C-N | 7.00 | 1.43 | 1.33 |
| 2 | Q | 118 | THR | CA-C | 7.00 | 1.61 | 1.52 |
| 2 | R | 359 | SER | N-CA | -7.00 | 1.37 | 1.46 |
| 2 | C | 391 | VAL | C-N | -7.00 | 1.25 | 1.33 |
| 2 | H | 430 | ALA | C-O | -7.00 | 1.15 | 1.24 |
| 3 | D | 58 | TRP | N-CA | -6.99 | 1.38 | 1.46 |
| 2 | G | 342 | THR | C-O | -6.99 | 1.16 | 1.24 |
| 2 | Q | 134 | ARG | C-N | -6.99 | 1.24 | 1.33 |
| 2 | S | 21 | LYS | C-N | 6.99 | 1.43 | 1.34 |
| 2 | G | 211 | PHE | C-N | -6.99 | 1.24 | 1.33 |
| 2 | S | 307 | HIS | CD2-NE2 | 6.98 | 1.45 | 1.37 |
| 2 | C | 356 | ALA | CA-C | -6.98 | 1.44 | 1.52 |
| 2 | G | 116 | ILE | CA-C | -6.98 | 1.44 | 1.52 |
| 2 | H | 284 | CYS | C-O | -6.98 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | H | 304 | GLN | CA-C | -6.98 | 1.43 | 1.53 |
| 2 | J | 385 | TRP | C-N | -6.98 | 1.24 | 1.33 |
| 2 | Q | 86 | HIS | ND1-CE1 | 6.98 | 1.39 | 1.32 |
| 2 | C | 297 | MET | SD-CE | -6.97 | 1.62 | 1.79 |
| 1 | F | 247 | HIS | ND1-CE1 | 6.97 | 1.39 | 1.32 |
| 2 | R | 165 | TYR | C-N | 6.97 | 1.42 | 1.33 |
| 2 | S | 436 | ASP | C-O | -6.97 | 1.15 | 1.24 |
| 2 | Q | 248 | GLU | C-N | -6.97 | 1.25 | 1.33 |
| 2 | C | 265 | ILE | CA-CB | -6.97 | 1.45 | 1.54 |
| 2 | I | 281 | ALA | N-CA | -6.97 | 1.38 | 1.46 |
| 2 | C | 192 | CYS | N-CA | -6.96 | 1.37 | 1.46 |
| 2 | G | 119 | SER | CA-C | -6.96 | 1.44 | 1.52 |
| 2 | I | 383 | HIS | CD2-NE2 | 6.96 | 1.45 | 1.37 |
| 2 | J | 361 | GLY | C-N | -6.96 | 1.26 | 1.33 |
| 2 | J | 298 | HIS | CA-C | -6.95 | 1.43 | 1.52 |
| 2 | G | 118 | THR | CA-C | 6.95 | 1.61 | 1.52 |
| 2 | G | 445 | LEU | C-O | -6.95 | 1.16 | 1.24 |
| 2 | I | 400 | LEU | CA-C | -6.95 | 1.44 | 1.52 |
| 3 | O | 39 | HIS | ND1-CE1 | 6.95 | 1.39 | 1.32 |
| 2 | H | 321 | SER | N-CA | -6.94 | 1.38 | 1.46 |
| 2 | I | 77 | MET | SD-CE | -6.94 | 1.62 | 1.79 |
| 2 | I | 264 | ILE | CA-CB | -6.94 | 1.48 | 1.55 |
| 2 | J | 306 | ASN | CA-C | 6.94 | 1.62 | 1.52 |
| 1 | B | 287 | TYR | C-N | 6.94 | 1.43 | 1.33 |
| 2 | G | 394 | PHE | CA-C | -6.94 | 1.44 | 1.52 |
| 2 | S | 187 | ARG | C-N | 6.94 | 1.42 | 1.33 |
| 2 | Q | 265 | ILE | C-N | -6.94 | 1.24 | 1.33 |
| 2 | S | 240 | LEU | CA-C | -6.94 | 1.44 | 1.52 |
| 2 | Q | 423 | ALA | CA-C | 6.93 | 1.62 | 1.52 |
| 1 | T | 279 | CYS | C-N | -6.93 | 1.24 | 1.33 |
| 2 | G | 242 | VAL | CA-CB | -6.93 | 1.46 | 1.54 |
| 2 | G | 132 | SER | N-CA | 6.93 | 1.54 | 1.46 |
| 2 | C | 87 | ILE | C-N | 6.93 | 1.40 | 1.33 |
| 2 | C | 425 | GLU | N-CA | -6.93 | 1.38 | 1.46 |
| 3 | E | 24 | ARG | N-CA | -6.93 | 1.38 | 1.46 |
| 2 | G | 37 | LEU | CA-C | 6.92 | 1.61 | 1.52 |
| 2 | G | 214 | TRP | N-CA | -6.92 | 1.38 | 1.46 |
| 2 | C | 58 | ALA | C-O | -6.92 | 1.16 | 1.24 |
| 2 | R | 165 | TYR | C-O | -6.92 | 1.15 | 1.23 |
| 2 | G | 184 | ASN | N-CA | -6.91 | 1.37 | 1.46 |
| 2 | J | 146 | LYS | C-N | -6.91 | 1.24 | 1.34 |
| 2 | G | 49 | PRO | C-O | -6.91 | 1.15 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 53 | ALA | C-O | -6.91 | 1.16 | 1.24 |
| 2 | G | 224 | ALA | CA-C | 6.91 | 1.61 | 1.52 |
| 2 | H | 276 | ALA | CA-C | 6.91 | 1.61 | 1.52 |
| 2 | I | 346 | VAL | CA-C | 6.90 | 1.61 | 1.52 |
| 2 | Q | 242 | VAL | CA-C | 6.90 | 1.59 | 1.52 |
| 2 | G | 95 | ASN | CA-C | 6.89 | 1.63 | 1.52 |
| 2 | R | 287 | ASN | CA-CB | -6.89 | 1.42 | 1.53 |
| 3 | D | 99 | GLN | N-CA | -6.89 | 1.37 | 1.46 |
| 3 | M | 86 | TYR | N-CA | -6.89 | 1.37 | 1.45 |
| 2 | Q | 377 | VAL | CA-C | -6.89 | 1.44 | 1.52 |
| 2 | S | 149 | GLN | CA-C | -6.89 | 1.43 | 1.52 |
| 2 | H | 315 | ALA | C-N | -6.89 | 1.24 | 1.33 |
| 3 | K | 33 | MET | N-CA | -6.88 | 1.38 | 1.46 |
| 2 | G | 215 | ARG | N-CA | -6.88 | 1.37 | 1.46 |
| 3 | M | 41 | LEU | CA-C | 6.88 | 1.60 | 1.52 |
| 2 | S | 320 | LEU | CA-C | -6.88 | 1.44 | 1.52 |
| 1 | F | 228 | GLU | CA-C | 6.88 | 1.61 | 1.52 |
| 2 | J | 229 | GLN | C-N | -6.88 | 1.25 | 1.33 |
| 2 | C | 223 | ASP | C-O | -6.87 | 1.16 | 1.24 |
| 1 | T | 283 | HIS | ND1-CE1 | 6.87 | 1.39 | 1.32 |
| 2 | C | 279 | THR | C-N | -6.87 | 1.24 | 1.33 |
| 3 | E | 43 | GLU | C-N | 6.86 | 1.42 | 1.33 |
| 2 | H | 235 | ILE | CA-C | -6.86 | 1.44 | 1.52 |
| 2 | C | 417 | ALA | CA-C | 6.86 | 1.61 | 1.52 |
| 2 | G | 121 | VAL | C-N | 6.86 | 1.42 | 1.33 |
| 2 | I | 180 | LEU | N-CA | 6.86 | 1.54 | 1.46 |
| 3 | K | 58 | TRP | CA-C | -6.85 | 1.45 | 1.53 |
| 2 | Q | 426 | ALA | N-CA | -6.85 | 1.38 | 1.46 |
| 2 | R | 130 | ILE | C-N | -6.85 | 1.25 | 1.33 |
| 2 | H | 330 | THR | CA-C | -6.84 | 1.44 | 1.52 |
| 2 | G | 324 | ASP | CA-C | -6.84 | 1.44 | 1.52 |
| 2 | H | 172 | CYS | CA-C | -6.84 | 1.44 | 1.52 |
| 2 | R | 183 | LYS | CA-C | 6.84 | 1.61 | 1.52 |
| 2 | C | 189 | VAL | CA-C | -6.84 | 1.45 | 1.52 |
| 2 | J | 326 | LEU | CB-CG | -6.84 | 1.39 | 1.53 |
| 2 | R | 362 | VAL | CA-C | 6.84 | 1.59 | 1.53 |
| 2 | S | 289 | VAL | CA-C | -6.83 | 1.44 | 1.52 |
| 2 | H | 160 | ASP | CA-C | -6.83 | 1.44 | 1.52 |
| 2 | S | 95 | ASN | CA-C | -6.83 | 1.43 | 1.53 |
| 2 | C | 350 | ARG | CA-C | 6.83 | 1.59 | 1.53 |
| 2 | J | 39 | ALA | N-CA | -6.83 | 1.37 | 1.46 |
| 2 | R | 51 | ASP | C-N | -6.83 | 1.24 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 72 | ASP | CA-C | -6.83 | 1.44 | 1.52 |
| 3 | L | 36 | GLN | CA-C | 6.81 | 1.62 | 1.52 |
| 2 | I | 128 | LYS | C-N | 6.81 | 1.43 | 1.33 |
| 2 | Q | 269 | PHE | CA-C | -6.81 | 1.43 | 1.52 |
| 2 | J | 316 | LYS | CA-C | 6.81 | 1.61 | 1.52 |
| 2 | J | 428 | VAL | C-N | -6.81 | 1.25 | 1.33 |
| 2 | R | 347 | ASP | C-N | 6.80 | 1.42 | 1.33 |
| 2 | G | 191 | GLU | C-N | -6.80 | 1.25 | 1.33 |
| 2 | I | 244 | ALA | CA-C | 6.80 | 1.58 | 1.52 |
| 2 | I | 390 | LEU | N-CA | -6.80 | 1.38 | 1.46 |
| 2 | C | 256 | PHE | N-CA | -6.80 | 1.38 | 1.46 |
| 2 | S | 395 | GLY | C-N | 6.79 | 1.43 | 1.34 |
| 2 | C | 271 | THR | C-O | -6.79 | 1.16 | 1.24 |
| 2 | S | 130 | ILE | CA-CB | 6.79 | 1.62 | 1.54 |
| 2 | G | 253 | ARG | CA-C | 6.78 | 1.61 | 1.52 |
| 3 | O | 63 | PHE | C-O | -6.77 | 1.15 | 1.24 |
| 2 | S | 230 | ALA | C-O | -6.77 | 1.16 | 1.24 |
| 2 | I | 179 | GLY | C-N | -6.77 | 1.24 | 1.33 |
| 3 | E | 23 | ASP | C-N | 6.77 | 1.42 | 1.33 |
| 2 | S | 276 | ALA | CA-C | -6.77 | 1.44 | 1.52 |
| 2 | G | 199 | PHE | CA-C | -6.76 | 1.44 | 1.52 |
| 2 | J | 325 | HIS | ND1-CE1 | -6.76 | 1.25 | 1.32 |
| 2 | S | 366 | GLN | CA-C | -6.76 | 1.44 | 1.52 |
| 2 | G | 149 | GLN | C-N | 6.76 | 1.43 | 1.33 |
| 2 | C | 309 | ILE | CA-C | 6.75 | 1.60 | 1.52 |
| 2 | G | 197 | LEU | CA-C | -6.75 | 1.44 | 1.52 |
| 2 | S | 286 | ASP | CA-C | -6.75 | 1.43 | 1.52 |
| 2 | R | 226 | HIS | CD2-NE2 | 6.75 | 1.45 | 1.37 |
| 2 | C | 298 | HIS | CA-C | -6.75 | 1.44 | 1.52 |
| 2 | H | 21 | LYS | CA-C | -6.75 | 1.44 | 1.52 |
| 2 | H | 194 | ARG | N-CA | 6.75 | 1.55 | 1.46 |
| 2 | S | 118 | THR | CA-CB | -6.75 | 1.42 | 1.53 |
| 2 | J | 397 | ASP | CA-C | 6.75 | 1.61 | 1.52 |
| 2 | G | 45 | GLN | CA-C | -6.75 | 1.44 | 1.52 |
| 2 | R | 125 | PHE | CA-C | -6.75 | 1.43 | 1.52 |
| 2 | G | 63 | THR | CA-C | 6.74 | 1.61 | 1.52 |
| 2 | I | 387 | MET | SD-CE | 6.74 | 1.96 | 1.79 |
| 2 | S | 284 | CYS | CA-C | 6.74 | 1.61 | 1.52 |
| 2 | J | 100 | PHE | CA-C | -6.74 | 1.44 | 1.52 |
| 2 | R | 61 | SER | CA-C | -6.74 | 1.43 | 1.52 |
| 2 | I | 273 | GLY | C-N | -6.74 | 1.24 | 1.33 |
| 2 | J | 298 | HIS | C-N | -6.74 | 1.25 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 213 | ARG | CA-CB | 6.74 | 1.63 | 1.53 |
| 2 | C | 76 | ASP | N-CA | -6.74 | 1.37 | 1.46 |
| 2 | R | 89 | PRO | CA-C | -6.74 | 1.44 | 1.52 |
| 1 | A | 232 | GLN | CA-C | -6.73 | 1.43 | 1.52 |
| 2 | I | 224 | ALA | CA-C | 6.73 | 1.61 | 1.52 |
| 3 | K | 33 | MET | C-N | 6.73 | 1.42 | 1.34 |
| 3 | L | 41 | LEU | C-O | -6.73 | 1.16 | 1.24 |
| 3 | L | 67 | SER | CA-C | -6.73 | 1.45 | 1.52 |
| 2 | R | 313 | VAL | CA-C | -6.73 | 1.44 | 1.52 |
| 2 | C | 252 | LYS | N-CA | -6.72 | 1.38 | 1.46 |
| 3 | D | 25 | GLN | N-CA | 6.72 | 1.54 | 1.46 |
| 2 | G | 311 | PHE | C-N | -6.72 | 1.25 | 1.33 |
| 3 | L | 9 | GLU | CA-C | -6.72 | 1.44 | 1.52 |
| 2 | J | 114 | THR | C-N | -6.72 | 1.25 | 1.33 |
| 1 | T | 262 | ALA | C-N | -6.72 | 1.25 | 1.33 |
| 2 | R | 389 | ALA | C-N | -6.71 | 1.25 | 1.33 |
| 3 | D | 80 | SER | CA-C | -6.71 | 1.44 | 1.52 |
| 2 | J | 345 | PHE | C-N | 6.71 | 1.42 | 1.34 |
| 2 | J | 438 | TYR | CA-C | -6.71 | 1.44 | 1.52 |
| 2 | H | 144 | LEU | CA-C | 6.71 | 1.61 | 1.52 |
| 2 | C | 221 | VAL | N-CA | -6.71 | 1.38 | 1.46 |
| 2 | S | 326 | LEU | N-CA | -6.71 | 1.38 | 1.46 |
| 2 | H | 421 | ARG | N-CA | 6.71 | 1.54 | 1.46 |
| 2 | J | 145 | VAL | CA-C | -6.70 | 1.44 | 1.52 |
| 2 | J | 189 | VAL | C-N | -6.70 | 1.25 | 1.33 |
| 2 | C | 294 | HIS | CE1-NE2 | -6.70 | 1.25 | 1.32 |
| 2 | C | 312 | ARG | C-O | -6.70 | 1.16 | 1.24 |
| 2 | R | 269 | PHE | C-O | -6.70 | 1.16 | 1.24 |
| 3 | L | 33 | MET | SD-CE | -6.70 | 1.62 | 1.79 |
| 2 | H | 353 | HIS | N-CA | 6.70 | 1.54 | 1.46 |
| 3 | O | 51 | GLU | C-O | -6.69 | 1.15 | 1.24 |
| 1 | B | 302 | PHE | C-N | -6.69 | 1.23 | 1.33 |
| 2 | R | 209 | GLN | CA-C | 6.69 | 1.60 | 1.53 |
| 2 | S | 268 | ASP | N-CA | 6.69 | 1.54 | 1.46 |
| 2 | G | 444 | ILE | CA-CB | 6.69 | 1.61 | 1.54 |
| 2 | H | 436 | ASP | C-O | -6.69 | 1.15 | 1.23 |
| 2 | Q | 413 | ASN | CA-C | -6.68 | 1.44 | 1.52 |
| 2 | S | 121 | VAL | C-N | 6.68 | 1.42 | 1.33 |
| 2 | C | 206 | ILE | CA-CB | 6.68 | 1.60 | 1.53 |
| 2 | C | 263 | PRO | C-N | 6.68 | 1.42 | 1.33 |
| 2 | J | 143 | ALA | CA-C | -6.68 | 1.44 | 1.52 |
| 2 | S | 84 | CYS | CA-C | 6.68 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 313 | VAL | C-O | -6.68 | 1.16 | 1.24 |
| 2 | Q | 397 | ASP | C-N | 6.68 | 1.42 | 1.33 |
| 2 | Q | 229 | GLN | CA-C | -6.68 | 1.44 | 1.52 |
| 2 | R | 133 | LEU | C-O | -6.68 | 1.15 | 1.23 |
| 2 | G | 80 | TYR | C-N | 6.67 | 1.42 | 1.33 |
| 2 | S | 295 | ARG | CA-C | 6.67 | 1.62 | 1.53 |
| 2 | G | 79 | ARG | C-N | 6.67 | 1.42 | 1.33 |
| 2 | I | 281 | ALA | C-N | 6.67 | 1.42 | 1.33 |
| 2 | S | 130 | ILE | C-O | -6.67 | 1.16 | 1.24 |
| 2 | C | 221 | VAL | C-O | -6.67 | 1.16 | 1.24 |
| 2 | S | 199 | PHE | N-CA | -6.67 | 1.37 | 1.45 |
| 2 | H | 209 | GLN | N-CA | -6.66 | 1.38 | 1.45 |
| 2 | J | 132 | SER | C-N | 6.66 | 1.43 | 1.33 |
| 2 | J | 143 | ALA | C-O | 6.66 | 1.31 | 1.24 |
| 2 | Q | 81 | LYS | C-N | 6.66 | 1.38 | 1.33 |
| 2 | H | 101 | ILE | CA-CB | 6.66 | 1.63 | 1.54 |
| 3 | P | 79 | ARG | C-O | -6.66 | 1.16 | 1.24 |
| 2 | S | 90 | VAL | C-O | 6.66 | 1.31 | 1.24 |
| 2 | R | 326 | LEU | CA-C | -6.66 | 1.45 | 1.52 |
| 1 | B | 256 | SER | CA-C | 6.66 | 1.62 | 1.53 |
| 2 | G | 30 | THR | CA-C | 6.66 | 1.59 | 1.52 |
| 2 | J | 40 | PHE | CA-C | -6.65 | 1.44 | 1.52 |
| 3 | L | 39 | HIS | CE1-NE2 | -6.65 | 1.25 | 1.32 |
| 2 | Q | 393 | ILE | C-N | 6.65 | 1.42 | 1.33 |
| 2 | C | 277 | ASN | CA-C | -6.65 | 1.44 | 1.52 |
| 2 | I | 115 | ASN | CA-C | -6.65 | 1.43 | 1.52 |
| 2 | C | 387 | MET | CA-C | 6.64 | 1.61 | 1.52 |
| 2 | G | 437 | LEU | CA-C | -6.64 | 1.44 | 1.52 |
| 2 | J | 266 | MET | SD-CE | -6.64 | 1.62 | 1.79 |
| 2 | H | 270 | LEU | CB-CG | -6.64 | 1.40 | 1.53 |
| 2 | I | 47 | GLY | C-N | 6.64 | 1.39 | 1.33 |
| 2 | I | 233 | GLY | C-N | -6.64 | 1.25 | 1.33 |
| 2 | J | 57 | ILE | CA-CB | 6.63 | 1.62 | 1.54 |
| 1 | A | 230 | ILE | C-O | -6.63 | 1.16 | 1.24 |
| 2 | I | 60 | GLU | C-N | -6.63 | 1.25 | 1.33 |
| 2 | C | 251 | MET | CA-C | -6.63 | 1.44 | 1.52 |
| 2 | G | 448 | ALA | CA-C | 6.63 | 1.61 | 1.52 |
| 2 | J | 97 | TYR | CA-C | 6.63 | 1.60 | 1.52 |
| 3 | E | 94 | ASN | CA-C | 6.63 | 1.61 | 1.52 |
| 2 | I | 228 | SER | C-N | 6.63 | 1.42 | 1.33 |
| 2 | Q | 269 | PHE | N-CA | 6.63 | 1.54 | 1.46 |
| 2 | G | 304 | GLN | C-N | -6.62 | 1.25 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | M | 101 | VAL | N-CA | -6.62 | 1.38 | 1.46 |
| 2 | Q | 264 | ILE | C-O | -6.62 | 1.17 | 1.23 |
| 2 | H | 33 | ASP | CA-C | 6.62 | 1.61 | 1.52 |
| 2 | H | 244 | ALA | CA-CB | -6.62 | 1.45 | 1.54 |
| 2 | H | 152 | PRO | C-N | -6.62 | 1.24 | 1.33 |
| 3 | P | 75 | VAL | N-CA | -6.62 | 1.38 | 1.46 |
| 3 | K | 53 | PHE | CA-C | -6.61 | 1.44 | 1.52 |
| 2 | S | 248 | GLU | C-O | -6.61 | 1.16 | 1.24 |
| 2 | R | 326 | LEU | C-N | 6.61 | 1.42 | 1.33 |
| 2 | I | 139 | ARG | CA-C | 6.61 | 1.62 | 1.53 |
| 1 | A | 264 | ILE | C-N | 6.61 | 1.42 | 1.33 |
| 2 | Q | 265 | ILE | C-O | -6.61 | 1.15 | 1.23 |
| 2 | S | 116 | ILE | CA-C | -6.61 | 1.45 | 1.52 |
| 3 | K | 32 | TYR | C-O | 6.61 | 1.31 | 1.24 |
| 2 | G | 382 | ILE | C-N | 6.60 | 1.41 | 1.33 |
| 2 | J | 38 | ALA | CA-C | 6.60 | 1.60 | 1.52 |
| 2 | Q | 234 | GLU | CA-C | -6.60 | 1.44 | 1.52 |
| 3 | E | 17 | TYR | C-N | 6.60 | 1.43 | 1.33 |
| 2 | S | 417 | ALA | C-N | -6.59 | 1.25 | 1.33 |
| 2 | S | 274 | PHE | CA-C | -6.59 | 1.44 | 1.52 |
| 2 | H | 276 | ALA | C-N | -6.59 | 1.25 | 1.33 |
| 2 | I | 116 | ILE | C-N | -6.59 | 1.25 | 1.33 |
| 2 | I | 142 | VAL | C-N | -6.59 | 1.25 | 1.33 |
| 2 | S | 223 | ASP | C-N | 6.59 | 1.42 | 1.33 |
| 3 | N | 54 | TYR | CA-C | -6.59 | 1.44 | 1.52 |
| 2 | I | 143 | ALA | N-CA | -6.58 | 1.38 | 1.46 |
| 2 | I | 153 | HIS | ND1-CE1 | 6.58 | 1.39 | 1.32 |
| 2 | G | 359 | SER | C-O | 6.58 | 1.31 | 1.24 |
| 2 | I | 244 | ALA | N-CA | -6.58 | 1.39 | 1.45 |
| 2 | S | 46 | PRO | C-O | 6.58 | 1.31 | 1.23 |
| 3 | P | 51 | GLU | CA-C | 6.58 | 1.61 | 1.52 |
| 3 | D | 18 | LEU | CA-C | -6.58 | 1.43 | 1.53 |
| 2 | H | 437 | LEU | CA-C | -6.58 | 1.44 | 1.52 |
| 2 | I | 24 | TYR | CA-C | 6.57 | 1.60 | 1.52 |
| 2 | I | 129 | ALA | N-CA | -6.57 | 1.37 | 1.46 |
| 2 | J | 302 | ASP | CA-C | -6.57 | 1.44 | 1.52 |
| 3 | E | 54 | TYR | C-O | -6.57 | 1.16 | 1.23 |
| 1 | F | 267 | THR | CA-C | 6.57 | 1.61 | 1.52 |
| 2 | G | 382 | ILE | CA-C | -6.57 | 1.44 | 1.52 |
| 2 | Q | 390 | LEU | C-N | 6.57 | 1.42 | 1.33 |
| 2 | Q | 451 | TRP | N-CA | -6.57 | 1.37 | 1.46 |
| 1 | F | 227 | SER | C-N | 6.57 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 149 | GLN | N-CA | -6.57 | 1.37 | 1.46 |
| 2 | Q | 222 | ALA | N-CA | 6.57 | 1.54 | 1.46 |
| 2 | I | 221 | VAL | C-O | -6.57 | 1.16 | 1.24 |
| 2 | H | 455 | LEU | C-N | 6.56 | 1.42 | 1.33 |
| 2 | R | 343 | LEU | CA-C | 6.56 | 1.61 | 1.52 |
| 2 | R | 369 | ALA | CA-C | -6.56 | 1.45 | 1.53 |
| 2 | G | 23 | THR | CA-C | 6.56 | 1.61 | 1.52 |
| 2 | H | 360 | ARG | N-CA | 6.56 | 1.55 | 1.46 |
| 3 | M | 30 | ILE | C-O | -6.56 | 1.16 | 1.24 |
| 2 | Q | 316 | LYS | C-N | -6.56 | 1.25 | 1.33 |
| 2 | I | 194 | ARG | C-N | 6.55 | 1.41 | 1.33 |
| 2 | R | 163 | ASN | N-CA | -6.55 | 1.38 | 1.46 |
| 3 | N | 91 | GLY | C-N | 6.55 | 1.42 | 1.33 |
| 1 | B | 234 | ARG | C-O | -6.55 | 1.16 | 1.24 |
| 2 | Q | 228 | SER | C-N | -6.55 | 1.25 | 1.33 |
| 2 | R | 200 | THR | C-O | -6.55 | 1.16 | 1.23 |
| 2 | J | 437 | LEU | CA-C | -6.54 | 1.43 | 1.52 |
| 2 | R | 346 | VAL | C-N | -6.54 | 1.25 | 1.33 |
| 2 | I | 347 | ASP | C-N | -6.54 | 1.25 | 1.33 |
| 2 | R | 260 | LEU | C-N | 6.54 | 1.42 | 1.33 |
| 1 | F | 257 | SER | C-N | 6.54 | 1.42 | 1.33 |
| 2 | J | 30 | THR | C-N | -6.54 | 1.26 | 1.33 |
| 2 | Q | 217 | ARG | C-O | -6.54 | 1.16 | 1.24 |
| 2 | S | 124 | VAL | C-O | -6.54 | 1.16 | 1.24 |
| 1 | T | 252 | ARG | CA-CB | 6.54 | 1.63 | 1.53 |
| 3 | P | 78 | CYS | C-O | -6.53 | 1.16 | 1.24 |
| 2 | C | 230 | ALA | C-N | -6.53 | 1.24 | 1.33 |
| 2 | S | 103 | TYR | C-N | 6.53 | 1.42 | 1.33 |
| 2 | S | 267 | HIS | N-CA | -6.53 | 1.38 | 1.46 |
| 2 | I | 199 | PHE | CA-C | -6.53 | 1.44 | 1.52 |
| 2 | S | 238 | HIS | ND1-CE1 | -6.53 | 1.26 | 1.32 |
| 2 | S | 369 | ALA | CA-C | -6.53 | 1.44 | 1.53 |
| 2 | C | 361 | GLY | C-N | 6.52 | 1.39 | 1.33 |
| 2 | C | 446 | ARG | N-CA | -6.52 | 1.38 | 1.46 |
| 3 | K | 52 | GLU | CA-CB | -6.52 | 1.44 | 1.53 |
| 2 | I | 399 | VAL | C-N | 6.52 | 1.42 | 1.33 |
| 3 | K | 39 | HIS | CG-CD2 | 6.52 | 1.43 | 1.35 |
| 2 | G | 89 | PRO | C-N | -6.52 | 1.25 | 1.33 |
| 2 | S | 375 | LEU | CB-CG | -6.52 | 1.40 | 1.53 |
| 3 | O | 63 | PHE | C-N | 6.52 | 1.42 | 1.33 |
| 2 | G | 419 | ALA | N-CA | -6.51 | 1.38 | 1.46 |
| 2 | H | 156 | GLN | N-CA | 6.51 | 1.54 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 142 | VAL | C-N | -6.51 | 1.25 | 1.33 |
| 2 | S | 293 | ILE | CA-C | -6.51 | 1.44 | 1.52 |
| 1 | A | 308 | ARG | C-O | -6.51 | 1.17 | 1.24 |
| 2 | I | 292 | HIS | CE1-NE2 | -6.51 | 1.26 | 1.32 |
| 2 | R | 349 | MET | SD-CE | -6.51 | 1.63 | 1.79 |
| 2 | I | 184 | ASN | C-O | -6.51 | 1.15 | 1.24 |
| 2 | C | 175 | LYS | CA-C | 6.51 | 1.58 | 1.52 |
| 1 | F | 231 | THR | CA-CB | -6.51 | 1.43 | 1.53 |
| 2 | G | 353 | HIS | CD2-NE2 | 6.50 | 1.45 | 1.37 |
| 2 | R | 357 | ASP | C-N | -6.50 | 1.25 | 1.33 |
| 2 | I | 276 | ALA | N-CA | 6.50 | 1.54 | 1.46 |
| 2 | S | 283 | TRP | CA-C | -6.50 | 1.44 | 1.52 |
| 3 | O | 95 | ILE | CA-C | -6.50 | 1.44 | 1.52 |
| 2 | H | 86 | HIS | C-O | -6.50 | 1.16 | 1.23 |
| 2 | R | 90 | VAL | C-N | -6.50 | 1.24 | 1.33 |
| 2 | S | 378 | ALA | CA-C | 6.49 | 1.60 | 1.52 |
| 2 | R | 158 | GLU | C-O | 6.49 | 1.31 | 1.24 |
| 2 | S | 76 | ASP | CA-C | -6.49 | 1.44 | 1.52 |
| 2 | H | 22 | LEU | CA-C | 6.49 | 1.61 | 1.52 |
| 2 | R | 276 | ALA | C-N | 6.49 | 1.42 | 1.33 |
| 2 | H | 120 | ILE | C-O | -6.49 | 1.16 | 1.24 |
| 2 | J | 315 | ALA | CA-C | -6.48 | 1.44 | 1.52 |
| 3 | M | 69 | GLN | CA-C | 6.48 | 1.61 | 1.52 |
| 2 | H | 138 | ILE | C-O | -6.47 | 1.16 | 1.23 |
| 2 | S | 51 | ASP | CA-C | 6.47 | 1.61 | 1.52 |
| 1 | A | 288 | VAL | C-N | 6.47 | 1.43 | 1.33 |
| 3 | E | 13 | GLU | C-O | -6.47 | 1.16 | 1.24 |
| 3 | O | 76 | ARG | CA-C | -6.47 | 1.44 | 1.52 |
| 2 | Q | 148 | PHE | C-N | -6.47 | 1.24 | 1.33 |
| 1 | B | 245 | THR | C-N | -6.47 | 1.24 | 1.33 |
| 2 | S | 238 | HIS | N-CA | 6.47 | 1.53 | 1.45 |
| 1 | T | 237 | LEU | CA-CB | 6.47 | 1.64 | 1.53 |
| 3 | L | 38 | PHE | CA-CB | 6.47 | 1.62 | 1.53 |
| 2 | Q | 206 | ILE | C-N | 6.47 | 1.42 | 1.33 |
| 2 | R | 330 | THR | CA-CB | 6.47 | 1.64 | 1.53 |
| 2 | J | 458 | ALA | C-N | 6.46 | 1.42 | 1.33 |
| 2 | Q | 354 | ILE | C-O | -6.46 | 1.17 | 1.24 |
| 2 | R | 84 | CYS | N-CA | 6.46 | 1.54 | 1.46 |
| 2 | H | 446 | ARG | C-O | -6.46 | 1.16 | 1.24 |
| 3 | P | 75 | VAL | CA-C | 6.46 | 1.60 | 1.52 |
| 3 | O | 10 | ARG | N-CA | 6.46 | 1.54 | 1.46 |
| 3 | D | 59 | LYS | C-N | 6.46 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | H | 387 | MET | C-N | 6.46 | 1.42 | 1.33 |
| 2 | Q | 193 | LEU | CA-C | -6.46 | 1.44 | 1.52 |
| 2 | G | 207 | ASN | N-CA | -6.46 | 1.39 | 1.46 |
| 2 | J | 317 | CYS | C-N | -6.46 | 1.25 | 1.33 |
| 3 | K | 9 | GLU | CA-C | 6.46 | 1.61 | 1.52 |
| 3 | M | 77 | GLU | N-CA | 6.46 | 1.54 | 1.46 |
| 1 | T | 257 | SER | CA-C | -6.46 | 1.44 | 1.52 |
| 1 | B | 284 | GLU | CA-C | -6.46 | 1.44 | 1.52 |
| 2 | C | 223 | ASP | CA-C | 6.46 | 1.61 | 1.52 |
| 2 | C | 386 | HIS | CE1-NE2 | -6.45 | 1.26 | 1.32 |
| 3 | E | 43 | GLU | CA-C | -6.45 | 1.44 | 1.52 |
| 1 | T | 281 | SER | N-CA | 6.45 | 1.54 | 1.46 |
| 2 | S | 244 | ALA | CA-CB | -6.45 | 1.46 | 1.53 |
| 3 | O | 82 | TYR | CA-C | 6.45 | 1.61 | 1.53 |
| 3 | M | 39 | HIS | CG-CD2 | 6.45 | 1.43 | 1.35 |
| 2 | R | 120 | ILE | C-O | 6.44 | 1.31 | 1.24 |
| 2 | S | 28 | ASP | C-O | -6.44 | 1.15 | 1.24 |
| 1 | A | 252 | ARG | N-CA | 6.44 | 1.54 | 1.46 |
| 2 | H | 391 | VAL | CA-C | 6.43 | 1.61 | 1.53 |
| 2 | S | 289 | VAL | CA-CB | 6.43 | 1.61 | 1.54 |
| 2 | G | 125 | PHE | CA-C | -6.43 | 1.43 | 1.52 |
| 2 | S | 106 | ASP | C-N | 6.43 | 1.42 | 1.33 |
| 2 | S | 319 | ARG | CA-C | 6.43 | 1.61 | 1.52 |
| 2 | I | 190 | TYR | C-N | -6.43 | 1.25 | 1.33 |
| 2 | I | 98 | PHE | C-O | -6.43 | 1.16 | 1.24 |
| 2 | I | 262 | MET | C-O | -6.43 | 1.16 | 1.24 |
| 1 | T | 250 | LYS | C-O | -6.43 | 1.16 | 1.24 |
| 2 | Q | 147 | THR | C-N | 6.42 | 1.42 | 1.33 |
| 2 | Q | 263 | PRO | C-N | 6.42 | 1.42 | 1.33 |
| 3 | D | 98 | CYS | CA-C | -6.42 | 1.44 | 1.52 |
| 2 | S | 440 | GLU | CA-C | 6.42 | 1.62 | 1.52 |
| 2 | G | 240 | LEU | CA-C | -6.42 | 1.44 | 1.53 |
| 3 | K | 26 | ILE | C-N | -6.42 | 1.25 | 1.33 |
| 2 | R | 83 | LYS | CA-C | -6.42 | 1.44 | 1.53 |
| 3 | E | 107 | ARG | CA-C | 6.42 | 1.58 | 1.52 |
| 2 | H | 125 | PHE | C-O | -6.42 | 1.16 | 1.24 |
| 3 | N | 104 | ILE | CA-CB | 6.42 | 1.60 | 1.54 |
| 2 | C | 317 | CYS | C-N | -6.42 | 1.25 | 1.33 |
| 1 | A | 305 | LEU | N-CA | -6.42 | 1.38 | 1.46 |
| 2 | S | 51 | ASP | N-CA | -6.41 | 1.38 | 1.46 |
| 3 | E | 45 | ASN | CA-C | -6.41 | 1.44 | 1.52 |
| 2 | C | 356 | ALA | C-O | -6.41 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | M | 71 | VAL | CA-C | -6.41 | 1.44 | 1.52 |
| 2 | R | 362 | VAL | C-N | -6.40 | 1.25 | 1.33 |
| 2 | C | 58 | ALA | CA-C | -6.40 | 1.44 | 1.52 |
| 2 | R | 258 | LYS | N-CA | -6.40 | 1.38 | 1.46 |
| 2 | J | 447 | GLU | CA-C | -6.40 | 1.44 | 1.52 |
| 2 | I | 391 | VAL | CA-C | 6.40 | 1.60 | 1.52 |
| 2 | R | 157 | VAL | CA-C | 6.40 | 1.61 | 1.52 |
| 2 | R | 447 | GLU | C-O | 6.40 | 1.31 | 1.24 |
| 2 | R | 330 | THR | C-O | 6.39 | 1.31 | 1.23 |
| 3 | K | 30 | ILE | C-O | -6.39 | 1.16 | 1.24 |
| 3 | P | 70 | GLN | C-N | -6.39 | 1.25 | 1.33 |
| 2 | R | 187 | ARG | C-N | 6.39 | 1.42 | 1.33 |
| 2 | S | 132 | SER | C-O | -6.39 | 1.16 | 1.23 |
| 2 | H | 222 | ALA | C-O | -6.39 | 1.16 | 1.24 |
| 2 | J | 343 | LEU | CA-C | -6.39 | 1.44 | 1.52 |
| 2 | G | 105 | LEU | C-N | 6.39 | 1.43 | 1.33 |
| 2 | S | 87 | ILE | CA-C | -6.39 | 1.45 | 1.52 |
| 2 | S | 255 | GLU | CA-CB | 6.39 | 1.63 | 1.53 |
| 2 | H | 135 | LEU | CA-CB | -6.39 | 1.45 | 1.53 |
| 1 | T | 234 | ARG | CA-C | -6.39 | 1.44 | 1.52 |
| 1 | T | 249 | ASP | CA-C | 6.38 | 1.61 | 1.53 |
| 3 | E | 47 | HIS | CD2-NE2 | 6.38 | 1.44 | 1.37 |
| 2 | H | 135 | LEU | CA-C | -6.38 | 1.44 | 1.52 |
| 2 | I | 132 | SER | CA-C | -6.38 | 1.44 | 1.52 |
| 2 | I | 153 | HIS | CG-CD2 | -6.38 | 1.28 | 1.35 |
| 3 | N | 19 | PRO | C-O | 6.38 | 1.31 | 1.24 |
| 3 | P | 16 | SER | C-O | -6.38 | 1.16 | 1.24 |
| 2 | G | 444 | ILE | CA-C | -6.38 | 1.45 | 1.52 |
| 2 | Q | 354 | ILE | CB-CG1 | 6.38 | 1.66 | 1.53 |
| 2 | I | 161 | LEU | N-CA | 6.38 | 1.53 | 1.46 |
| 2 | Q | 292 | HIS | C-O | -6.38 | 1.16 | 1.23 |
| 3 | P | 77 | GLU | C-N | -6.38 | 1.25 | 1.33 |
| 2 | Q | 353 | HIS | ND1-CE1 | 6.37 | 1.39 | 1.32 |
| 2 | S | 206 | ILE | N-CA | -6.37 | 1.38 | 1.46 |
| 2 | S | 339 | LYS | CA-C | 6.37 | 1.61 | 1.52 |
| 3 | E | 36 | GLN | C-N | 6.37 | 1.41 | 1.33 |
| 2 | Q | 357 | ASP | N-CA | 6.36 | 1.54 | 1.46 |
| 2 | H | 106 | ASP | C-N | -6.36 | 1.25 | 1.33 |
| 3 | P | 106 | HIS | CA-C | -6.36 | 1.44 | 1.52 |
| 2 | R | 207 | ASN | C-O | -6.36 | 1.16 | 1.24 |
| 2 | Q | 204 | GLU | N-CA | -6.36 | 1.38 | 1.46 |
| 2 | I | 178 | LEU | CA-C | 6.36 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 33 | ASP | N-CA | -6.36 | 1.38 | 1.46 |
| 3 | M | 70 | GLN | N-CA | -6.35 | 1.38 | 1.46 |
| 2 | Q | 383 | HIS | CE1-NE2 | 6.35 | 1.39 | 1.32 |
| 2 | S | 120 | ILE | C-N | 6.35 | 1.41 | 1.33 |
| 2 | C | 201 | LYS | C-N | -6.35 | 1.25 | 1.33 |
| 2 | I | 310 | HIS | ND1-CE1 | -6.35 | 1.26 | 1.32 |
| 2 | J | 383 | HIS | CA-C | -6.35 | 1.47 | 1.53 |
| 2 | C | 447 | GLU | N-CA | -6.35 | 1.38 | 1.46 |
| 2 | J | 444 | ILE | N-CA | 6.35 | 1.54 | 1.46 |
| 2 | G | 292 | HIS | CD2-NE2 | 6.35 | 1.44 | 1.37 |
| 2 | H | 203 | ASP | CA-C | 6.35 | 1.60 | 1.52 |
| 2 | Q | 305 | ARG | C-O | -6.35 | 1.16 | 1.24 |
| 2 | C | 177 | LYS | C-O | -6.34 | 1.16 | 1.24 |
| 2 | H | 374 | VAL | N-CA | -6.34 | 1.38 | 1.46 |
| 2 | J | 438 | TYR | C-N | -6.34 | 1.25 | 1.33 |
| 2 | R | 431 | ARG | CA-C | -6.34 | 1.44 | 1.52 |
| 3 | D | 31 | GLU | N-CA | 6.34 | 1.53 | 1.46 |
| 2 | I | 130 | ILE | C-N | -6.34 | 1.25 | 1.33 |
| 2 | G | 446 | ARG | N-CA | -6.34 | 1.38 | 1.46 |
| 2 | H | 255 | GLU | C-N | 6.34 | 1.42 | 1.33 |
| 2 | G | 53 | ALA | N-CA | -6.33 | 1.38 | 1.46 |
| 2 | H | 358 | ARG | CA-C | -6.33 | 1.44 | 1.52 |
| 2 | Q | 257 | ALA | C-O | -6.33 | 1.16 | 1.24 |
| 2 | H | 236 | LYS | C-N | 6.33 | 1.41 | 1.33 |
| 2 | R | 325 | HIS | CD2-NE2 | 6.33 | 1.44 | 1.37 |
| 2 | S | 80 | TYR | CA-C | 6.33 | 1.61 | 1.52 |
| 2 | S | 99 | ALA | CA-CB | -6.33 | 1.43 | 1.53 |
| 1 | F | 246 | GLU | C-N | 6.33 | 1.43 | 1.33 |
| 2 | I | 454 | GLU | C-N | 6.33 | 1.42 | 1.34 |
| 2 | G | 136 | GLU | N-CA | -6.32 | 1.38 | 1.46 |
| 2 | Q | 439 | ARG | C-O | -6.32 | 1.15 | 1.23 |
| 2 | S | 227 | LYS | N-CA | -6.32 | 1.38 | 1.46 |
| 2 | J | 64 | GLY | C-N | 6.32 | 1.42 | 1.33 |
| 2 | G | 138 | ILE | C-N | 6.32 | 1.41 | 1.33 |
| 2 | J | 258 | LYS | N-CA | 6.32 | 1.54 | 1.46 |
| 2 | R | 202 | ASP | CA-C | -6.32 | 1.44 | 1.52 |
| 2 | S | 178 | LEU | CA-C | 6.32 | 1.60 | 1.52 |
| 2 | C | 283 | TRP | CA-C | 6.31 | 1.60 | 1.52 |
| 2 | C | 325 | HIS | CG-CD2 | -6.31 | 1.28 | 1.35 |
| 3 | L | 84 | ASP | CA-C | 6.31 | 1.63 | 1.52 |
| 3 | E | 84 | ASP | N-CA | -6.31 | 1.39 | 1.46 |
| 2 | H | 143 | ALA | C-N | -6.31 | 1.25 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 56 | ALA | CA-C | -6.31 | 1.44 | 1.52 |
| 2 | H | 212 | GLN | C-O | 6.31 | 1.31 | 1.23 |
| 3 | L | 31 | GLU | CA-C | 6.30 | 1.60 | 1.52 |
| 2 | S | 246 | THR | CA-C | 6.30 | 1.60 | 1.52 |
| 2 | H | 253 | ARG | CA-C | -6.30 | 1.44 | 1.52 |
| 2 | J | 353 | HIS | C-N | 6.30 | 1.42 | 1.33 |
| 2 | I | 215 | ARG | C-O | -6.30 | 1.16 | 1.24 |
| 3 | P | 35 | GLU | N-CA | 6.30 | 1.54 | 1.46 |
| 2 | Q | 189 | VAL | C-O | -6.30 | 1.17 | 1.24 |
| 2 | C | 298 | HIS | CD2-NE2 | 6.29 | 1.44 | 1.37 |
| 2 | G | 321 | SER | C-O | -6.29 | 1.16 | 1.24 |
| 2 | G | 341 | SER | C-N | 6.29 | 1.41 | 1.33 |
| 2 | Q | 424 | LEU | CB-CG | -6.29 | 1.40 | 1.53 |
| 3 | D | 67 | SER | C-N | -6.29 | 1.26 | 1.34 |
| 2 | C | 393 | ILE | CA-CB | 6.29 | 1.61 | 1.54 |
| 3 | E | 87 | ILE | N-CA | 6.29 | 1.54 | 1.46 |
| 3 | O | 72 | LEU | CA-CB | 6.29 | 1.63 | 1.53 |
| 2 | S | 256 | PHE | CA-C | 6.29 | 1.61 | 1.52 |
| 2 | Q | 175 | LYS | N-CA | -6.28 | 1.38 | 1.45 |
| 2 | S | 416 | GLY | C-N | -6.28 | 1.25 | 1.33 |
| 1 | B | 304 | ALA | N-CA | -6.28 | 1.39 | 1.46 |
| 2 | C | 392 | GLU | CA-C | -6.28 | 1.44 | 1.52 |
| 2 | I | 203 | ASP | C-O | 6.28 | 1.31 | 1.23 |
| 2 | S | 30 | THR | CA-C | 6.28 | 1.59 | 1.52 |
| 2 | C | 124 | VAL | CA-C | -6.28 | 1.44 | 1.52 |
| 2 | J | 243 | THR | C-O | -6.28 | 1.16 | 1.24 |
| 2 | H | 232 | THR | CA-C | 6.28 | 1.61 | 1.52 |
| 2 | S | 127 | PHE | N-CA | -6.28 | 1.38 | 1.46 |
| 3 | O | 74 | GLU | C-O | 6.27 | 1.31 | 1.24 |
| 3 | E | 106 | HIS | N-CA | -6.27 | 1.38 | 1.45 |
| 2 | C | 29 | TYR | C-O | -6.27 | 1.16 | 1.23 |
| 2 | C | 201 | LYS | CA-C | -6.27 | 1.45 | 1.52 |
| 2 | S | 37 | LEU | CA-CB | 6.27 | 1.62 | 1.53 |
| 1 | F | 265 | GLN | C-N | 6.26 | 1.42 | 1.33 |
| 2 | J | 138 | ILE | C-O | -6.26 | 1.17 | 1.24 |
| 2 | R | 85 | TYR | C-N | 6.26 | 1.41 | 1.33 |
| 2 | S | 149 | GLN | N-CA | -6.26 | 1.38 | 1.46 |
| 3 | D | 44 | PHE | C-N | -6.26 | 1.24 | 1.33 |
| 2 | I | 81 | LYS | CA-C | -6.26 | 1.45 | 1.52 |
| 2 | J | 370 | SER | CA-C | -6.26 | 1.43 | 1.52 |
| 3 | N | 17 | TYR | CA-C | 6.26 | 1.61 | 1.52 |
| 2 | R | 130 | ILE | C-O | -6.26 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 266 | MET | SD-CE | -6.26 | 1.64 | 1.79 |
| 2 | C | 383 | HIS | CG-CD2 | -6.26 | 1.28 | 1.35 |
| 2 | G | 143 | ALA | CA-CB | -6.25 | 1.43 | 1.53 |
| 2 | S | 181 | SER | CA-C | -6.25 | 1.45 | 1.52 |
| 2 | H | 387 | MET | SD-CE | -6.25 | 1.64 | 1.79 |
| 2 | S | 304 | GLN | C-N | -6.25 | 1.24 | 1.33 |
| 2 | I | 125 | PHE | CA-C | -6.25 | 1.44 | 1.52 |
| 2 | S | 267 | HIS | ND1-CE1 | 6.25 | 1.38 | 1.32 |
| 3 | D | 9 | GLU | C-N | 6.25 | 1.41 | 1.33 |
| 2 | R | 172 | CYS | CA-C | -6.25 | 1.45 | 1.52 |
| 2 | S | 39 | ALA | CA-C | -6.25 | 1.45 | 1.52 |
| 2 | R | 44 | PRO | CA-CB | -6.24 | 1.45 | 1.53 |
| 2 | I | 159 | ARG | C-N | 6.24 | 1.42 | 1.33 |
| 2 | S | 62 | SER | CA-C | -6.24 | 1.46 | 1.52 |
| 2 | S | 265 | ILE | CA-CB | 6.24 | 1.62 | 1.54 |
| 2 | C | 102 | ALA | N-CA | 6.24 | 1.53 | 1.46 |
| 2 | J | 390 | LEU | CA-C | 6.24 | 1.60 | 1.52 |
| 2 | S | 158 | GLU | CA-C | -6.24 | 1.44 | 1.52 |
| 3 | M | 85 | CYS | N-CA | 6.23 | 1.54 | 1.46 |
| 2 | S | 118 | THR | CA-C | 6.23 | 1.60 | 1.52 |
| 2 | H | 443 | ASP | CA-C | -6.23 | 1.45 | 1.52 |
| 3 | D | 39 | HIS | CD2-NE2 | 6.23 | 1.44 | 1.37 |
| 3 | N | 47 | HIS | CG-CD2 | 6.23 | 1.42 | 1.35 |
| 2 | S | 269 | PHE | CA-CB | 6.23 | 1.63 | 1.53 |
| 1 | B | 283 | HIS | CD2-NE2 | 6.22 | 1.44 | 1.37 |
| 2 | J | 394 | PHE | CA-C | -6.22 | 1.44 | 1.52 |
| 2 | H | 31 | PRO | C-N | -6.22 | 1.25 | 1.33 |
| 2 | S | 285 | ARG | C-O | 6.22 | 1.31 | 1.24 |
| 3 | E | 21 | LEU | CA-C | -6.22 | 1.44 | 1.52 |
| 2 | S | 78 | ASP | CA-C | -6.22 | 1.45 | 1.52 |
| 2 | J | 296 | ALA | C-O | -6.21 | 1.16 | 1.23 |
| 3 | P | 39 | HIS | CG-ND1 | -6.21 | 1.31 | 1.38 |
| 1 | F | 309 | PRO | C-N | -6.21 | 1.24 | 1.33 |
| 2 | I | 310 | HIS | CE1-NE2 | -6.21 | 1.26 | 1.32 |
| 2 | I | 256 | PHE | N-CA | -6.21 | 1.38 | 1.46 |
| 1 | T | 238 | ASN | CA-CB | -6.21 | 1.43 | 1.53 |
| 3 | N | 67 | SER | CA-C | 6.20 | 1.58 | 1.52 |
| 2 | R | 391 | VAL | C-O | -6.20 | 1.17 | 1.24 |
| 1 | B | 250 | LYS | C-N | -6.20 | 1.26 | 1.33 |
| 2 | H | 368 | TRP | N-CA | 6.20 | 1.53 | 1.46 |
| 2 | H | 450 | LYS | C-N | 6.20 | 1.43 | 1.33 |
| 3 | L | 13 | GLU | N-CA | -6.20 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 102 | ALA | CA-C | 6.20 | 1.60 | 1.52 |
| 2 | Q | 119 | SER | N-CA | 6.20 | 1.53 | 1.46 |
| 2 | J | 252 | LYS | CA-CB | 6.20 | 1.62 | 1.53 |
| 2 | Q | 453 | PRO | C-O | -6.20 | 1.16 | 1.24 |
| 2 | G | 101 | ILE | C-O | 6.20 | 1.30 | 1.24 |
| 2 | Q | 402 | PHE | N-CA | 6.20 | 1.53 | 1.45 |
| 2 | J | 356 | ALA | C-N | -6.19 | 1.25 | 1.33 |
| 3 | M | 58 | TRP | CA-C | -6.19 | 1.46 | 1.53 |
| 1 | T | 245 | THR | CA-C | 6.19 | 1.60 | 1.52 |
| 2 | J | 238 | HIS | CA-C | 6.19 | 1.59 | 1.52 |
| 2 | S | 101 | ILE | C-O | 6.19 | 1.30 | 1.24 |
| 3 | E | 76 | ARG | C-N | -6.18 | 1.26 | 1.33 |
| 2 | G | 376 | PRO | N-CA | -6.18 | 1.40 | 1.46 |
| 3 | M | 89 | VAL | N-CA | -6.18 | 1.39 | 1.46 |
| 2 | H | 254 | ALA | C-N | 6.18 | 1.41 | 1.33 |
| 3 | K | 36 | GLN | CA-C | 6.18 | 1.61 | 1.52 |
| 2 | S | 131 | ARG | N-CA | -6.18 | 1.39 | 1.46 |
| 2 | S | 329 | GLY | C-N | -6.18 | 1.25 | 1.33 |
| 2 | G | 205 | ASN | CA-C | 6.18 | 1.61 | 1.52 |
| 2 | H | 386 | HIS | C-N | -6.18 | 1.26 | 1.33 |
| 3 | M | 81 | GLU | C-N | 6.18 | 1.41 | 1.33 |
| 1 | T | 305 | LEU | CA-CB | 6.18 | 1.61 | 1.53 |
| 2 | C | 78 | ASP | C-O | 6.18 | 1.31 | 1.24 |
| 2 | C | 180 | LEU | C-N | 6.18 | 1.42 | 1.33 |
| 2 | J | 128 | LYS | CA-C | 6.18 | 1.61 | 1.52 |
| 1 | A | 241 | TYR | C-N | 6.17 | 1.42 | 1.33 |
| 2 | C | 348 | LEU | CA-C | -6.17 | 1.44 | 1.52 |
| 2 | I | 97 | TYR | CA-C | -6.17 | 1.45 | 1.52 |
| 2 | J | 56 | ALA | C-O | -6.17 | 1.17 | 1.24 |
| 2 | Q | 205 | ASN | CA-C | 6.17 | 1.60 | 1.52 |
| 2 | Q | 436 | ASP | N-CA | 6.17 | 1.54 | 1.46 |
| 2 | C | 115 | ASN | C-N | -6.17 | 1.26 | 1.33 |
| 2 | G | 278 | THR | N-CA | -6.17 | 1.38 | 1.46 |
| 2 | I | 344 | GLY | C-N | 6.17 | 1.42 | 1.33 |
| 2 | R | 166 | GLY | C-N | -6.17 | 1.26 | 1.33 |
| 2 | H | 27 | PRO | C-O | -6.17 | 1.16 | 1.24 |
| 2 | H | 429 | GLN | C-N | -6.17 | 1.25 | 1.33 |
| 2 | R | 306 | ASN | C-N | 6.17 | 1.42 | 1.33 |
| 1 | T | 230 | ILE | C-O | -6.17 | 1.17 | 1.24 |
| 1 | A | 263 | PRO | CA-C | -6.17 | 1.44 | 1.52 |
| 1 | A | 306 | ILE | N-CA | -6.17 | 1.38 | 1.46 |
| 2 | G | 257 | ALA | N-CA | -6.17 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 276 | ALA | CA-CB | -6.17 | 1.43 | 1.53 |
| 2 | H | 421 | ARG | CA-C | -6.16 | 1.44 | 1.52 |
| 2 | S | 203 | ASP | CA-C | -6.16 | 1.44 | 1.52 |
| 2 | G | 192 | CYS | CA-C | -6.16 | 1.44 | 1.52 |
| 2 | J | 432 | ASN | C-O | 6.16 | 1.31 | 1.24 |
| 1 | T | 230 | ILE | N-CA | 6.16 | 1.53 | 1.46 |
| 3 | D | 30 | ILE | CA-C | -6.16 | 1.45 | 1.52 |
| 2 | I | 367 | ASP | CA-C | 6.16 | 1.59 | 1.52 |
| 2 | I | 185 | TYR | C-N | 6.15 | 1.42 | 1.33 |
| 2 | J | 402 | PHE | C-N | -6.15 | 1.24 | 1.33 |
| 2 | H | 174 | ILE | N-CA | -6.15 | 1.39 | 1.46 |
| 2 | Q | 58 | ALA | CA-C | -6.15 | 1.45 | 1.52 |
| 2 | R | 47 | GLY | C-N | 6.15 | 1.40 | 1.33 |
| 2 | J | 248 | GLU | CA-C | 6.15 | 1.60 | 1.52 |
| 1 | F | 303 | GLU | N-CA | -6.15 | 1.38 | 1.46 |
| 2 | H | 348 | LEU | CA-C | -6.15 | 1.44 | 1.52 |
| 3 | L | 103 | PHE | CA-C | -6.15 | 1.45 | 1.52 |
| 2 | S | 203 | ASP | CA-CB | 6.15 | 1.62 | 1.53 |
| 3 | O | 68 | PRO | C-N | -6.14 | 1.25 | 1.33 |
| 2 | H | 27 | PRO | C-N | 6.14 | 1.42 | 1.33 |
| 2 | Q | 445 | LEU | CA-CB | -6.14 | 1.43 | 1.53 |
| 2 | C | 299 | ALA | C-O | -6.14 | 1.16 | 1.24 |
| 3 | N | 66 | LYS | CA-C | -6.14 | 1.44 | 1.52 |
| 2 | S | 242 | VAL | C-N | -6.14 | 1.25 | 1.33 |
| 1 | T | 238 | ASN | C-N | -6.14 | 1.25 | 1.33 |
| 3 | O | 60 | LEU | C-N | 6.14 | 1.41 | 1.33 |
| 2 | I | 428 | VAL | CA-CB | -6.13 | 1.47 | 1.54 |
| 2 | J | 221 | VAL | C-O | -6.13 | 1.17 | 1.24 |
| 2 | R | 94 | GLU | CA-C | 6.13 | 1.60 | 1.52 |
| 2 | C | 167 | ARG | CA-C | -6.13 | 1.46 | 1.52 |
| 2 | G | 29 | TYR | N-CA | 6.13 | 1.54 | 1.46 |
| 2 | I | 422 | VAL | CA-CB | 6.13 | 1.60 | 1.54 |
| 2 | J | 208 | SER | C-N | -6.13 | 1.25 | 1.33 |
| 3 | M | 47 | HIS | ND1-CE1 | 6.13 | 1.38 | 1.32 |
| 2 | G | 73 | LEU | N-CA | -6.13 | 1.38 | 1.46 |
| 2 | Q | 363 | PHE | C-N | 6.13 | 1.40 | 1.33 |
| 2 | H | 236 | LYS | C-O | -6.12 | 1.16 | 1.23 |
| 2 | H | 314 | LEU | C-O | -6.12 | 1.17 | 1.24 |
| 2 | I | 49 | PRO | N-CA | -6.12 | 1.39 | 1.47 |
| 2 | I | 55 | ALA | C-N | 6.12 | 1.41 | 1.33 |
| 2 | I | 265 | ILE | CA-C | 6.12 | 1.60 | 1.52 |
| 2 | J | 242 | VAL | N-CA | -6.12 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 445 | LEU | C-N | -6.12 | 1.26 | 1.33 |
| 3 | N | 46 | GLU | N-CA | -6.12 | 1.38 | 1.46 |
| 2 | S | 221 | VAL | C-O | -6.12 | 1.16 | 1.24 |
| 2 | C | 354 | ILE | C-O | -6.12 | 1.17 | 1.24 |
| 2 | I | 302 | ASP | N-CA | 6.12 | 1.53 | 1.45 |
| 2 | G | 238 | HIS | CA-C | -6.12 | 1.45 | 1.52 |
| 2 | G | 293 | ILE | CA-CB | 6.12 | 1.64 | 1.55 |
| 2 | G | 256 | PHE | N-CA | 6.12 | 1.54 | 1.46 |
| 1 | B | 262 | ALA | CA-C | 6.11 | 1.59 | 1.53 |
| 2 | C | 107 | LEU | C-N | 6.11 | 1.41 | 1.33 |
| 1 | F | 295 | THR | CA-C | 6.11 | 1.60 | 1.52 |
| 2 | Q | 145 | VAL | C-N | -6.11 | 1.24 | 1.33 |
| 2 | R | 185 | TYR | C-O | -6.11 | 1.17 | 1.24 |
| 2 | Q | 184 | ASN | CA-C | -6.11 | 1.44 | 1.52 |
| 3 | D | 107 | ARG | N-CA | 6.11 | 1.52 | 1.45 |
| 2 | C | 264 | ILE | N-CA | -6.11 | 1.39 | 1.46 |
| 2 | H | 309 | ILE | CA-CB | 6.10 | 1.62 | 1.54 |
| 2 | J | 120 | ILE | N-CA | -6.10 | 1.38 | 1.46 |
| 3 | N | 75 | VAL | C-N | -6.10 | 1.26 | 1.33 |
| 2 | G | 326 | LEU | C-N | -6.10 | 1.25 | 1.33 |
| 2 | I | 301 | ILE | CA-C | 6.09 | 1.60 | 1.53 |
| 2 | G | 451 | TRP | C-N | -6.09 | 1.26 | 1.33 |
| 2 | I | 245 | PRO | C-O | -6.09 | 1.16 | 1.24 |
| 2 | S | 143 | ALA | C-N | -6.09 | 1.25 | 1.34 |
| 2 | G | 84 | CYS | C-N | 6.09 | 1.41 | 1.33 |
| 2 | I | 293 | ILE | CA-CB | 6.09 | 1.61 | 1.54 |
| 3 | L | 76 | ARG | C-N | -6.09 | 1.26 | 1.33 |
| 2 | S | 120 | ILE | CA-C | -6.09 | 1.45 | 1.52 |
| 3 | O | 13 | GLU | C-O | -6.09 | 1.16 | 1.24 |
| 2 | Q | 151 | PRO | C-N | 6.09 | 1.41 | 1.33 |
| 2 | S | 106 | ASP | N-CA | 6.09 | 1.54 | 1.46 |
| 2 | J | 292 | HIS | C-N | 6.09 | 1.43 | 1.33 |
| 3 | L | 57 | MET | N-CA | 6.08 | 1.53 | 1.45 |
| 2 | R | 183 | LYS | N-CA | -6.08 | 1.39 | 1.46 |
| 2 | S | 89 | PRO | C-O | -6.08 | 1.17 | 1.23 |
| 2 | S | 139 | ARG | N-CA | -6.08 | 1.39 | 1.46 |
| 2 | R | 302 | ASP | C-N | 6.08 | 1.42 | 1.33 |
| 2 | C | 152 | PRO | C-O | -6.08 | 1.16 | 1.24 |
| 2 | H | 80 | TYR | C-N | 6.08 | 1.42 | 1.33 |
| 2 | J | 327 | HIS | CA-C | -6.08 | 1.44 | 1.52 |
| 2 | Q | 132 | SER | C-N | 6.08 | 1.42 | 1.33 |
| 1 | F | 253 | PHE | CA-C | 6.07 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 387 | MET | N-CA | -6.07 | 1.41 | 1.46 |
| 2 | R | 129 | ALA | C-N | 6.07 | 1.40 | 1.33 |
| 2 | C | 29 | TYR | CA-C | 6.07 | 1.60 | 1.52 |
| 2 | J | 118 | THR | CA-C | 6.07 | 1.60 | 1.52 |
| 2 | G | 446 | ARG | C-O | -6.07 | 1.17 | 1.24 |
| 2 | G | 298 | HIS | CA-C | -6.07 | 1.45 | 1.52 |
| 2 | S | 396 | ASP | N-CA | -6.06 | 1.38 | 1.46 |
| 3 | D | 29 | GLN | C-N | -6.06 | 1.26 | 1.33 |
| 2 | R | 391 | VAL | CA-C | 6.06 | 1.60 | 1.52 |
| 2 | R | 371 | MET | CA-C | -6.06 | 1.46 | 1.52 |
| 3 | M | 53 | PHE | CA-C | -6.05 | 1.45 | 1.52 |
| 2 | H | 267 | HIS | CA-C | -6.05 | 1.45 | 1.52 |
| 3 | M | 84 | ASP | C-N | 6.05 | 1.42 | 1.33 |
| 2 | G | 110 | GLU | C-O | -6.05 | 1.16 | 1.23 |
| 2 | Q | 459 | LEU | CA-C | -6.05 | 1.44 | 1.52 |
| 2 | G | 258 | LYS | C-O | -6.05 | 1.17 | 1.24 |
| 2 | H | 77 | MET | CA-C | -6.05 | 1.44 | 1.52 |
| 3 | O | 49 | ASN | C-N | -6.05 | 1.25 | 1.34 |
| 2 | Q | 420 | ASN | CA-CB | -6.05 | 1.44 | 1.53 |
| 2 | R | 258 | LYS | CA-C | 6.05 | 1.60 | 1.52 |
| 2 | S | 270 | LEU | C-N | -6.04 | 1.26 | 1.33 |
| 3 | M | 11 | ARG | CA-C | 6.04 | 1.62 | 1.53 |
| 3 | N | 69 | GLN | N-CA | -6.04 | 1.38 | 1.46 |
| 3 | P | 83 | GLY | C-N | 6.04 | 1.43 | 1.33 |
| 1 | F | 260 | PRO | CA-CB | 6.04 | 1.61 | 1.53 |
| 2 | I | 117 | LEU | C-O | -6.04 | 1.17 | 1.24 |
| 2 | G | 183 | LYS | C-O | -6.04 | 1.17 | 1.24 |
| 2 | S | 320 | LEU | N-CA | -6.04 | 1.39 | 1.46 |
| 2 | R | 317 | CYS | C-N | 6.04 | 1.41 | 1.33 |
| 2 | C | 298 | HIS | N-CA | 6.04 | 1.53 | 1.46 |
| 2 | J | 357 | ASP | CA-C | 6.04 | 1.59 | 1.52 |
| 2 | I | 259 | GLU | N-CA | -6.03 | 1.38 | 1.46 |
| 2 | I | 126 | GLY | C-O | -6.03 | 1.17 | 1.23 |
| 2 | I | 392 | GLU | C-N | 6.03 | 1.41 | 1.33 |
| 3 | L | 38 | PHE | CA-C | -6.03 | 1.45 | 1.52 |
| 2 | C | 86 | HIS | CD2-NE2 | 6.03 | 1.44 | 1.37 |
| 3 | L | 106 | HIS | C-N | 6.02 | 1.39 | 1.33 |
| 2 | J | 191 | GLU | N-CA | 6.02 | 1.53 | 1.46 |
| 2 | S | 22 | LEU | C-N | 6.02 | 1.41 | 1.33 |
| 3 | D | 75 | VAL | C-N | 6.02 | 1.41 | 1.33 |
| 2 | H | 188 | ALA | CA-C | -6.02 | 1.45 | 1.52 |
| 2 | Q | 416 | GLY | C-O | -6.02 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 232 | THR | CA-C | -6.02 | 1.45 | 1.52 |
| 3 | E | 105 | VAL | N-CA | -6.02 | 1.40 | 1.46 |
| 2 | S | 74 | LEU | CA-C | 6.02 | 1.61 | 1.52 |
| 2 | H | 321 | SER | C-N | -6.02 | 1.26 | 1.33 |
| 2 | J | 424 | LEU | CA-C | -6.01 | 1.45 | 1.52 |
| 2 | J | 265 | ILE | C-O | -6.01 | 1.17 | 1.24 |
| 2 | C | 232 | THR | C-N | 6.01 | 1.41 | 1.33 |
| 2 | H | 368 | TRP | C-N | 6.01 | 1.42 | 1.33 |
| 3 | L | 42 | ILE | CB-CG1 | 6.01 | 1.65 | 1.53 |
| 2 | Q | 290 | LEU | C-N | -6.01 | 1.24 | 1.33 |
| 2 | R | 345 | PHE | CA-C | 6.01 | 1.60 | 1.52 |
| 2 | H | 278 | THR | N-CA | -6.00 | 1.39 | 1.46 |
| 2 | S | 148 | PHE | CA-C | 6.00 | 1.60 | 1.52 |
| 3 | E | 102 | SER | CA-C | -6.00 | 1.46 | 1.52 |
| 2 | I | 452 | SER | C-O | -6.00 | 1.18 | 1.24 |
| 2 | R | 204 | GLU | CA-C | 6.00 | 1.60 | 1.52 |
| 2 | R | 221 | VAL | CA-C | -6.00 | 1.45 | 1.52 |
| 2 | J | 117 | LEU | C-O | -6.00 | 1.17 | 1.24 |
| 3 | E | 91 | GLY | C-N | 6.00 | 1.41 | 1.33 |
| 2 | J | 254 | ALA | CA-CB | -6.00 | 1.44 | 1.53 |
| 1 | T | 273 | LEU | C-O | 6.00 | 1.31 | 1.24 |
| 2 | G | 293 | ILE | CB-CG1 | 6.00 | 1.65 | 1.53 |
| 3 | K | 87 | ILE | N-CA | -6.00 | 1.39 | 1.46 |
| 2 | S | 265 | ILE | C-O | -6.00 | 1.17 | 1.24 |
| 3 | E | 31 | GLU | CA-CB | -5.99 | 1.44 | 1.53 |
| 1 | F | 232 | GLN | CA-CB | 5.99 | 1.62 | 1.53 |
| 2 | I | 310 | HIS | C-O | -5.99 | 1.16 | 1.23 |
| 3 | P | 60 | LEU | N-CA | -5.99 | 1.37 | 1.46 |
| 3 | M | 61 | PRO | C-N | -5.99 | 1.25 | 1.33 |
| 2 | C | 220 | PHE | N-CA | -5.99 | 1.39 | 1.46 |
| 3 | O | 92 | PHE | N-CA | 5.99 | 1.53 | 1.46 |
| 2 | Q | 99 | ALA | CA-C | 5.99 | 1.60 | 1.53 |
| 2 | I | 230 | ALA | N-CA | -5.99 | 1.39 | 1.46 |
| 1 | A | 299 | SER | CA-C | -5.98 | 1.45 | 1.52 |
| 2 | H | 428 | VAL | C-N | -5.98 | 1.26 | 1.33 |
| 3 | L | 82 | TYR | C-N | -5.98 | 1.26 | 1.33 |
| 2 | R | 443 | ASP | C-O | -5.98 | 1.17 | 1.24 |
| 2 | G | 229 | GLN | CA-C | 5.98 | 1.60 | 1.52 |
| 2 | Q | 415 | PRO | C-O | -5.98 | 1.16 | 1.24 |
| 2 | J | 436 | ASP | C-N | 5.98 | 1.41 | 1.34 |
| 3 | D | 17 | TYR | CA-C | -5.98 | 1.44 | 1.52 |
| 2 | J | 414 | ALA | C-O | -5.98 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 284 | CYS | C-N | 5.98 | 1.41 | 1.33 |
| 2 | G | 39 | ALA | N-CA | -5.98 | 1.38 | 1.46 |
| 2 | S | 185 | TYR | C-O | -5.97 | 1.16 | 1.23 |
| 2 | I | 180 | LEU | CA-C | -5.97 | 1.45 | 1.52 |
| 2 | H | 384 | VAL | C-N | -5.97 | 1.26 | 1.34 |
| 2 | G | 56 | ALA | N-CA | 5.97 | 1.53 | 1.46 |
| 2 | Q | 276 | ALA | C-O | -5.97 | 1.17 | 1.24 |
| 2 | Q | 432 | ASN | CA-C | -5.97 | 1.45 | 1.52 |
| 2 | S | 225 | ILE | CA-C | -5.97 | 1.45 | 1.52 |
| 2 | G | 81 | LYS | C-N | 5.97 | 1.38 | 1.33 |
| 2 | H | 191 | GLU | N-CA | 5.97 | 1.53 | 1.46 |
| 3 | N | 35 | GLU | C-O | 5.97 | 1.31 | 1.24 |
| 1 | B | 295 | THR | C-N | 5.96 | 1.41 | 1.33 |
| 2 | H | 448 | ALA | CA-CB | -5.96 | 1.44 | 1.53 |
| 3 | N | 18 | LEU | C-N | 5.96 | 1.40 | 1.33 |
| 3 | P | 23 | ASP | C-O | 5.96 | 1.31 | 1.24 |
| 1 | A | 280 | LEU | C-N | -5.96 | 1.25 | 1.34 |
| 2 | C | 368 | TRP | CA-C | -5.96 | 1.45 | 1.52 |
| 2 | H | 431 | ARG | N-CA | 5.96 | 1.53 | 1.46 |
| 3 | O | 78 | CYS | C-N | 5.96 | 1.41 | 1.33 |
| 2 | Q | 202 | ASP | C-O | -5.96 | 1.16 | 1.23 |
| 2 | G | 189 | VAL | CA-CB | 5.96 | 1.60 | 1.54 |
| 3 | L | 24 | ARG | CA-C | 5.96 | 1.60 | 1.52 |
| 2 | I | 299 | ALA | N-CA | -5.96 | 1.38 | 1.46 |
| 2 | Q | 267 | HIS | CD2-NE2 | 5.95 | 1.44 | 1.37 |
| 3 | P | 58 | TRP | N-CA | -5.95 | 1.39 | 1.46 |
| 2 | Q | 23 | THR | N-CA | 5.95 | 1.53 | 1.46 |
| 2 | Q | 77 | MET | SD-CE | 5.95 | 1.94 | 1.79 |
| 2 | H | 25 | TYR | C-O | -5.95 | 1.17 | 1.24 |
| 2 | Q | 238 | HIS | C-O | -5.95 | 1.16 | 1.23 |
| 2 | R | 357 | ASP | N-CA | -5.95 | 1.39 | 1.46 |
| 2 | I | 265 | ILE | C-N | -5.95 | 1.25 | 1.33 |
| 2 | C | 36 | LEU | N-CA | -5.95 | 1.38 | 1.46 |
| 2 | C | 294 | HIS | CD2-NE2 | 5.95 | 1.44 | 1.37 |
| 2 | R | 113 | VAL | C-N | -5.95 | 1.26 | 1.33 |
| 2 | S | 394 | PHE | N-CA | -5.95 | 1.38 | 1.46 |
| 2 | H | 131 | ARG | CA-CB | 5.94 | 1.62 | 1.53 |
| 2 | I | 77 | MET | N-CA | -5.94 | 1.39 | 1.46 |
| 1 | B | 288 | VAL | C-O | 5.94 | 1.29 | 1.24 |
| 3 | D | 33 | MET | N-CA | -5.94 | 1.39 | 1.46 |
| 2 | G | 45 | GLN | C-N | 5.94 | 1.41 | 1.33 |
| 3 | K | 28 | ALA | CA-CB | -5.94 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 70 | TRP | N-CA | 5.94 | 1.53 | 1.46 |
| 2 | H | 200 | THR | CA-C | -5.94 | 1.45 | 1.52 |
| 3 | L | 18 | LEU | C-O | -5.94 | 1.16 | 1.23 |
| 2 | R | 146 | LYS | CA-C | 5.94 | 1.60 | 1.52 |
| 2 | G | 103 | TYR | CA-C | 5.94 | 1.59 | 1.52 |
| 2 | I | 52 | GLU | N-CA | -5.94 | 1.39 | 1.46 |
| 2 | J | 153 | HIS | C-O | -5.94 | 1.16 | 1.24 |
| 2 | R | 212 | GLN | N-CA | -5.94 | 1.39 | 1.46 |
| 2 | C | 296 | ALA | CA-C | 5.94 | 1.60 | 1.52 |
| 2 | C | 391 | VAL | N-CA | 5.93 | 1.53 | 1.46 |
| 2 | H | 38 | ALA | CA-C | -5.93 | 1.45 | 1.52 |
| 1 | T | 306 | ILE | C-N | -5.93 | 1.26 | 1.33 |
| 2 | J | 207 | ASN | N-CA | -5.93 | 1.39 | 1.46 |
| 2 | Q | 422 | VAL | N-CA | -5.93 | 1.39 | 1.46 |
| 1 | A | 308 | ARG | CA-C | -5.93 | 1.46 | 1.52 |
| 3 | E | 107 | ARG | N-CA | -5.93 | 1.38 | 1.45 |
| 2 | R | 152 | PRO | C-O | 5.93 | 1.31 | 1.24 |
| 2 | R | 200 | THR | CA-C | -5.93 | 1.45 | 1.52 |
| 2 | J | 124 | VAL | CA-C | 5.93 | 1.60 | 1.52 |
| 2 | J | 215 | ARG | CA-C | 5.93 | 1.60 | 1.52 |
| 2 | S | 199 | PHE | CA-C | 5.92 | 1.59 | 1.52 |
| 1 | B | 230 | ILE | C-N | -5.92 | 1.25 | 1.33 |
| 2 | H | 367 | ASP | C-N | -5.92 | 1.25 | 1.33 |
| 2 | Q | 127 | PHE | C-O | -5.92 | 1.16 | 1.23 |
| 2 | G | 227 | LYS | CA-C | -5.92 | 1.44 | 1.52 |
| 2 | C | 37 | LEU | N-CA | -5.92 | 1.39 | 1.46 |
| 2 | J | 445 | LEU | C-O | -5.92 | 1.17 | 1.24 |
| 2 | C | 71 | THR | CA-C | 5.92 | 1.61 | 1.52 |
| 2 | I | 313 | VAL | CA-C | -5.92 | 1.45 | 1.52 |
| 3 | D | 24 | ARG | CA-C | 5.91 | 1.60 | 1.52 |
| 3 | P | 22 | SER | C-N | -5.91 | 1.26 | 1.33 |
| 2 | R | 390 | LEU | N-CA | 5.91 | 1.53 | 1.46 |
| 2 | I | 209 | GLN | C-O | -5.91 | 1.16 | 1.24 |
| 2 | I | 427 | CYS | N-CA | -5.91 | 1.39 | 1.46 |
| 2 | I | 439 | ARG | CA-C | -5.91 | 1.44 | 1.52 |
| 2 | I | 345 | PHE | N-CA | -5.91 | 1.38 | 1.46 |
| 2 | C | 307 | HIS | CE1-NE2 | -5.91 | 1.26 | 1.32 |
| 2 | J | 114 | THR | N-CA | 5.91 | 1.53 | 1.46 |
| 3 | N | 57 | MET | C-O | 5.90 | 1.31 | 1.23 |
| 1 | A | 265 | GLN | CA-C | -5.90 | 1.47 | 1.53 |
| 2 | G | 221 | VAL | C-O | -5.90 | 1.17 | 1.24 |
| 2 | J | 191 | GLU | CA-C | -5.90 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 443 | ASP | N-CA | 5.90 | 1.53 | 1.46 |
| 2 | Q | 213 | ARG | N-CA | -5.90 | 1.38 | 1.46 |
| 2 | R | 56 | ALA | N-CA | -5.90 | 1.39 | 1.46 |
| 2 | C | 243 | THR | C-O | -5.89 | 1.16 | 1.23 |
| 2 | R | 207 | ASN | CA-C | 5.89 | 1.58 | 1.52 |
| 2 | S | 87 | ILE | N-CA | 5.89 | 1.52 | 1.46 |
| 2 | S | 124 | VAL | CA-CB | 5.89 | 1.61 | 1.54 |
| 2 | S | 249 | GLU | C-O | -5.89 | 1.17 | 1.24 |
| 2 | G | 226 | HIS | CD2-NE2 | 5.89 | 1.44 | 1.37 |
| 2 | G | 346 | VAL | CA-C | 5.89 | 1.59 | 1.52 |
| 2 | J | 169 | MET | CA-C | -5.89 | 1.45 | 1.52 |
| 3 | L | 17 | TYR | CA-C | 5.89 | 1.61 | 1.52 |
| 2 | R | 419 | ALA | N-CA | -5.89 | 1.39 | 1.46 |
| 1 | F | 293 | ILE | CA-CB | 5.89 | 1.62 | 1.54 |
| 2 | J | 25 | TYR | C-N | 5.89 | 1.41 | 1.33 |
| 3 | O | 51 | GLU | CA-C | 5.89 | 1.60 | 1.52 |
| 1 | T | 297 | THR | C-N | -5.89 | 1.25 | 1.33 |
| 2 | C | 237 | GLY | C-O | -5.89 | 1.18 | 1.24 |
| 3 | O | 84 | ASP | C-N | -5.89 | 1.24 | 1.33 |
| 2 | C | 326 | LEU | CA-C | -5.88 | 1.45 | 1.52 |
| 2 | G | 307 | HIS | CD2-NE2 | 5.88 | 1.44 | 1.37 |
| 2 | H | 384 | VAL | CA-CB | 5.88 | 1.63 | 1.54 |
| 2 | J | 178 | LEU | CA-CB | 5.88 | 1.61 | 1.53 |
| 3 | K | 33 | MET | CA-C | 5.88 | 1.60 | 1.52 |
| 3 | K | 64 | ASP | C-O | -5.88 | 1.16 | 1.23 |
| 2 | R | 218 | PHE | CA-C | -5.88 | 1.45 | 1.52 |
| 3 | O | 37 | GLY | C-N | 5.88 | 1.41 | 1.33 |
| 2 | S | 114 | THR | CA-CB | -5.88 | 1.44 | 1.53 |
| 2 | C | 113 | VAL | N-CA | -5.88 | 1.39 | 1.46 |
| 2 | G | 199 | PHE | N-CA | 5.88 | 1.53 | 1.46 |
| 2 | J | 164 | LYS | C-O | 5.88 | 1.31 | 1.24 |
| 3 | N | 51 | GLU | C-O | 5.88 | 1.31 | 1.24 |
| 2 | H | 93 | GLU | C-N | 5.88 | 1.41 | 1.33 |
| 3 | N | 102 | SER | C-N | -5.88 | 1.26 | 1.33 |
| 2 | C | 221 | VAL | CA-C | 5.88 | 1.60 | 1.52 |
| 2 | G | 386 | HIS | CD2-NE2 | 5.88 | 1.44 | 1.37 |
| 2 | J | 205 | ASN | CA-CB | 5.88 | 1.62 | 1.53 |
| 2 | Q | 326 | LEU | C-O | -5.88 | 1.17 | 1.23 |
| 2 | R | 115 | ASN | C-N | 5.88 | 1.41 | 1.33 |
| 1 | T | 293 | ILE | CA-C | 5.88 | 1.59 | 1.52 |
| 2 | H | 360 | ARG | CA-C | -5.88 | 1.42 | 1.52 |
| 2 | I | 213 | ARG | C-N | -5.87 | 1.25 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | P | 24 | ARG | CA-CB | 5.87 | 1.62 | 1.53 |
| 3 | E | 99 | GLN | CA-CB | -5.87 | 1.45 | 1.53 |
| 3 | P | 12 | PHE | CA-CB | 5.87 | 1.63 | 1.53 |
| 2 | C | 110 | GLU | N-CA | 5.87 | 1.53 | 1.46 |
| 1 | B | 276 | LEU | CA-C | -5.87 | 1.45 | 1.52 |
| 2 | C | 173 | THR | CA-C | 5.87 | 1.60 | 1.52 |
| 2 | C | 389 | ALA | C-O | -5.87 | 1.17 | 1.24 |
| 2 | R | 461 | LEU | CB-CG | 5.87 | 1.65 | 1.53 |
| 2 | C | 43 | SER | C-O | -5.86 | 1.17 | 1.24 |
| 2 | C | 163 | ASN | CA-C | -5.86 | 1.45 | 1.52 |
| 2 | J | 185 | TYR | CA-C | 5.86 | 1.60 | 1.52 |
| 3 | K | 78 | CYS | C-N | 5.86 | 1.41 | 1.33 |
| 3 | O | 25 | GLN | N-CA | -5.86 | 1.39 | 1.46 |
| 2 | S | 207 | ASN | N-CA | -5.86 | 1.39 | 1.46 |
| 2 | Q | 81 | LYS | N-CA | 5.86 | 1.53 | 1.46 |
| 2 | I | 459 | LEU | C-O | -5.86 | 1.16 | 1.24 |
| 1 | A | 271 | GLN | CA-C | 5.86 | 1.60 | 1.52 |
| 2 | C | 426 | ALA | C-O | -5.86 | 1.17 | 1.24 |
| 2 | I | 76 | ASP | C-O | -5.86 | 1.17 | 1.24 |
| 3 | O | 94 | ASN | N-CA | -5.86 | 1.38 | 1.46 |
| 2 | S | 222 | ALA | CA-C | -5.86 | 1.45 | 1.52 |
| 2 | Q | 28 | ASP | CA-C | 5.86 | 1.60 | 1.52 |
| 3 | E | 92 | PHE | N-CA | -5.85 | 1.39 | 1.46 |
| 3 | P | 33 | MET | C-O | -5.85 | 1.17 | 1.24 |
| 3 | P | 34 | ILE | CA-C | 5.85 | 1.59 | 1.52 |
| 2 | I | 133 | LEU | CA-C | 5.85 | 1.59 | 1.52 |
| 2 | J | 445 | LEU | N-CA | 5.85 | 1.53 | 1.46 |
| 3 | P | 72 | LEU | C-O | -5.85 | 1.17 | 1.24 |
| 2 | S | 354 | ILE | CB-CG1 | 5.85 | 1.65 | 1.53 |
| 2 | G | 239 | TYR | CA-CB | -5.85 | 1.45 | 1.53 |
| 2 | Q | 211 | PHE | C-N | 5.85 | 1.41 | 1.33 |
| 2 | G | 366 | GLN | C-N | -5.85 | 1.25 | 1.33 |
| 2 | I | 355 | GLU | CA-C | -5.85 | 1.45 | 1.52 |
| 2 | S | 267 | HIS | CD2-NE2 | 5.85 | 1.44 | 1.37 |
| 2 | C | 394 | PHE | C-O | -5.84 | 1.16 | 1.24 |
| 2 | R | 365 | THR | C-O | -5.84 | 1.16 | 1.24 |
| 2 | R | 329 | GLY | C-N | -5.84 | 1.25 | 1.33 |
| 2 | R | 443 | ASP | N-CA | -5.84 | 1.39 | 1.46 |
| 2 | S | 234 | GLU | C-N | 5.84 | 1.39 | 1.33 |
| 1 | A | 295 | THR | C-N | 5.84 | 1.41 | 1.33 |
| 2 | C | 300 | VAL | CA-CB | 5.84 | 1.62 | 1.54 |
| 2 | I | 77 | MET | CA-C | -5.84 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 320 | LEU | C-N | -5.84 | 1.26 | 1.33 |
| 2 | R | 149 | GLN | CA-C | -5.84 | 1.45 | 1.52 |
| 3 | N | 65 | CYS | C-N | -5.84 | 1.25 | 1.33 |
| 1 | A | 283 | HIS | C-N | 5.84 | 1.41 | 1.33 |
| 2 | H | 109 | GLU | N-CA | -5.84 | 1.38 | 1.46 |
| 2 | C | 190 | TYR | CA-C | -5.83 | 1.45 | 1.52 |
| 2 | C | 226 | HIS | CE1-NE2 | 5.83 | 1.38 | 1.32 |
| 3 | L | 89 | VAL | CA-CB | -5.83 | 1.47 | 1.54 |
| 2 | G | 29 | TYR | CA-C | -5.83 | 1.45 | 1.52 |
| 2 | G | 141 | PRO | CA-CB | -5.83 | 1.45 | 1.53 |
| 1 | A | 245 | THR | CA-C | 5.83 | 1.59 | 1.52 |
| 2 | H | 374 | VAL | CA-C | -5.83 | 1.45 | 1.52 |
| 2 | S | 185 | TYR | C-N | 5.83 | 1.42 | 1.33 |
| 2 | C | 354 | ILE | CA-C | 5.82 | 1.59 | 1.52 |
| 3 | E | 47 | HIS | CE1-NE2 | -5.82 | 1.26 | 1.32 |
| 2 | H | 322 | GLY | CA-C | -5.82 | 1.48 | 1.52 |
| 2 | J | 99 | ALA | CA-CB | -5.82 | 1.45 | 1.53 |
| 3 | O | 78 | CYS | C-O | -5.82 | 1.17 | 1.24 |
| 2 | R | 297 | MET | CA-CB | -5.82 | 1.46 | 1.54 |
| 2 | S | 451 | TRP | C-N | -5.82 | 1.26 | 1.33 |
| 2 | G | 445 | LEU | CA-CB | -5.82 | 1.44 | 1.53 |
| 2 | I | 354 | ILE | N-CA | 5.82 | 1.53 | 1.46 |
| 1 | T | 276 | LEU | C-O | -5.82 | 1.17 | 1.24 |
| 2 | I | 286 | ASP | C-O | -5.82 | 1.17 | 1.24 |
| 3 | M | 48 | SER | C-N | -5.82 | 1.26 | 1.33 |
| 2 | R | 34 | THR | CA-C | 5.82 | 1.60 | 1.52 |
| 2 | H | 85 | TYR | C-N | 5.81 | 1.41 | 1.33 |
| 2 | R | 205 | ASN | CA-CB | -5.81 | 1.43 | 1.53 |
| 2 | R | 343 | LEU | C-N | 5.81 | 1.41 | 1.33 |
| 3 | E | 99 | GLN | C-O | -5.81 | 1.17 | 1.24 |
| 1 | A | 247 | HIS | CA-C | 5.81 | 1.59 | 1.52 |
| 2 | C | 294 | HIS | CA-C | 5.81 | 1.59 | 1.52 |
| 2 | H | 426 | ALA | CA-C | -5.81 | 1.45 | 1.52 |
| 2 | S | 198 | ASP | CA-C | -5.81 | 1.44 | 1.52 |
| 2 | S | 387 | MET | SD-CE | -5.81 | 1.65 | 1.79 |
| 2 | Q | 289 | VAL | C-O | -5.80 | 1.18 | 1.24 |
| 2 | G | 175 | LYS | CA-CB | -5.80 | 1.45 | 1.53 |
| 2 | H | 328 | SER | C-N | 5.80 | 1.42 | 1.33 |
| 3 | P | 84 | ASP | N-CA | -5.80 | 1.38 | 1.46 |
| 2 | S | 271 | THR | C-N | -5.80 | 1.25 | 1.33 |
| 2 | C | 386 | HIS | CD2-NE2 | 5.80 | 1.44 | 1.37 |
| 1 | B | 280 | LEU | CA-C | -5.80 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | L | 39 | HIS | CD2-NE2 | 5.80 | 1.44 | 1.37 |
| 3 | N | 69 | GLN | C-N | 5.80 | 1.41 | 1.33 |
| 2 | S | 348 | LEU | C-O | -5.80 | 1.17 | 1.24 |
| 2 | Q | 28 | ASP | C-O | -5.80 | 1.16 | 1.24 |
| 2 | S | 375 | LEU | CA-CB | 5.80 | 1.63 | 1.53 |
| 2 | I | 269 | PHE | C-O | -5.80 | 1.17 | 1.24 |
| 3 | D | 22 | SER | N-CA | -5.79 | 1.38 | 1.45 |
| 2 | J | 423 | ALA | C-O | 5.79 | 1.31 | 1.24 |
| 2 | R | 306 | ASN | CA-CB | -5.79 | 1.45 | 1.54 |
| 3 | E | 73 | ASP | C-O | -5.79 | 1.17 | 1.24 |
| 2 | H | 402 | PHE | CA-C | -5.79 | 1.46 | 1.52 |
| 2 | I | 193 | LEU | CA-C | -5.79 | 1.45 | 1.52 |
| 3 | P | 61 | PRO | C-N | 5.79 | 1.42 | 1.33 |
| 1 | F | 267 | THR | C-O | -5.79 | 1.16 | 1.24 |
| 2 | R | 79 | ARG | CA-C | 5.79 | 1.60 | 1.52 |
| 2 | C | 286 | ASP | CA-C | -5.79 | 1.44 | 1.52 |
| 1 | B | 267 | THR | C-N | 5.78 | 1.41 | 1.33 |
| 2 | G | 45 | GLN | C-O | -5.78 | 1.16 | 1.24 |
| 2 | I | 183 | LYS | CA-C | 5.78 | 1.60 | 1.52 |
| 2 | I | 212 | GLN | N-CA | 5.78 | 1.53 | 1.46 |
| 2 | Q | 207 | ASN | CA-C | 5.78 | 1.58 | 1.52 |
| 2 | Q | 438 | TYR | CA-C | -5.78 | 1.44 | 1.52 |
| 2 | S | 233 | GLY | C-N | -5.78 | 1.25 | 1.33 |
| 3 | D | 76 | ARG | CA-C | -5.78 | 1.45 | 1.52 |
| 2 | J | 32 | LYS | C-N | 5.78 | 1.41 | 1.33 |
| 2 | S | 230 | ALA | CA-C | 5.78 | 1.60 | 1.52 |
| 1 | T | 230 | ILE | C-N | 5.78 | 1.41 | 1.33 |
| 2 | H | 273 | GLY | C-N | 5.77 | 1.41 | 1.33 |
| 2 | J | 70 | TRP | CA-C | 5.77 | 1.60 | 1.52 |
| 2 | Q | 177 | LYS | CA-C | -5.77 | 1.44 | 1.52 |
| 2 | R | 103 | TYR | CA-C | -5.77 | 1.45 | 1.52 |
| 1 | B | 303 | GLU | N-CA | 5.77 | 1.53 | 1.46 |
| 2 | H | 217 | ARG | N-CA | -5.77 | 1.39 | 1.46 |
| 2 | I | 274 | PHE | CA-CB | -5.77 | 1.44 | 1.53 |
| 2 | C | 41 | ARG | C-N | -5.77 | 1.26 | 1.33 |
| 2 | G | 140 | PHE | CA-CB | -5.77 | 1.45 | 1.53 |
| 2 | G | 330 | THR | CA-CB | 5.77 | 1.62 | 1.53 |
| 2 | I | 55 | ALA | CA-C | -5.77 | 1.45 | 1.52 |
| 2 | R | 101 | ILE | C-N | 5.77 | 1.41 | 1.33 |
| 2 | S | 57 | ILE | C-N | -5.77 | 1.26 | 1.33 |
| 2 | S | 275 | THR | C-N | 5.77 | 1.41 | 1.33 |
| 3 | D | 10 | ARG | N-CA | -5.76 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 148 | PHE | C-N | 5.76 | 1.41 | 1.34 |
| 3 | M | 13 | GLU | N-CA | -5.76 | 1.39 | 1.46 |
| 2 | S | 399 | VAL | CA-C | 5.76 | 1.59 | 1.52 |
| 2 | C | 441 | GLY | C-N | -5.76 | 1.26 | 1.33 |
| 2 | R | 110 | GLU | CA-C | 5.76 | 1.60 | 1.52 |
| 2 | Q | 383 | HIS | CG-CD2 | -5.76 | 1.29 | 1.35 |
| 2 | R | 118 | THR | C-N | 5.76 | 1.42 | 1.33 |
| 2 | S | 86 | HIS | CA-CB | -5.76 | 1.44 | 1.53 |
| 2 | S | 77 | MET | C-O | 5.76 | 1.31 | 1.24 |
| 2 | R | 127 | PHE | CA-C | 5.76 | 1.60 | 1.52 |
| 3 | D | 33 | MET | C-N | 5.75 | 1.40 | 1.33 |
| 2 | S | 275 | THR | CA-CB | -5.75 | 1.44 | 1.53 |
| 3 | L | 101 | VAL | CA-C | -5.75 | 1.45 | 1.52 |
| 2 | I | 302 | ASP | CA-CB | -5.75 | 1.46 | 1.54 |
| 2 | J | 125 | PHE | C-O | 5.75 | 1.31 | 1.24 |
| 3 | K | 73 | ASP | CA-C | -5.75 | 1.45 | 1.52 |
| 2 | Q | 292 | HIS | CA-C | -5.75 | 1.45 | 1.52 |
| 2 | R | 86 | HIS | CE1-NE2 | 5.75 | 1.38 | 1.32 |
| 2 | H | 28 | ASP | N-CA | -5.75 | 1.38 | 1.46 |
| 3 | K | 71 | VAL | CA-C | 5.75 | 1.60 | 1.52 |
| 2 | Q | 432 | ASN | C-O | -5.75 | 1.17 | 1.24 |
| 2 | I | 255 | GLU | C-O | -5.75 | 1.17 | 1.24 |
| 3 | N | 18 | LEU | CA-CB | 5.75 | 1.61 | 1.53 |
| 2 | R | 157 | VAL | CA-CB | -5.75 | 1.47 | 1.54 |
| 2 | S | 283 | TRP | CA-CB | -5.75 | 1.44 | 1.53 |
| 2 | C | 246 | THR | CA-CB | -5.74 | 1.42 | 1.54 |
| 2 | G | 422 | VAL | CA-CB | 5.74 | 1.60 | 1.54 |
| 2 | C | 107 | LEU | CB-CG | 5.74 | 1.65 | 1.53 |
| 2 | C | 383 | HIS | C-N | -5.74 | 1.26 | 1.34 |
| 3 | K | 46 | GLU | N-CA | -5.74 | 1.39 | 1.46 |
| 2 | Q | 29 | TYR | C-O | -5.74 | 1.17 | 1.23 |
| 2 | J | 194 | ARG | N-CA | -5.74 | 1.39 | 1.46 |
| 2 | R | 303 | ARG | C-N | -5.74 | 1.25 | 1.33 |
| 2 | S | 394 | PHE | CA-CB | -5.74 | 1.44 | 1.53 |
| 2 | C | 126 | GLY | C-O | -5.74 | 1.16 | 1.23 |
| 2 | C | 155 | ILE | C-O | -5.74 | 1.17 | 1.24 |
| 2 | C | 356 | ALA | C-N | 5.74 | 1.41 | 1.34 |
| 3 | D | 21 | LEU | CA-CB | -5.74 | 1.44 | 1.53 |
| 2 | G | 173 | THR | CA-C | -5.74 | 1.45 | 1.52 |
| 2 | R | 50 | ALA | CA-C | -5.74 | 1.45 | 1.52 |
| 2 | S | 294 | HIS | C-O | -5.74 | 1.16 | 1.23 |
| 2 | G | 77 | MET | C-N | -5.73 | 1.26 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 234 | GLU | CA-CB | -5.73 | 1.44 | 1.53 |
| 2 | H | 271 | THR | CA-C | 5.73 | 1.60 | 1.52 |
| 2 | H | 418 | THR | C-O | -5.73 | 1.17 | 1.24 |
| 2 | G | 346 | VAL | C-O | -5.73 | 1.17 | 1.24 |
| 3 | K | 45 | ASN | C-O | -5.73 | 1.17 | 1.23 |
| 2 | S | 262 | MET | CA-C | -5.73 | 1.46 | 1.52 |
| 2 | H | 400 | LEU | CA-C | 5.73 | 1.59 | 1.53 |
| 2 | I | 385 | TRP | C-N | -5.73 | 1.26 | 1.33 |
| 2 | S | 353 | HIS | N-CA | -5.73 | 1.39 | 1.46 |
| 3 | P | 72 | LEU | N-CA | -5.72 | 1.39 | 1.46 |
| 3 | E | 69 | GLN | N-CA | -5.72 | 1.39 | 1.46 |
| 2 | I | 247 | CYS | N-CA | -5.72 | 1.39 | 1.46 |
| 3 | E | 20 | PRO | C-N | 5.72 | 1.41 | 1.33 |
| 2 | Q | 233 | GLY | C-N | 5.72 | 1.41 | 1.33 |
| 2 | R | 149 | GLN | N-CA | -5.72 | 1.39 | 1.46 |
| 2 | I | 149 | GLN | N-CA | -5.72 | 1.39 | 1.46 |
| 2 | I | 382 | ILE | C-O | 5.72 | 1.30 | 1.24 |
| 3 | D | 57 | MET | CA-C | 5.71 | 1.59 | 1.52 |
| 2 | H | 165 | TYR | CA-C | -5.71 | 1.45 | 1.52 |
| 2 | H | 290 | LEU | CA-C | -5.71 | 1.45 | 1.52 |
| 2 | I | 49 | PRO | C-N | -5.71 | 1.26 | 1.33 |
| 2 | Q | 164 | LYS | N-CA | 5.71 | 1.53 | 1.46 |
| 2 | Q | 200 | THR | CA-C | -5.71 | 1.46 | 1.52 |
| 3 | L | 56 | THR | N-CA | -5.71 | 1.39 | 1.46 |
| 1 | T | 295 | THR | N-CA | -5.71 | 1.39 | 1.46 |
| 1 | F | 306 | ILE | CA-CB | -5.71 | 1.46 | 1.54 |
| 2 | I | 386 | HIS | N-CA | 5.71 | 1.53 | 1.46 |
| 3 | K | 106 | HIS | ND1-CE1 | 5.71 | 1.38 | 1.32 |
| 2 | C | 270 | LEU | CA-C | -5.71 | 1.44 | 1.52 |
| 3 | M | 18 | LEU | C-N | 5.71 | 1.38 | 1.33 |
| 2 | G | 82 | GLY | CA-C | -5.70 | 1.46 | 1.52 |
| 2 | Q | 148 | PHE | C-O | -5.70 | 1.16 | 1.23 |
| 2 | R | 397 | ASP | N-CA | 5.70 | 1.54 | 1.46 |
| 2 | C | 306 | ASN | CA-CB | -5.70 | 1.45 | 1.53 |
| 2 | H | 110 | GLU | C-N | -5.70 | 1.27 | 1.33 |
| 2 | I | 72 | ASP | CA-C | -5.70 | 1.45 | 1.52 |
| 2 | J | 118 | THR | CA-CB | -5.70 | 1.44 | 1.53 |
| 3 | P | 99 | GLN | N-CA | -5.70 | 1.39 | 1.46 |
| 2 | Q | 125 | PHE | CA-C | -5.70 | 1.44 | 1.52 |
| 2 | R | 226 | HIS | CG-CD2 | -5.70 | 1.29 | 1.35 |
| 2 | S | 150 | GLY | C-N | 5.70 | 1.40 | 1.33 |
| 2 | S | 213 | ARG | CA-CB | 5.70 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 383 | HIS | CA-C | -5.70 | 1.46 | 1.53 |
| 3 | N | 63 | PHE | C-N | 5.70 | 1.41 | 1.33 |
| 2 | C | 312 | ARG | N-CA | -5.70 | 1.39 | 1.46 |
| 1 | F | 233 | VAL | C-N | -5.70 | 1.26 | 1.33 |
| 2 | H | 187 | ARG | C-N | -5.70 | 1.26 | 1.33 |
| 3 | D | 70 | GLN | N-CA | -5.69 | 1.39 | 1.46 |
| 2 | Q | 36 | LEU | C-N | 5.69 | 1.41 | 1.33 |
| 2 | H | 313 | VAL | C-O | -5.69 | 1.17 | 1.24 |
| 2 | R | 23 | THR | C-O | -5.69 | 1.15 | 1.23 |
| 3 | M | 71 | VAL | C-O | 5.69 | 1.30 | 1.24 |
| 3 | P | 49 | ASN | CA-C | 5.69 | 1.57 | 1.52 |
| 2 | Q | 302 | ASP | C-O | -5.69 | 1.17 | 1.24 |
| 1 | T | 276 | LEU | C-N | 5.69 | 1.41 | 1.33 |
| 2 | G | 97 | TYR | CA-C | 5.69 | 1.59 | 1.52 |
| 2 | I | 297 | MET | SD-CE | -5.69 | 1.65 | 1.79 |
| 2 | R | 212 | GLN | C-N | 5.69 | 1.41 | 1.33 |
| 1 | T | 293 | ILE | C-N | -5.69 | 1.24 | 1.33 |
| 3 | D | 104 | ILE | CA-C | -5.69 | 1.46 | 1.52 |
| 2 | H | 43 | SER | C-O | -5.68 | 1.19 | 1.24 |
| 2 | H | 201 | LYS | CA-C | -5.68 | 1.45 | 1.52 |
| 2 | S | 279 | THR | CA-C | -5.68 | 1.45 | 1.52 |
| 2 | C | 435 | ARG | C-N | 5.68 | 1.41 | 1.33 |
| 2 | C | 340 | ALA | C-N | 5.68 | 1.41 | 1.33 |
| 3 | D | 39 | HIS | CA-C | 5.68 | 1.58 | 1.52 |
| 2 | I | 458 | ALA | C-N | -5.68 | 1.26 | 1.34 |
| 2 | J | 92 | GLY | C-N | 5.68 | 1.40 | 1.33 |
| 2 | Q | 183 | LYS | CA-C | 5.68 | 1.60 | 1.52 |
| 3 | M | 106 | HIS | ND1-CE1 | -5.68 | 1.26 | 1.32 |
| 2 | H | 118 | THR | N-CA | 5.68 | 1.53 | 1.46 |
| 2 | H | 317 | CYS | CA-C | -5.68 | 1.45 | 1.52 |
| 3 | P | 105 | VAL | CA-C | 5.68 | 1.59 | 1.52 |
| 2 | Q | 247 | CYS | CA-C | 5.68 | 1.60 | 1.52 |
| 2 | S | 292 | HIS | CA-CB | 5.68 | 1.62 | 1.53 |
| 2 | C | 151 | PRO | CA-C | -5.67 | 1.48 | 1.52 |
| 2 | C | 174 | ILE | CA-CB | 5.67 | 1.60 | 1.54 |
| 2 | G | 227 | LYS | C-N | 5.67 | 1.41 | 1.33 |
| 2 | J | 371 | MET | SD-CE | -5.67 | 1.65 | 1.79 |
| 2 | Q | 247 | CYS | N-CA | -5.67 | 1.38 | 1.46 |
| 3 | N | 44 | PHE | C-N | -5.67 | 1.26 | 1.33 |
| 2 | H | 278 | THR | C-O | -5.67 | 1.17 | 1.24 |
| 2 | C | 194 | ARG | C-N | 5.67 | 1.41 | 1.33 |
| 2 | I | 314 | LEU | CB-CG | 5.67 | 1.64 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | M | 11 | ARG | CA-CB | -5.67 | 1.44 | 1.53 |
| 2 | H | 298 | HIS | ND1-CE1 | 5.67 | 1.38 | 1.32 |
| 2 | R | 100 | PHE | C-O | -5.67 | 1.17 | 1.24 |
| 2 | C | 33 | ASP | CA-C | -5.67 | 1.44 | 1.52 |
| 2 | C | 454 | GLU | C-N | 5.67 | 1.41 | 1.34 |
| 2 | G | 348 | LEU | C-O | -5.67 | 1.17 | 1.24 |
| 3 | D | 21 | LEU | C-O | -5.66 | 1.17 | 1.23 |
| 2 | H | 227 | LYS | C-N | 5.66 | 1.41 | 1.33 |
| 3 | O | 67 | SER | C-N | 5.66 | 1.41 | 1.33 |
| 3 | D | 33 | MET | C-O | -5.66 | 1.17 | 1.24 |
| 2 | G | 330 | THR | CA-C | -5.66 | 1.45 | 1.52 |
| 2 | G | 348 | LEU | CA-CB | 5.66 | 1.62 | 1.53 |
| 2 | I | 98 | PHE | CA-C | 5.66 | 1.59 | 1.52 |
| 2 | J | 425 | GLU | CA-C | 5.66 | 1.60 | 1.52 |
| 1 | A | 267 | THR | C-N | 5.66 | 1.41 | 1.33 |
| 3 | E | 103 | PHE | C-O | -5.66 | 1.17 | 1.23 |
| 2 | R | 262 | MET | CA-C | -5.66 | 1.46 | 1.52 |
| 3 | L | 84 | ASP | N-CA | -5.66 | 1.39 | 1.46 |
| 2 | I | 137 | ASP | C-O | 5.66 | 1.30 | 1.23 |
| 2 | C | 211 | PHE | CA-C | 5.65 | 1.60 | 1.52 |
| 2 | C | 278 | THR | CA-C | 5.65 | 1.60 | 1.52 |
| 2 | G | 49 | PRO | CA-C | 5.65 | 1.59 | 1.52 |
| 2 | H | 45 | GLN | CA-C | 5.65 | 1.60 | 1.52 |
| 2 | H | 48 | VAL | CA-C | 5.65 | 1.58 | 1.52 |
| 2 | J | 397 | ASP | C-O | -5.65 | 1.16 | 1.23 |
| 2 | S | 153 | HIS | CD2-NE2 | 5.65 | 1.44 | 1.37 |
| 3 | E | 74 | GLU | CA-C | -5.65 | 1.45 | 1.52 |
| 2 | G | 459 | LEU | CB-CG | -5.65 | 1.42 | 1.53 |
| 2 | C | 131 | ARG | CA-C | 5.65 | 1.60 | 1.52 |
| 3 | E | 80 | SER | C-N | 5.65 | 1.41 | 1.33 |
| 2 | S | 345 | PHE | C-N | 5.65 | 1.41 | 1.33 |
| 2 | I | 58 | ALA | CA-C | -5.65 | 1.45 | 1.52 |
| 2 | Q | 108 | PHE | C-O | 5.65 | 1.30 | 1.23 |
| 2 | C | 105 | LEU | CA-C | -5.64 | 1.45 | 1.52 |
| 2 | G | 171 | GLY | N-CA | -5.64 | 1.39 | 1.45 |
| 2 | R | 454 | GLU | CA-CB | 5.64 | 1.62 | 1.53 |
| 2 | H | 161 | LEU | CA-CB | -5.64 | 1.44 | 1.53 |
| 2 | H | 328 | SER | N-CA | -5.64 | 1.39 | 1.46 |
| 2 | J | 430 | ALA | CA-CB | -5.64 | 1.44 | 1.53 |
| 3 | N | 84 | ASP | CA-C | -5.64 | 1.43 | 1.52 |
| 2 | R | 93 | GLU | C-O | -5.64 | 1.17 | 1.23 |
| 2 | J | 249 | GLU | C-O | -5.64 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | T | 228 | GLU | C-O | -5.64 | 1.17 | 1.24 |
| 3 | E | 39 | HIS | C-N | 5.64 | 1.40 | 1.33 |
| 2 | S | 307 | HIS | CA-C | 5.64 | 1.59 | 1.52 |
| 3 | O | 15 | PHE | C-N | -5.64 | 1.25 | 1.33 |
| 3 | K | 61 | PRO | N-CA | -5.64 | 1.40 | 1.47 |
| 3 | M | 62 | LEU | C-N | 5.64 | 1.43 | 1.33 |
| 2 | Q | 399 | VAL | C-O | 5.64 | 1.29 | 1.23 |
| 2 | G | 397 | ASP | C-O | 5.63 | 1.29 | 1.23 |
| 2 | H | 253 | ARG | C-O | 5.63 | 1.30 | 1.24 |
| 3 | L | 107 | ARG | C-O | 5.63 | 1.29 | 1.24 |
| 2 | J | 458 | ALA | C-O | -5.63 | 1.17 | 1.24 |
| 2 | R | 21 | LYS | CA-C | -5.63 | 1.45 | 1.52 |
| 2 | R | 164 | LYS | CA-C | -5.63 | 1.46 | 1.52 |
| 2 | C | 172 | CYS | CA-C | -5.63 | 1.46 | 1.52 |
| 2 | G | 314 | LEU | CB-CG | 5.63 | 1.64 | 1.53 |
| 2 | J | 226 | HIS | CD2-NE2 | 5.63 | 1.44 | 1.37 |
| 2 | S | 292 | HIS | CA-C | -5.63 | 1.45 | 1.52 |
| 2 | H | 371 | MET | N-CA | -5.62 | 1.38 | 1.46 |
| 2 | I | 137 | ASP | N-CA | 5.62 | 1.52 | 1.46 |
| 2 | J | 402 | PHE | CA-CB | 5.62 | 1.61 | 1.53 |
| 2 | S | 423 | ALA | C-O | -5.62 | 1.17 | 1.24 |
| 2 | J | 175 | LYS | N-CA | -5.62 | 1.41 | 1.45 |
| 2 | J | 213 | ARG | N-CA | -5.62 | 1.38 | 1.46 |
| 2 | R | 53 | ALA | CA-C | 5.62 | 1.59 | 1.52 |
| 3 | P | 43 | GLU | C-O | -5.62 | 1.16 | 1.23 |
| 2 | C | 28 | ASP | C-N | -5.62 | 1.26 | 1.33 |
| 2 | S | 330 | THR | CA-C | -5.62 | 1.45 | 1.52 |
| 2 | H | 88 | GLU | CA-C | -5.61 | 1.46 | 1.52 |
| 3 | M | 67 | SER | CA-C | 5.61 | 1.58 | 1.52 |
| 1 | A | 266 | SER | N-CA | -5.61 | 1.39 | 1.46 |
| 1 | A | 276 | LEU | CB-CG | -5.61 | 1.42 | 1.53 |
| 1 | A | 298 | ARG | C-O | -5.61 | 1.16 | 1.23 |
| 2 | G | 312 | ARG | C-N | -5.61 | 1.26 | 1.33 |
| 2 | G | 392 | GLU | CA-CB | 5.61 | 1.62 | 1.53 |
| 2 | Q | 350 | ARG | C-O | 5.61 | 1.30 | 1.24 |
| 2 | I | 298 | HIS | C-N | 5.61 | 1.41 | 1.34 |
| 2 | J | 97 | TYR | N-CA | -5.61 | 1.38 | 1.45 |
| 2 | C | 215 | ARG | N-CA | 5.61 | 1.53 | 1.46 |
| 2 | J | 440 | GLU | CA-CB | 5.61 | 1.60 | 1.53 |
| 2 | Q | 229 | GLN | N-CA | 5.61 | 1.53 | 1.46 |
| 2 | Q | 240 | LEU | CB-CG | -5.61 | 1.42 | 1.53 |
| 2 | R | 133 | LEU | N-CA | -5.61 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 145 | VAL | CA-C | -5.61 | 1.46 | 1.52 |
| 2 | J | 37 | LEU | C-N | -5.60 | 1.26 | 1.33 |
| 2 | J | 91 | GLN | C-N | -5.60 | 1.26 | 1.33 |
| 2 | H | 223 | ASP | C-N | -5.60 | 1.25 | 1.33 |
| 2 | Q | 112 | SER | CA-C | -5.60 | 1.45 | 1.53 |
| 2 | R | 31 | PRO | C-O | 5.60 | 1.30 | 1.23 |
| 2 | I | 131 | ARG | CA-C | -5.60 | 1.45 | 1.52 |
| 2 | Q | 383 | HIS | CD2-NE2 | 5.60 | 1.44 | 1.37 |
| 2 | C | 77 | MET | SD-CE | 5.60 | 1.93 | 1.79 |
| 2 | J | 230 | ALA | N-CA | -5.60 | 1.39 | 1.46 |
| 2 | J | 344 | GLY | C-N | 5.60 | 1.41 | 1.34 |
| 2 | Q | 170 | LEU | CA-C | -5.60 | 1.45 | 1.52 |
| 2 | I | 218 | PHE | C-O | -5.60 | 1.17 | 1.24 |
| 2 | J | 222 | ALA | N-CA | -5.60 | 1.39 | 1.46 |
| 2 | C | 423 | ALA | C-N | 5.59 | 1.40 | 1.33 |
| 2 | G | 301 | ILE | CB-CG1 | 5.59 | 1.64 | 1.53 |
| 2 | G | 438 | TYR | C-N | -5.59 | 1.26 | 1.33 |
| 2 | I | 359 | SER | CA-C | -5.59 | 1.45 | 1.52 |
| 2 | R | 397 | ASP | CA-CB | -5.59 | 1.45 | 1.52 |
| 2 | S | 176 | PRO | C-N | 5.59 | 1.41 | 1.33 |
| 2 | G | 396 | ASP | CA-C | 5.59 | 1.60 | 1.52 |
| 2 | I | 160 | ASP | CA-C | -5.59 | 1.45 | 1.52 |
| 2 | J | 86 | HIS | C-O | -5.59 | 1.17 | 1.23 |
| 1 | F | 297 | THR | C-N | -5.59 | 1.25 | 1.33 |
| 2 | G | 23 | THR | C-N | -5.59 | 1.26 | 1.33 |
| 2 | H | 301 | ILE | CB-CG1 | -5.59 | 1.42 | 1.53 |
| 2 | I | 187 | ARG | N-CA | -5.59 | 1.39 | 1.46 |
| 2 | I | 327 | HIS | CA-C | 5.59 | 1.60 | 1.52 |
| 2 | R | 396 | ASP | N-CA | 5.59 | 1.53 | 1.46 |
| 2 | S | 435 | ARG | N-CA | -5.59 | 1.39 | 1.46 |
| 2 | I | 193 | LEU | CB-CG | -5.59 | 1.42 | 1.53 |
| 2 | G | 340 | ALA | C-O | -5.59 | 1.17 | 1.24 |
| 2 | S | 383 | HIS | N-CA | -5.59 | 1.38 | 1.46 |
| 2 | C | 346 | VAL | C-O | -5.59 | 1.17 | 1.24 |
| 2 | G | 24 | TYR | N-CA | 5.59 | 1.53 | 1.46 |
| 2 | G | 329 | GLY | C-N | 5.59 | 1.41 | 1.33 |
| 2 | H | 197 | LEU | C-O | -5.59 | 1.17 | 1.23 |
| 3 | M | 19 | PRO | CA-C | 5.59 | 1.54 | 1.51 |
| 2 | Q | 182 | ALA | C-O | -5.59 | 1.17 | 1.24 |
| 2 | C | 147 | THR | C-O | -5.58 | 1.17 | 1.24 |
| 2 | G | 300 | VAL | N-CA | -5.58 | 1.38 | 1.46 |
| 3 | K | 56 | THR | CA-CB | 5.58 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | T | 228 | GLU | CA-CB | -5.58 | 1.44 | 1.53 |
| 2 | G | 249 | GLU | N-CA | -5.58 | 1.39 | 1.46 |
| 3 | L | 77 | GLU | CA-C | 5.58 | 1.59 | 1.52 |
| 3 | D | 28 | ALA | C-N | 5.58 | 1.41 | 1.33 |
| 3 | O | 77 | GLU | C-N | 5.58 | 1.41 | 1.33 |
| 2 | G | 443 | ASP | C-N | 5.58 | 1.40 | 1.33 |
| 2 | I | 64 | GLY | C-N | 5.58 | 1.41 | 1.33 |
| 3 | N | 34 | ILE | C-N | 5.58 | 1.41 | 1.34 |
| 2 | R | 190 | TYR | N-CA | 5.58 | 1.53 | 1.46 |
| 2 | S | 83 | LYS | CA-C | -5.58 | 1.45 | 1.52 |
| 2 | S | 182 | ALA | CA-C | -5.58 | 1.45 | 1.52 |
| 2 | G | 273 | GLY | C-N | 5.57 | 1.41 | 1.33 |
| 2 | J | 460 | ASP | CA-C | -5.57 | 1.45 | 1.52 |
| 2 | Q | 75 | THR | N-CA | -5.57 | 1.39 | 1.45 |
| 2 | I | 122 | GLY | C-O | -5.57 | 1.17 | 1.23 |
| 2 | Q | 238 | HIS | C-N | 5.57 | 1.41 | 1.33 |
| 2 | I | 249 | GLU | C-N | -5.57 | 1.26 | 1.33 |
| 2 | J | 168 | PRO | C-N | 5.57 | 1.41 | 1.33 |
| 3 | D | 42 | ILE | C-O | -5.57 | 1.17 | 1.24 |
| 2 | H | 86 | HIS | C-N | -5.57 | 1.26 | 1.33 |
| 1 | T | 283 | HIS | CG-CD2 | -5.57 | 1.29 | 1.35 |
| 1 | A | 283 | HIS | CA-C | 5.57 | 1.60 | 1.52 |
| 3 | D | 61 | PRO | N-CA | 5.57 | 1.53 | 1.46 |
| 2 | H | 24 | TYR | N-CA | 5.57 | 1.52 | 1.46 |
| 2 | H | 229 | GLN | CA-C | -5.57 | 1.45 | 1.52 |
| 3 | K | 88 | ARG | C-N | 5.57 | 1.42 | 1.33 |
| 2 | G | 458 | ALA | C-N | -5.56 | 1.26 | 1.33 |
| 2 | J | 443 | ASP | C-O | -5.56 | 1.17 | 1.24 |
| 3 | M | 82 | TYR | CA-CB | -5.56 | 1.45 | 1.53 |
| 2 | G | 239 | TYR | N-CA | -5.56 | 1.39 | 1.46 |
| 2 | I | 455 | LEU | C-O | -5.56 | 1.17 | 1.24 |
| 2 | Q | 146 | LYS | CA-C | 5.56 | 1.60 | 1.52 |
| 2 | S | 139 | ARG | C-N | -5.56 | 1.24 | 1.33 |
| 2 | H | 121 | VAL | CA-CB | -5.56 | 1.48 | 1.54 |
| 2 | J | 77 | MET | CA-C | -5.56 | 1.45 | 1.52 |
| 2 | R | 281 | ALA | CA-C | -5.56 | 1.45 | 1.52 |
| 2 | S | 56 | ALA | CA-CB | -5.56 | 1.44 | 1.53 |
| 2 | C | 135 | LEU | CA-C | 5.55 | 1.59 | 1.52 |
| 2 | C | 318 | LEU | C-O | -5.55 | 1.17 | 1.24 |
| 2 | J | 103 | TYR | C-O | -5.55 | 1.16 | 1.25 |
| 2 | R | 117 | LEU | CA-CB | -5.55 | 1.44 | 1.53 |
| 2 | R | 129 | ALA | C-O | -5.55 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 294 | HIS | N-CA | -5.55 | 1.38 | 1.46 |
| 1 | B | 242 | ARG | C-N | 5.55 | 1.40 | 1.33 |
| 1 | B | 276 | LEU | C-N | 5.55 | 1.41 | 1.34 |
| 1 | B | 278 | ASN | CA-C | 5.55 | 1.59 | 1.52 |
| 1 | F | 278 | ASN | C-N | 5.55 | 1.41 | 1.33 |
| 2 | Q | 155 | ILE | C-N | -5.55 | 1.26 | 1.33 |
| 2 | C | 427 | CYS | CA-C | -5.55 | 1.45 | 1.52 |
| 3 | E | 40 | PRO | C-N | -5.55 | 1.25 | 1.33 |
| 2 | G | 436 | ASP | N-CA | -5.55 | 1.39 | 1.46 |
| 3 | M | 51 | GLU | N-CA | -5.55 | 1.38 | 1.46 |
| 3 | L | 74 | GLU | C-N | -5.55 | 1.26 | 1.33 |
| 2 | R | 163 | ASN | C-N | 5.55 | 1.41 | 1.33 |
| 2 | R | 299 | ALA | C-N | 5.55 | 1.40 | 1.34 |
| 2 | C | 319 | ARG | CA-C | -5.55 | 1.45 | 1.52 |
| 3 | L | 107 | ARG | N-CA | -5.54 | 1.40 | 1.45 |
| 2 | Q | 63 | THR | CA-C | 5.54 | 1.60 | 1.52 |
| 2 | C | 270 | LEU | N-CA | -5.54 | 1.39 | 1.46 |
| 2 | I | 120 | ILE | CB-CG1 | 5.54 | 1.64 | 1.53 |
| 2 | I | 151 | PRO | C-N | -5.54 | 1.26 | 1.34 |
| 3 | O | 86 | TYR | C-N | 5.54 | 1.40 | 1.33 |
| 2 | S | 49 | PRO | CA-CB | -5.54 | 1.46 | 1.53 |
| 2 | J | 61 | SER | CA-C | 5.54 | 1.60 | 1.52 |
| 2 | J | 389 | ALA | CA-C | -5.54 | 1.45 | 1.52 |
| 3 | L | 74 | GLU | N-CA | -5.54 | 1.39 | 1.46 |
| 2 | R | 161 | LEU | CB-CG | -5.54 | 1.42 | 1.53 |
| 2 | C | 51 | ASP | CA-C | 5.54 | 1.59 | 1.52 |
| 2 | H | 231 | GLU | CA-C | 5.54 | 1.60 | 1.52 |
| 2 | J | 163 | ASN | N-CA | -5.54 | 1.39 | 1.46 |
| 2 | C | 156 | GLN | C-N | -5.54 | 1.27 | 1.33 |
| 2 | H | 389 | ALA | CA-CB | -5.54 | 1.44 | 1.53 |
| 2 | C | 322 | GLY | C-N | 5.54 | 1.40 | 1.33 |
| 2 | J | 421 | ARG | C-N | 5.54 | 1.40 | 1.33 |
| 3 | P | 63 | PHE | C-N | 5.54 | 1.40 | 1.33 |
| 2 | Q | 298 | HIS | CE1-NE2 | 5.54 | 1.38 | 1.32 |
| 2 | S | 148 | PHE | N-CA | 5.54 | 1.52 | 1.45 |
| 1 | B | 279 | CYS | CA-C | 5.53 | 1.59 | 1.52 |
| 3 | D | 49 | ASN | C-O | 5.53 | 1.30 | 1.24 |
| 2 | G | 310 | HIS | ND1-CE1 | 5.53 | 1.38 | 1.32 |
| 2 | R | 189 | VAL | CA-C | -5.53 | 1.46 | 1.52 |
| 2 | H | 88 | GLU | C-O | -5.53 | 1.18 | 1.24 |
| 3 | O | 39 | HIS | CD2-NE2 | 5.53 | 1.44 | 1.37 |
| 2 | I | 163 | ASN | C-N | 5.53 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 278 | THR | C-O | -5.53 | 1.17 | 1.24 |
| 2 | C | 145 | VAL | C-N | -5.53 | 1.26 | 1.33 |
| 2 | C | 200 | THR | CA-C | -5.53 | 1.46 | 1.52 |
| 2 | H | 180 | LEU | CA-C | -5.53 | 1.45 | 1.53 |
| 2 | J | 382 | ILE | CA-C | 5.53 | 1.59 | 1.52 |
| 1 | B | 234 | ARG | CA-C | -5.53 | 1.45 | 1.52 |
| 2 | J | 76 | ASP | CA-C | -5.53 | 1.47 | 1.53 |
| 2 | I | 188 | ALA | C-O | -5.52 | 1.17 | 1.24 |
| 3 | N | 42 | ILE | CA-C | -5.52 | 1.45 | 1.52 |
| 3 | O | 48 | SER | N-CA | 5.52 | 1.53 | 1.46 |
| 3 | P | 52 | GLU | CA-C | -5.52 | 1.46 | 1.53 |
| 1 | A | 228 | GLU | C-N | 5.52 | 1.40 | 1.33 |
| 1 | F | 277 | GLU | CA-C | 5.52 | 1.59 | 1.52 |
| 2 | I | 43 | SER | N-CA | 5.52 | 1.52 | 1.46 |
| 2 | J | 35 | ASP | N-CA | 5.52 | 1.53 | 1.45 |
| 2 | J | 451 | TRP | N-CA | 5.52 | 1.53 | 1.46 |
| 2 | R | 414 | ALA | CA-CB | -5.52 | 1.46 | 1.53 |
| 2 | C | 420 | ASN | C-O | 5.52 | 1.30 | 1.24 |
| 2 | H | 207 | ASN | C-O | -5.52 | 1.16 | 1.24 |
| 3 | L | 79 | ARG | CA-CB | -5.52 | 1.44 | 1.53 |
| 2 | R | 180 | LEU | N-CA | 5.52 | 1.52 | 1.46 |
| 2 | S | 238 | HIS | CD2-NE2 | 5.52 | 1.44 | 1.37 |
| 2 | I | 208 | SER | N-CA | -5.52 | 1.38 | 1.46 |
| 3 | P | 47 | HIS | CG-CD2 | 5.52 | 1.42 | 1.35 |
| 2 | R | 76 | ASP | N-CA | -5.52 | 1.39 | 1.46 |
| 1 | T | 246 | GLU | C-O | 5.52 | 1.30 | 1.23 |
| 2 | I | 223 | ASP | C-N | 5.51 | 1.40 | 1.33 |
| 2 | I | 326 | LEU | CA-CB | -5.51 | 1.44 | 1.53 |
| 2 | J | 56 | ALA | C-N | -5.51 | 1.27 | 1.34 |
| 2 | J | 321 | SER | N-CA | -5.51 | 1.39 | 1.46 |
| 2 | R | 328 | SER | N-CA | -5.51 | 1.40 | 1.46 |
| 2 | S | 169 | MET | C-N | 5.51 | 1.41 | 1.33 |
| 2 | C | 71 | THR | C-O | -5.51 | 1.17 | 1.24 |
| 2 | C | 327 | HIS | CD2-NE2 | 5.51 | 1.44 | 1.37 |
| 3 | D | 72 | LEU | C-N | -5.51 | 1.26 | 1.33 |
| 2 | I | 329 | GLY | C-N | -5.51 | 1.25 | 1.33 |
| 3 | O | 44 | PHE | CA-C | 5.51 | 1.59 | 1.52 |
| 2 | Q | 219 | LEU | N-CA | -5.51 | 1.39 | 1.46 |
| 1 | T | 282 | GLU | C-O | 5.51 | 1.30 | 1.24 |
| 2 | C | 187 | ARG | CA-C | -5.51 | 1.45 | 1.52 |
| 2 | C | 290 | LEU | C-O | -5.51 | 1.16 | 1.23 |
| 2 | G | 125 | PHE | N-CA | -5.51 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 45 | GLN | N-CA | 5.51 | 1.53 | 1.45 |
| 2 | S | 42 | PHE | CA-C | 5.51 | 1.59 | 1.52 |
| 2 | S | 222 | ALA | N-CA | -5.51 | 1.39 | 1.46 |
| 2 | H | 185 | TYR | CA-C | 5.51 | 1.60 | 1.52 |
| 2 | R | 295 | ARG | CA-C | 5.51 | 1.60 | 1.52 |
| 2 | I | 366 | GLN | CA-C | 5.51 | 1.59 | 1.52 |
| 3 | L | 34 | ILE | CA-C | -5.51 | 1.46 | 1.52 |
| 3 | P | 21 | LEU | CA-C | -5.51 | 1.45 | 1.52 |
| 2 | I | 421 | ARG | N-CA | 5.50 | 1.52 | 1.46 |
| 3 | K | 93 | ASP | N-CA | -5.50 | 1.39 | 1.46 |
| 2 | Q | 125 | PHE | C-O | -5.50 | 1.17 | 1.24 |
| 2 | R | 79 | ARG | C-N | 5.50 | 1.41 | 1.33 |
| 2 | J | 148 | PHE | CA-C | -5.50 | 1.45 | 1.52 |
| 2 | I | 169 | MET | N-CA | 5.50 | 1.52 | 1.45 |
| 2 | Q | 119 | SER | C-O | 5.50 | 1.30 | 1.24 |
| 1 | B | 242 | ARG | CD-NE | 5.50 | 1.53 | 1.46 |
| 1 | B | 273 | LEU | N-CA | -5.50 | 1.39 | 1.46 |
| 2 | I | 116 | ILE | N-CA | -5.50 | 1.40 | 1.46 |
| 2 | I | 349 | MET | SD-CE | -5.50 | 1.65 | 1.79 |
| 2 | I | 414 | ALA | N-CA | -5.50 | 1.41 | 1.46 |
| 2 | H | 52 | GLU | CA-CB | 5.50 | 1.62 | 1.53 |
| 2 | H | 454 | GLU | C-O | -5.49 | 1.17 | 1.24 |
| 2 | Q | 136 | GLU | C-N | -5.49 | 1.26 | 1.33 |
| 2 | Q | 443 | ASP | N-CA | 5.49 | 1.52 | 1.46 |
| 2 | G | 135 | LEU | CA-CB | 5.49 | 1.60 | 1.53 |
| 2 | Q | 29 | TYR | C-N | 5.49 | 1.43 | 1.33 |
| 2 | C | 255 | GLU | N-CA | 5.49 | 1.52 | 1.46 |
| 3 | N | 17 | TYR | C-N | 5.49 | 1.43 | 1.33 |
| 2 | R | 165 | TYR | CA-C | -5.49 | 1.46 | 1.52 |
| 3 | D | 95 | ILE | CA-CB | 5.49 | 1.60 | 1.54 |
| 2 | H | 34 | THR | N-CA | 5.49 | 1.53 | 1.46 |
| 2 | J | 390 | LEU | CA-CB | 5.49 | 1.61 | 1.53 |
| 2 | G | 398 | SER | CA-C | 5.49 | 1.59 | 1.52 |
| 2 | H | 194 | ARG | CA-C | 5.49 | 1.60 | 1.52 |
| 2 | Q | 353 | HIS | CD2-NE2 | 5.49 | 1.43 | 1.37 |
| 3 | O | 75 | VAL | CA-C | 5.49 | 1.61 | 1.52 |
| 2 | R | 255 | GLU | N-CA | 5.49 | 1.52 | 1.46 |
| 2 | C | 228 | SER | CA-C | -5.48 | 1.45 | 1.52 |
| 3 | D | 70 | GLN | C-O | -5.48 | 1.17 | 1.24 |
| 2 | S | 156 | GLN | N-CA | -5.48 | 1.39 | 1.46 |
| 2 | Q | 135 | LEU | C-N | -5.48 | 1.26 | 1.33 |
| 2 | G | 24 | TYR | CA-C | -5.48 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 130 | ILE | CA-CB | 5.48 | 1.60 | 1.54 |
| 2 | R | 259 | GLU | N-CA | 5.48 | 1.53 | 1.46 |
| 2 | G | 123 | ASN | C-N | -5.48 | 1.26 | 1.33 |
| 2 | Q | 303 | ARG | C-O | 5.48 | 1.30 | 1.24 |
| 2 | J | 123 | ASN | N-CA | 5.47 | 1.52 | 1.46 |
| 3 | O | 93 | ASP | CA-CB | 5.47 | 1.59 | 1.52 |
| 3 | D | 13 | GLU | C-N | 5.47 | 1.42 | 1.33 |
| 3 | E | 30 | ILE | C-O | -5.47 | 1.18 | 1.24 |
| 2 | J | 292 | HIS | CE1-NE2 | -5.47 | 1.27 | 1.32 |
| 2 | S | 253 | ARG | C-N | -5.47 | 1.27 | 1.33 |
| 2 | H | 308 | GLY | C-N | 5.47 | 1.40 | 1.33 |
| 3 | D | 60 | LEU | CA-C | 5.47 | 1.61 | 1.53 |
| 2 | I | 101 | ILE | N-CA | -5.47 | 1.39 | 1.46 |
| 2 | Q | 342 | THR | CA-CB | -5.47 | 1.44 | 1.53 |
| 2 | G | 186 | GLY | C-N | -5.47 | 1.26 | 1.33 |
| 2 | C | 443 | ASP | C-N | 5.47 | 1.40 | 1.33 |
| 2 | G | 275 | THR | N-CA | -5.47 | 1.39 | 1.46 |
| 2 | I | 255 | GLU | CA-C | 5.47 | 1.59 | 1.52 |
| 2 | J | 209 | GLN | N-CA | -5.47 | 1.38 | 1.45 |
| 2 | H | 173 | THR | CA-C | -5.46 | 1.45 | 1.52 |
| 2 | H | 290 | LEU | C-O | 5.46 | 1.30 | 1.23 |
| 1 | F | 283 | HIS | CA-C | 5.46 | 1.60 | 1.52 |
| 2 | Q | 101 | ILE | CB-CG1 | 5.46 | 1.64 | 1.53 |
| 2 | R | 44 | PRO | C-N | -5.46 | 1.25 | 1.33 |
| 2 | Q | 301 | ILE | C-O | -5.46 | 1.18 | 1.24 |
| 2 | R | 254 | ALA | CA-C | 5.46 | 1.59 | 1.52 |
| 2 | H | 311 | PHE | N-CA | -5.46 | 1.39 | 1.46 |
| 2 | S | 108 | PHE | CA-C | -5.46 | 1.46 | 1.52 |
| 2 | J | 302 | ASP | CA-CB | -5.45 | 1.45 | 1.54 |
| 1 | A | 294 | ASP | C-O | 5.45 | 1.30 | 1.24 |
| 2 | G | 371 | MET | SD-CE | 5.45 | 1.93 | 1.79 |
| 2 | I | 263 | PRO | C-N | -5.45 | 1.28 | 1.33 |
| 2 | J | 377 | VAL | C-O | -5.45 | 1.17 | 1.24 |
| 1 | B | 260 | PRO | CA-CB | -5.45 | 1.46 | 1.53 |
| 2 | C | 194 | ARG | CA-C | -5.45 | 1.45 | 1.52 |
| 2 | H | 383 | HIS | CA-C | -5.45 | 1.47 | 1.53 |
| 3 | N | 52 | GLU | C-O | 5.45 | 1.30 | 1.23 |
| 2 | Q | 56 | ALA | CA-C | 5.45 | 1.59 | 1.52 |
| 2 | Q | 203 | ASP | CA-CB | -5.45 | 1.45 | 1.53 |
| 2 | S | 319 | ARG | N-CA | -5.45 | 1.39 | 1.46 |
| 2 | J | 85 | TYR | C-O | -5.45 | 1.16 | 1.24 |
| 3 | O | 26 | ILE | CB-CG1 | -5.45 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 88 | GLU | C-N | 5.45 | 1.40 | 1.33 |
| 2 | H | 226 | HIS | CG-ND1 | -5.44 | 1.32 | 1.38 |
| 2 | R | 327 | HIS | CA-CB | 5.44 | 1.62 | 1.53 |
| 2 | S | 63 | THR | C-N | -5.44 | 1.25 | 1.33 |
| 2 | C | 131 | ARG | C-O | -5.44 | 1.17 | 1.24 |
| 2 | G | 236 | LYS | C-O | -5.44 | 1.16 | 1.23 |
| 2 | Q | 281 | ALA | CA-C | 5.44 | 1.59 | 1.52 |
| 1 | T | 238 | ASN | CA-C | 5.44 | 1.59 | 1.52 |
| 2 | G | 101 | ILE | CB-CG1 | 5.44 | 1.64 | 1.53 |
| 2 | I | 437 | LEU | CA-C | -5.44 | 1.45 | 1.52 |
| 2 | J | 285 | ARG | C-N | -5.44 | 1.26 | 1.33 |
| 2 | J | 303 | ARG | CA-CB | -5.44 | 1.45 | 1.53 |
| 3 | M | 33 | MET | CA-CB | -5.44 | 1.45 | 1.53 |
| 2 | S | 115 | ASN | CA-CB | -5.44 | 1.44 | 1.53 |
| 2 | Q | 320 | LEU | CA-C | -5.44 | 1.46 | 1.52 |
| 2 | I | 271 | THR | CA-CB | 5.43 | 1.61 | 1.53 |
| 2 | S | 180 | LEU | CA-CB | 5.43 | 1.61 | 1.53 |
| 2 | J | 239 | TYR | CA-CB | 5.43 | 1.60 | 1.52 |
| 2 | Q | 210 | PRO | C-O | 5.43 | 1.31 | 1.24 |
| 2 | I | 100 | PHE | N-CA | -5.43 | 1.39 | 1.46 |
| 3 | D | 39 | HIS | ND1-CE1 | 5.43 | 1.38 | 1.32 |
| 2 | H | 285 | ARG | C-N | 5.43 | 1.41 | 1.33 |
| 2 | J | 35 | ASP | CA-CB | -5.43 | 1.45 | 1.53 |
| 2 | R | 400 | LEU | C-N | 5.42 | 1.40 | 1.33 |
| 2 | I | 267 | HIS | CD2-NE2 | 5.42 | 1.43 | 1.37 |
| 2 | G | 369 | ALA | CA-CB | -5.42 | 1.44 | 1.53 |
| 2 | I | 383 | HIS | ND1-CE1 | 5.42 | 1.38 | 1.32 |
| 2 | C | 235 | ILE | CA-CB | 5.42 | 1.61 | 1.54 |
| 2 | I | 340 | ALA | CA-C | 5.42 | 1.59 | 1.52 |
| 1 | A | 296 | ASN | CA-CB | 5.41 | 1.61 | 1.53 |
| 3 | E | 106 | HIS | CA-C | -5.41 | 1.46 | 1.52 |
| 2 | J | 143 | ALA | N-CA | -5.41 | 1.40 | 1.46 |
| 2 | R | 292 | HIS | CA-C | -5.41 | 1.46 | 1.52 |
| 2 | S | 275 | THR | N-CA | 5.41 | 1.52 | 1.46 |
| 2 | G | 460 | ASP | CA-C | -5.41 | 1.45 | 1.52 |
| 2 | I | 357 | ASP | C-N | -5.41 | 1.25 | 1.33 |
| 3 | P | 78 | CYS | C-N | 5.41 | 1.41 | 1.33 |
| 2 | Q | 414 | ALA | CA-CB | -5.41 | 1.46 | 1.53 |
| 2 | R | 174 | ILE | C-N | 5.41 | 1.40 | 1.33 |
| 1 | B | 294 | ASP | CA-C | -5.41 | 1.46 | 1.52 |
| 2 | G | 138 | ILE | N-CA | -5.41 | 1.39 | 1.46 |
| 2 | I | 86 | HIS | CE1-NE2 | 5.41 | 1.38 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 302 | PHE | N-CA | -5.41 | 1.39 | 1.46 |
| 2 | J | 352 | ASP | CA-C | 5.41 | 1.59 | 1.52 |
| 3 | O | 46 | GLU | C-N | -5.41 | 1.25 | 1.33 |
| 2 | C | 138 | ILE | CB-CG1 | 5.41 | 1.64 | 1.53 |
| 3 | D | 99 | GLN | CA-C | 5.41 | 1.59 | 1.52 |
| 2 | H | 138 | ILE | C-N | 5.41 | 1.42 | 1.33 |
| 2 | C | 292 | HIS | N-CA | -5.40 | 1.39 | 1.45 |
| 2 | I | 298 | HIS | C-O | -5.40 | 1.17 | 1.24 |
| 2 | J | 226 | HIS | ND1-CE1 | -5.40 | 1.27 | 1.32 |
| 2 | H | 397 | ASP | C-N | -5.40 | 1.26 | 1.33 |
| 2 | J | 247 | CYS | CA-C | -5.40 | 1.45 | 1.52 |
| 2 | J | 100 | PHE | C-N | -5.40 | 1.26 | 1.33 |
| 2 | J | 158 | GLU | CA-CB | -5.40 | 1.45 | 1.53 |
| 2 | J | 171 | GLY | C-N | -5.40 | 1.25 | 1.33 |
| 1 | A | 297 | THR | CA-CB | -5.39 | 1.44 | 1.53 |
| 2 | H | 53 | ALA | CA-CB | -5.39 | 1.45 | 1.53 |
| 3 | N | 44 | PHE | C-O | -5.39 | 1.17 | 1.23 |
| 2 | Q | 269 | PHE | C-N | 5.39 | 1.40 | 1.33 |
| 2 | Q | 295 | ARG | CA-C | 5.39 | 1.59 | 1.53 |
| 2 | S | 455 | LEU | CA-CB | -5.39 | 1.44 | 1.53 |
| 2 | Q | 426 | ALA | CA-C | -5.39 | 1.45 | 1.52 |
| 2 | C | 289 | VAL | C-O | -5.39 | 1.18 | 1.24 |
| 2 | I | 21 | LYS | CA-C | -5.39 | 1.45 | 1.52 |
| 2 | J | 251 | MET | C-O | -5.39 | 1.18 | 1.24 |
| 1 | F | 299 | SER | C-N | 5.39 | 1.41 | 1.33 |
| 2 | G | 318 | LEU | C-O | -5.39 | 1.18 | 1.24 |
| 2 | Q | 284 | CYS | C-O | -5.39 | 1.17 | 1.24 |
| 2 | Q | 348 | LEU | N-CA | -5.39 | 1.39 | 1.46 |
| 2 | G | 125 | PHE | C-O | -5.39 | 1.17 | 1.24 |
| 2 | G | 221 | VAL | C-N | 5.39 | 1.40 | 1.33 |
| 2 | H | 358 | ARG | N-CA | 5.39 | 1.52 | 1.46 |
| 2 | Q | 192 | CYS | C-N | 5.39 | 1.41 | 1.33 |
| 2 | C | 421 | ARG | C-O | -5.39 | 1.17 | 1.24 |
| 2 | I | 235 | ILE | N-CA | -5.39 | 1.39 | 1.46 |
| 2 | Q | 251 | MET | CA-CB | 5.39 | 1.61 | 1.53 |
| 2 | Q | 383 | HIS | C-O | -5.39 | 1.15 | 1.23 |
| 2 | Q | 396 | ASP | CA-C | 5.39 | 1.60 | 1.52 |
| 2 | S | 345 | PHE | CA-CB | -5.38 | 1.44 | 1.53 |
| 3 | E | 95 | ILE | C-N | -5.38 | 1.26 | 1.33 |
| 2 | J | 230 | ALA | C-N | -5.38 | 1.25 | 1.33 |
| 3 | O | 22 | SER | C-N | 5.38 | 1.41 | 1.33 |
| 2 | R | 267 | HIS | CG-CD2 | -5.38 | 1.29 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 230 | ALA | C-O | 5.38 | 1.30 | 1.24 |
| 3 | L | 49 | ASN | C-N | -5.38 | 1.26 | 1.34 |
| 2 | H | 340 | ALA | C-N | -5.38 | 1.26 | 1.34 |
| 3 | K | 102 | SER | C-O | 5.38 | 1.30 | 1.24 |
| 2 | G | 86 | HIS | CG-CD2 | -5.38 | 1.29 | 1.35 |
| 2 | J | 174 | ILE | C-O | -5.38 | 1.17 | 1.24 |
| 2 | H | 139 | ARG | N-CA | -5.38 | 1.39 | 1.46 |
| 2 | R | 445 | LEU | C-O | 5.38 | 1.30 | 1.24 |
| 2 | S | 180 | LEU | CA-C | -5.38 | 1.45 | 1.52 |
| 2 | G | 344 | GLY | C-N | 5.38 | 1.41 | 1.33 |
| 2 | J | 82 | GLY | C-N | -5.38 | 1.26 | 1.33 |
| 1 | A | 255 | THR | CB-OG1 | -5.37 | 1.35 | 1.43 |
| 2 | J | 90 | VAL | CA-CB | -5.37 | 1.47 | 1.54 |
| 3 | K | 94 | ASN | CA-C | -5.37 | 1.46 | 1.52 |
| 2 | S | 398 | SER | C-N | -5.37 | 1.26 | 1.33 |
| 2 | G | 382 | ILE | C-O | 5.37 | 1.31 | 1.24 |
| 2 | G | 440 | GLU | C-O | -5.37 | 1.16 | 1.24 |
| 3 | O | 33 | MET | C-N | -5.37 | 1.27 | 1.33 |
| 2 | Q | 23 | THR | C-O | -5.37 | 1.17 | 1.23 |
| 2 | Q | 302 | ASP | C-N | -5.37 | 1.27 | 1.33 |
| 2 | C | 103 | TYR | C-O | -5.37 | 1.17 | 1.24 |
| 3 | D | 47 | HIS | CG-CD2 | -5.37 | 1.29 | 1.35 |
| 2 | Q | 159 | ARG | CA-C | 5.37 | 1.59 | 1.52 |
| 2 | G | 147 | THR | CA-CB | 5.37 | 1.62 | 1.53 |
| 2 | S | 300 | VAL | CA-CB | -5.37 | 1.46 | 1.54 |
| 2 | C | 116 | ILE | CB-CG1 | 5.37 | 1.64 | 1.53 |
| 2 | I | 30 | THR | CA-C | 5.37 | 1.57 | 1.52 |
| 1 | A | 242 | ARG | C-N | 5.36 | 1.40 | 1.33 |
| 2 | R | 230 | ALA | C-N | -5.36 | 1.27 | 1.33 |
| 3 | N | 102 | SER | C-O | 5.36 | 1.30 | 1.24 |
| 2 | Q | 187 | ARG | CA-C | 5.36 | 1.59 | 1.52 |
| 2 | J | 22 | LEU | C-N | 5.36 | 1.42 | 1.33 |
| 2 | J | 226 | HIS | CA-C | -5.36 | 1.45 | 1.52 |
| 2 | Q | 133 | LEU | CB-CG | -5.36 | 1.42 | 1.53 |
| 2 | Q | 183 | LYS | N-CA | -5.36 | 1.40 | 1.46 |
| 2 | Q | 360 | ARG | CA-CB | -5.36 | 1.45 | 1.53 |
| 2 | G | 180 | LEU | C-O | -5.36 | 1.17 | 1.23 |
| 3 | O | 31 | GLU | N-CA | -5.36 | 1.40 | 1.46 |
| 3 | P | 32 | TYR | C-N | -5.36 | 1.27 | 1.33 |
| 2 | Q | 123 | ASN | C-N | 5.36 | 1.40 | 1.33 |
| 2 | G | 370 | SER | N-CA | 5.36 | 1.53 | 1.46 |
| 3 | O | 87 | ILE | CA-CB | -5.36 | 1.47 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 180 | LEU | C-O | -5.36 | 1.17 | 1.23 |
| 1 | A | 239 | GLN | CA-C | 5.35 | 1.60 | 1.52 |
| 3 | M | 47 | HIS | CE1-NE2 | 5.35 | 1.38 | 1.32 |
| 2 | H | 458 | ALA | C-O | 5.35 | 1.30 | 1.24 |
| 2 | I | 63 | THR | CA-CB | -5.35 | 1.46 | 1.54 |
| 2 | I | 136 | GLU | C-N | -5.35 | 1.26 | 1.33 |
| 2 | S | 247 | CYS | N-CA | -5.35 | 1.39 | 1.46 |
| 2 | R | 126 | GLY | C-O | -5.35 | 1.17 | 1.23 |
| 2 | H | 107 | LEU | C-N | 5.35 | 1.40 | 1.33 |
| 3 | K | 51 | GLU | CA-CB | -5.35 | 1.44 | 1.53 |
| 2 | S | 99 | ALA | CA-C | -5.35 | 1.46 | 1.52 |
| 2 | G | 86 | HIS | CG-ND1 | -5.35 | 1.32 | 1.38 |
| 3 | L | 87 | ILE | CA-C | 5.35 | 1.59 | 1.52 |
| 3 | M | 107 | ARG | C-O | -5.35 | 1.17 | 1.24 |
| 3 | L | 102 | SER | N-CA | -5.34 | 1.40 | 1.46 |
| 2 | C | 163 | ASN | C-N | 5.34 | 1.40 | 1.33 |
| 2 | G | 229 | GLN | C-N | -5.34 | 1.27 | 1.33 |
| 2 | R | 217 | ARG | CA-C | -5.34 | 1.46 | 1.52 |
| 2 | C | 288 | GLY | CA-C | 5.34 | 1.57 | 1.51 |
| 1 | F | 305 | LEU | C-N | -5.34 | 1.26 | 1.33 |
| 2 | H | 79 | ARG | CA-CB | -5.34 | 1.45 | 1.53 |
| 2 | H | 397 | ASP | C-O | 5.34 | 1.29 | 1.23 |
| 2 | G | 310 | HIS | CG-ND1 | -5.34 | 1.32 | 1.38 |
| 2 | I | 265 | ILE | C-O | -5.34 | 1.17 | 1.24 |
| 2 | J | 217 | ARG | CA-CB | -5.34 | 1.45 | 1.53 |
| 2 | Q | 371 | MET | SD-CE | 5.34 | 1.93 | 1.79 |
| 2 | R | 243 | THR | C-N | -5.34 | 1.27 | 1.33 |
| 2 | S | 137 | ASP | CA-C | 5.34 | 1.59 | 1.52 |
| 2 | H | 60 | GLU | C-N | 5.34 | 1.41 | 1.34 |
| 2 | Q | 382 | ILE | C-N | 5.34 | 1.40 | 1.33 |
| 2 | I | 99 | ALA | C-N | 5.34 | 1.40 | 1.33 |
| 1 | B | 304 | ALA | CA-C | -5.33 | 1.46 | 1.52 |
| 1 | T | 295 | THR | C-O | -5.33 | 1.17 | 1.24 |
| 2 | C | 127 | PHE | CA-CB | -5.33 | 1.45 | 1.53 |
| 2 | H | 448 | ALA | N-CA | 5.33 | 1.52 | 1.46 |
| 3 | N | 56 | THR | C-N | -5.33 | 1.26 | 1.33 |
| 3 | P | 67 | SER | N-CA | -5.33 | 1.39 | 1.46 |
| 2 | R | 202 | ASP | CG-OD1 | -5.33 | 1.15 | 1.25 |
| 2 | G | 133 | LEU | CA-C | 5.33 | 1.59 | 1.52 |
| 1 | A | 286 | GLU | C-O | -5.33 | 1.17 | 1.23 |
| 2 | S | 441 | GLY | C-N | 5.33 | 1.40 | 1.33 |
| 2 | C | 50 | ALA | C-O | -5.33 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 109 | GLU | C-N | -5.33 | 1.25 | 1.33 |
| 3 | E | 56 | THR | C-N | -5.33 | 1.26 | 1.33 |
| 2 | Q | 324 | ASP | CA-CB | -5.33 | 1.44 | 1.53 |
| 2 | C | 181 | SER | C-O | -5.33 | 1.16 | 1.23 |
| 2 | J | 433 | GLU | C-O | -5.33 | 1.17 | 1.24 |
| 3 | L | 90 | ALA | C-N | 5.33 | 1.40 | 1.32 |
| 1 | F | 244 | GLY | C-N | 5.33 | 1.40 | 1.33 |
| 2 | H | 420 | ASN | N-CA | -5.33 | 1.39 | 1.46 |
| 2 | S | 214 | TRP | CA-CB | -5.33 | 1.45 | 1.53 |
| 3 | E | 28 | ALA | C-O | -5.32 | 1.18 | 1.24 |
| 2 | I | 309 | ILE | CB-CG1 | 5.32 | 1.64 | 1.53 |
| 3 | L | 25 | GLN | C-N | -5.32 | 1.27 | 1.33 |
| 2 | R | 281 | ALA | C-O | 5.32 | 1.30 | 1.24 |
| 2 | S | 246 | THR | C-N | 5.32 | 1.40 | 1.33 |
| 1 | F | 259 | GLN | N-CA | -5.32 | 1.39 | 1.45 |
| 2 | G | 20 | TYR | CA-C | -5.32 | 1.41 | 1.52 |
| 3 | O | 77 | GLU | N-CA | -5.32 | 1.39 | 1.46 |
| 2 | S | 325 | HIS | CA-C | -5.32 | 1.46 | 1.52 |
| 2 | H | 292 | HIS | C-N | 5.32 | 1.40 | 1.33 |
| 2 | G | 127 | PHE | CA-CB | 5.32 | 1.62 | 1.53 |
| 2 | G | 445 | LEU | C-N | 5.32 | 1.40 | 1.33 |
| 2 | I | 171 | GLY | CA-C | 5.32 | 1.56 | 1.51 |
| 2 | J | 144 | LEU | CA-CB | -5.32 | 1.44 | 1.53 |
| 3 | N | 101 | VAL | CA-C | -5.32 | 1.46 | 1.52 |
| 2 | Q | 357 | ASP | CA-C | -5.32 | 1.47 | 1.53 |
| 2 | R | 358 | ARG | N-CA | 5.32 | 1.52 | 1.46 |
| 2 | G | 193 | LEU | C-O | 5.32 | 1.30 | 1.24 |
| 3 | O | 94 | ASN | CA-CB | -5.32 | 1.44 | 1.53 |
| 2 | H | 173 | THR | CA-CB | 5.31 | 1.61 | 1.53 |
| 2 | I | 342 | THR | CA-CB | -5.31 | 1.45 | 1.53 |
| 2 | H | 141 | PRO | C-O | -5.31 | 1.17 | 1.23 |
| 3 | K | 95 | ILE | N-CA | -5.31 | 1.40 | 1.46 |
| 3 | M | 106 | HIS | CG-CD2 | -5.31 | 1.30 | 1.35 |
| 3 | O | 20 | PRO | N-CA | -5.31 | 1.40 | 1.47 |
| 2 | Q | 284 | CYS | C-N | -5.31 | 1.27 | 1.33 |
| 3 | L | 96 | LYS | C-O | -5.31 | 1.17 | 1.24 |
| 1 | A | 253 | PHE | CA-C | -5.31 | 1.46 | 1.52 |
| 2 | C | 367 | ASP | N-CA | -5.31 | 1.39 | 1.45 |
| 2 | J | 392 | GLU | C-N | -5.31 | 1.27 | 1.33 |
| 3 | P | 10 | ARG | CA-CB | 5.31 | 1.62 | 1.53 |
| 3 | D | 107 | ARG | CA-C | -5.31 | 1.47 | 1.52 |
| 2 | G | 148 | PHE | C-O | 5.31 | 1.30 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 294 | HIS | CA-C | 5.31 | 1.59 | 1.52 |
| 2 | H | 189 | VAL | CA-CB | 5.31 | 1.60 | 1.54 |
| 2 | C | 318 | LEU | CA-CB | -5.31 | 1.45 | 1.53 |
| 3 | L | 96 | LYS | N-CA | 5.31 | 1.53 | 1.46 |
| 3 | M | 64 | ASP | C-N | 5.31 | 1.41 | 1.33 |
| 2 | Q | 214 | TRP | C-N | 5.31 | 1.40 | 1.33 |
| 2 | Q | 341 | SER | CA-C | 5.31 | 1.59 | 1.52 |
| 1 | B | 294 | ASP | C-O | -5.30 | 1.17 | 1.24 |
| 2 | I | 224 | ALA | C-O | -5.30 | 1.18 | 1.24 |
| 2 | R | 121 | VAL | CA-CB | 5.30 | 1.61 | 1.54 |
| 2 | R | 177 | LYS | C-O | -5.30 | 1.17 | 1.24 |
| 1 | B | 291 | LEU | C-N | 5.30 | 1.41 | 1.33 |
| 2 | G | 422 | VAL | C-O | -5.30 | 1.18 | 1.24 |
| 2 | Q | 263 | PRO | C-O | -5.30 | 1.17 | 1.24 |
| 2 | I | 211 | PHE | N-CA | -5.30 | 1.39 | 1.46 |
| 1 | F | 291 | LEU | C-N | -5.30 | 1.28 | 1.33 |
| 2 | G | 236 | LYS | CA-C | -5.30 | 1.45 | 1.53 |
| 1 | T | 261 | CYS | C-N | 5.30 | 1.41 | 1.33 |
| 2 | H | 31 | PRO | C-O | -5.30 | 1.17 | 1.23 |
| 2 | H | 207 | ASN | C-N | 5.30 | 1.43 | 1.34 |
| 2 | J | 212 | GLN | CA-C | 5.30 | 1.58 | 1.53 |
| 2 | G | 75 | THR | C-N | -5.29 | 1.26 | 1.33 |
| 2 | S | 296 | ALA | CA-C | 5.29 | 1.60 | 1.53 |
| 2 | J | 223 | ASP | CA-C | 5.29 | 1.59 | 1.52 |
| 2 | C | 146 | LYS | CA-C | -5.29 | 1.45 | 1.52 |
| 3 | P | 100 | THR | CA-C | 5.29 | 1.60 | 1.52 |
| 2 | R | 253 | ARG | N-CA | 5.29 | 1.52 | 1.46 |
| 2 | S | 460 | ASP | C-N | 5.29 | 1.40 | 1.33 |
| 2 | R | 224 | ALA | CA-C | 5.29 | 1.59 | 1.52 |
| 2 | C | 430 | ALA | C-O | -5.29 | 1.18 | 1.24 |
| 2 | J | 160 | ASP | CA-C | -5.29 | 1.46 | 1.52 |
| 2 | J | 363 | PHE | CA-C | 5.29 | 1.60 | 1.52 |
| 2 | J | 235 | ILE | CA-C | -5.29 | 1.46 | 1.52 |
| 2 | C | 167 | ARG | C-N | 5.29 | 1.39 | 1.33 |
| 2 | G | 289 | VAL | C-N | -5.29 | 1.26 | 1.33 |
| 2 | Q | 181 | SER | CA-C | -5.29 | 1.46 | 1.52 |
| 2 | Q | 207 | ASN | N-CA | -5.29 | 1.40 | 1.46 |
| 2 | C | 177 | LYS | CA-C | 5.28 | 1.59 | 1.52 |
| 2 | C | 327 | HIS | CG-CD2 | -5.28 | 1.30 | 1.35 |
| 2 | I | 212 | GLN | C-N | 5.28 | 1.41 | 1.33 |
| 2 | C | 137 | ASP | CA-C | 5.28 | 1.58 | 1.52 |
| 3 | O | 40 | PRO | C-O | 5.28 | 1.30 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | O | 54 | TYR | CA-C | -5.28 | 1.46 | 1.52 |
| 2 | R | 285 | ARG | N-CA | -5.28 | 1.40 | 1.46 |
| 1 | T | 239 | GLN | C-N | 5.28 | 1.39 | 1.33 |
| 3 | E | 60 | LEU | C-N | -5.28 | 1.27 | 1.33 |
| 2 | C | 113 | VAL | CA-C | 5.28 | 1.59 | 1.52 |
| 2 | R | 293 | ILE | C-N | -5.28 | 1.26 | 1.33 |
| 2 | C | 460 | ASP | CA-C | 5.28 | 1.60 | 1.52 |
| 2 | G | 278 | THR | C-N | -5.28 | 1.26 | 1.33 |
| 2 | H | 41 | ARG | CA-C | -5.28 | 1.46 | 1.52 |
| 2 | I | 175 | LYS | CA-CB | -5.28 | 1.47 | 1.54 |
| 3 | M | 101 | VAL | C-O | 5.28 | 1.29 | 1.24 |
| 3 | N | 31 | GLU | C-N | 5.28 | 1.40 | 1.33 |
| 2 | G | 180 | LEU | CA-C | -5.27 | 1.46 | 1.52 |
| 2 | H | 83 | LYS | C-O | -5.27 | 1.17 | 1.24 |
| 2 | Q | 71 | THR | CA-C | 5.27 | 1.60 | 1.52 |
| 3 | L | 94 | ASN | C-N | 5.27 | 1.40 | 1.33 |
| 2 | Q | 58 | ALA | N-CA | 5.27 | 1.52 | 1.46 |
| 2 | R | 263 | PRO | C-O | -5.27 | 1.17 | 1.24 |
| 2 | R | 426 | ALA | C-O | -5.27 | 1.18 | 1.24 |
| 2 | I | 317 | CYS | CA-C | -5.27 | 1.46 | 1.52 |
| 2 | J | 117 | LEU | N-CA | -5.27 | 1.40 | 1.46 |
| 3 | O | 72 | LEU | CA-C | -5.27 | 1.45 | 1.52 |
| 2 | R | 439 | ARG | N-CA | 5.27 | 1.53 | 1.46 |
| 2 | G | 383 | HIS | CG-CD2 | 5.27 | 1.41 | 1.35 |
| 2 | Q | 209 | GLN | N-CA | 5.27 | 1.53 | 1.46 |
| 1 | A | 236 | LEU | C-O | 5.26 | 1.30 | 1.24 |
| 2 | C | 138 | ILE | CA-C | 5.26 | 1.58 | 1.52 |
| 2 | G | 69 | VAL | CA-C | 5.26 | 1.58 | 1.52 |
| 2 | J | 455 | LEU | C-N | -5.26 | 1.27 | 1.33 |
| 3 | K | 55 | TRP | CA-CB | -5.26 | 1.45 | 1.54 |
| 3 | O | 16 | SER | CA-C | 5.26 | 1.59 | 1.52 |
| 2 | R | 32 | LYS | N-CA | 5.26 | 1.52 | 1.46 |
| 2 | S | 297 | MET | SD-CE | 5.26 | 1.92 | 1.79 |
| 3 | D | 79 | ARG | NE-CZ | -5.26 | 1.27 | 1.33 |
| 2 | I | 50 | ALA | CA-C | -5.26 | 1.46 | 1.52 |
| 2 | C | 37 | LEU | CA-C | -5.25 | 1.46 | 1.52 |
| 2 | G | 50 | ALA | CA-C | 5.25 | 1.59 | 1.52 |
| 2 | G | 399 | VAL | CA-CB | -5.25 | 1.47 | 1.54 |
| 3 | O | 47 | HIS | ND1-CE1 | 5.25 | 1.37 | 1.32 |
| 3 | P | 65 | CYS | C-N | -5.25 | 1.25 | 1.33 |
| 2 | S | 279 | THR | C-N | -5.25 | 1.26 | 1.33 |
| 2 | H | 163 | ASN | C-O | -5.25 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 99 | ALA | C-O | -5.25 | 1.17 | 1.24 |
| 2 | R | 442 | GLY | C-N | 5.25 | 1.40 | 1.33 |
| 2 | S | 181 | SER | C-O | -5.25 | 1.17 | 1.23 |
| 1 | F | 268 | ASN | C-N | 5.25 | 1.40 | 1.33 |
| 3 | P | 60 | LEU | C-N | 5.25 | 1.40 | 1.33 |
| 2 | Q | 137 | ASP | C-O | -5.25 | 1.17 | 1.23 |
| 2 | R | 73 | LEU | CB-CG | -5.25 | 1.43 | 1.53 |
| 2 | Q | 114 | THR | C-O | 5.25 | 1.30 | 1.24 |
| 2 | G | 243 | THR | CA-C | 5.24 | 1.59 | 1.52 |
| 2 | Q | 123 | ASN | CA-C | 5.24 | 1.59 | 1.52 |
| 2 | G | 187 | ARG | N-CA | 5.24 | 1.52 | 1.46 |
| 3 | E | 13 | GLU | CA-C | -5.24 | 1.45 | 1.52 |
| 3 | L | 21 | LEU | CA-C | -5.24 | 1.46 | 1.52 |
| 3 | O | 58 | TRP | C-O | -5.24 | 1.15 | 1.23 |
| 2 | R | 286 | ASP | CA-C | -5.24 | 1.45 | 1.52 |
| 2 | S | 132 | SER | N-CA | -5.24 | 1.39 | 1.46 |
| 3 | D | 29 | GLN | CA-C | 5.24 | 1.59 | 1.52 |
| 2 | I | 419 | ALA | N-CA | -5.24 | 1.40 | 1.46 |
| 3 | N | 101 | VAL | C-O | 5.24 | 1.29 | 1.24 |
| 2 | G | 133 | LEU | C-O | 5.24 | 1.30 | 1.23 |
| 2 | H | 294 | HIS | N-CA | -5.24 | 1.39 | 1.45 |
| 2 | I | 247 | CYS | CA-C | 5.24 | 1.60 | 1.52 |
| 3 | N | 68 | PRO | CA-CB | -5.24 | 1.46 | 1.53 |
| 2 | R | 283 | TRP | C-N | -5.24 | 1.27 | 1.33 |
| 2 | R | 458 | ALA | C-N | 5.24 | 1.41 | 1.34 |
| 2 | S | 96 | SER | C-O | 5.24 | 1.30 | 1.23 |
| 1 | B | 225 | LEU | C-N | 5.23 | 1.40 | 1.33 |
| 2 | C | 293 | ILE | N-CA | -5.23 | 1.40 | 1.46 |
| 2 | Q | 212 | GLN | CA-C | -5.23 | 1.46 | 1.52 |
| 2 | S | 105 | LEU | C-O | 5.23 | 1.30 | 1.24 |
| 2 | I | 209 | GLN | CA-C | 5.23 | 1.58 | 1.53 |
| 2 | I | 220 | PHE | C-O | -5.23 | 1.18 | 1.24 |
| 2 | S | 107 | LEU | CA-C | 5.23 | 1.60 | 1.52 |
| 1 | T | 229 | VAL | C-N | -5.23 | 1.27 | 1.33 |
| 3 | M | 104 | ILE | C-N | -5.23 | 1.27 | 1.33 |
| 3 | N | 86 | TYR | CA-C | 5.23 | 1.59 | 1.52 |
| 1 | T | 280 | LEU | C-N | -5.23 | 1.27 | 1.33 |
| 2 | C | 347 | ASP | N-CA | -5.23 | 1.40 | 1.46 |
| 3 | N | 33 | MET | SD-CE | -5.23 | 1.66 | 1.79 |
| 2 | R | 187 | ARG | NE-CZ | -5.23 | 1.27 | 1.33 |
| 2 | Q | 305 | ARG | CD-NE | 5.23 | 1.53 | 1.46 |
| 2 | R | 244 | ALA | CA-C | 5.23 | 1.57 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 262 | ALA | C-N | 5.22 | 1.40 | 1.33 |
| 2 | I | 388 | PRO | CA-C | 5.22 | 1.59 | 1.52 |
| 2 | R | 296 | ALA | C-N | 5.22 | 1.40 | 1.33 |
| 1 | T | 239 | GLN | CA-C | 5.22 | 1.60 | 1.52 |
| 2 | I | 349 | MET | C-O | -5.22 | 1.17 | 1.24 |
| 2 | Q | 425 | GLU | CA-C | 5.22 | 1.59 | 1.52 |
| 2 | G | 371 | MET | CA-C | 5.22 | 1.58 | 1.52 |
| 3 | L | 84 | ASP | C-N | -5.22 | 1.25 | 1.33 |
| 2 | C | 267 | HIS | CG-CD2 | 5.22 | 1.41 | 1.35 |
| 1 | F | 301 | VAL | N-CA | 5.22 | 1.52 | 1.46 |
| 2 | H | 212 | GLN | CD-NE2 | -5.22 | 1.22 | 1.33 |
| 2 | S | 221 | VAL | N-CA | 5.22 | 1.52 | 1.46 |
| 2 | I | 444 | ILE | C-N | -5.22 | 1.27 | 1.33 |
| 3 | P | 53 | PHE | C-O | 5.22 | 1.30 | 1.24 |
| 2 | R | 317 | CYS | N-CA | -5.22 | 1.40 | 1.46 |
| 2 | R | 433 | GLU | C-N | 5.22 | 1.41 | 1.33 |
| 2 | R | 440 | GLU | N-CA | -5.22 | 1.39 | 1.46 |
| 2 | S | 110 | GLU | N-CA | -5.22 | 1.39 | 1.46 |
| 2 | C | 91 | GLN | C-N | -5.21 | 1.26 | 1.33 |
| 2 | C | 217 | ARG | CD-NE | -5.21 | 1.39 | 1.46 |
| 2 | J | 190 | TYR | CA-C | -5.21 | 1.45 | 1.52 |
| 2 | Q | 338 | ASP | CG-OD1 | 5.21 | 1.35 | 1.25 |
| 2 | S | 26 | THR | CB-OG1 | 5.21 | 1.52 | 1.43 |
| 2 | S | 360 | ARG | CA-C | 5.21 | 1.60 | 1.52 |
| 1 | T | 250 | LYS | C-N | -5.21 | 1.27 | 1.33 |
| 2 | C | 118 | THR | CA-CB | 5.21 | 1.61 | 1.53 |
| 2 | I | 72 | ASP | C-O | 5.21 | 1.30 | 1.24 |
| 3 | M | 69 | GLN | C-O | -5.21 | 1.17 | 1.24 |
| 3 | N | 88 | ARG | N-CA | -5.21 | 1.39 | 1.45 |
| 2 | S | 231 | GLU | CA-C | -5.21 | 1.46 | 1.52 |
| 3 | K | 102 | SER | CA-C | -5.21 | 1.46 | 1.52 |
| 2 | I | 402 | PHE | CA-C | -5.21 | 1.46 | 1.52 |
| 3 | K | 38 | PHE | N-CA | 5.21 | 1.52 | 1.46 |
| 2 | C | 452 | SER | N-CA | -5.21 | 1.40 | 1.46 |
| 2 | G | 418 | THR | C-O | -5.21 | 1.18 | 1.24 |
| 3 | O | 36 | GLN | CA-C | 5.21 | 1.59 | 1.52 |
| 2 | R | 280 | LEU | C-N | 5.21 | 1.40 | 1.33 |
| 2 | C | 225 | ILE | N-CA | -5.20 | 1.40 | 1.46 |
| 2 | G | 250 | MET | CA-C | 5.20 | 1.59 | 1.52 |
| 3 | N | 79 | ARG | N-CA | 5.20 | 1.52 | 1.46 |
| 3 | D | 47 | HIS | CA-C | 5.20 | 1.60 | 1.53 |
| 3 | D | 84 | ASP | CA-CB | -5.20 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | N | 30 | ILE | CB-CG1 | 5.20 | 1.63 | 1.53 |
| 2 | Q | 389 | ALA | C-O | -5.20 | 1.18 | 1.24 |
| 3 | L | 13 | GLU | C-O | -5.20 | 1.18 | 1.24 |
| 2 | R | 134 | ARG | C-O | 5.20 | 1.30 | 1.23 |
| 2 | S | 385 | TRP | CA-C | 5.20 | 1.59 | 1.52 |
| 2 | J | 202 | ASP | C-O | 5.20 | 1.30 | 1.23 |
| 2 | R | 277 | ASN | C-N | -5.20 | 1.26 | 1.33 |
| 2 | C | 239 | TYR | N-CA | -5.20 | 1.40 | 1.46 |
| 2 | I | 389 | ALA | C-N | 5.20 | 1.41 | 1.33 |
| 3 | M | 57 | MET | CA-C | -5.20 | 1.46 | 1.52 |
| 2 | R | 87 | ILE | C-N | 5.19 | 1.40 | 1.33 |
| 2 | C | 305 | ARG | CA-C | 5.19 | 1.59 | 1.52 |
| 2 | H | 245 | PRO | CA-C | -5.19 | 1.44 | 1.52 |
| 2 | J | 105 | LEU | CB-CG | -5.19 | 1.43 | 1.53 |
| 2 | J | 444 | ILE | CA-CB | 5.19 | 1.60 | 1.54 |
| 3 | M | 17 | TYR | CA-C | 5.19 | 1.59 | 1.52 |
| 3 | O | 107 | ARG | C-O | -5.19 | 1.17 | 1.24 |
| 2 | C | 430 | ALA | CA-C | -5.19 | 1.46 | 1.52 |
| 3 | O | 11 | ARG | CA-C | 5.19 | 1.59 | 1.52 |
| 2 | R | 220 | PHE | CA-C | -5.19 | 1.46 | 1.52 |
| 2 | S | 442 | GLY | C-N | -5.19 | 1.27 | 1.33 |
| 2 | C | 72 | ASP | CA-CB | -5.19 | 1.45 | 1.53 |
| 2 | J | 240 | LEU | CG-CD1 | -5.19 | 1.35 | 1.52 |
| 2 | J | 359 | SER | CA-C | -5.19 | 1.45 | 1.52 |
| 3 | K | 34 | ILE | CB-CG1 | 5.19 | 1.63 | 1.53 |
| 1 | T | 259 | GLN | C-O | -5.19 | 1.17 | 1.24 |
| 3 | E | 94 | ASN | CA-CB | -5.19 | 1.44 | 1.53 |
| 3 | P | 54 | TYR | CA-C | 5.19 | 1.59 | 1.52 |
| 2 | I | 87 | ILE | C-N | 5.18 | 1.38 | 1.33 |
| 3 | L | 86 | TYR | N-CA | 5.18 | 1.52 | 1.45 |
| 3 | M | 75 | VAL | C-N | -5.18 | 1.27 | 1.33 |
| 2 | R | 159 | ARG | N-CA | -5.18 | 1.40 | 1.46 |
| 2 | G | 156 | GLN | CA-C | -5.18 | 1.46 | 1.52 |
| 2 | G | 205 | ASN | C-O | -5.18 | 1.17 | 1.24 |
| 2 | G | 240 | LEU | CA-CB | -5.18 | 1.45 | 1.53 |
| 3 | M | 40 | PRO | C-N | 5.18 | 1.41 | 1.33 |
| 2 | C | 130 | ILE | CA-CB | 5.18 | 1.60 | 1.54 |
| 2 | J | 71 | THR | N-CA | -5.18 | 1.39 | 1.46 |
| 3 | K | 15 | PHE | N-CA | -5.18 | 1.39 | 1.46 |
| 2 | G | 287 | ASN | CG-ND2 | -5.18 | 1.22 | 1.33 |
| 2 | I | 443 | ASP | CA-C | 5.18 | 1.59 | 1.52 |
| 2 | J | 113 | VAL | CA-C | -5.18 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 270 | LEU | C-O | 5.18 | 1.30 | 1.24 |
| 2 | J | 443 | ASP | C-N | -5.18 | 1.27 | 1.33 |
| 2 | R | 358 | ARG | C-N | 5.18 | 1.40 | 1.33 |
| 2 | C | 435 | ARG | CD-NE | -5.18 | 1.39 | 1.46 |
| 2 | G | 206 | ILE | CA-CB | 5.18 | 1.59 | 1.53 |
| 2 | R | 22 | LEU | CA-C | 5.18 | 1.59 | 1.52 |
| 2 | G | 207 | ASN | CG-ND2 | 5.18 | 1.44 | 1.33 |
| 2 | Q | 126 | GLY | N-CA | 5.18 | 1.51 | 1.45 |
| 2 | R | 459 | LEU | C-O | 5.18 | 1.30 | 1.24 |
| 1 | B | 229 | VAL | C-N | -5.17 | 1.27 | 1.33 |
| 2 | C | 382 | ILE | C-N | 5.17 | 1.41 | 1.33 |
| 2 | G | 267 | HIS | CE1-NE2 | -5.17 | 1.27 | 1.32 |
| 2 | G | 320 | LEU | C-N | -5.17 | 1.27 | 1.33 |
| 2 | G | 420 | ASN | N-CA | -5.17 | 1.40 | 1.46 |
| 2 | H | 357 | ASP | CA-C | -5.17 | 1.48 | 1.53 |
| 2 | I | 216 | ASP | CA-C | 5.17 | 1.59 | 1.52 |
| 2 | S | 423 | ALA | C-N | 5.17 | 1.40 | 1.33 |
| 2 | C | 394 | PHE | CA-C | -5.17 | 1.45 | 1.52 |
| 2 | G | 244 | ALA | CA-C | -5.17 | 1.46 | 1.52 |
| 1 | A | 247 | HIS | N-CA | -5.17 | 1.39 | 1.45 |
| 2 | G | 190 | TYR | CA-C | -5.17 | 1.45 | 1.52 |
| 2 | G | 235 | ILE | CA-C | -5.17 | 1.46 | 1.52 |
| 2 | I | 183 | LYS | CA-CB | 5.17 | 1.61 | 1.53 |
| 2 | R | 160 | ASP | N-CA | -5.17 | 1.40 | 1.46 |
| 2 | R | 278 | THR | N-CA | 5.17 | 1.52 | 1.46 |
| 1 | T | 306 | ILE | CA-CB | -5.17 | 1.48 | 1.54 |
| 2 | C | 341 | SER | C-O | -5.16 | 1.18 | 1.24 |
| 2 | J | 203 | ASP | C-O | 5.16 | 1.30 | 1.23 |
| 2 | R | 271 | THR | CA-C | 5.16 | 1.59 | 1.52 |
| 1 | B | 299 | SER | CA-C | -5.16 | 1.46 | 1.52 |
| 2 | R | 170 | LEU | N-CA | -5.16 | 1.39 | 1.46 |
| 2 | S | 46 | PRO | N-CA | 5.16 | 1.53 | 1.47 |
| 2 | H | 235 | ILE | CA-CB | 5.16 | 1.61 | 1.54 |
| 2 | S | 437 | LEU | CA-CB | -5.16 | 1.45 | 1.53 |
| 3 | E | 44 | PHE | CA-CB | 5.16 | 1.62 | 1.53 |
| 2 | I | 92 | GLY | C-N | 5.16 | 1.40 | 1.33 |
| 2 | S | 158 | GLU | C-N | -5.16 | 1.27 | 1.34 |
| 2 | S | 316 | LYS | CA-CB | 5.16 | 1.61 | 1.53 |
| 1 | A | 229 | VAL | N-CA | 5.15 | 1.52 | 1.46 |
| 1 | A | 286 | GLU | C-N | 5.15 | 1.40 | 1.33 |
| 3 | K | 15 | PHE | C-N | 5.15 | 1.40 | 1.34 |
| 2 | Q | 86 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 307 | HIS | C-O | 5.15 | 1.29 | 1.23 |
| 3 | K | 16 | SER | CA-C | -5.15 | 1.45 | 1.52 |
| 3 | M | 24 | ARG | CD-NE | 5.15 | 1.53 | 1.46 |
| 3 | N | 107 | ARG | CA-C | 5.15 | 1.57 | 1.52 |
| 3 | P | 46 | GLU | N-CA | -5.15 | 1.39 | 1.46 |
| 2 | R | 346 | VAL | C-O | 5.15 | 1.30 | 1.24 |
| 2 | H | 400 | LEU | CB-CG | -5.15 | 1.43 | 1.53 |
| 2 | R | 355 | GLU | CA-C | -5.15 | 1.46 | 1.52 |
| 2 | I | 101 | ILE | CA-CB | 5.15 | 1.61 | 1.54 |
| 2 | I | 129 | ALA | CA-C | -5.15 | 1.45 | 1.52 |
| 2 | R | 340 | ALA | C-O | -5.15 | 1.18 | 1.24 |
| 2 | I | 103 | TYR | C-N | -5.15 | 1.26 | 1.33 |
| 2 | G | 351 | GLU | C-N | -5.14 | 1.26 | 1.33 |
| 2 | I | 194 | ARG | NE-CZ | -5.14 | 1.27 | 1.33 |
| 2 | I | 340 | ALA | N-CA | -5.14 | 1.40 | 1.46 |
| 2 | C | 59 | ALA | CA-C | -5.14 | 1.46 | 1.52 |
| 2 | G | 321 | SER | CA-C | 5.14 | 1.59 | 1.52 |
| 2 | J | 93 | GLU | C-N | 5.14 | 1.41 | 1.33 |
| 2 | C | 425 | GLU | C-O | -5.14 | 1.18 | 1.24 |
| 2 | G | 352 | ASP | CA-CB | 5.14 | 1.61 | 1.53 |
| 2 | I | 338 | ASP | CG-OD1 | 5.14 | 1.35 | 1.25 |
| 2 | I | 432 | ASN | N-CA | -5.14 | 1.40 | 1.46 |
| 3 | L | 45 | ASN | C-N | -5.14 | 1.27 | 1.33 |
| 3 | O | 86 | TYR | CA-C | -5.14 | 1.46 | 1.52 |
| 2 | R | 416 | GLY | CA-C | 5.14 | 1.57 | 1.52 |
| 2 | G | 427 | CYS | CA-C | -5.14 | 1.46 | 1.52 |
| 2 | H | 33 | ASP | N-CA | -5.14 | 1.40 | 1.46 |
| 2 | R | 453 | PRO | C-N | 5.14 | 1.41 | 1.33 |
| 2 | S | 357 | ASP | CA-C | -5.14 | 1.47 | 1.53 |
| 3 | D | 79 | ARG | CA-CB | 5.13 | 1.61 | 1.53 |
| 2 | G | 52 | GLU | C-N | -5.13 | 1.27 | 1.33 |
| 3 | P | 79 | ARG | CA-C | 5.13 | 1.59 | 1.52 |
| 2 | S | 181 | SER | C-N | -5.13 | 1.27 | 1.33 |
| 2 | H | 422 | VAL | CA-C | -5.13 | 1.46 | 1.52 |
| 2 | Q | 76 | ASP | C-O | -5.13 | 1.17 | 1.23 |
| 2 | S | 130 | ILE | CA-C | -5.13 | 1.46 | 1.52 |
| 2 | I | 147 | THR | CA-C | 5.13 | 1.61 | 1.52 |
| 2 | J | 441 | GLY | C-O | 5.13 | 1.30 | 1.23 |
| 2 | H | 238 | HIS | C-N | 5.13 | 1.40 | 1.33 |
| 2 | C | 136 | GLU | C-N | 5.13 | 1.39 | 1.33 |
| 2 | C | 149 | GLN | C-N | 5.13 | 1.41 | 1.33 |
| 2 | I | 374 | VAL | CA-C | 5.13 | 1.58 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 303 | ARG | N-CA | -5.13 | 1.40 | 1.46 |
| 2 | C | 319 | ARG | CD-NE | 5.13 | 1.53 | 1.46 |
| 2 | G | 154 | GLY | N-CA | 5.13 | 1.50 | 1.45 |
| 2 | G | 293 | ILE | C-O | -5.13 | 1.18 | 1.24 |
| 2 | I | 229 | GLN | CA-C | -5.13 | 1.45 | 1.52 |
| 3 | M | 39 | HIS | CA-C | 5.13 | 1.59 | 1.52 |
| 2 | S | 55 | ALA | C-O | -5.13 | 1.18 | 1.24 |
| 1 | T | 249 | ASP | C-N | -5.13 | 1.27 | 1.33 |
| 3 | L | 53 | PHE | C-O | 5.12 | 1.30 | 1.24 |
| 1 | B | 227 | SER | C-O | -5.12 | 1.18 | 1.24 |
| 1 | F | 264 | ILE | CA-C | -5.12 | 1.47 | 1.53 |
| 2 | I | 383 | HIS | CA-CB | 5.12 | 1.61 | 1.53 |
| 2 | J | 168 | PRO | C-O | -5.12 | 1.17 | 1.24 |
| 3 | L | 13 | GLU | CA-C | -5.12 | 1.46 | 1.52 |
| 2 | I | 53 | ALA | CA-C | 5.12 | 1.59 | 1.52 |
| 2 | I | 57 | ILE | C-N | -5.12 | 1.27 | 1.33 |
| 2 | I | 156 | GLN | C-O | -5.12 | 1.18 | 1.24 |
| 2 | Q | 242 | VAL | C-N | 5.12 | 1.40 | 1.33 |
| 2 | Q | 438 | TYR | C-N | -5.12 | 1.27 | 1.33 |
| 2 | H | 26 | THR | CA-CB | -5.12 | 1.47 | 1.53 |
| 2 | H | 325 | HIS | CE1-NE2 | -5.12 | 1.27 | 1.32 |
| 3 | M | 74 | GLU | C-N | 5.12 | 1.40 | 1.33 |
| 2 | G | 175 | LYS | CA-C | -5.12 | 1.46 | 1.52 |
| 2 | I | 249 | GLU | CA-C | -5.12 | 1.45 | 1.52 |
| 3 | M | 72 | LEU | CA-C | -5.12 | 1.46 | 1.52 |
| 2 | R | 184 | ASN | CA-C | -5.12 | 1.46 | 1.52 |
| 2 | S | 362 | VAL | CA-CB | 5.12 | 1.59 | 1.53 |
| 2 | S | 431 | ARG | CA-C | -5.12 | 1.46 | 1.52 |
| 3 | E | 93 | ASP | CA-CB | -5.12 | 1.46 | 1.52 |
| 2 | G | 391 | VAL | C-N | -5.12 | 1.27 | 1.33 |
| 2 | J | 213 | ARG | C-N | 5.12 | 1.40 | 1.33 |
| 2 | Q | 187 | ARG | CA-CB | 5.12 | 1.61 | 1.53 |
| 2 | R | 120 | ILE | C-N | 5.12 | 1.40 | 1.33 |
| 2 | G | 319 | ARG | CA-CB | 5.11 | 1.61 | 1.53 |
| 2 | H | 48 | VAL | CA-CB | -5.11 | 1.47 | 1.54 |
| 2 | H | 59 | ALA | C-O | -5.11 | 1.18 | 1.24 |
| 2 | H | 362 | VAL | C-N | -5.11 | 1.26 | 1.33 |
| 2 | Q | 121 | VAL | C-N | 5.11 | 1.40 | 1.33 |
| 2 | Q | 168 | PRO | N-CA | 5.11 | 1.52 | 1.47 |
| 2 | R | 298 | HIS | N-CA | 5.11 | 1.52 | 1.46 |
| 2 | G | 229 | GLN | N-CA | -5.11 | 1.40 | 1.46 |
| 2 | S | 134 | ARG | CA-CB | 5.11 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 250 | LYS | C-O | -5.11 | 1.18 | 1.24 |
| 2 | C | 21 | LYS | C-O | -5.11 | 1.18 | 1.24 |
| 2 | G | 293 | ILE | N-CA | -5.11 | 1.40 | 1.46 |
| 2 | J | 34 | THR | CA-C | 5.11 | 1.59 | 1.52 |
| 3 | L | 32 | TYR | CA-C | 5.11 | 1.59 | 1.52 |
| 2 | Q | 401 | GLN | CA-C | 5.11 | 1.58 | 1.52 |
| 2 | S | 108 | PHE | C-N | 5.11 | 1.40 | 1.33 |
| 2 | C | 166 | GLY | C-O | -5.11 | 1.17 | 1.23 |
| 2 | G | 119 | SER | C-O | 5.11 | 1.30 | 1.24 |
| 3 | M | 63 | PHE | C-N | 5.11 | 1.40 | 1.33 |
| 3 | P | 89 | VAL | N-CA | -5.11 | 1.40 | 1.46 |
| 1 | T | 244 | GLY | N-CA | -5.11 | 1.39 | 1.45 |
| 2 | J | 318 | LEU | CA-C | -5.11 | 1.46 | 1.52 |
| 3 | M | 93 | ASP | N-CA | -5.11 | 1.39 | 1.46 |
| 3 | O | 10 | ARG | C-O | -5.11 | 1.17 | 1.23 |
| 2 | Q | 83 | LYS | CA-CB | -5.11 | 1.46 | 1.53 |
| 2 | R | 367 | ASP | C-N | -5.11 | 1.26 | 1.33 |
| 2 | C | 249 | GLU | CA-C | -5.11 | 1.46 | 1.52 |
| 2 | J | 35 | ASP | C-N | 5.11 | 1.40 | 1.33 |
| 2 | Q | 444 | ILE | CB-CG1 | 5.11 | 1.63 | 1.53 |
| 2 | S | 153 | HIS | CG-ND1 | -5.11 | 1.32 | 1.38 |
| 3 | D | 88 | ARG | CA-C | -5.10 | 1.46 | 1.52 |
| 2 | H | 299 | ALA | C-O | -5.10 | 1.17 | 1.24 |
| 2 | H | 307 | HIS | ND1-CE1 | -5.10 | 1.27 | 1.32 |
| 2 | I | 313 | VAL | C-N | -5.10 | 1.27 | 1.33 |
| 3 | P | 94 | ASN | C-N | -5.10 | 1.27 | 1.33 |
| 2 | Q | 267 | HIS | CA-C | 5.10 | 1.58 | 1.52 |
| 2 | R | 134 | ARG | C-N | -5.10 | 1.26 | 1.33 |
| 2 | R | 148 | PHE | C-O | -5.10 | 1.17 | 1.23 |
| 2 | S | 106 | ASP | CA-C | 5.10 | 1.59 | 1.52 |
| 3 | E | 94 | ASN | N-CA | -5.10 | 1.40 | 1.46 |
| 2 | J | 330 | THR | C-N | -5.10 | 1.26 | 1.33 |
| 3 | M | 13 | GLU | C-O | -5.10 | 1.18 | 1.24 |
| 2 | C | 299 | ALA | CA-C | -5.10 | 1.45 | 1.52 |
| 2 | G | 283 | TRP | C-O | -5.10 | 1.18 | 1.24 |
| 2 | I | 109 | GLU | C-O | -5.10 | 1.17 | 1.23 |
| 2 | G | 245 | PRO | CA-CB | -5.10 | 1.46 | 1.53 |
| 2 | I | 58 | ALA | C-N | -5.10 | 1.27 | 1.33 |
| 3 | K | 24 | ARG | CA-C | 5.10 | 1.59 | 1.52 |
| 3 | L | 35 | GLU | N-CA | -5.10 | 1.39 | 1.46 |
| 2 | S | 24 | TYR | N-CA | 5.10 | 1.52 | 1.46 |
| 2 | S | 327 | HIS | CD2-NE2 | 5.10 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | S | 435 | ARG | CA-CB | 5.10 | 1.61 | 1.53 |
| 2 | G | 48 | VAL | CA-C | 5.10 | 1.57 | 1.53 |
| 1 | A | 267 | THR | CA-C | 5.09 | 1.59 | 1.52 |
| 2 | H | 184 | ASN | C-N | -5.09 | 1.26 | 1.33 |
| 3 | M | 30 | ILE | CA-CB | -5.09 | 1.48 | 1.54 |
| 2 | C | 59 | ALA | C-O | -5.09 | 1.18 | 1.24 |
| 2 | G | 449 | GLY | C-N | 5.09 | 1.40 | 1.34 |
| 2 | I | 152 | PRO | C-N | 5.09 | 1.42 | 1.33 |
| 2 | I | 423 | ALA | CA-C | -5.09 | 1.46 | 1.52 |
| 3 | K | 32 | TYR | N-CA | 5.09 | 1.52 | 1.46 |
| 1 | T | 302 | PHE | N-CA | -5.09 | 1.39 | 1.45 |
| 3 | D | 80 | SER | C-N | 5.09 | 1.41 | 1.33 |
| 2 | G | 222 | ALA | C-N | -5.09 | 1.27 | 1.33 |
| 2 | H | 453 | PRO | N-CA | 5.09 | 1.54 | 1.47 |
| 2 | I | 432 | ASN | C-N | 5.09 | 1.41 | 1.33 |
| 2 | J | 295 | ARG | CD-NE | 5.09 | 1.53 | 1.46 |
| 3 | N | 102 | SER | CA-C | 5.09 | 1.58 | 1.52 |
| 2 | S | 209 | GLN | CD-NE2 | -5.09 | 1.22 | 1.33 |
| 3 | O | 96 | LYS | N-CA | -5.09 | 1.39 | 1.46 |
| 2 | C | 169 | MET | SD-CE | 5.09 | 1.92 | 1.79 |
| 2 | C | 423 | ALA | CA-C | -5.09 | 1.46 | 1.52 |
| 2 | C | 454 | GLU | CA-CB | -5.09 | 1.45 | 1.53 |
| 2 | G | 217 | ARG | CA-C | -5.09 | 1.46 | 1.52 |
| 3 | K | 13 | GLU | CA-C | -5.09 | 1.46 | 1.52 |
| 2 | C | 226 | HIS | N-CA | -5.08 | 1.40 | 1.46 |
| 3 | M | 99 | GLN | CA-C | -5.08 | 1.46 | 1.52 |
| 3 | D | 56 | THR | C-O | -5.08 | 1.18 | 1.23 |
| 2 | I | 453 | PRO | CA-C | -5.08 | 1.45 | 1.52 |
| 2 | G | 235 | ILE | CB-CG1 | 5.08 | 1.63 | 1.53 |
| 2 | I | 316 | LYS | C-O | -5.08 | 1.18 | 1.24 |
| 2 | J | 265 | ILE | C-N | 5.08 | 1.40 | 1.33 |
| 2 | Q | 57 | ILE | CA-CB | 5.08 | 1.60 | 1.54 |
| 3 | E | 66 | LYS | C-N | 5.08 | 1.39 | 1.33 |
| 2 | H | 434 | GLY | C-N | -5.08 | 1.26 | 1.33 |
| 2 | S | 384 | VAL | C-O | -5.08 | 1.18 | 1.24 |
| 2 | I | 285 | ARG | CA-C | 5.08 | 1.59 | 1.52 |
| 2 | I | 387 | MET | CA-C | 5.08 | 1.59 | 1.52 |
| 2 | J | 400 | LEU | C-O | -5.08 | 1.17 | 1.23 |
| 2 | Q | 84 | CYS | CA-C | -5.08 | 1.46 | 1.52 |
| 2 | H | 129 | ALA | CA-CB | -5.07 | 1.45 | 1.53 |
| 2 | I | 254 | ALA | C-O | 5.07 | 1.30 | 1.24 |
| 3 | K | 9 | GLU | C-N | 5.07 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | R | 372 | PRO | C-N | 5.07 | 1.40 | 1.33 |
| 2 | I | 29 | TYR | CA-C | -5.07 | 1.46 | 1.52 |
| 2 | S | 123 | ASN | C-O | -5.07 | 1.17 | 1.24 |
| 2 | G | 184 | ASN | CA-C | 5.07 | 1.59 | 1.52 |
| 2 | G | 428 | VAL | CA-C | -5.07 | 1.46 | 1.52 |
| 2 | H | 163 | ASN | CA-C | 5.07 | 1.60 | 1.53 |
| 2 | I | 146 | LYS | C-O | 5.07 | 1.30 | 1.24 |
| 2 | I | 213 | ARG | CA-C | 5.07 | 1.59 | 1.52 |
| 3 | L | 31 | GLU | C-O | -5.07 | 1.18 | 1.24 |
| 3 | L | 104 | ILE | C-N | 5.07 | 1.38 | 1.33 |
| 2 | Q | 340 | ALA | CA-C | 5.07 | 1.59 | 1.52 |
| 1 | A | 277 | GLU | N-CA | -5.06 | 1.40 | 1.46 |
| 2 | C | 168 | PRO | N-CA | -5.06 | 1.41 | 1.47 |
| 2 | I | 378 | ALA | CA-CB | -5.06 | 1.45 | 1.53 |
| 3 | N | 92 | PHE | N-CA | -5.06 | 1.40 | 1.46 |
| 2 | R | 48 | VAL | C-O | 5.06 | 1.31 | 1.24 |
| 2 | S | 371 | MET | SD-CE | -5.06 | 1.66 | 1.79 |
| 2 | J | 265 | ILE | CA-C | -5.06 | 1.46 | 1.52 |
| 2 | R | 108 | PHE | C-O | -5.06 | 1.17 | 1.24 |
| 2 | I | 118 | THR | CA-C | 5.06 | 1.59 | 1.52 |
| 3 | P | 40 | PRO | CA-C | 5.06 | 1.58 | 1.52 |
| 2 | Q | 253 | ARG | CA-CB | -5.06 | 1.45 | 1.53 |
| 2 | C | 198 | ASP | C-N | 5.06 | 1.40 | 1.33 |
| 3 | D | 83 | GLY | C-N | 5.06 | 1.40 | 1.33 |
| 2 | G | 302 | ASP | CA-C | -5.06 | 1.45 | 1.52 |
| 2 | R | 436 | ASP | CA-CB | -5.06 | 1.45 | 1.53 |
| 2 | S | 43 | SER | C-N | -5.06 | 1.27 | 1.33 |
| 3 | E | 86 | TYR | CA-C | -5.06 | 1.45 | 1.53 |
| 2 | Q | 171 | GLY | C-O | -5.06 | 1.17 | 1.23 |
| 2 | R | 398 | SER | N-CA | -5.06 | 1.40 | 1.46 |
| 2 | S | 58 | ALA | CA-C | -5.06 | 1.46 | 1.52 |
| 2 | C | 134 | ARG | N-CA | -5.05 | 1.39 | 1.45 |
| 2 | H | 260 | LEU | CA-C | -5.05 | 1.45 | 1.52 |
| 2 | C | 87 | ILE | C-O | -5.05 | 1.18 | 1.24 |
| 2 | I | 372 | PRO | CA-CB | 5.05 | 1.60 | 1.53 |
| 2 | S | 33 | ASP | CA-CB | -5.05 | 1.44 | 1.53 |
| 2 | C | 86 | HIS | ND1-CE1 | -5.05 | 1.27 | 1.32 |
| 2 | H | 202 | ASP | CA-C | -5.05 | 1.46 | 1.53 |
| 2 | H | 380 | GLY | C-N | 5.05 | 1.40 | 1.33 |
| 2 | I | 53 | ALA | N-CA | -5.05 | 1.40 | 1.46 |
| 2 | Q | 132 | SER | CA-C | -5.05 | 1.47 | 1.53 |
| 2 | R | 37 | LEU | C-O | -5.05 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 307 | GLN | C-O | 5.05 | 1.29 | 1.23 |
| 2 | C | 359 | SER | C-O | 5.05 | 1.29 | 1.24 |
| 2 | J | 318 | LEU | C-N | -5.05 | 1.27 | 1.33 |
| 3 | L | 80 | SER | CA-C | -5.05 | 1.45 | 1.52 |
| 2 | S | 450 | LYS | CA-CB | 5.05 | 1.61 | 1.53 |
| 2 | C | 100 | PHE | C-N | 5.04 | 1.40 | 1.33 |
| 2 | H | 264 | ILE | CA-C | 5.04 | 1.58 | 1.52 |
| 2 | H | 285 | ARG | C-O | -5.04 | 1.18 | 1.24 |
| 2 | J | 419 | ALA | CA-CB | -5.04 | 1.45 | 1.53 |
| 2 | S | 170 | LEU | C-N | -5.04 | 1.26 | 1.33 |
| 2 | C | 206 | ILE | CB-CG1 | -5.04 | 1.43 | 1.53 |
| 2 | C | 321 | SER | CA-C | 5.04 | 1.59 | 1.52 |
| 2 | H | 342 | THR | N-CA | -5.04 | 1.40 | 1.46 |
| 2 | J | 325 | HIS | CE1-NE2 | -5.04 | 1.27 | 1.32 |
| 2 | R | 78 | ASP | N-CA | 5.04 | 1.52 | 1.46 |
| 2 | R | 278 | THR | C-N | 5.04 | 1.40 | 1.33 |
| 3 | D | 21 | LEU | C-N | 5.04 | 1.40 | 1.33 |
| 2 | G | 260 | LEU | N-CA | 5.04 | 1.52 | 1.46 |
| 2 | G | 214 | TRP | CA-C | 5.04 | 1.59 | 1.52 |
| 2 | G | 286 | ASP | C-N | 5.04 | 1.40 | 1.33 |
| 2 | J | 161 | LEU | CA-C | -5.04 | 1.46 | 1.52 |
| 2 | J | 258 | LYS | C-O | -5.04 | 1.17 | 1.24 |
| 2 | Q | 425 | GLU | C-N | 5.04 | 1.40 | 1.33 |
| 1 | B | 307 | GLN | C-N | -5.04 | 1.26 | 1.32 |
| 2 | G | 310 | HIS | C-O | 5.04 | 1.30 | 1.23 |
| 1 | F | 233 | VAL | N-CA | -5.03 | 1.40 | 1.46 |
| 2 | I | 363 | PHE | C-O | 5.03 | 1.30 | 1.24 |
| 3 | P | 9 | GLU | N-CA | -5.03 | 1.40 | 1.46 |
| 2 | G | 445 | LEU | CB-CG | 5.03 | 1.63 | 1.53 |
| 2 | H | 347 | ASP | C-N | -5.03 | 1.27 | 1.34 |
| 2 | H | 356 | ALA | CA-CB | -5.03 | 1.45 | 1.53 |
| 2 | S | 452 | SER | N-CA | -5.03 | 1.41 | 1.46 |
| 3 | E | 67 | SER | N-CA | -5.03 | 1.39 | 1.45 |
| 2 | S | 80 | TYR | CA-CB | -5.03 | 1.46 | 1.53 |
| 2 | J | 326 | LEU | CA-C | -5.03 | 1.46 | 1.52 |
| 2 | G | 277 | ASN | CA-C | -5.03 | 1.46 | 1.52 |
| 2 | H | 74 | LEU | C-N | 5.03 | 1.41 | 1.33 |
| 3 | M | 22 | SER | C-N | 5.03 | 1.40 | 1.33 |
| 1 | B | 266 | SER | CA-C | -5.02 | 1.46 | 1.52 |
| 1 | F | 301 | VAL | CA-CB | 5.02 | 1.60 | 1.54 |
| 1 | F | 304 | ALA | N-CA | -5.02 | 1.40 | 1.46 |
| 2 | H | 37 | LEU | CA-C | -5.02 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 182 | ALA | CA-C | 5.02 | 1.59 | 1.52 |
| 2 | Q | 165 | TYR | CA-C | -5.02 | 1.46 | 1.52 |
| 3 | L | 31 | GLU | CA-CB | -5.02 | 1.45 | 1.53 |
| 3 | N | 65 | CYS | CA-C | 5.02 | 1.59 | 1.52 |
| 2 | Q | 30 | THR | N-CA | -5.02 | 1.40 | 1.46 |
| 2 | S | 306 | ASN | C-O | -5.02 | 1.17 | 1.23 |
| 3 | D | 91 | GLY | C-N | 5.02 | 1.40 | 1.33 |
| 2 | G | 325 | HIS | CA-CB | -5.02 | 1.45 | 1.54 |
| 2 | I | 387 | MET | N-CA | 5.02 | 1.51 | 1.46 |
| 2 | I | 86 | HIS | CB-CG | -5.02 | 1.43 | 1.50 |
| 2 | H | 347 | ASP | CG-OD1 | -5.01 | 1.15 | 1.25 |
| 2 | J | 284 | CYS | C-O | -5.01 | 1.18 | 1.24 |
| 3 | M | 25 | GLN | C-O | -5.01 | 1.17 | 1.24 |
| 2 | Q | 401 | GLN | C-O | 5.01 | 1.29 | 1.23 |
| 2 | R | 327 | HIS | ND1-CE1 | -5.01 | 1.27 | 1.32 |
| 3 | D | 56 | THR | CA-C | 5.01 | 1.59 | 1.53 |
| 2 | C | 379 | SER | CA-C | 5.01 | 1.59 | 1.53 |
| 2 | C | 437 | LEU | CA-CB | -5.01 | 1.45 | 1.53 |
| 2 | H | 212 | GLN | N-CA | -5.01 | 1.40 | 1.46 |
| 2 | J | 329 | GLY | C-O | -5.01 | 1.17 | 1.23 |
| 2 | J | 436 | ASP | C-O | -5.01 | 1.17 | 1.24 |
| 2 | R | 365 | THR | CA-C | -5.01 | 1.46 | 1.52 |
| 2 | G | 61 | SER | C-N | 5.01 | 1.40 | 1.33 |
| 3 | L | 24 | ARG | CD-NE | 5.01 | 1.53 | 1.46 |
| 3 | O | 72 | LEU | CB-CG | -5.01 | 1.43 | 1.53 |
| 2 | R | 22 | LEU | C-N | 5.01 | 1.40 | 1.33 |
| 2 | R | 317 | CYS | C-O | 5.01 | 1.29 | 1.24 |
| 2 | Q | 258 | LYS | CA-CB | -5.01 | 1.45 | 1.53 |
| 2 | Q | 391 | VAL | C-N | -5.01 | 1.27 | 1.33 |
| 2 | Q | 441 | GLY | C-O | -5.01 | 1.17 | 1.23 |
| 3 | E | 57 | MET | CA-C | -5.00 | 1.46 | 1.52 |
| 3 | E | 33 | MET | SD-CE | -5.00 | 1.67 | 1.79 |
| 2 | J | 310 | HIS | CA-C | -5.00 | 1.46 | 1.52 |
| 2 | S | 327 | HIS | CG-ND1 | -5.00 | 1.32 | 1.38 |
| 2 | C | 160 | ASP | C-O | -5.00 | 1.18 | 1.24 |
| 2 | J | 422 | VAL | C-N | -5.00 | 1.27 | 1.34 |
| 3 | L | 45 | ASN | CA-CB | 5.00 | 1.62 | 1.53 |
| 3 | L | 70 | GLN | C-O | -5.00 | 1.18 | 1.24 |
| 3 | N | 24 | ARG | N-CA | -5.00 | 1.40 | 1.46 |

All (2018) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 151 | PRO | CA-C-O | -13.89 | 109.75 | 120.73 |
| 2 | I | 444 | ILE | N-CA-C | -11.46 | 99.42 | 110.42 |
| 2 | G | 86 | HIS | CE1-NE2-CD2 | -11.22 | 97.78 | 109.00 |
| 2 | C | 253 | ARG | N-CA-C | -11.13 | 99.12 | 111.14 |
| 1 | B | 228 | GLU | N-CA-C | -11.10 | 99.26 | 111.36 |
| 2 | J | 256 | PHE | N-CA-C | -11.01 | 99.35 | 111.36 |
| 2 | R | 157 | VAL | N-CA-C | -10.98 | 99.63 | 110.72 |
| 3 | L | 19 | PRO | O-C-N | 10.80 | 126.28 | 121.31 |
| 2 | C | 151 | PRO | O-C-N | 10.79 | 126.22 | 121.15 |
| 3 | L | 97 | GLN | OE1-CD-NE2 | -10.78 | 111.82 | 122.60 |
| 2 | R | 229 | GLN | OE1-CD-NE2 | -10.75 | 111.85 | 122.60 |
| 1 | B | 271 | GLN | OE1-CD-NE2 | -10.73 | 111.87 | 122.60 |
| 2 | J | 212 | GLN | OE1-CD-NE2 | -10.69 | 111.92 | 122.60 |
| 3 | O | 92 | PHE | CA-CB-CG | -10.68 | 103.12 | 113.80 |
| 2 | Q | 52 | GLU | N-CA-C | -10.65 | 99.75 | 111.36 |
| 2 | J | 394 | PHE | CA-CB-CG | 10.65 | 124.45 | 113.80 |
| 2 | J | 185 | TYR | N-CA-C | -10.63 | 99.66 | 111.14 |
| 3 | D | 12 | PHE | CA-CB-CG | -10.51 | 103.29 | 113.80 |
| 2 | C | 184 | ASN | OD1-CG-ND2 | -10.49 | 112.11 | 122.60 |
| 3 | O | 97 | GLN | OE1-CD-NE2 | -10.47 | 112.13 | 122.60 |
| 2 | S | 106 | ASP | N-CA-C | -10.37 | 100.63 | 113.18 |
| 1 | A | 236 | LEU | N-CA-C | 10.32 | 122.11 | 111.07 |
| 3 | L | 45 | ASN | OD1-CG-ND2 | -10.26 | 112.34 | 122.60 |
| 2 | Q | 116 | ILE | N-CA-C | -10.25 | 100.79 | 110.42 |
| 2 | I | 231 | GLU | N-CA-C | 10.18 | 121.96 | 111.07 |
| 2 | J | 270 | LEU | N-CA-C | 10.11 | 121.89 | 111.07 |
| 2 | H | 432 | ASN | OD1-CG-ND2 | -10.07 | 112.53 | 122.60 |
| 1 | F | 228 | GLU | N-CA-C | -10.07 | 100.39 | 111.36 |
| 3 | D | 97 | GLN | OE1-CD-NE2 | -10.00 | 112.60 | 122.60 |
| 3 | E | 70 | GLN | N-CA-C | -9.99 | 100.47 | 111.36 |
| 2 | H | 277 | ASN | CA-CB-CG | 9.99 | 122.59 | 112.60 |
| 2 | G | 185 | TYR | N-CA-C | -9.97 | 99.24 | 111.40 |
| 2 | H | 198 | ASP | N-CA-C | -9.96 | 100.50 | 111.36 |
| 2 | C | 401 | GLN | OE1-CD-NE2 | -9.96 | 112.64 | 122.60 |
| 2 | H | 363 | PHE | CA-CB-CG | -9.94 | 103.86 | 113.80 |
| 2 | H | 352 | ASP | N-CA-C | -9.94 | 100.80 | 113.72 |
| 3 | M | 19 | PRO | O-C-N | 9.91 | 125.87 | 121.31 |
| 2 | J | 116 | ILE | N-CA-C | -9.91 | 100.72 | 110.72 |
| 2 | R | 298 | HIS | N-CA-C | -9.87 | 100.60 | 111.36 |
| 3 | L | 47 | HIS | CE1-NE2-CD2 | -9.85 | 99.16 | 109.00 |
| 2 | R | 343 | LEU | N-CA-C | -9.82 | 99.61 | 111.69 |
| 2 | C | 256 | PHE | N-CA-C | 9.81 | 122.89 | 111.11 |
| 3 | M | 19 | PRO | CA-C-O | -9.81 | 113.84 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 294 | HIS | CE1-NE2-CD2 | -9.81 | 99.19 | 109.00 |
| 2 | H | 185 | TYR | N-CA-C | -9.79 | 99.65 | 111.69 |
| 3 | N | 99 | GLN | OE1-CD-NE2 | -9.78 | 112.82 | 122.60 |
| 3 | K | 26 | ILE | N-CA-C | -9.78 | 100.65 | 110.62 |
| 3 | L | 31 | GLU | N-CA-C | -9.74 | 100.64 | 111.07 |
| 2 | H | 217 | ARG | N-CA-C | 9.70 | 123.06 | 111.33 |
| 3 | N | 53 | PHE | CA-CB-CG | -9.68 | 104.12 | 113.80 |
| 2 | S | 163 | ASN | OD1-CG-ND2 | -9.68 | 112.92 | 122.60 |
| 2 | I | 42 | PHE | CA-CB-CG | -9.64 | 104.16 | 113.80 |
| 2 | S | 294 | HIS | CG-CD2-NE2 | 9.64 | 116.84 | 107.20 |
| 2 | G | 292 | HIS | CB-CG-CD2 | -9.62 | 118.69 | 131.20 |
| 2 | Q | 432 | ASN | OD1-CG-ND2 | -9.60 | 113.00 | 122.60 |
| 1 | A | 239 | GLN | OE1-CD-NE2 | -9.59 | 113.01 | 122.60 |
| 2 | G | 45 | GLN | OE1-CD-NE2 | -9.58 | 113.02 | 122.60 |
| 3 | D | 99 | GLN | OE1-CD-NE2 | -9.53 | 113.07 | 122.60 |
| 2 | H | 229 | GLN | OE1-CD-NE2 | -9.53 | 113.07 | 122.60 |
| 3 | O | 63 | PHE | N-CA-C | -9.53 | 99.97 | 111.69 |
| 2 | C | 302 | ASP | CA-CB-CG | 9.49 | 122.09 | 112.60 |
| 3 | E | 18 | LEU | N-CA-C | -9.47 | 99.24 | 110.13 |
| 3 | M | 13 | GLU | CA-C-O | -9.46 | 110.78 | 120.90 |
| 2 | C | 277 | ASN | OD1-CG-ND2 | -9.44 | 113.16 | 122.60 |
| 2 | R | 209 | GLN | OE1-CD-NE2 | 9.39 | 132.00 | 122.60 |
| 2 | S | 238 | HIS | CB-CG-CD2 | -9.39 | 118.99 | 131.20 |
| 2 | J | 202 | ASP | CA-CB-CG | 9.39 | 121.99 | 112.60 |
| 2 | H | 160 | ASP | N-CA-C | 9.37 | 121.10 | 111.07 |
| 2 | R | 324 | ASP | CA-CB-CG | 9.37 | 121.97 | 112.60 |
| 2 | I | 115 | ASN | OD1-CG-ND2 | -9.36 | 113.24 | 122.60 |
| 2 | I | 417 | ALA | N-CA-C | -9.36 | 101.04 | 111.14 |
| 2 | J | 248 | GLU | N-CA-C | -9.34 | 101.06 | 111.14 |
| 2 | G | 348 | LEU | N-CA-C | 9.31 | 121.43 | 111.28 |
| 2 | Q | 294 | HIS | CG-CD2-NE2 | 9.31 | 116.51 | 107.20 |
| 2 | C | 425 | GLU | N-CA-C | 9.30 | 122.37 | 111.02 |
| 2 | I | 59 | ALA | CA-C-O | -9.30 | 111.05 | 120.82 |
| 2 | S | 118 | THR | N-CA-C | -9.30 | 101.15 | 111.28 |
| 2 | R | 161 | LEU | N-CA-C | 9.29 | 122.25 | 111.11 |
| 2 | H | 58 | ALA | N-CA-C | 9.28 | 122.24 | 111.11 |
| 2 | R | 216 | ASP | N-CA-C | -9.26 | 101.27 | 111.36 |
| 2 | S | 256 | PHE | N-CA-C | -9.26 | 101.08 | 111.82 |
| 2 | C | 86 | HIS | CE1-NE2-CD2 | -9.25 | 99.75 | 109.00 |
| 2 | H | 428 | VAL | N-CA-C | -9.23 | 101.35 | 110.30 |
| 3 | L | 19 | PRO | CA-C-O | -9.22 | 114.26 | 120.90 |
| 2 | G | 205 | ASN | N-CA-C | -9.21 | 101.30 | 112.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 238 | HIS | CB-CG-CD2 | -9.19 | 119.25 | 131.20 |
| 2 | Q | 345 | PHE | CA-CB-CG | 9.19 | 122.99 | 113.80 |
| 2 | I | 103 | TYR | CA-C-O | -9.18 | 112.43 | 119.59 |
| 2 | G | 394 | PHE | N-CA-C | 9.17 | 123.07 | 111.24 |
| 2 | G | 432 | ASN | CA-CB-CG | 9.16 | 121.76 | 112.60 |
| 2 | G | 256 | PHE | N-CA-C | -9.15 | 100.70 | 112.23 |
| 2 | H | 417 | ALA | N-CA-C | -9.13 | 101.28 | 111.14 |
| 2 | J | 427 | CYS | N-CA-C | 9.12 | 120.83 | 111.07 |
| 3 | O | 54 | TYR | CA-C-O | -9.12 | 110.86 | 121.16 |
| 2 | S | 268 | ASP | N-CA-C | 9.11 | 122.27 | 109.15 |
| 2 | C | 220 | PHE | N-CA-C | 9.10 | 120.81 | 111.07 |
| 2 | I | 217 | ARG | N-CA-C | -9.10 | 101.33 | 111.07 |
| 2 | H | 287 | ASN | OD1-CG-ND2 | -9.10 | 113.50 | 122.60 |
| 3 | O | 63 | PHE | CA-CB-CG | -9.07 | 104.73 | 113.80 |
| 2 | S | 306 | ASN | OD1-CG-ND2 | -9.07 | 113.53 | 122.60 |
| 3 | D | 69 | GLN | N-CA-C | 9.06 | 122.33 | 111.82 |
| 2 | R | 77 | MET | N-CA-C | -9.05 | 100.25 | 111.11 |
| 2 | H | 420 | ASN | N-CA-C | -9.05 | 101.50 | 111.36 |
| 3 | L | 47 | HIS | ND1-CE1-NE2 | 9.04 | 117.44 | 108.40 |
| 2 | R | 121 | VAL | CA-C-N | 9.04 | 129.97 | 119.94 |
| 2 | R | 121 | VAL | C-N-CA | 9.04 | 129.97 | 119.94 |
| 2 | Q | 298 | HIS | N-CA-C | -9.03 | 101.52 | 111.36 |
| 2 | I | 98 | PHE | CA-CB-CG | -9.01 | 104.79 | 113.80 |
| 2 | I | 223 | ASP | N-CA-C | -9.01 | 101.55 | 111.36 |
| 3 | K | 25 | GLN | OE1-CD-NE2 | -8.98 | 113.62 | 122.60 |
| 1 | F | 253 | PHE | N-CA-C | 8.97 | 121.06 | 111.28 |
| 2 | H | 226 | HIS | CE1-NE2-CD2 | -8.96 | 100.04 | 109.00 |
| 2 | H | 95 | ASN | OD1-CG-ND2 | -8.95 | 113.65 | 122.60 |
| 2 | Q | 142 | VAL | N-CA-C | 8.94 | 119.75 | 110.36 |
| 2 | J | 438 | TYR | N-CA-C | 8.92 | 121.90 | 111.02 |
| 3 | L | 49 | ASN | OD1-CG-ND2 | -8.91 | 113.69 | 122.60 |
| 2 | S | 185 | TYR | N-CA-C | -8.91 | 99.21 | 112.04 |
| 2 | S | 438 | TYR | N-CA-C | 8.90 | 121.79 | 111.11 |
| 2 | C | 277 | ASN | N-CA-C | 8.88 | 120.58 | 111.07 |
| 2 | H | 347 | ASP | N-CA-C | 8.87 | 122.06 | 111.33 |
| 2 | C | 342 | THR | N-CA-C | -8.87 | 101.58 | 111.07 |
| 2 | S | 216 | ASP | N-CA-C | -8.85 | 100.81 | 111.69 |
| 2 | H | 193 | LEU | N-CA-C | 8.84 | 120.53 | 111.07 |
| 2 | C | 327 | HIS | CE1-NE2-CD2 | -8.83 | 100.17 | 109.00 |
| 2 | Q | 127 | PHE | CA-CB-CG | -8.83 | 104.97 | 113.80 |
| 2 | S | 51 | ASP | N-CA-C | 8.81 | 120.88 | 111.28 |
| 3 | M | 29 | GLN | OE1-CD-NE2 | -8.81 | 113.79 | 122.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 437 | LEU | N-CA-C | 8.79 | 120.86 | 111.28 |
| 2 | Q | 187 | ARG | N-CA-C | -8.77 | 100.70 | 111.40 |
| 2 | Q | 277 | ASN | N-CA-C | -8.77 | 101.80 | 111.36 |
| 2 | I | 212 | GLN | OE1-CD-NE2 | -8.76 | 113.84 | 122.60 |
| 2 | I | 35 | ASP | N-CA-C | 8.74 | 122.07 | 110.53 |
| 2 | J | 53 | ALA | N-CA-C | -8.72 | 101.47 | 110.97 |
| 2 | H | 367 | ASP | CA-CB-CG | 8.71 | 121.31 | 112.60 |
| 2 | S | 447 | GLU | N-CA-C | -8.71 | 101.86 | 111.36 |
| 2 | R | 226 | HIS | CE1-NE2-CD2 | -8.71 | 100.29 | 109.00 |
| 2 | J | 189 | VAL | N-CA-C | 8.70 | 119.50 | 110.36 |
| 3 | K | 16 | SER | N-CA-C | 8.69 | 121.71 | 111.71 |
| 2 | S | 348 | LEU | N-CA-C | -8.69 | 100.03 | 111.24 |
| 2 | H | 276 | ALA | N-CA-C | 8.68 | 120.36 | 111.07 |
| 2 | J | 215 | ARG | N-CA-C | -8.67 | 101.78 | 111.14 |
| 2 | G | 347 | ASP | N-CA-C | -8.66 | 101.77 | 111.82 |
| 2 | S | 229 | GLN | OE1-CD-NE2 | -8.66 | 113.94 | 122.60 |
| 1 | B | 304 | ALA | N-CA-C | 8.66 | 122.52 | 108.32 |
| 2 | S | 254 | ALA | N-CA-C | 8.65 | 121.49 | 111.11 |
| 3 | M | 94 | ASN | OD1-CG-ND2 | -8.64 | 113.96 | 122.60 |
| 2 | G | 353 | HIS | CB-CG-CD2 | -8.64 | 119.97 | 131.20 |
| 2 | I | 225 | ILE | N-CA-C | -8.59 | 101.86 | 110.62 |
| 3 | P | 47 | HIS | CB-CG-CD2 | -8.59 | 120.04 | 131.20 |
| 2 | G | 95 | ASN | OD1-CG-ND2 | -8.58 | 114.02 | 122.60 |
| 2 | R | 277 | ASN | OD1-CG-ND2 | -8.55 | 114.05 | 122.60 |
| 2 | H | 59 | ALA | N-CA-C | 8.55 | 120.29 | 110.97 |
| 2 | J | 393 | ILE | N-CA-C | 8.55 | 118.57 | 110.53 |
| 2 | J | 287 | ASN | CA-CB-CG | 8.54 | 121.14 | 112.60 |
| 2 | I | 444 | ILE | CA-C-O | -8.54 | 112.12 | 121.17 |
| 2 | J | 269 | PHE | N-CA-C | 8.53 | 121.65 | 111.33 |
| 2 | R | 167 | ARG | N-CA-C | 8.53 | 115.80 | 108.13 |
| 1 | T | 251 | ARG | CA-C-O | -8.53 | 111.78 | 120.90 |
| 2 | S | 304 | GLN | OE1-CD-NE2 | -8.52 | 114.08 | 122.60 |
| 2 | G | 86 | HIS | ND1-CE1-NE2 | 8.51 | 116.91 | 108.40 |
| 1 | F | 271 | GLN | OE1-CD-NE2 | -8.49 | 114.11 | 122.60 |
| 2 | J | 271 | THR | N-CA-C | -8.49 | 102.51 | 113.12 |
| 2 | I | 63 | THR | CB-CA-C | 8.48 | 122.37 | 109.13 |
| 2 | G | 437 | LEU | N-CA-C | 8.45 | 120.48 | 111.28 |
| 2 | H | 303 | ARG | N-CA-C | 8.44 | 120.10 | 111.07 |
| 2 | C | 197 | LEU | N-CA-C | 8.44 | 122.14 | 110.24 |
| 2 | S | 454 | GLU | N-CA-C | -8.43 | 101.32 | 111.69 |
| 2 | H | 391 | VAL | N-CA-C | -8.41 | 100.48 | 112.35 |
| 2 | S | 242 | VAL | CA-C-O | -8.41 | 112.06 | 119.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | G | 268 | ASP | N-CA-C | 8.41 | 122.33 | 108.96 |
| 3 | E | 67 | SER | CA-C-O | -8.41 | 111.62 | 120.28 |
| 3 | E | 32 | TYR | N-CA-C | -8.39 | 102.09 | 111.07 |
| 2 | Q | 305 | ARG | N-CA-C | 8.39 | 120.43 | 111.28 |
| 1 | F | 232 | GLN | CA-C-O | -8.39 | 111.92 | 120.90 |
| 2 | H | 86 | HIS | CE1-NE2-CD2 | -8.39 | 100.61 | 109.00 |
| 2 | R | 215 | ARG | N-CA-C | -8.39 | 102.08 | 111.14 |
| 2 | H | 37 | LEU | CA-C-O | -8.38 | 111.31 | 120.36 |
| 2 | I | 149 | GLN | OE1-CD-NE2 | -8.38 | 114.22 | 122.60 |
| 2 | H | 238 | HIS | CB-CG-CD2 | -8.38 | 120.31 | 131.20 |
| 2 | S | 294 | HIS | CE1-NE2-CD2 | -8.38 | 100.62 | 109.00 |
| 2 | I | 363 | PHE | N-CA-C | 8.36 | 121.52 | 111.82 |
| 3 | D | 31 | GLU | CA-C-O | -8.36 | 112.23 | 121.00 |
| 1 | T | 283 | HIS | CG-CD2-NE2 | 8.35 | 115.55 | 107.20 |
| 2 | G | 166 | GLY | CA-C-O | 8.34 | 127.46 | 119.20 |
| 2 | R | 130 | ILE | N-CA-C | 8.34 | 119.84 | 108.84 |
| 2 | J | 327 | HIS | CG-CD2-NE2 | 8.33 | 115.53 | 107.20 |
| 2 | I | 302 | ASP | CA-CB-CG | 8.33 | 120.93 | 112.60 |
| 2 | I | 432 | ASN | OD1-CG-ND2 | -8.33 | 114.27 | 122.60 |
| 2 | J | 383 | HIS | CA-C-O | -8.33 | 111.45 | 122.44 |
| 3 | L | 36 | GLN | OE1-CD-NE2 | -8.32 | 114.28 | 122.60 |
| 2 | H | 250 | MET | N-CA-C | 8.31 | 119.97 | 111.07 |
| 3 | L | 81 | GLU | N-CA-C | -8.29 | 103.29 | 113.41 |
| 2 | S | 157 | VAL | N-CA-C | -8.29 | 102.16 | 110.62 |
| 2 | C | 212 | GLN | N-CA-C | 8.29 | 122.02 | 108.26 |
| 2 | G | 89 | PRO | CA-C-O | -8.29 | 112.00 | 121.36 |
| 3 | O | 105 | VAL | N-CA-CB | -8.28 | 102.47 | 112.33 |
| 2 | G | 295 | ARG | N-CA-C | 8.26 | 122.70 | 113.21 |
| 3 | L | 32 | TYR | N-CA-C | -8.26 | 102.28 | 111.28 |
| 2 | J | 327 | HIS | CE1-NE2-CD2 | -8.25 | 100.75 | 109.00 |
| 2 | H | 58 | ALA | CA-C-O | 8.24 | 129.72 | 120.90 |
| 3 | M | 26 | ILE | N-CA-C | -8.24 | 102.51 | 110.42 |
| 2 | S | 217 | ARG | CA-C-O | -8.24 | 112.17 | 120.82 |
| 3 | L | 18 | LEU | CA-C-N | -8.22 | 113.66 | 119.66 |
| 3 | L | 18 | LEU | C-N-CA | -8.22 | 113.66 | 119.66 |
| 2 | Q | 348 | LEU | CA-C-O | -8.22 | 111.83 | 120.55 |
| 3 | O | 104 | ILE | CA-C-O | -8.21 | 111.05 | 121.48 |
| 2 | S | 119 | SER | N-CA-C | -8.20 | 101.61 | 111.69 |
| 2 | G | 341 | SER | N-CA-C | -8.19 | 102.32 | 111.82 |
| 2 | I | 208 | SER | CA-C-O | -8.19 | 112.69 | 121.20 |
| 2 | G | 118 | THR | N-CA-C | -8.17 | 102.46 | 111.36 |
| 2 | C | 86 | HIS | ND1-CE1-NE2 | 8.16 | 116.56 | 108.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 75 | VAL | N-CA-C | -8.16 | 102.30 | 110.62 |
| 2 | S | 327 | HIS | CB-CG-CD2 | -8.16 | 120.59 | 131.20 |
| 2 | Q | 446 | ARG | N-CA-C | 8.16 | 120.97 | 111.02 |
| 2 | J | 401 | GLN | OE1-CD-NE2 | -8.15 | 114.45 | 122.60 |
| 2 | Q | 119 | SER | CA-C-O | -8.14 | 112.27 | 120.82 |
| 3 | E | 15 | PHE | CA-CB-CG | 8.14 | 121.94 | 113.80 |
| 2 | R | 303 | ARG | N-CA-C | -8.13 | 102.36 | 111.14 |
| 2 | G | 215 | ARG | N-CA-C | -8.13 | 102.50 | 111.36 |
| 2 | R | 401 | GLN | OE1-CD-NE2 | -8.12 | 114.48 | 122.60 |
| 2 | R | 417 | ALA | N-CA-C | -8.12 | 102.52 | 111.36 |
| 3 | N | 81 | GLU | N-CA-C | -8.11 | 102.98 | 113.12 |
| 2 | R | 223 | ASP | N-CA-C | -8.10 | 101.72 | 111.69 |
| 2 | G | 274 | PHE | N-CA-C | -8.08 | 103.37 | 113.55 |
| 3 | P | 27 | ALA | CA-C-O | 8.07 | 129.11 | 120.55 |
| 3 | D | 76 | ARG | N-CA-C | 8.07 | 119.70 | 111.07 |
| 2 | R | 320 | LEU | N-CA-C | 8.05 | 119.69 | 111.07 |
| 2 | C | 274 | PHE | CA-CB-CG | 8.04 | 121.84 | 113.80 |
| 2 | C | 299 | ALA | N-CA-C | 8.02 | 121.03 | 111.33 |
| 1 | F | 251 | ARG | CA-C-O | -8.02 | 112.05 | 120.55 |
| 2 | G | 205 | ASN | CA-CB-CG | -8.02 | 104.58 | 112.60 |
| 2 | H | 127 | PHE | CA-CB-CG | -8.01 | 105.79 | 113.80 |
| 2 | Q | 225 | ILE | N-CA-C | -8.01 | 102.73 | 110.42 |
| 2 | J | 79 | ARG | N-CA-C | 8.01 | 120.92 | 111.71 |
| 2 | H | 86 | HIS | ND1-CE1-NE2 | 7.99 | 116.39 | 108.40 |
| 2 | S | 348 | LEU | CA-C-O | -7.97 | 112.43 | 120.80 |
| 2 | R | 321 | SER | N-CA-C | 7.96 | 119.59 | 111.07 |
| 2 | J | 145 | VAL | N-CA-C | 7.96 | 118.72 | 110.36 |
| 2 | J | 193 | LEU | N-CA-C | 7.95 | 119.58 | 111.07 |
| 2 | Q | 424 | LEU | N-CA-C | -7.95 | 102.56 | 111.07 |
| 2 | S | 402 | PHE | N-CA-C | 7.95 | 121.42 | 109.25 |
| 3 | E | 94 | ASN | CA-CB-CG | 7.94 | 120.54 | 112.60 |
| 2 | J | 441 | GLY | N-CA-C | 7.94 | 121.71 | 112.50 |
| 2 | Q | 118 | THR | N-CA-C | -7.92 | 102.72 | 111.36 |
| 3 | N | 39 | HIS | CE1-NE2-CD2 | -7.92 | 101.08 | 109.00 |
| 2 | R | 108 | PHE | CA-CB-CG | -7.92 | 105.88 | 113.80 |
| 2 | J | 45 | GLN | N-CA-C | -7.92 | 99.15 | 110.08 |
| 3 | K | 29 | GLN | OE1-CD-NE2 | -7.92 | 114.68 | 122.60 |
| 2 | R | 155 | ILE | N-CA-C | -7.92 | 102.62 | 110.30 |
| 2 | G | 274 | PHE | CA-CB-CG | -7.90 | 105.90 | 113.80 |
| 2 | R | 125 | PHE | CA-C-O | -7.88 | 111.37 | 120.20 |
| 2 | H | 346 | VAL | N-CA-C | 7.88 | 118.42 | 110.23 |
| 2 | C | 287 | ASN | OD1-CG-ND2 | -7.87 | 114.73 | 122.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 244 | ALA | CA-C-O | -7.87 | 112.99 | 120.94 |
| 2 | R | 421 | ARG | N-CA-C | 7.86 | 119.48 | 111.07 |
| 3 | N | 84 | ASP | N-CA-C | 7.86 | 122.54 | 113.19 |
| 2 | J | 160 | ASP | N-CA-C | 7.85 | 119.84 | 111.28 |
| 2 | C | 298 | HIS | CB-CG-CD2 | 7.85 | 141.41 | 131.20 |
| 2 | C | 311 | PHE | N-CA-C | 7.85 | 119.83 | 111.28 |
| 1 | F | 272 | VAL | N-CA-C | 7.85 | 118.39 | 110.23 |
| 3 | P | 63 | PHE | N-CA-C | -7.83 | 101.57 | 112.45 |
| 2 | S | 292 | HIS | CA-C-O | -7.82 | 113.04 | 121.56 |
| 2 | J | 37 | LEU | CA-C-O | -7.81 | 112.06 | 121.28 |
| 2 | I | 385 | TRP | CA-C-O | -7.81 | 111.45 | 120.20 |
| 2 | Q | 204 | GLU | N-CA-C | -7.81 | 102.85 | 111.36 |
| 2 | S | 223 | ASP | N-CA-C | -7.80 | 102.86 | 111.36 |
| 2 | R | 95 | ASN | OD1-CG-ND2 | -7.80 | 114.80 | 122.60 |
| 2 | G | 325 | HIS | CB-CG-CD2 | -7.79 | 121.07 | 131.20 |
| 2 | H | 318 | LEU | N-CA-C | 7.79 | 119.78 | 111.28 |
| 2 | H | 163 | ASN | OD1-CG-ND2 | -7.78 | 114.82 | 122.60 |
| 2 | R | 157 | VAL | CA-C-O | -7.78 | 112.61 | 120.85 |
| 3 | N | 64 | ASP | N-CA-C | -7.77 | 99.88 | 110.68 |
| 2 | H | 223 | ASP | CA-CB-CG | 7.77 | 120.37 | 112.60 |
| 2 | R | 163 | ASN | N-CA-C | 7.76 | 122.46 | 113.38 |
| 2 | J | 292 | HIS | CB-CG-CD2 | -7.76 | 121.11 | 131.20 |
| 2 | I | 156 | GLN | N-CA-C | 7.74 | 119.35 | 111.07 |
| 2 | Q | 248 | GLU | N-CA-C | 7.73 | 119.78 | 111.36 |
| 2 | G | 269 | PHE | CA-CB-CG | 7.73 | 121.53 | 113.80 |
| 2 | C | 264 | ILE | CA-C-O | -7.72 | 113.73 | 121.45 |
| 2 | Q | 223 | ASP | N-CA-C | -7.72 | 102.94 | 111.36 |
| 2 | C | 352 | ASP | N-CA-C | 7.71 | 119.69 | 111.28 |
| 2 | G | 51 | ASP | N-CA-C | 7.71 | 119.31 | 111.07 |
| 2 | C | 353 | HIS | CA-CB-CG | -7.70 | 106.11 | 113.80 |
| 3 | O | 36 | GLN | OE1-CD-NE2 | -7.70 | 114.91 | 122.60 |
| 2 | R | 151 | PRO | N-CA-C | 7.69 | 120.08 | 110.70 |
| 2 | Q | 133 | LEU | CA-C-O | -7.69 | 112.13 | 121.36 |
| 2 | I | 450 | LYS | N-CA-C | 7.68 | 120.33 | 111.11 |
| 2 | H | 183 | LYS | N-CA-C | 7.68 | 120.62 | 111.33 |
| 2 | H | 369 | ALA | N-CA-C | 7.67 | 122.06 | 112.24 |
| 2 | Q | 48 | VAL | N-CA-C | -7.67 | 98.99 | 107.73 |
| 2 | R | 127 | PHE | CA-CB-CG | -7.66 | 106.14 | 113.80 |
| 2 | S | 363 | PHE | N-CA-C | 7.66 | 120.30 | 111.11 |
| 1 | A | 278 | ASN | OD1-CG-ND2 | -7.66 | 114.94 | 122.60 |
| 2 | S | 113 | VAL | N-CA-C | -7.66 | 102.81 | 110.62 |
| 2 | H | 262 | MET | CA-C-O | -7.66 | 112.14 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | G | 157 | VAL | N-CA-C | -7.65 | 102.99 | 110.72 |
| 2 | G | 383 | HIS | CA-C-O | -7.65 | 112.34 | 122.44 |
| 2 | G | 157 | VAL | CA-C-O | -7.64 | 112.76 | 120.85 |
| 2 | S | 441 | GLY | N-CA-C | -7.64 | 103.64 | 112.50 |
| 3 | D | 59 | LYS | N-CA-CB | -7.63 | 105.47 | 114.17 |
| 2 | R | 345 | PHE | N-CA-C | -7.63 | 102.61 | 112.23 |
| 2 | J | 226 | HIS | N-CA-C | 7.63 | 120.27 | 111.11 |
| 2 | G | 125 | PHE | N-CA-C | 7.61 | 121.50 | 111.75 |
| 2 | R | 276 | ALA | N-CA-C | -7.61 | 102.98 | 111.28 |
| 2 | I | 277 | ASN | OD1-CG-ND2 | -7.61 | 114.99 | 122.60 |
| 3 | D | 60 | LEU | N-CA-CB | 7.60 | 118.42 | 111.27 |
| 2 | J | 100 | PHE | CA-CB-CG | 7.60 | 121.40 | 113.80 |
| 2 | J | 127 | PHE | CA-CB-CG | -7.60 | 106.20 | 113.80 |
| 3 | K | 63 | PHE | CA-CB-CG | -7.60 | 106.20 | 113.80 |
| 2 | H | 256 | PHE | CA-CB-CG | -7.59 | 106.21 | 113.80 |
| 2 | J | 385 | TRP | CA-C-O | -7.59 | 112.50 | 120.55 |
| 2 | H | 291 | LEU | CA-C-O | -7.59 | 112.11 | 120.38 |
| 2 | Q | 438 | TYR | N-CA-C | 7.59 | 121.46 | 111.75 |
| 2 | I | 324 | ASP | N-CA-C | 7.58 | 122.36 | 113.18 |
| 2 | R | 307 | HIS | ND1-CE1-NE2 | 7.58 | 115.98 | 108.40 |
| 2 | Q | 50 | ALA | N-CA-C | 7.58 | 119.19 | 111.07 |
| 3 | L | 53 | PHE | CA-C-O | -7.58 | 112.51 | 120.55 |
| 2 | C | 151 | PRO | N-CA-CB | -7.58 | 99.28 | 103.22 |
| 3 | N | 19 | PRO | CA-C-O | -7.58 | 109.58 | 120.56 |
| 3 | M | 63 | PHE | CA-CB-CG | -7.57 | 106.23 | 113.80 |
| 3 | D | 49 | ASN | CA-C-O | -7.56 | 112.29 | 119.55 |
| 2 | H | 117 | LEU | CA-C-O | -7.56 | 112.88 | 120.82 |
| 3 | L | 106 | HIS | CB-CG-CD2 | 7.54 | 141.01 | 131.20 |
| 2 | H | 105 | LEU | N-CA-C | 7.54 | 121.40 | 111.75 |
| 2 | J | 180 | LEU | N-CA-C | 7.54 | 120.87 | 110.24 |
| 2 | H | 180 | LEU | N-CA-C | 7.54 | 120.30 | 110.43 |
| 2 | S | 157 | VAL | CA-C-O | -7.54 | 113.11 | 120.95 |
| 2 | Q | 139 | ARG | CA-C-N | 7.53 | 130.76 | 120.67 |
| 2 | Q | 139 | ARG | C-N-CA | 7.53 | 130.76 | 120.67 |
| 2 | C | 189 | VAL | N-CA-C | 7.53 | 118.06 | 110.23 |
| 2 | G | 86 | HIS | CG-CD2-NE2 | 7.53 | 114.73 | 107.20 |
| 2 | J | 287 | ASN | OD1-CG-ND2 | -7.51 | 115.09 | 122.60 |
| 3 | O | 15 | PHE | CA-CB-CG | 7.51 | 121.31 | 113.80 |
| 2 | H | 33 | ASP | CA-C-O | 7.51 | 128.51 | 120.55 |
| 2 | I | 184 | ASN | OD1-CG-ND2 | -7.50 | 115.10 | 122.60 |
| 3 | M | 106 | HIS | CE1-NE2-CD2 | -7.50 | 101.50 | 109.00 |
| 2 | R | 238 | HIS | CB-CG-CD2 | -7.50 | 121.45 | 131.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 232 | GLN | CA-C-O | -7.50 | 112.88 | 120.90 |
| 2 | I | 129 | ALA | N-CA-C | 7.50 | 121.52 | 112.38 |
| 3 | D | 64 | ASP | N-CA-C | -7.49 | 101.21 | 110.65 |
| 2 | R | 326 | LEU | N-CA-C | 7.49 | 120.52 | 107.49 |
| 3 | M | 57 | MET | N-CA-C | 7.48 | 119.97 | 110.24 |
| 2 | C | 167 | ARG | N-CA-C | 7.48 | 120.22 | 108.55 |
| 2 | Q | 148 | PHE | CA-CB-CG | -7.47 | 106.33 | 113.80 |
| 3 | K | 39 | HIS | CA-CB-CG | -7.47 | 106.33 | 113.80 |
| 3 | M | 79 | ARG | N-CA-C | 7.47 | 119.42 | 111.28 |
| 3 | D | 32 | TYR | CA-C-O | -7.46 | 112.56 | 120.92 |
| 2 | S | 311 | PHE | N-CA-C | 7.46 | 120.36 | 111.33 |
| 3 | M | 46 | GLU | N-CA-C | 7.46 | 119.41 | 111.28 |
| 2 | C | 62 | SER | N-CA-C | 7.46 | 119.49 | 111.36 |
| 3 | N | 92 | PHE | CA-CB-CG | -7.46 | 106.34 | 113.80 |
| 2 | S | 158 | GLU | N-CA-C | 7.46 | 120.06 | 111.11 |
| 2 | I | 423 | ALA | N-CA-C | -7.45 | 103.10 | 111.07 |
| 2 | C | 251 | MET | N-CA-C | 7.43 | 119.02 | 111.07 |
| 2 | I | 274 | PHE | CA-C-O | -7.43 | 112.55 | 120.42 |
| 2 | S | 59 | ALA | N-CA-C | 7.42 | 119.01 | 111.07 |
| 2 | G | 420 | ASN | OD1-CG-ND2 | -7.42 | 115.18 | 122.60 |
| 2 | Q | 95 | ASN | OD1-CG-ND2 | -7.42 | 115.18 | 122.60 |
| 1 | F | 237 | LEU | CA-C-N | 7.42 | 130.22 | 120.28 |
| 1 | F | 237 | LEU | C-N-CA | 7.42 | 130.22 | 120.28 |
| 2 | J | 113 | VAL | N-CA-C | 7.42 | 118.19 | 110.62 |
| 1 | B | 253 | PHE | N-CA-C | 7.41 | 119.00 | 111.07 |
| 2 | Q | 367 | ASP | N-CA-C | 7.40 | 120.96 | 108.90 |
| 2 | H | 401 | GLN | CB-CG-CD | -7.40 | 100.02 | 112.60 |
| 2 | Q | 399 | VAL | CA-C-O | -7.40 | 114.31 | 121.63 |
| 1 | T | 284 | GLU | N-CA-C | 7.40 | 121.22 | 110.42 |
| 3 | E | 33 | MET | N-CA-C | 7.39 | 120.28 | 111.33 |
| 2 | G | 429 | GLN | OE1-CD-NE2 | -7.38 | 115.22 | 122.60 |
| 3 | P | 63 | PHE | CA-CB-CG | -7.38 | 106.42 | 113.80 |
| 2 | H | 311 | PHE | N-CA-C | -7.38 | 103.32 | 111.36 |
| 2 | C | 301 | ILE | CA-C-O | -7.37 | 111.39 | 118.98 |
| 2 | J | 52 | GLU | CA-C-N | 7.37 | 130.38 | 120.65 |
| 2 | J | 52 | GLU | C-N-CA | 7.37 | 130.38 | 120.65 |
| 2 | Q | 341 | SER | N-CA-C | -7.36 | 103.28 | 111.82 |
| 2 | S | 148 | PHE | CA-C-N | 7.36 | 130.47 | 120.38 |
| 2 | S | 148 | PHE | C-N-CA | 7.36 | 130.47 | 120.38 |
| 2 | Q | 212 | GLN | OE1-CD-NE2 | -7.36 | 115.24 | 122.60 |
| 2 | J | 40 | PHE | CA-CB-CG | 7.35 | 121.15 | 113.80 |
| 2 | J | 171 | GLY | CA-C-O | -7.35 | 114.50 | 121.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 125 | PHE | N-CA-C | 7.35 | 121.16 | 111.75 |
| 2 | J | 298 | HIS | N-CA-C | 7.33 | 119.91 | 111.11 |
| 2 | I | 125 | PHE | CA-CB-CG | -7.33 | 106.47 | 113.80 |
| 2 | I | 327 | HIS | CA-CB-CG | -7.32 | 106.48 | 113.80 |
| 3 | L | 44 | PHE | O-C-N | -7.32 | 115.59 | 123.42 |
| 3 | L | 80 | SER | CA-C-O | -7.31 | 112.01 | 120.20 |
| 2 | R | 119 | SER | N-CA-C | -7.31 | 102.29 | 112.45 |
| 2 | C | 30 | THR | CA-C-O | -7.31 | 113.22 | 119.36 |
| 2 | Q | 238 | HIS | CB-CG-ND1 | 7.30 | 133.65 | 122.70 |
| 2 | G | 349 | MET | N-CA-C | 7.30 | 121.45 | 112.54 |
| 1 | A | 232 | GLN | CB-CG-CD | -7.30 | 100.19 | 112.60 |
| 2 | C | 301 | ILE | CB-CA-C | 7.29 | 117.80 | 110.65 |
| 3 | O | 67 | SER | CA-C-O | 7.29 | 127.79 | 120.28 |
| 2 | H | 107 | LEU | N-CA-C | 7.29 | 121.61 | 112.87 |
| 2 | Q | 29 | TYR | N-CA-C | 7.29 | 120.51 | 110.24 |
| 2 | R | 147 | THR | N-CA-C | 7.28 | 121.42 | 112.54 |
| 3 | P | 40 | PRO | CB-CA-C | -7.28 | 102.59 | 111.11 |
| 3 | N | 71 | VAL | N-CA-C | -7.28 | 103.69 | 110.53 |
| 2 | C | 318 | LEU | CA-C-O | -7.28 | 113.36 | 121.00 |
| 2 | R | 375 | LEU | N-CA-C | 7.28 | 122.31 | 109.58 |
| 2 | H | 215 | ARG | N-CA-C | -7.27 | 102.75 | 111.69 |
| 1 | F | 284 | GLU | N-CA-C | 7.27 | 121.03 | 110.42 |
| 2 | C | 446 | ARG | N-CA-C | 7.27 | 119.28 | 111.36 |
| 2 | Q | 100 | PHE | N-CA-C | 7.27 | 120.27 | 109.59 |
| 2 | G | 60 | GLU | N-CA-C | 7.27 | 119.83 | 111.11 |
| 2 | Q | 425 | GLU | N-CA-C | -7.26 | 103.09 | 112.23 |
| 2 | G | 375 | LEU | N-CA-C | 7.25 | 118.84 | 109.64 |
| 2 | H | 77 | MET | CA-C-O | -7.25 | 113.14 | 120.90 |
| 3 | N | 27 | ALA | N-CA-C | -7.24 | 103.47 | 111.36 |
| 2 | J | 125 | PHE | CA-C-O | -7.24 | 112.09 | 120.20 |
| 2 | Q | 125 | PHE | N-CA-C | 7.23 | 121.74 | 112.34 |
| 2 | I | 148 | PHE | CA-CB-CG | -7.23 | 106.57 | 113.80 |
| 2 | Q | 346 | VAL | CA-C-O | 7.23 | 128.79 | 121.27 |
| 3 | E | 103 | PHE | CA-CB-CG | 7.23 | 121.03 | 113.80 |
| 3 | L | 91 | GLY | CA-C-O | -7.22 | 115.31 | 120.94 |
| 2 | S | 45 | GLN | OE1-CD-NE2 | -7.22 | 115.38 | 122.60 |
| 2 | J | 70 | TRP | N-CA-C | -7.21 | 103.42 | 111.71 |
| 2 | C | 170 | LEU | CA-C-N | 7.21 | 128.31 | 121.46 |
| 2 | C | 170 | LEU | C-N-CA | 7.21 | 128.31 | 121.46 |
| 2 | R | 238 | HIS | CE1-NE2-CD2 | 7.21 | 116.21 | 109.00 |
| 3 | K | 26 | ILE | CA-C-O | -7.20 | 113.46 | 120.95 |
| 3 | M | 12 | PHE | CA-CB-CG | -7.20 | 106.60 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 359 | SER | N-CA-C | 7.20 | 119.13 | 111.28 |
| 2 | G | 131 | ARG | N-CA-C | 7.20 | 118.77 | 111.07 |
| 3 | N | 106 | HIS | N-CA-C | 7.20 | 120.63 | 108.90 |
| 2 | I | 231 | GLU | O-C-N | 7.19 | 129.48 | 122.07 |
| 3 | M | 63 | PHE | N-CA-C | -7.18 | 104.38 | 113.43 |
| 2 | C | 304 | GLN | N-CA-C | -7.18 | 101.03 | 110.43 |
| 2 | S | 214 | TRP | N-CA-C | -7.18 | 103.39 | 111.14 |
| 1 | B | 287 | TYR | CA-C-O | -7.16 | 113.79 | 120.95 |
| 2 | J | 207 | ASN | N-CA-C | 7.15 | 121.70 | 112.12 |
| 2 | I | 220 | PHE | N-CA-C | 7.14 | 119.68 | 111.11 |
| 2 | C | 287 | ASN | CA-CB-CG | 7.13 | 119.73 | 112.60 |
| 1 | B | 232 | GLN | N-CA-C | 7.13 | 119.67 | 111.11 |
| 2 | Q | 205 | ASN | N-CA-C | -7.13 | 103.59 | 111.36 |
| 2 | J | 314 | LEU | CA-C-O | -7.12 | 113.34 | 120.82 |
| 2 | S | 207 | ASN | CA-CB-CG | -7.12 | 105.48 | 112.60 |
| 2 | R | 153 | HIS | CB-CG-CD2 | 7.11 | 140.45 | 131.20 |
| 2 | I | 379 | SER | CA-C-O | -7.11 | 113.82 | 121.14 |
| 2 | I | 221 | VAL | N-CA-C | -7.11 | 103.25 | 111.00 |
| 2 | C | 307 | HIS | N-CA-C | 7.11 | 120.48 | 108.90 |
| 3 | E | 16 | SER | N-CA-C | 7.10 | 119.02 | 111.28 |
| 2 | I | 44 | PRO | CA-C-N | 7.10 | 130.80 | 120.51 |
| 2 | I | 44 | PRO | C-N-CA | 7.10 | 130.80 | 120.51 |
| 2 | J | 304 | GLN | CA-C-O | -7.09 | 113.78 | 121.44 |
| 3 | O | 39 | HIS | CA-CB-CG | -7.09 | 106.71 | 113.80 |
| 1 | F | 262 | ALA | O-C-N | 7.08 | 127.60 | 121.30 |
| 2 | G | 353 | HIS | CB-CG-ND1 | 7.08 | 133.32 | 122.70 |
| 2 | S | 327 | HIS | CB-CG-ND1 | 7.08 | 133.31 | 122.70 |
| 2 | Q | 383 | HIS | CA-C-O | -7.08 | 113.19 | 122.03 |
| 3 | E | 22 | SER | N-CA-C | -7.07 | 99.41 | 110.36 |
| 3 | E | 107 | ARG | CA-C-O | -7.07 | 112.48 | 120.46 |
| 2 | C | 366 | GLN | OE1-CD-NE2 | -7.06 | 115.54 | 122.60 |
| 1 | F | 232 | GLN | N-CA-C | 7.05 | 119.57 | 111.11 |
| 2 | J | 307 | HIS | N-CA-C | 7.05 | 119.97 | 108.55 |
| 2 | R | 225 | ILE | N-CA-C | -7.05 | 103.65 | 110.42 |
| 2 | S | 40 | PHE | CA-CB-CG | -7.05 | 106.75 | 113.80 |
| 2 | Q | 24 | TYR | N-CA-C | 7.05 | 118.96 | 111.28 |
| 2 | S | 347 | ASP | N-CA-C | -7.04 | 103.95 | 112.54 |
| 2 | Q | 153 | HIS | CB-CG-CD2 | 7.04 | 140.35 | 131.20 |
| 1 | B | 273 | LEU | N-CA-C | 7.03 | 119.84 | 111.33 |
| 2 | H | 238 | HIS | CE1-NE2-CD2 | 7.03 | 116.03 | 109.00 |
| 2 | C | 303 | ARG | N-CA-C | 7.03 | 118.59 | 111.07 |
| 2 | R | 423 | ALA | N-CA-C | -7.03 | 103.62 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | G | 148 | PHE | CA-CB-CG | -7.03 | 106.77 | 113.80 |
| 2 | Q | 363 | PHE | CA-CB-CG | 7.03 | 120.83 | 113.80 |
| 2 | S | 372 | PRO | N-CA-C | 7.03 | 122.10 | 111.14 |
| 2 | H | 72 | ASP | N-CA-C | 7.02 | 118.62 | 110.97 |
| 2 | R | 137 | ASP | CA-CB-CG | 7.01 | 119.61 | 112.60 |
| 2 | C | 148 | PHE | CA-CB-CG | -7.01 | 106.79 | 113.80 |
| 2 | I | 185 | TYR | N-CA-C | -7.00 | 103.58 | 111.14 |
| 2 | C | 115 | ASN | OD1-CG-ND2 | -7.00 | 115.60 | 122.60 |
| 2 | S | 312 | ARG | CA-C-O | -7.00 | 113.07 | 120.63 |
| 1 | T | 239 | GLN | OE1-CD-NE2 | -7.00 | 115.60 | 122.60 |
| 2 | I | 42 | PHE | N-CA-C | 7.00 | 120.95 | 109.06 |
| 3 | D | 71 | VAL | CA-C-O | -6.99 | 113.44 | 120.85 |
| 2 | J | 362 | VAL | N-CA-CB | -6.99 | 105.28 | 112.06 |
| 2 | S | 444 | ILE | N-CA-C | -6.99 | 103.52 | 110.30 |
| 3 | D | 95 | ILE | N-CA-C | 6.99 | 117.08 | 110.30 |
| 3 | L | 64 | ASP | CA-CB-CG | -6.99 | 105.61 | 112.60 |
| 3 | M | 12 | PHE | CA-C-N | 6.98 | 129.97 | 120.54 |
| 3 | M | 12 | PHE | C-N-CA | 6.98 | 129.97 | 120.54 |
| 2 | Q | 318 | LEU | CA-C-O | -6.98 | 113.49 | 120.82 |
| 2 | H | 135 | LEU | N-CA-C | 6.98 | 119.20 | 109.15 |
| 2 | C | 41 | ARG | CA-C-O | -6.97 | 112.83 | 120.43 |
| 2 | G | 61 | SER | N-CA-C | 6.97 | 121.62 | 113.18 |
| 2 | S | 23 | THR | N-CA-C | 6.97 | 121.68 | 112.13 |
| 3 | N | 79 | ARG | N-CA-C | 6.97 | 119.52 | 111.02 |
| 2 | H | 274 | PHE | N-CA-C | 6.96 | 118.76 | 111.03 |
| 2 | C | 342 | THR | CA-C-O | -6.96 | 113.51 | 120.82 |
| 2 | Q | 421 | ARG | N-CA-C | 6.96 | 119.46 | 111.11 |
| 1 | A | 284 | GLU | N-CA-C | 6.95 | 120.09 | 110.35 |
| 3 | E | 75 | VAL | N-CA-C | 6.95 | 117.66 | 110.36 |
| 2 | Q | 444 | ILE | N-CA-CB | -6.95 | 102.42 | 110.55 |
| 2 | C | 270 | LEU | N-CA-C | 6.94 | 120.64 | 111.75 |
| 2 | I | 51 | ASP | N-CA-C | 6.93 | 118.84 | 111.28 |
| 3 | E | 71 | VAL | N-CA-C | -6.93 | 103.55 | 110.62 |
| 2 | H | 201 | LYS | N-CA-C | 6.93 | 119.87 | 108.99 |
| 3 | N | 82 | TYR | CA-C-N | 6.93 | 129.02 | 120.22 |
| 3 | N | 82 | TYR | C-N-CA | 6.93 | 129.02 | 120.22 |
| 3 | P | 17 | TYR | N-CA-C | 6.92 | 119.70 | 111.33 |
| 2 | C | 255 | GLU | N-CA-C | 6.91 | 118.47 | 111.07 |
| 2 | Q | 119 | SER | N-CA-C | -6.91 | 103.67 | 111.07 |
| 2 | R | 120 | ILE | CA-C-O | -6.91 | 114.09 | 121.27 |
| 2 | J | 198 | ASP | N-CA-C | -6.90 | 102.10 | 112.04 |
| 2 | H | 84 | CYS | CA-C-O | -6.90 | 113.74 | 120.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 241 | ASN | CA-CB-CG | 6.90 | 119.50 | 112.60 |
| 2 | G | 36 | LEU | CA-C-O | -6.89 | 113.41 | 120.71 |
| 2 | J | 139 | ARG | CA-C-O | -6.89 | 113.21 | 120.58 |
| 3 | M | 59 | LYS | CA-C-O | -6.88 | 112.12 | 119.00 |
| 2 | S | 325 | HIS | CE1-NE2-CD2 | 6.88 | 115.88 | 109.00 |
| 2 | G | 250 | MET | N-CA-C | -6.88 | 103.71 | 111.07 |
| 1 | F | 251 | ARG | N-CA-C | 6.88 | 118.78 | 111.28 |
| 3 | M | 86 | TYR | N-CA-C | -6.87 | 99.11 | 110.17 |
| 2 | H | 253 | ARG | N-CA-C | 6.87 | 118.77 | 111.28 |
| 3 | N | 15 | PHE | CA-C-O | -6.86 | 112.50 | 121.08 |
| 2 | R | 340 | ALA | N-CA-C | 6.86 | 118.41 | 111.07 |
| 3 | D | 9 | GLU | CB-CG-CD | 6.85 | 124.24 | 112.60 |
| 2 | R | 310 | HIS | CA-C-O | -6.85 | 113.14 | 121.36 |
| 2 | H | 160 | ASP | CA-CB-CG | 6.84 | 119.44 | 112.60 |
| 2 | G | 325 | HIS | CA-CB-CG | 6.84 | 120.64 | 113.80 |
| 2 | C | 306 | ASN | N-CA-C | 6.83 | 121.60 | 111.96 |
| 2 | R | 30 | THR | N-CA-C | -6.83 | 98.98 | 109.64 |
| 3 | M | 45 | ASN | CA-CB-CG | 6.83 | 119.43 | 112.60 |
| 2 | Q | 145 | VAL | O-C-N | 6.82 | 128.76 | 121.94 |
| 3 | E | 53 | PHE | CA-CB-CG | 6.82 | 120.62 | 113.80 |
| 2 | H | 209 | GLN | CA-C-O | -6.82 | 113.98 | 119.71 |
| 2 | C | 200 | THR | CA-C-O | -6.81 | 113.14 | 121.11 |
| 2 | C | 422 | VAL | CA-C-O | -6.81 | 113.97 | 121.05 |
| 2 | G | 444 | ILE | N-CA-CB | -6.81 | 102.95 | 110.51 |
| 3 | M | 16 | SER | N-CA-C | 6.80 | 119.56 | 111.33 |
| 1 | T | 232 | GLN | N-CA-C | 6.80 | 122.59 | 111.37 |
| 1 | T | 282 | GLU | CA-C-O | -6.80 | 112.41 | 120.10 |
| 2 | R | 225 | ILE | CA-C-O | -6.80 | 113.96 | 121.17 |
| 2 | S | 270 | LEU | N-CA-C | 6.80 | 119.27 | 111.11 |
| 2 | Q | 383 | HIS | CE1-NE2-CD2 | -6.79 | 102.20 | 109.00 |
| 2 | C | 274 | PHE | N-CA-C | 6.79 | 122.58 | 111.37 |
| 2 | I | 341 | SER | N-CA-C | -6.79 | 103.94 | 111.82 |
| 2 | C | 292 | HIS | CB-CG-ND1 | 6.79 | 132.89 | 122.70 |
| 2 | Q | 185 | TYR | N-CA-C | -6.79 | 103.11 | 111.40 |
| 2 | G | 58 | ALA | N-CA-C | -6.79 | 103.88 | 111.28 |
| 2 | J | 279 | THR | N-CA-C | 6.78 | 119.25 | 111.11 |
| 2 | Q | 437 | LEU | N-CA-C | 6.77 | 122.54 | 111.37 |
| 2 | J | 220 | PHE | N-CA-C | 6.77 | 118.73 | 111.36 |
| 3 | N | 95 | ILE | N-CA-C | -6.76 | 104.17 | 110.53 |
| 1 | B | 247 | HIS | CA-CB-CG | 6.76 | 120.56 | 113.80 |
| 2 | C | 320 | LEU | N-CA-C | 6.75 | 122.51 | 111.37 |
| 2 | J | 299 | ALA | N-CA-C | 6.75 | 120.39 | 111.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 190 | TYR | O-C-N | 6.75 | 129.87 | 122.11 |
| 2 | H | 44 | PRO | N-CA-C | 6.74 | 121.26 | 110.40 |
| 2 | C | 298 | HIS | CB-CG-ND1 | -6.74 | 112.59 | 122.70 |
| 2 | I | 310 | HIS | CB-CG-CD2 | 6.74 | 139.96 | 131.20 |
| 2 | Q | 145 | VAL | CA-C-O | -6.74 | 114.26 | 121.27 |
| 1 | T | 252 | ARG | N-CA-C | -6.74 | 104.02 | 111.36 |
| 2 | R | 365 | THR | CA-C-O | -6.73 | 113.00 | 120.60 |
| 2 | S | 262 | MET | N-CA-C | -6.73 | 101.17 | 109.65 |
| 2 | S | 187 | ARG | N-CA-C | -6.73 | 104.03 | 111.36 |
| 2 | I | 385 | TRP | N-CA-C | 6.72 | 120.35 | 111.75 |
| 2 | Q | 327 | HIS | CE1-NE2-CD2 | -6.72 | 102.28 | 109.00 |
| 2 | H | 56 | ALA | CA-C-O | -6.71 | 113.77 | 120.82 |
| 2 | C | 425 | GLU | CA-C-N | 6.71 | 129.16 | 120.44 |
| 2 | C | 425 | GLU | C-N-CA | 6.71 | 129.16 | 120.44 |
| 3 | D | 12 | PHE | N-CA-C | -6.71 | 98.87 | 109.07 |
| 2 | I | 88 | GLU | CA-C-O | -6.71 | 114.33 | 120.50 |
| 2 | I | 359 | SER | N-CA-C | 6.71 | 118.25 | 111.07 |
| 1 | T | 297 | THR | N-CA-C | 6.71 | 119.60 | 111.82 |
| 2 | Q | 108 | PHE | CA-C-O | -6.71 | 113.58 | 121.16 |
| 1 | T | 300 | ARG | CA-C-N | 6.70 | 129.82 | 121.85 |
| 1 | T | 300 | ARG | C-N-CA | 6.70 | 129.82 | 121.85 |
| 3 | E | 9 | GLU | CA-C-N | 6.70 | 130.22 | 120.71 |
| 3 | E | 9 | GLU | C-N-CA | 6.70 | 130.22 | 120.71 |
| 3 | M | 93 | ASP | CA-CB-CG | 6.70 | 119.30 | 112.60 |
| 2 | R | 375 | LEU | CA-C-O | -6.70 | 112.95 | 119.51 |
| 2 | G | 166 | GLY | N-CA-C | 6.69 | 123.92 | 115.42 |
| 2 | J | 401 | GLN | CB-CG-CD | -6.69 | 101.22 | 112.60 |
| 2 | C | 460 | ASP | N-CA-C | -6.69 | 104.38 | 112.54 |
| 2 | C | 438 | TYR | N-CA-C | 6.68 | 118.56 | 111.28 |
| 2 | C | 199 | PHE | CA-CB-CG | -6.68 | 107.12 | 113.80 |
| 2 | I | 207 | ASN | OD1-CG-ND2 | -6.68 | 115.92 | 122.60 |
| 2 | Q | 382 | ILE | CA-C-N | -6.68 | 113.01 | 122.63 |
| 2 | Q | 382 | ILE | C-N-CA | -6.68 | 113.01 | 122.63 |
| 2 | G | 182 | ALA | N-CA-C | -6.67 | 103.94 | 111.07 |
| 2 | J | 422 | VAL | O-C-N | 6.67 | 128.45 | 121.91 |
| 2 | Q | 451 | TRP | N-CA-C | 6.67 | 121.27 | 113.20 |
| 2 | R | 242 | VAL | N-CA-C | 6.67 | 118.56 | 112.43 |
| 2 | J | 394 | PHE | N-CA-C | 6.67 | 121.41 | 113.28 |
| 3 | O | 12 | PHE | N-CA-C | 6.66 | 120.54 | 109.95 |
| 2 | C | 180 | LEU | N-CA-C | 6.66 | 120.14 | 110.42 |
| 2 | Q | 393 | ILE | CA-C-O | -6.66 | 114.11 | 121.17 |
| 2 | G | 306 | ASN | CA-C-O | -6.66 | 111.73 | 119.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 303 | ARG | N-CA-C | 6.65 | 119.38 | 111.33 |
| 2 | G | 116 | ILE | N-CA-CB | -6.64 | 103.38 | 110.62 |
| 2 | J | 71 | THR | N-CA-C | 6.64 | 119.35 | 111.71 |
| 2 | J | 226 | HIS | CE1-NE2-CD2 | -6.64 | 102.36 | 109.00 |
| 1 | B | 233 | VAL | N-CA-C | 6.64 | 117.43 | 110.72 |
| 2 | H | 259 | GLU | N-CA-C | 6.64 | 120.97 | 112.34 |
| 2 | S | 221 | VAL | N-CA-C | -6.64 | 104.01 | 110.72 |
| 2 | H | 190 | TYR | CA-C-O | -6.64 | 113.49 | 120.92 |
| 2 | S | 414 | ALA | CA-C-O | -6.64 | 112.23 | 118.73 |
| 2 | C | 185 | TYR | N-CA-C | 6.63 | 119.11 | 111.02 |
| 2 | Q | 423 | ALA | N-CA-C | 6.63 | 119.35 | 111.33 |
| 2 | S | 250 | MET | N-CA-C | -6.63 | 104.05 | 111.28 |
| 2 | G | 417 | ALA | N-CA-C | -6.63 | 103.98 | 111.07 |
| 2 | S | 437 | LEU | N-CA-C | 6.63 | 118.16 | 111.07 |
| 2 | C | 342 | THR | CA-C-N | 6.62 | 129.69 | 120.29 |
| 2 | C | 342 | THR | C-N-CA | 6.62 | 129.69 | 120.29 |
| 2 | G | 292 | HIS | CA-CB-CG | 6.62 | 120.42 | 113.80 |
| 3 | E | 105 | VAL | N-CA-CB | -6.62 | 104.46 | 112.33 |
| 2 | H | 393 | ILE | N-CA-C | 6.61 | 117.36 | 110.62 |
| 2 | H | 134 | ARG | N-CA-C | 6.60 | 120.28 | 109.06 |
| 2 | J | 438 | TYR | O-C-N | 6.60 | 129.14 | 122.08 |
| 2 | R | 181 | SER | CA-C-O | -6.60 | 114.02 | 121.81 |
| 1 | A | 273 | LEU | O-C-N | 6.59 | 129.11 | 122.12 |
| 3 | P | 31 | GLU | CA-C-O | -6.59 | 113.54 | 120.92 |
| 2 | G | 122 | GLY | O-C-N | 6.59 | 128.58 | 122.19 |
| 3 | K | 39 | HIS | CA-C-O | -6.59 | 113.90 | 119.76 |
| 2 | C | 286 | ASP | N-CA-C | 6.58 | 120.41 | 112.38 |
| 2 | Q | 447 | GLU | CB-CG-CD | 6.58 | 123.78 | 112.60 |
| 2 | S | 225 | ILE | CA-C-O | -6.58 | 114.11 | 120.95 |
| 2 | S | 277 | ASN | OD1-CG-ND2 | -6.58 | 116.02 | 122.60 |
| 2 | Q | 421 | ARG | CA-C-N | 6.58 | 128.85 | 120.56 |
| 2 | Q | 421 | ARG | C-N-CA | 6.58 | 128.85 | 120.56 |
| 2 | R | 383 | HIS | CG-CD2-NE2 | 6.58 | 113.78 | 107.20 |
| 2 | J | 188 | ALA | N-CA-C | 6.58 | 118.11 | 111.07 |
| 1 | A | 253 | PHE | N-CA-C | 6.57 | 118.10 | 111.07 |
| 3 | O | 45 | ASN | OD1-CG-ND2 | -6.57 | 116.03 | 122.60 |
| 2 | H | 102 | ALA | N-CA-C | 6.57 | 120.57 | 110.20 |
| 2 | S | 241 | ASN | OD1-CG-ND2 | -6.57 | 116.03 | 122.60 |
| 2 | Q | 277 | ASN | CA-C-O | -6.56 | 113.46 | 120.42 |
| 2 | G | 175 | LYS | CA-C-O | -6.56 | 112.60 | 120.41 |
| 2 | H | 52 | GLU | N-CA-C | -6.56 | 103.62 | 111.69 |
| 2 | H | 319 | ARG | N-CA-C | -6.56 | 104.06 | 111.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | N | 63 | PHE | N-CA-C | -6.56 | 103.40 | 111.40 |
| 2 | C | 58 | ALA | N-CA-C | 6.55 | 118.08 | 111.07 |
| 2 | H | 249 | GLU | CA-C-N | 6.54 | 128.94 | 120.44 |
| 2 | H | 249 | GLU | C-N-CA | 6.54 | 128.94 | 120.44 |
| 2 | G | 226 | HIS | CB-CG-ND1 | -6.54 | 112.90 | 122.70 |
| 1 | A | 228 | GLU | N-CA-C | -6.53 | 103.66 | 111.69 |
| 2 | C | 204 | GLU | CA-C-O | -6.53 | 112.89 | 120.20 |
| 2 | G | 167 | ARG | N-CA-C | 6.53 | 120.68 | 109.06 |
| 2 | S | 379 | SER | CA-C-O | -6.52 | 113.62 | 121.32 |
| 2 | G | 89 | PRO | CA-C-N | 6.52 | 129.84 | 120.98 |
| 2 | G | 89 | PRO | C-N-CA | 6.52 | 129.84 | 120.98 |
| 3 | L | 67 | SER | O-C-N | -6.52 | 116.19 | 121.80 |
| 3 | P | 47 | HIS | N-CA-C | -6.51 | 99.65 | 108.24 |
| 3 | L | 23 | ASP | N-CA-C | -6.51 | 104.18 | 111.28 |
| 2 | H | 28 | ASP | N-CA-C | -6.51 | 104.97 | 113.17 |
| 2 | Q | 351 | GLU | CB-CG-CD | 6.50 | 123.66 | 112.60 |
| 2 | G | 281 | ALA | O-C-N | 6.50 | 128.77 | 122.07 |
| 3 | D | 67 | SER | N-CA-C | 6.50 | 118.91 | 110.40 |
| 2 | I | 436 | ASP | CA-C-O | 6.50 | 128.35 | 120.62 |
| 2 | J | 351 | GLU | CA-C-O | -6.50 | 113.48 | 121.67 |
| 2 | C | 363 | PHE | CA-C-O | -6.49 | 112.77 | 120.10 |
| 2 | G | 127 | PHE | CA-CB-CG | -6.49 | 107.31 | 113.80 |
| 2 | I | 327 | HIS | N-CA-C | -6.49 | 100.30 | 109.96 |
| 2 | J | 98 | PHE | N-CA-C | 6.48 | 119.40 | 107.99 |
| 2 | J | 70 | TRP | CA-C-O | -6.48 | 112.78 | 120.10 |
| 2 | Q | 50 | ALA | CA-C-O | 6.48 | 127.63 | 120.82 |
| 2 | S | 330 | THR | N-CA-C | 6.48 | 118.34 | 111.28 |
| 2 | C | 237 | GLY | O-C-N | -6.48 | 118.35 | 123.27 |
| 2 | H | 184 | ASN | CB-CG-ND2 | 6.48 | 126.12 | 116.40 |
| 2 | S | 302 | ASP | CA-CB-CG | 6.47 | 119.07 | 112.60 |
| 2 | H | 348 | LEU | CA-C-O | -6.46 | 112.80 | 120.10 |
| 2 | C | 327 | HIS | ND1-CE1-NE2 | 6.46 | 114.86 | 108.40 |
| 2 | C | 420 | ASN | CB-CG-ND2 | -6.46 | 106.72 | 116.40 |
| 2 | J | 251 | MET | N-CA-C | -6.46 | 104.16 | 111.07 |
| 2 | I | 243 | THR | CA-C-O | 6.46 | 126.95 | 120.88 |
| 2 | I | 345 | PHE | N-CA-C | 6.46 | 120.42 | 112.54 |
| 2 | J | 446 | ARG | N-CA-C | 6.45 | 118.86 | 111.11 |
| 2 | I | 364 | PHE | N-CA-C | -6.45 | 99.24 | 109.23 |
| 3 | K | 44 | PHE | CA-CB-CG | -6.45 | 107.35 | 113.80 |
| 2 | R | 89 | PRO | N-CA-C | 6.45 | 121.46 | 111.21 |
| 2 | J | 160 | ASP | CA-CB-CG | 6.44 | 119.04 | 112.60 |
| 2 | S | 352 | ASP | CA-C-O | -6.44 | 114.06 | 120.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 31 | PRO | N-CA-C | 6.44 | 120.53 | 110.80 |
| 2 | C | 385 | TRP | N-CA-C | 6.43 | 119.11 | 111.33 |
| 2 | J | 244 | ALA | CA-C-O | -6.43 | 114.27 | 120.64 |
| 2 | G | 200 | THR | CB-CA-C | 6.43 | 121.65 | 109.37 |
| 2 | I | 35 | ASP | CA-CB-CG | 6.43 | 119.03 | 112.60 |
| 2 | I | 127 | PHE | N-CA-C | -6.43 | 101.27 | 110.59 |
| 2 | Q | 180 | LEU | N-CA-C | 6.43 | 119.69 | 110.24 |
| 3 | L | 42 | ILE | CA-C-O | -6.42 | 113.67 | 120.48 |
| 2 | C | 40 | PHE | CA-C-O | -6.42 | 113.38 | 120.38 |
| 2 | I | 364 | PHE | CA-CB-CG | -6.42 | 107.38 | 113.80 |
| 3 | O | 17 | TYR | N-CA-C | 6.42 | 120.82 | 113.19 |
| 2 | I | 206 | ILE | N-CA-CB | 6.41 | 118.32 | 111.46 |
| 2 | I | 238 | HIS | CB-CG-ND1 | 6.41 | 132.32 | 122.70 |
| 3 | M | 21 | LEU | CA-C-O | -6.41 | 113.98 | 121.16 |
| 2 | I | 387 | MET | CA-C-O | -6.41 | 112.43 | 118.33 |
| 2 | C | 391 | VAL | CA-C-O | -6.41 | 114.28 | 120.95 |
| 2 | H | 28 | ASP | CA-CB-CG | -6.41 | 106.19 | 112.60 |
| 2 | I | 160 | ASP | N-CA-C | 6.41 | 118.34 | 111.36 |
| 2 | R | 140 | PHE | O-C-N | 6.41 | 127.14 | 121.18 |
| 2 | H | 323 | GLY | CA-C-N | 6.41 | 128.86 | 120.28 |
| 2 | H | 323 | GLY | C-N-CA | 6.41 | 128.86 | 120.28 |
| 2 | S | 198 | ASP | CA-C-O | -6.41 | 112.86 | 120.10 |
| 1 | A | 251 | ARG | N-CA-C | 6.40 | 117.92 | 111.07 |
| 3 | E | 44 | PHE | CA-CB-CG | -6.40 | 107.40 | 113.80 |
| 1 | F | 307 | GLN | CA-C-O | 6.40 | 128.49 | 121.06 |
| 2 | G | 204 | GLU | CB-CG-CD | 6.40 | 123.48 | 112.60 |
| 2 | I | 151 | PRO | CA-C-O | -6.40 | 111.28 | 120.56 |
| 2 | Q | 366 | GLN | OE1-CD-NE2 | -6.39 | 116.21 | 122.60 |
| 1 | B | 250 | LYS | N-CA-C | -6.39 | 103.61 | 111.40 |
| 2 | J | 138 | ILE | CA-C-N | -6.39 | 113.93 | 122.42 |
| 2 | J | 138 | ILE | C-N-CA | -6.39 | 113.93 | 122.42 |
| 2 | J | 238 | HIS | CG-CD2-NE2 | -6.39 | 100.81 | 107.20 |
| 2 | R | 330 | THR | N-CA-C | -6.39 | 102.84 | 112.04 |
| 2 | S | 212 | GLN | CG-CD-NE2 | -6.38 | 106.83 | 116.40 |
| 2 | S | 358 | ARG | N-CA-C | 6.38 | 119.05 | 111.71 |
| 2 | H | 419 | ALA | N-CA-C | -6.38 | 104.33 | 111.28 |
| 3 | E | 94 | ASN | OD1-CG-ND2 | -6.38 | 116.22 | 122.60 |
| 2 | I | 440 | GLU | CA-C-O | -6.38 | 112.10 | 119.56 |
| 2 | Q | 218 | PHE | CA-CB-CG | 6.37 | 120.17 | 113.80 |
| 2 | G | 296 | ALA | N-CA-C | 6.37 | 119.47 | 110.23 |
| 2 | J | 31 | PRO | CB-CA-C | -6.37 | 103.66 | 111.11 |
| 3 | K | 46 | GLU | N-CA-C | 6.37 | 119.03 | 111.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | K | 10 | ARG | CA-C-O | -6.36 | 114.20 | 121.19 |
| 2 | Q | 229 | GLN | OE1-CD-NE2 | -6.35 | 116.25 | 122.60 |
| 1 | T | 262 | ALA | CA-C-O | -6.35 | 113.28 | 119.51 |
| 2 | C | 292 | HIS | CB-CG-CD2 | -6.35 | 122.94 | 131.20 |
| 2 | C | 202 | ASP | N-CA-C | 6.35 | 118.75 | 110.43 |
| 3 | D | 89 | VAL | N-CA-C | 6.35 | 117.06 | 108.17 |
| 2 | J | 384 | VAL | N-CA-CB | -6.35 | 102.53 | 110.47 |
| 2 | J | 437 | LEU | N-CA-C | 6.35 | 119.87 | 111.75 |
| 1 | T | 304 | ALA | CA-C-N | -6.34 | 114.33 | 122.77 |
| 1 | T | 304 | ALA | C-N-CA | -6.34 | 114.33 | 122.77 |
| 2 | I | 220 | PHE | CA-CB-CG | -6.34 | 107.46 | 113.80 |
| 2 | H | 184 | ASN | OD1-CG-ND2 | -6.34 | 116.26 | 122.60 |
| 2 | S | 61 | SER | N-CA-C | 6.34 | 120.87 | 113.20 |
| 3 | P | 32 | TYR | N-CA-C | 6.34 | 121.83 | 111.37 |
| 2 | R | 252 | LYS | N-CA-C | 6.34 | 118.72 | 111.11 |
| 3 | E | 63 | PHE | N-CA-C | 6.33 | 121.76 | 111.37 |
| 2 | H | 24 | TYR | CA-C-O | -6.33 | 112.28 | 119.95 |
| 3 | L | 10 | ARG | N-CA-C | 6.33 | 119.80 | 110.30 |
| 2 | J | 443 | ASP | CA-C-O | -6.33 | 114.17 | 120.82 |
| 2 | C | 199 | PHE | CA-C-O | 6.33 | 128.22 | 121.45 |
| 2 | G | 348 | LEU | O-C-N | 6.33 | 128.83 | 122.12 |
| 3 | M | 59 | LYS | N-CA-CB | -6.33 | 106.96 | 114.17 |
| 2 | S | 339 | LYS | N-CA-C | -6.33 | 104.38 | 111.28 |
| 2 | I | 127 | PHE | CA-C-O | -6.33 | 114.49 | 121.89 |
| 1 | F | 282 | GLU | N-CA-C | -6.32 | 104.39 | 111.28 |
| 2 | H | 226 | HIS | ND1-CE1-NE2 | 6.32 | 114.72 | 108.40 |
| 2 | J | 392 | GLU | CA-C-N | 6.32 | 128.65 | 120.56 |
| 2 | J | 392 | GLU | C-N-CA | 6.32 | 128.65 | 120.56 |
| 2 | S | 371 | MET | CA-C-O | -6.32 | 114.59 | 119.46 |
| 2 | Q | 161 | LEU | N-CA-C | 6.32 | 118.69 | 111.11 |
| 2 | I | 375 | LEU | N-CA-C | 6.32 | 118.79 | 109.50 |
| 1 | A | 307 | GLN | OE1-CD-NE2 | -6.31 | 116.29 | 122.60 |
| 3 | P | 54 | TYR | N-CA-C | 6.31 | 119.53 | 109.24 |
| 3 | K | 79 | ARG | N-CA-C | 6.31 | 121.72 | 111.37 |
| 2 | I | 199 | PHE | CA-CB-CG | 6.31 | 120.11 | 113.80 |
| 2 | R | 62 | SER | N-CA-C | 6.31 | 120.57 | 112.12 |
| 2 | I | 384 | VAL | CB-CA-C | -6.30 | 102.84 | 112.05 |
| 2 | J | 455 | LEU | CA-C-O | -6.30 | 113.87 | 120.55 |
| 2 | S | 205 | ASN | OD1-CG-ND2 | -6.30 | 116.30 | 122.60 |
| 2 | R | 383 | HIS | ND1-CE1-NE2 | -6.30 | 102.10 | 108.40 |
| 2 | I | 58 | ALA | CA-C-N | 6.30 | 128.63 | 120.44 |
| 2 | I | 58 | ALA | C-N-CA | 6.30 | 128.63 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 191 | GLU | N-CA-C | -6.30 | 104.30 | 112.23 |
| 2 | R | 432 | ASN | CA-CB-CG | 6.29 | 118.89 | 112.60 |
| 2 | J | 33 | ASP | CA-CB-CG | -6.29 | 106.31 | 112.60 |
| 2 | G | 45 | GLN | CB-CG-CD | -6.28 | 101.92 | 112.60 |
| 3 | P | 71 | VAL | N-CA-C | -6.28 | 104.38 | 110.72 |
| 2 | H | 308 | GLY | CA-C-N | -6.27 | 113.65 | 122.75 |
| 2 | H | 308 | GLY | C-N-CA | -6.27 | 113.65 | 122.75 |
| 3 | L | 97 | GLN | CB-CG-CD | -6.27 | 101.94 | 112.60 |
| 2 | C | 208 | SER | CA-C-O | -6.27 | 114.68 | 121.20 |
| 2 | J | 327 | HIS | CB-CG-ND1 | 6.27 | 132.10 | 122.70 |
| 2 | C | 343 | LEU | N-CA-C | -6.26 | 104.53 | 111.36 |
| 3 | E | 57 | MET | N-CA-C | 6.26 | 119.33 | 110.50 |
| 2 | Q | 235 | ILE | CA-C-O | -6.26 | 114.47 | 121.36 |
| 2 | J | 439 | ARG | N-CA-C | 6.26 | 117.77 | 111.07 |
| 2 | R | 401 | GLN | N-CA-C | -6.26 | 100.00 | 109.95 |
| 2 | R | 98 | PHE | CA-CB-CG | -6.26 | 107.54 | 113.80 |
| 2 | I | 160 | ASP | CA-CB-CG | 6.25 | 118.85 | 112.60 |
| 3 | O | 32 | TYR | N-CA-C | -6.25 | 104.55 | 111.36 |
| 2 | I | 56 | ALA | CA-C-N | 6.25 | 128.66 | 120.60 |
| 2 | I | 56 | ALA | C-N-CA | 6.25 | 128.66 | 120.60 |
| 3 | K | 97 | GLN | OE1-CD-NE2 | -6.25 | 116.36 | 122.60 |
| 2 | R | 116 | ILE | N-CA-C | -6.24 | 104.42 | 110.42 |
| 2 | S | 151 | PRO | O-C-N | 6.24 | 128.83 | 121.46 |
| 1 | T | 300 | ARG | N-CA-C | -6.24 | 99.53 | 109.76 |
| 2 | H | 113 | VAL | N-CA-CB | 6.23 | 119.50 | 110.52 |
| 2 | S | 310 | HIS | CB-CG-CD2 | 6.23 | 139.31 | 131.20 |
| 2 | Q | 379 | SER | CA-C-O | -6.22 | 113.98 | 121.32 |
| 3 | D | 76 | ARG | CA-C-O | 6.22 | 127.35 | 120.82 |
| 2 | Q | 348 | LEU | O-C-N | 6.22 | 128.71 | 122.12 |
| 2 | G | 384 | VAL | O-C-N | -6.22 | 115.62 | 121.90 |
| 2 | Q | 310 | HIS | N-CA-C | -6.22 | 100.16 | 110.17 |
| 2 | R | 77 | MET | CA-C-O | -6.22 | 114.25 | 120.90 |
| 2 | G | 372 | PRO | CA-C-N | 6.21 | 130.62 | 121.05 |
| 2 | G | 372 | PRO | C-N-CA | 6.21 | 130.62 | 121.05 |
| 2 | J | 171 | GLY | O-C-N | 6.21 | 128.26 | 123.23 |
| 2 | I | 42 | PHE | CA-C-N | -6.21 | 114.36 | 123.30 |
| 2 | I | 42 | PHE | C-N-CA | -6.21 | 114.36 | 123.30 |
| 3 | P | 74 | GLU | N-CA-C | 6.21 | 118.56 | 111.11 |
| 2 | S | 119 | SER | CA-C-N | 6.20 | 128.50 | 120.56 |
| 2 | S | 119 | SER | C-N-CA | 6.20 | 128.50 | 120.56 |
| 3 | K | 63 | PHE | CA-C-O | 6.20 | 127.28 | 119.78 |
| 2 | H | 370 | SER | N-CA-C | 6.20 | 122.17 | 113.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 197 | LEU | CA-C-N | 6.20 | 128.49 | 120.44 |
| 2 | R | 197 | LEU | C-N-CA | 6.20 | 128.49 | 120.44 |
| 2 | C | 264 | ILE | O-C-N | 6.19 | 129.57 | 122.82 |
| 2 | J | 32 | LYS | CA-C-O | -6.19 | 115.06 | 121.87 |
| 3 | D | 35 | GLU | N-CA-C | 6.19 | 118.82 | 111.33 |
| 2 | C | 198 | ASP | N-CA-C | -6.19 | 104.08 | 111.69 |
| 2 | G | 193 | LEU | CA-C-O | -6.19 | 114.53 | 120.90 |
| 2 | C | 310 | HIS | N-CA-C | -6.18 | 101.34 | 110.48 |
| 2 | R | 115 | ASN | OD1-CG-ND2 | 6.18 | 128.78 | 122.60 |
| 2 | H | 302 | ASP | CA-CB-CG | 6.17 | 118.77 | 112.60 |
| 2 | J | 448 | ALA | N-CA-C | 6.17 | 118.81 | 111.71 |
| 2 | Q | 321 | SER | N-CA-C | 6.17 | 117.67 | 111.07 |
| 2 | I | 452 | SER | CA-C-O | -6.17 | 114.05 | 120.09 |
| 1 | B | 271 | GLN | N-CA-C | -6.16 | 104.65 | 111.36 |
| 2 | I | 270 | LEU | N-CA-C | -6.16 | 104.12 | 111.69 |
| 2 | J | 60 | GLU | CB-CG-CD | 6.16 | 123.06 | 112.60 |
| 2 | G | 191 | GLU | CA-C-O | -6.15 | 113.90 | 120.42 |
| 3 | K | 104 | ILE | CA-C-N | 6.15 | 128.97 | 122.14 |
| 3 | K | 104 | ILE | C-N-CA | 6.15 | 128.97 | 122.14 |
| 2 | G | 140 | PHE | N-CA-C | 6.15 | 117.45 | 109.64 |
| 3 | N | 39 | HIS | CA-CB-CG | -6.14 | 107.66 | 113.80 |
| 3 | E | 37 | GLY | CA-C-N | -6.14 | 114.45 | 123.05 |
| 3 | E | 37 | GLY | C-N-CA | -6.14 | 114.45 | 123.05 |
| 2 | H | 224 | ALA | N-CA-C | -6.14 | 104.14 | 111.69 |
| 2 | S | 447 | GLU | CA-C-O | -6.14 | 113.91 | 120.42 |
| 2 | G | 218 | PHE | CA-C-O | -6.13 | 114.34 | 120.90 |
| 2 | S | 313 | VAL | O-C-N | 6.13 | 127.92 | 121.91 |
| 2 | J | 35 | ASP | CA-C-N | -6.13 | 114.36 | 123.00 |
| 2 | J | 35 | ASP | C-N-CA | -6.13 | 114.36 | 123.00 |
| 2 | J | 137 | ASP | CA-C-O | -6.13 | 114.47 | 121.40 |
| 3 | K | 53 | PHE | CA-C-O | -6.13 | 113.92 | 120.42 |
| 2 | C | 319 | ARG | O-C-N | -6.13 | 115.63 | 122.12 |
| 2 | C | 200 | THR | CB-CA-C | 6.12 | 122.17 | 109.38 |
| 2 | G | 327 | HIS | CB-CG-CD2 | 6.12 | 139.16 | 131.20 |
| 2 | H | 45 | GLN | N-CA-C | -6.12 | 101.21 | 110.39 |
| 2 | Q | 213 | ARG | N-CA-C | 6.12 | 119.10 | 110.23 |
| 2 | R | 171 | GLY | CA-C-O | -6.12 | 116.17 | 120.94 |
| 2 | R | 294 | HIS | N-CA-C | 6.12 | 119.86 | 110.20 |
| 2 | I | 181 | SER | CA-C-O | -6.11 | 114.90 | 121.56 |
| 2 | I | 238 | HIS | CB-CG-CD2 | -6.11 | 123.25 | 131.20 |
| 2 | J | 177 | LYS | CA-C-O | -6.11 | 113.19 | 120.10 |
| 2 | Q | 203 | ASP | N-CA-C | -6.11 | 100.94 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 443 | ASP | CA-C-N | 6.11 | 128.25 | 120.56 |
| 2 | H | 443 | ASP | C-N-CA | 6.11 | 128.25 | 120.56 |
| 2 | S | 252 | LYS | CA-C-O | 6.10 | 127.02 | 120.55 |
| 2 | Q | 36 | LEU | CA-C-O | -6.10 | 114.08 | 121.28 |
| 2 | G | 144 | LEU | N-CA-C | 6.10 | 118.00 | 111.36 |
| 3 | O | 84 | ASP | CA-C-O | -6.10 | 112.09 | 119.59 |
| 2 | J | 51 | ASP | N-CA-C | 6.09 | 117.92 | 111.28 |
| 2 | R | 238 | HIS | CG-CD2-NE2 | -6.09 | 101.11 | 107.20 |
| 2 | J | 396 | ASP | N-CA-C | 6.09 | 121.36 | 111.37 |
| 3 | P | 31 | GLU | O-C-N | 6.09 | 129.12 | 122.11 |
| 3 | L | 65 | CYS | O-C-N | -6.09 | 116.28 | 123.22 |
| 2 | S | 120 | ILE | N-CA-C | -6.09 | 104.81 | 110.53 |
| 3 | M | 17 | TYR | CA-C-O | -6.09 | 111.14 | 119.05 |
| 2 | R | 120 | ILE | O-C-N | 6.09 | 128.03 | 121.94 |
| 2 | S | 372 | PRO | CA-C-O | -6.09 | 114.40 | 121.34 |
| 2 | H | 43 | SER | CA-C-N | -6.08 | 114.47 | 120.98 |
| 2 | H | 43 | SER | C-N-CA | -6.08 | 114.47 | 120.98 |
| 2 | I | 56 | ALA | CA-C-O | -6.08 | 114.44 | 120.82 |
| 3 | N | 44 | PHE | CA-C-O | -6.08 | 114.76 | 121.33 |
| 2 | R | 419 | ALA | N-CA-C | -6.08 | 104.73 | 111.36 |
| 2 | G | 246 | THR | CA-C-N | 6.08 | 128.74 | 120.54 |
| 2 | G | 246 | THR | C-N-CA | 6.08 | 128.74 | 120.54 |
| 2 | R | 205 | ASN | CA-C-N | -6.08 | 114.78 | 122.43 |
| 2 | R | 205 | ASN | C-N-CA | -6.08 | 114.78 | 122.43 |
| 2 | H | 202 | ASP | CA-C-O | -6.07 | 114.83 | 121.87 |
| 3 | E | 15 | PHE | CA-C-N | 6.07 | 128.42 | 120.28 |
| 3 | E | 15 | PHE | C-N-CA | 6.07 | 128.42 | 120.28 |
| 2 | S | 264 | ILE | N-CA-C | 6.07 | 116.36 | 108.35 |
| 2 | C | 199 | PHE | N-CA-C | -6.07 | 99.92 | 108.96 |
| 2 | G | 292 | HIS | CG-CD2-NE2 | -6.07 | 101.13 | 107.20 |
| 2 | H | 109 | GLU | N-CA-C | -6.07 | 99.81 | 109.76 |
| 2 | Q | 267 | HIS | CE1-NE2-CD2 | -6.07 | 102.93 | 109.00 |
| 2 | R | 260 | LEU | N-CA-C | 6.06 | 120.36 | 113.15 |
| 2 | R | 293 | ILE | CA-C-N | 6.05 | 130.08 | 121.42 |
| 2 | R | 293 | ILE | C-N-CA | 6.05 | 130.08 | 121.42 |
| 2 | H | 293 | ILE | CA-C-O | -6.05 | 114.10 | 120.39 |
| 3 | K | 30 | ILE | O-C-N | 6.05 | 127.74 | 121.87 |
| 2 | Q | 277 | ASN | OD1-CG-ND2 | -6.05 | 116.55 | 122.60 |
| 2 | H | 401 | GLN | N-CA-C | -6.05 | 99.84 | 109.76 |
| 2 | S | 256 | PHE | CA-C-O | -6.05 | 113.02 | 119.97 |
| 1 | B | 242 | ARG | N-CA-C | -6.04 | 102.73 | 110.53 |
| 2 | G | 339 | LYS | N-CA-C | 6.04 | 121.34 | 111.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 52 | GLU | N-CA-C | -6.04 | 104.26 | 111.69 |
| 2 | J | 363 | PHE | CA-CB-CG | -6.04 | 107.76 | 113.80 |
| 3 | N | 12 | PHE | CA-C-O | 6.04 | 127.78 | 121.38 |
| 3 | M | 39 | HIS | CB-CG-CD2 | -6.03 | 123.36 | 131.20 |
| 2 | C | 402 | PHE | CA-CB-CG | 6.03 | 119.83 | 113.80 |
| 2 | Q | 361 | GLY | N-CA-C | 6.03 | 123.37 | 115.47 |
| 2 | H | 30 | THR | CA-C-N | -6.03 | 113.55 | 119.76 |
| 2 | H | 30 | THR | C-N-CA | -6.03 | 113.55 | 119.76 |
| 2 | I | 140 | PHE | O-C-N | 6.03 | 126.44 | 121.31 |
| 2 | G | 100 | PHE | CA-C-O | -6.03 | 113.91 | 120.36 |
| 2 | Q | 270 | LEU | O-C-N | 6.03 | 128.54 | 122.03 |
| 3 | E | 50 | PRO | N-CA-C | 6.02 | 121.90 | 113.53 |
| 2 | R | 325 | HIS | CA-C-N | 6.02 | 130.55 | 121.40 |
| 2 | R | 325 | HIS | C-N-CA | 6.02 | 130.55 | 121.40 |
| 2 | C | 424 | LEU | CA-C-O | -6.02 | 114.46 | 120.90 |
| 2 | C | 364 | PHE | CA-CB-CG | -6.02 | 107.78 | 113.80 |
| 2 | J | 350 | ARG | N-CA-C | -6.02 | 104.06 | 112.12 |
| 1 | T | 254 | ARG | N-CA-C | 6.02 | 118.61 | 111.33 |
| 1 | F | 236 | LEU | N-CA-C | 6.01 | 117.50 | 111.07 |
| 3 | E | 99 | GLN | OE1-CD-NE2 | -6.01 | 116.59 | 122.60 |
| 2 | Q | 386 | HIS | CA-C-N | 6.01 | 128.32 | 120.26 |
| 2 | Q | 386 | HIS | C-N-CA | 6.01 | 128.32 | 120.26 |
| 2 | R | 364 | PHE | CA-CB-CG | 6.01 | 119.81 | 113.80 |
| 2 | J | 327 | HIS | CA-CB-CG | 6.01 | 119.81 | 113.80 |
| 2 | Q | 208 | SER | CA-C-O | -6.01 | 114.19 | 120.32 |
| 2 | J | 35 | ASP | CA-CB-CG | 6.01 | 118.61 | 112.60 |
| 2 | J | 428 | VAL | N-CA-C | 6.01 | 121.83 | 109.34 |
| 3 | O | 28 | ALA | N-CA-C | 6.01 | 117.91 | 111.36 |
| 1 | A | 262 | ALA | CA-C-N | -6.00 | 113.58 | 119.76 |
| 1 | A | 262 | ALA | C-N-CA | -6.00 | 113.58 | 119.76 |
| 2 | H | 30 | THR | CA-C-O | -6.00 | 114.84 | 119.46 |
| 2 | J | 152 | PRO | N-CA-C | 6.00 | 121.44 | 113.57 |
| 2 | Q | 98 | PHE | CA-CB-CG | -6.00 | 107.80 | 113.80 |
| 2 | Q | 413 | ASN | CA-C-O | -6.00 | 115.02 | 121.38 |
| 2 | H | 241 | ASN | OD1-CG-ND2 | -6.00 | 116.60 | 122.60 |
| 2 | Q | 143 | ALA | CA-C-O | 6.00 | 126.91 | 120.55 |
| 2 | R | 113 | VAL | N-CA-CB | 6.00 | 117.17 | 110.51 |
| 2 | R | 311 | PHE | N-CA-C | 6.00 | 117.82 | 111.28 |
| 2 | S | 209 | GLN | CG-CD-NE2 | -6.00 | 107.41 | 116.40 |
| 2 | R | 432 | ASN | CB-CG-ND2 | 5.99 | 125.39 | 116.40 |
| 2 | H | 363 | PHE | N-CA-C | 5.99 | 119.85 | 112.54 |
| 2 | S | 200 | THR | N-CA-CB | -5.99 | 101.78 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 200 | THR | CB-CA-C | 5.99 | 121.28 | 109.66 |
| 2 | I | 393 | ILE | CB-CA-C | 5.99 | 119.54 | 111.88 |
| 2 | G | 327 | HIS | CB-CG-ND1 | -5.98 | 113.73 | 122.70 |
| 2 | S | 417 | ALA | CA-C-O | -5.98 | 114.55 | 120.82 |
| 2 | G | 439 | ARG | CA-C-O | 5.97 | 126.75 | 120.42 |
| 3 | M | 106 | HIS | ND1-CE1-NE2 | 5.96 | 114.36 | 108.40 |
| 2 | Q | 423 | ALA | O-C-N | 5.96 | 128.44 | 122.12 |
| 2 | C | 364 | PHE | N-CA-C | -5.96 | 99.99 | 109.23 |
| 3 | N | 19 | PRO | CA-C-N | 5.96 | 127.29 | 119.84 |
| 3 | N | 19 | PRO | C-N-CA | 5.96 | 127.29 | 119.84 |
| 2 | G | 393 | ILE | CA-C-N | 5.96 | 130.53 | 120.88 |
| 2 | G | 393 | ILE | C-N-CA | 5.96 | 130.53 | 120.88 |
| 2 | J | 398 | SER | CA-CB-OG | -5.96 | 99.18 | 111.10 |
| 1 | B | 234 | ARG | N-CA-C | 5.96 | 121.14 | 111.37 |
| 2 | Q | 207 | ASN | CA-CB-CG | -5.96 | 106.64 | 112.60 |
| 2 | I | 281 | ALA | O-C-N | 5.95 | 128.28 | 122.09 |
| 2 | H | 287 | ASN | N-CA-C | 5.95 | 121.27 | 113.30 |
| 2 | I | 29 | TYR | N-CA-C | 5.95 | 118.63 | 110.24 |
| 3 | O | 93 | ASP | CA-C-O | -5.95 | 114.92 | 121.58 |
| 2 | C | 107 | LEU | N-CA-C | -5.95 | 105.28 | 112.54 |
| 2 | J | 419 | ALA | N-CA-C | -5.95 | 104.70 | 111.07 |
| 2 | S | 167 | ARG | CA-C-O | -5.95 | 114.61 | 120.26 |
| 2 | I | 190 | TYR | N-CA-C | 5.94 | 118.24 | 111.11 |
| 2 | R | 31 | PRO | CA-C-N | 5.94 | 129.72 | 120.75 |
| 2 | R | 31 | PRO | C-N-CA | 5.94 | 129.72 | 120.75 |
| 1 | A | 273 | LEU | CA-C-O | -5.94 | 114.25 | 120.55 |
| 2 | G | 98 | PHE | CA-C-O | -5.94 | 114.00 | 120.36 |
| 2 | I | 198 | ASP | O-C-N | 5.94 | 128.42 | 122.12 |
| 2 | I | 401 | GLN | CA-C-N | 5.94 | 130.57 | 122.19 |
| 2 | I | 401 | GLN | C-N-CA | 5.94 | 130.57 | 122.19 |
| 2 | J | 58 | ALA | N-CA-C | 5.94 | 117.43 | 111.07 |
| 2 | J | 191 | GLU | O-C-N | 5.94 | 128.19 | 122.07 |
| 2 | H | 317 | CYS | N-CA-C | 5.94 | 117.75 | 111.28 |
| 2 | R | 387 | MET | CA-C-O | -5.94 | 112.58 | 118.34 |
| 2 | H | 70 | TRP | N-CA-C | -5.93 | 104.89 | 111.71 |
| 3 | M | 53 | PHE | CA-C-N | -5.93 | 114.04 | 122.94 |
| 3 | M | 53 | PHE | C-N-CA | -5.93 | 114.04 | 122.94 |
| 2 | Q | 270 | LEU | CA-C-O | -5.93 | 114.79 | 120.90 |
| 2 | G | 226 | HIS | CB-CG-CD2 | 5.93 | 138.91 | 131.20 |
| 2 | J | 35 | ASP | O-C-N | 5.93 | 129.68 | 122.68 |
| 1 | T | 278 | ASN | OD1-CG-ND2 | -5.93 | 116.67 | 122.60 |
| 2 | C | 377 | VAL | CA-C-O | -5.93 | 114.08 | 120.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | M | 70 | GLN | CG-CD-NE2 | 5.93 | 125.29 | 116.40 |
| 3 | O | 72 | LEU | N-CA-C | 5.93 | 118.22 | 111.11 |
| 2 | H | 279 | THR | CA-CB-OG1 | -5.92 | 100.72 | 109.60 |
| 2 | H | 109 | GLU | CA-C-N | 5.92 | 129.78 | 121.02 |
| 2 | H | 109 | GLU | C-N-CA | 5.92 | 129.78 | 121.02 |
| 2 | H | 238 | HIS | CA-CB-CG | 5.92 | 119.72 | 113.80 |
| 3 | N | 31 | GLU | CA-C-O | -5.92 | 114.56 | 121.07 |
| 2 | R | 61 | SER | N-CA-C | 5.91 | 120.22 | 112.89 |
| 2 | C | 278 | THR | N-CA-C | -5.91 | 104.84 | 111.28 |
| 2 | C | 440 | GLU | CB-CG-CD | -5.91 | 102.55 | 112.60 |
| 2 | H | 356 | ALA | N-CA-C | -5.91 | 101.29 | 110.10 |
| 2 | J | 420 | ASN | CA-C-N | 5.91 | 128.12 | 120.44 |
| 2 | J | 420 | ASN | C-N-CA | 5.91 | 128.12 | 120.44 |
| 2 | Q | 241 | ASN | N-CA-C | -5.91 | 101.53 | 110.28 |
| 2 | S | 166 | GLY | N-CA-C | 5.91 | 124.00 | 114.90 |
| 2 | R | 427 | CYS | O-C-N | 5.91 | 128.16 | 122.07 |
| 2 | J | 111 | GLY | N-CA-C | 5.91 | 123.21 | 115.47 |
| 3 | L | 44 | PHE | CA-CB-CG | -5.91 | 107.89 | 113.80 |
| 2 | J | 270 | LEU | O-C-N | 5.90 | 128.15 | 122.07 |
| 3 | N | 28 | ALA | O-C-N | -5.90 | 115.86 | 122.12 |
| 2 | J | 85 | TYR | N-CA-C | 5.90 | 120.64 | 113.38 |
| 1 | T | 243 | ILE | CB-CA-C | 5.90 | 119.78 | 110.81 |
| 2 | H | 262 | MET | O-C-N | 5.90 | 127.18 | 121.28 |
| 2 | G | 294 | HIS | N-CA-C | 5.90 | 119.33 | 109.95 |
| 1 | B | 252 | ARG | CA-C-O | 5.89 | 126.80 | 120.55 |
| 2 | H | 120 | ILE | O-C-N | 5.89 | 127.90 | 121.83 |
| 2 | G | 220 | PHE | CA-CB-CG | 5.89 | 119.69 | 113.80 |
| 2 | R | 402 | PHE | CA-CB-CG | 5.89 | 119.69 | 113.80 |
| 2 | Q | 371 | MET | CA-C-O | -5.89 | 114.96 | 119.32 |
| 3 | D | 64 | ASP | CA-C-N | 5.89 | 130.25 | 122.30 |
| 3 | D | 64 | ASP | C-N-CA | 5.89 | 130.25 | 122.30 |
| 2 | I | 384 | VAL | CA-C-O | -5.89 | 114.22 | 120.64 |
| 2 | Q | 177 | LYS | CA-C-O | -5.89 | 113.45 | 120.10 |
| 2 | H | 305 | ARG | N-CA-C | 5.88 | 120.32 | 113.20 |
| 2 | J | 256 | PHE | CA-C-O | -5.88 | 114.18 | 120.42 |
| 2 | Q | 189 | VAL | N-CA-C | 5.88 | 116.54 | 110.36 |
| 1 | A | 279 | CYS | CA-C-O | 5.88 | 126.78 | 120.55 |
| 2 | C | 248 | GLU | CB-CG-CD | 5.88 | 122.60 | 112.60 |
| 2 | J | 218 | PHE | CA-CB-CG | 5.88 | 119.68 | 113.80 |
| 2 | H | 37 | LEU | CD1-CG-CD2 | 5.88 | 123.74 | 110.80 |
| 2 | C | 90 | VAL | N-CA-CB | 5.88 | 117.12 | 110.72 |
| 2 | I | 215 | ARG | N-CA-C | -5.88 | 104.95 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 238 | HIS | N-CA-C | -5.88 | 99.07 | 109.06 |
| 2 | S | 125 | PHE | CA-C-O | -5.88 | 113.62 | 120.20 |
| 2 | R | 309 | ILE | O-C-N | -5.88 | 117.15 | 123.14 |
| 3 | P | 26 | ILE | N-CA-C | -5.87 | 104.63 | 110.62 |
| 3 | N | 60 | LEU | CB-CA-C | -5.87 | 103.60 | 110.76 |
| 2 | S | 353 | HIS | CB-CG-CD2 | 5.87 | 138.83 | 131.20 |
| 2 | S | 293 | ILE | CB-CA-C | 5.87 | 119.31 | 110.63 |
| 2 | S | 460 | ASP | N-CA-C | -5.87 | 105.38 | 112.54 |
| 3 | E | 75 | VAL | CB-CA-C | 5.87 | 119.39 | 111.88 |
| 1 | A | 266 | SER | CA-C-O | -5.86 | 113.33 | 120.54 |
| 2 | G | 329 | GLY | CA-C-O | 5.86 | 126.28 | 122.23 |
| 2 | H | 83 | LYS | CA-C-O | -5.86 | 114.09 | 120.36 |
| 3 | P | 94 | ASN | CA-CB-CG | -5.86 | 106.74 | 112.60 |
| 2 | C | 280 | LEU | CA-C-N | 5.86 | 128.13 | 120.28 |
| 2 | C | 280 | LEU | C-N-CA | 5.86 | 128.13 | 120.28 |
| 1 | T | 283 | HIS | CE1-NE2-CD2 | -5.86 | 103.14 | 109.00 |
| 2 | C | 429 | GLN | O-C-N | 5.86 | 128.10 | 122.07 |
| 2 | R | 318 | LEU | CA-C-O | -5.86 | 114.87 | 120.90 |
| 2 | I | 256 | PHE | N-CA-C | -5.85 | 104.85 | 112.23 |
| 2 | Q | 243 | THR | CA-CB-OG1 | -5.85 | 100.82 | 109.60 |
| 2 | R | 81 | LYS | N-CA-C | 5.85 | 119.62 | 110.32 |
| 2 | C | 220 | PHE | O-C-N | 5.85 | 128.09 | 122.07 |
| 2 | C | 294 | HIS | CA-CB-CG | 5.85 | 119.65 | 113.80 |
| 2 | I | 417 | ALA | CA-C-O | -5.85 | 114.67 | 120.70 |
| 2 | Q | 153 | HIS | ND1-CG-CD2 | -5.85 | 100.25 | 106.10 |
| 2 | I | 105 | LEU | CA-C-O | -5.85 | 112.42 | 119.49 |
| 2 | Q | 383 | HIS | N-CA-C | 5.85 | 119.17 | 111.28 |
| 2 | C | 241 | ASN | OD1-CG-ND2 | -5.84 | 116.76 | 122.60 |
| 3 | K | 16 | SER | CA-C-O | 5.84 | 126.70 | 120.10 |
| 2 | S | 357 | ASP | O-C-N | -5.84 | 116.80 | 123.40 |
| 2 | Q | 43 | SER | CA-C-N | 5.83 | 125.77 | 119.76 |
| 2 | Q | 43 | SER | C-N-CA | 5.83 | 125.77 | 119.76 |
| 2 | I | 310 | HIS | N-CA-C | -5.83 | 101.85 | 110.48 |
| 1 | A | 294 | ASP | CA-C-O | -5.83 | 114.48 | 120.54 |
| 2 | I | 285 | ARG | O-C-N | 5.83 | 128.15 | 122.09 |
| 2 | Q | 61 | SER | N-CA-C | 5.83 | 121.30 | 113.72 |
| 2 | C | 376 | PRO | N-CA-C | -5.83 | 102.71 | 111.57 |
| 3 | K | 39 | HIS | ND1-CG-CD2 | -5.83 | 100.27 | 106.10 |
| 2 | R | 327 | HIS | CA-CB-CG | -5.83 | 107.97 | 113.80 |
| 2 | J | 225 | ILE | CA-C-O | -5.82 | 115.00 | 121.17 |
| 2 | S | 216 | ASP | CA-CB-CG | -5.82 | 106.78 | 112.60 |
| 3 | O | 65 | CYS | N-CA-C | 5.82 | 118.69 | 109.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 79 | ARG | CA-C-O | -5.82 | 112.74 | 119.61 |
| 2 | C | 98 | PHE | CA-CB-CG | -5.82 | 107.98 | 113.80 |
| 2 | R | 167 | ARG | CA-C-O | -5.82 | 115.13 | 120.13 |
| 1 | B | 293 | ILE | O-C-N | -5.81 | 116.92 | 123.20 |
| 2 | Q | 235 | ILE | O-C-N | 5.81 | 128.79 | 122.63 |
| 2 | H | 51 | ASP | N-CA-C | 5.81 | 118.39 | 111.71 |
| 2 | Q | 349 | MET | CA-C-O | -5.81 | 112.11 | 119.31 |
| 1 | T | 305 | LEU | N-CA-C | -5.81 | 99.27 | 108.73 |
| 2 | G | 153 | HIS | CB-CG-ND1 | -5.80 | 113.99 | 122.70 |
| 2 | G | 311 | PHE | CA-CB-CG | -5.80 | 108.00 | 113.80 |
| 2 | H | 341 | SER | N-CA-C | 5.80 | 119.18 | 111.75 |
| 2 | G | 304 | GLN | N-CA-C | -5.80 | 99.73 | 108.96 |
| 2 | R | 354 | ILE | N-CA-CB | -5.80 | 102.70 | 112.44 |
| 2 | C | 375 | LEU | N-CA-C | 5.79 | 116.95 | 109.65 |
| 3 | L | 44 | PHE | CA-C-O | 5.79 | 127.43 | 121.23 |
| 2 | H | 225 | ILE | CA-C-O | -5.79 | 114.62 | 121.05 |
| 2 | Q | 264 | ILE | CA-C-O | -5.79 | 115.14 | 121.28 |
| 2 | Q | 298 | HIS | ND1-CG-CD2 | 5.79 | 111.89 | 106.10 |
| 2 | S | 184 | ASN | CA-CB-CG | -5.79 | 106.81 | 112.60 |
| 2 | H | 137 | ASP | CA-C-O | -5.79 | 115.08 | 121.33 |
| 2 | Q | 305 | ARG | O-C-N | 5.79 | 128.25 | 122.12 |
| 1 | F | 286 | GLU | CB-CG-CD | -5.79 | 102.77 | 112.60 |
| 3 | P | 27 | ALA | N-CA-C | 5.79 | 117.59 | 111.28 |
| 2 | R | 41 | ARG | O-C-N | -5.79 | 116.42 | 122.96 |
| 3 | E | 32 | TYR | CA-C-O | -5.78 | 114.75 | 120.82 |
| 2 | J | 305 | ARG | CA-C-O | -5.78 | 112.44 | 119.43 |
| 2 | I | 97 | TYR | N-CA-C | -5.78 | 100.35 | 108.96 |
| 2 | Q | 165 | TYR | CA-C-O | 5.78 | 127.76 | 121.06 |
| 3 | O | 19 | PRO | CA-C-O | -5.78 | 112.18 | 120.56 |
| 3 | P | 69 | GLN | CB-CG-CD | -5.78 | 102.78 | 112.60 |
| 2 | S | 417 | ALA | N-CA-C | -5.78 | 104.89 | 111.07 |
| 2 | J | 243 | THR | CB-CA-C | -5.77 | 101.85 | 110.16 |
| 3 | M | 95 | ILE | N-CA-CB | 5.77 | 117.30 | 110.55 |
| 2 | Q | 163 | ASN | CB-CG-ND2 | -5.77 | 107.74 | 116.40 |
| 2 | Q | 320 | LEU | N-CA-C | 5.77 | 117.25 | 111.07 |
| 3 | K | 13 | GLU | N-CA-C | 5.77 | 117.65 | 111.36 |
| 2 | I | 329 | GLY | N-CA-C | -5.77 | 105.35 | 112.33 |
| 3 | K | 78 | CYS | CA-C-O | -5.77 | 114.31 | 120.42 |
| 3 | L | 69 | GLN | N-CA-C | -5.77 | 105.13 | 111.82 |
| 2 | G | 74 | LEU | N-CA-CB | -5.77 | 102.11 | 110.47 |
| 2 | J | 32 | LYS | CA-C-N | 5.77 | 128.01 | 120.28 |
| 2 | J | 32 | LYS | C-N-CA | 5.77 | 128.01 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | N | 97 | GLN | OE1-CD-NE2 | -5.77 | 116.83 | 122.60 |
| 2 | R | 275 | THR | CA-C-N | 5.77 | 128.01 | 120.28 |
| 2 | R | 275 | THR | C-N-CA | 5.77 | 128.01 | 120.28 |
| 2 | C | 234 | GLU | CB-CG-CD | 5.77 | 122.40 | 112.60 |
| 1 | T | 227 | SER | O-C-N | -5.76 | 116.14 | 122.07 |
| 2 | I | 108 | PHE | N-CA-C | -5.76 | 100.40 | 109.50 |
| 2 | S | 383 | HIS | CA-C-O | -5.76 | 114.83 | 122.03 |
| 2 | G | 303 | ARG | N-CA-C | 5.76 | 119.40 | 112.38 |
| 2 | Q | 42 | PHE | N-CA-C | -5.76 | 100.02 | 109.40 |
| 2 | Q | 267 | HIS | CA-C-N | 5.75 | 130.06 | 121.72 |
| 2 | Q | 267 | HIS | C-N-CA | 5.75 | 130.06 | 121.72 |
| 2 | G | 342 | THR | CA-C-O | 5.75 | 127.40 | 121.07 |
| 2 | H | 342 | THR | CA-C-O | 5.75 | 126.86 | 120.82 |
| 2 | J | 226 | HIS | ND1-CE1-NE2 | 5.75 | 114.15 | 108.40 |
| 2 | J | 294 | HIS | N-CA-C | 5.75 | 118.94 | 109.85 |
| 2 | C | 317 | CYS | N-CA-C | 5.75 | 117.22 | 111.07 |
| 3 | D | 84 | ASP | CA-C-O | -5.75 | 112.73 | 120.15 |
| 2 | C | 207 | ASN | N-CA-C | 5.75 | 119.82 | 112.12 |
| 2 | Q | 268 | ASP | N-CA-C | 5.75 | 118.04 | 109.25 |
| 2 | S | 58 | ALA | CA-C-O | -5.75 | 114.79 | 120.82 |
| 2 | S | 304 | GLN | N-CA-CB | 5.75 | 118.42 | 109.97 |
| 2 | G | 251 | MET | CA-C-O | -5.75 | 114.97 | 121.00 |
| 2 | S | 274 | PHE | CA-C-O | -5.75 | 113.06 | 119.67 |
| 3 | M | 48 | SER | CA-CB-OG | -5.74 | 99.61 | 111.10 |
| 2 | R | 46 | PRO | CB-CA-C | 5.74 | 118.87 | 111.46 |
| 2 | R | 202 | ASP | CA-CB-CG | 5.74 | 118.34 | 112.60 |
| 2 | Q | 452 | SER | O-C-N | 5.74 | 126.67 | 121.04 |
| 2 | H | 203 | ASP | N-CA-C | -5.74 | 100.32 | 109.96 |
| 2 | I | 422 | VAL | N-CA-C | -5.74 | 104.26 | 110.23 |
| 3 | M | 13 | GLU | O-C-N | 5.74 | 128.06 | 122.09 |
| 2 | Q | 181 | SER | CA-C-O | -5.73 | 115.47 | 121.55 |
| 2 | Q | 205 | ASN | CA-C-O | -5.73 | 114.35 | 120.42 |
| 3 | K | 18 | LEU | N-CA-C | -5.73 | 102.69 | 110.36 |
| 2 | J | 286 | ASP | N-CA-C | 5.72 | 119.78 | 112.34 |
| 2 | C | 139 | ARG | CB-CA-C | -5.72 | 101.53 | 110.74 |
| 3 | L | 26 | ILE | N-CA-CB | -5.72 | 103.86 | 110.55 |
| 2 | Q | 418 | THR | CA-C-O | -5.72 | 114.81 | 120.82 |
| 2 | G | 137 | ASP | CA-CB-CG | 5.72 | 118.32 | 112.60 |
| 3 | D | 71 | VAL | CB-CA-C | -5.72 | 104.33 | 112.22 |
| 3 | P | 15 | PHE | N-CA-C | 5.72 | 120.07 | 113.38 |
| 2 | Q | 158 | GLU | O-C-N | 5.72 | 128.20 | 122.08 |
| 2 | R | 31 | PRO | CB-CA-C | -5.72 | 104.54 | 111.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | K | 34 | ILE | O-C-N | -5.72 | 116.29 | 121.89 |
| 2 | H | 240 | LEU | CA-C-O | -5.71 | 114.50 | 121.36 |
| 2 | G | 348 | LEU | CA-C-O | -5.71 | 114.49 | 120.55 |
| 2 | S | 350 | ARG | CB-CA-C | -5.71 | 101.80 | 110.83 |
| 3 | O | 73 | ASP | CA-CB-CG | -5.71 | 106.89 | 112.60 |
| 2 | S | 88 | GLU | O-C-N | -5.71 | 117.83 | 121.88 |
| 2 | J | 229 | GLN | N-CA-C | 5.71 | 118.28 | 111.71 |
| 2 | J | 198 | ASP | CA-C-O | -5.71 | 113.18 | 120.31 |
| 2 | R | 447 | GLU | N-CA-CB | 5.71 | 118.51 | 110.12 |
| 1 | B | 307 | GLN | CB-CG-CD | 5.70 | 122.30 | 112.60 |
| 2 | Q | 385 | TRP | N-CA-C | 5.70 | 119.98 | 113.19 |
| 2 | R | 51 | ASP | CA-CB-CG | 5.70 | 118.30 | 112.60 |
| 2 | C | 162 | LEU | N-CA-C | 5.70 | 119.33 | 112.38 |
| 1 | F | 278 | ASN | OD1-CG-ND2 | -5.70 | 116.90 | 122.60 |
| 2 | J | 147 | THR | CA-C-O | 5.70 | 126.58 | 120.20 |
| 3 | N | 46 | GLU | N-CA-C | 5.70 | 119.33 | 112.38 |
| 2 | R | 205 | ASN | N-CA-C | -5.70 | 105.21 | 111.82 |
| 2 | H | 343 | LEU | N-CA-C | -5.70 | 105.07 | 111.28 |
| 3 | O | 62 | LEU | N-CA-CB | -5.70 | 102.88 | 110.57 |
| 2 | G | 238 | HIS | N-CA-C | 5.70 | 119.10 | 109.76 |
| 1 | A | 307 | GLN | CB-CG-CD | 5.70 | 122.28 | 112.60 |
| 2 | R | 432 | ASN | OD1-CG-ND2 | -5.70 | 116.90 | 122.60 |
| 3 | L | 57 | MET | N-CA-C | -5.69 | 102.06 | 110.48 |
| 3 | D | 90 | ALA | N-CA-C | 5.69 | 119.00 | 109.95 |
| 3 | E | 74 | GLU | N-CA-C | 5.69 | 117.48 | 111.28 |
| 2 | C | 142 | VAL | N-CA-C | 5.69 | 117.11 | 110.62 |
| 2 | H | 399 | VAL | N-CA-C | -5.69 | 100.14 | 108.11 |
| 2 | S | 441 | GLY | CA-C-N | -5.69 | 113.67 | 119.98 |
| 2 | S | 441 | GLY | C-N-CA | -5.69 | 113.67 | 119.98 |
| 3 | O | 36 | GLN | CB-CG-CD | 5.69 | 122.27 | 112.60 |
| 2 | I | 48 | VAL | N-CA-C | -5.68 | 101.25 | 107.73 |
| 2 | Q | 136 | GLU | N-CA-C | -5.68 | 105.12 | 112.68 |
| 2 | Q | 330 | THR | N-CA-C | 5.68 | 117.55 | 111.36 |
| 2 | C | 345 | PHE | CA-CB-CG | 5.68 | 119.48 | 113.80 |
| 3 | E | 87 | ILE | N-CA-C | -5.68 | 100.49 | 108.27 |
| 1 | F | 239 | GLN | OE1-CD-NE2 | -5.68 | 116.92 | 122.60 |
| 2 | I | 57 | ILE | N-CA-C | -5.67 | 104.40 | 110.36 |
| 2 | R | 51 | ASP | N-CA-C | 5.67 | 117.47 | 111.28 |
| 1 | T | 276 | LEU | N-CA-C | 5.67 | 117.47 | 111.28 |
| 2 | S | 454 | GLU | CA-C-O | -5.67 | 113.94 | 120.24 |
| 1 | A | 250 | LYS | CA-C-N | 5.67 | 127.81 | 120.44 |
| 1 | A | 250 | LYS | C-N-CA | 5.67 | 127.81 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 260 | PRO | CB-CA-C | -5.67 | 103.97 | 111.23 |
| 2 | H | 354 | ILE | CB-CA-C | 5.67 | 118.82 | 110.77 |
| 3 | L | 53 | PHE | O-C-N | 5.67 | 128.13 | 122.12 |
| 2 | H | 212 | GLN | CB-CA-C | -5.67 | 102.91 | 110.79 |
| 2 | G | 122 | GLY | CA-C-O | -5.67 | 114.66 | 120.66 |
| 3 | L | 64 | ASP | N-CA-C | -5.67 | 102.81 | 110.68 |
| 2 | R | 159 | ARG | CA-C-N | 5.66 | 127.80 | 120.44 |
| 2 | R | 159 | ARG | C-N-CA | 5.66 | 127.80 | 120.44 |
| 2 | G | 439 | ARG | N-CA-C | 5.66 | 117.53 | 111.36 |
| 2 | J | 361 | GLY | N-CA-C | 5.66 | 123.06 | 115.59 |
| 2 | S | 211 | PHE | CA-CB-CG | -5.66 | 108.14 | 113.80 |
| 2 | R | 238 | HIS | CA-CB-CG | 5.66 | 119.46 | 113.80 |
| 3 | D | 72 | LEU | N-CA-C | 5.66 | 117.90 | 111.11 |
| 2 | H | 271 | THR | N-CA-C | -5.66 | 104.59 | 112.45 |
| 2 | R | 56 | ALA | CA-C-N | 5.66 | 128.18 | 120.77 |
| 2 | R | 56 | ALA | C-N-CA | 5.66 | 128.18 | 120.77 |
| 2 | G | 101 | ILE | N-CA-C | -5.65 | 99.98 | 108.12 |
| 2 | G | 302 | ASP | CA-CB-CG | 5.65 | 118.25 | 112.60 |
| 2 | G | 326 | LEU | N-CA-C | 5.65 | 116.99 | 108.46 |
| 2 | I | 41 | ARG | N-CA-C | -5.65 | 100.08 | 109.46 |
| 2 | S | 179 | GLY | O-C-N | -5.65 | 116.77 | 122.65 |
| 2 | Q | 364 | PHE | N-CA-C | -5.65 | 101.33 | 108.45 |
| 2 | Q | 431 | ARG | O-C-N | 5.65 | 127.89 | 122.07 |
| 1 | A | 233 | VAL | CA-C-N | 5.65 | 128.16 | 120.54 |
| 1 | A | 233 | VAL | C-N-CA | 5.65 | 128.16 | 120.54 |
| 2 | I | 196 | GLY | CA-C-N | 5.65 | 128.85 | 120.95 |
| 2 | I | 196 | GLY | C-N-CA | 5.65 | 128.85 | 120.95 |
| 2 | I | 348 | LEU | N-CA-CB | 5.65 | 118.20 | 110.01 |
| 2 | C | 177 | LYS | CA-C-O | -5.64 | 114.86 | 121.07 |
| 2 | H | 79 | ARG | O-C-N | 5.64 | 128.10 | 122.12 |
| 2 | I | 37 | LEU | N-CA-C | -5.64 | 100.20 | 109.40 |
| 3 | O | 95 | ILE | N-CA-C | 5.64 | 116.30 | 110.82 |
| 2 | I | 431 | ARG | CA-C-O | -5.64 | 113.73 | 120.10 |
| 2 | Q | 378 | ALA | CA-C-O | -5.64 | 114.54 | 120.80 |
| 1 | F | 283 | HIS | CB-CA-C | -5.63 | 101.83 | 111.46 |
| 2 | R | 345 | PHE | CA-CB-CG | 5.63 | 119.44 | 113.80 |
| 3 | N | 39 | HIS | CB-CG-CD2 | -5.63 | 123.88 | 131.20 |
| 2 | R | 121 | VAL | O-C-N | -5.63 | 115.53 | 122.57 |
| 1 | A | 238 | ASN | N-CA-C | 5.63 | 117.42 | 111.28 |
| 1 | F | 287 | TYR | N-CA-C | 5.63 | 118.52 | 110.24 |
| 2 | J | 226 | HIS | CB-CA-C | -5.63 | 101.80 | 110.81 |
| 3 | K | 106 | HIS | CE1-NE2-CD2 | -5.63 | 103.37 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | O | 74 | GLU | N-CA-C | 5.63 | 118.14 | 111.33 |
| 2 | Q | 34 | THR | N-CA-C | 5.63 | 120.14 | 113.16 |
| 2 | S | 149 | GLN | N-CA-C | 5.63 | 118.14 | 111.33 |
| 2 | J | 384 | VAL | CA-C-N | 5.63 | 127.82 | 120.28 |
| 2 | J | 384 | VAL | C-N-CA | 5.63 | 127.82 | 120.28 |
| 2 | S | 80 | TYR | CA-C-O | -5.63 | 113.89 | 120.53 |
| 2 | G | 163 | ASN | CB-CG-ND2 | -5.63 | 107.96 | 116.40 |
| 2 | G | 203 | ASP | N-CA-C | -5.63 | 102.69 | 110.35 |
| 2 | G | 178 | LEU | N-CA-C | -5.62 | 100.93 | 108.86 |
| 2 | I | 24 | TYR | CB-CA-C | -5.62 | 101.63 | 110.85 |
| 3 | M | 15 | PHE | CA-C-N | 5.62 | 128.08 | 120.38 |
| 3 | M | 15 | PHE | C-N-CA | 5.62 | 128.08 | 120.38 |
| 2 | R | 283 | TRP | N-CA-C | -5.62 | 105.06 | 111.07 |
| 2 | H | 280 | LEU | CD1-CG-CD2 | 5.62 | 123.16 | 110.80 |
| 2 | J | 291 | LEU | CA-C-O | -5.62 | 113.34 | 120.20 |
| 3 | O | 85 | CYS | CA-C-N | 5.62 | 128.82 | 120.90 |
| 3 | O | 85 | CYS | C-N-CA | 5.62 | 128.82 | 120.90 |
| 2 | I | 36 | LEU | CA-C-N | -5.62 | 114.52 | 122.94 |
| 2 | I | 36 | LEU | C-N-CA | -5.62 | 114.52 | 122.94 |
| 3 | L | 99 | GLN | CB-CA-C | 5.62 | 117.87 | 110.06 |
| 2 | S | 114 | THR | N-CA-C | -5.62 | 105.06 | 111.07 |
| 2 | S | 372 | PRO | CB-CA-C | -5.62 | 104.22 | 111.46 |
| 2 | S | 205 | ASN | CA-CB-CG | -5.61 | 106.99 | 112.60 |
| 2 | S | 293 | ILE | CA-C-O | -5.61 | 114.50 | 120.39 |
| 2 | H | 320 | LEU | N-CA-C | 5.61 | 117.87 | 111.02 |
| 3 | P | 86 | TYR | N-CA-C | -5.61 | 101.14 | 110.17 |
| 2 | H | 180 | LEU | CD1-CG-CD2 | -5.61 | 98.46 | 110.80 |
| 3 | M | 39 | HIS | CA-CB-CG | -5.61 | 108.19 | 113.80 |
| 2 | I | 383 | HIS | CA-C-O | -5.61 | 115.02 | 122.03 |
| 2 | R | 39 | ALA | CA-C-O | -5.61 | 114.15 | 120.43 |
| 2 | I | 249 | GLU | N-CA-C | 5.60 | 120.62 | 111.37 |
| 2 | J | 53 | ALA | CA-C-O | -5.60 | 115.12 | 121.00 |
| 2 | R | 30 | THR | CA-C-O | -5.60 | 112.72 | 119.67 |
| 2 | J | 81 | LYS | N-CA-C | -5.60 | 101.42 | 110.32 |
| 3 | K | 74 | GLU | CA-C-O | 5.60 | 126.89 | 120.90 |
| 2 | H | 287 | ASN | CA-CB-CG | 5.60 | 118.20 | 112.60 |
| 2 | R | 267 | HIS | CA-C-O | -5.59 | 115.08 | 121.40 |
| 2 | G | 369 | ALA | CA-C-O | -5.59 | 115.35 | 121.84 |
| 2 | Q | 246 | THR | N-CA-CB | -5.59 | 101.82 | 111.55 |
| 2 | J | 430 | ALA | N-CA-C | -5.59 | 105.10 | 111.14 |
| 3 | D | 99 | GLN | CG-CD-NE2 | 5.59 | 124.78 | 116.40 |
| 2 | J | 52 | GLU | N-CA-C | -5.59 | 104.82 | 111.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | S | 24 | TYR | O-C-N | 5.59 | 128.76 | 122.22 |
| 2 | H | 101 | ILE | CB-CA-C | 5.59 | 118.48 | 110.33 |
| 3 | P | 80 | SER | N-CA-C | -5.59 | 105.09 | 111.07 |
| 2 | R | 327 | HIS | ND1-CG-CD2 | -5.59 | 100.51 | 106.10 |
| 2 | C | 128 | LYS | N-CA-C | 5.58 | 117.17 | 111.14 |
| 2 | G | 401 | GLN | CB-CG-CD | -5.58 | 103.11 | 112.60 |
| 3 | K | 71 | VAL | CB-CA-C | -5.58 | 104.76 | 112.24 |
| 2 | G | 217 | ARG | N-CA-C | 5.58 | 117.83 | 111.02 |
| 3 | N | 38 | PHE | CA-CB-CG | 5.58 | 119.38 | 113.80 |
| 2 | S | 120 | ILE | N-CA-CB | 5.58 | 117.71 | 110.57 |
| 2 | Q | 371 | MET | O-C-N | 5.58 | 126.48 | 121.35 |
| 3 | K | 105 | VAL | N-CA-C | 5.58 | 119.10 | 113.47 |
| 2 | C | 205 | ASN | CA-C-N | -5.58 | 116.18 | 122.93 |
| 2 | C | 205 | ASN | C-N-CA | -5.58 | 116.18 | 122.93 |
| 2 | H | 106 | ASP | CA-C-O | -5.57 | 112.75 | 119.49 |
| 2 | C | 116 | ILE | CB-CG1-CD1 | 5.57 | 125.50 | 113.80 |
| 1 | B | 287 | TYR | O-C-N | 5.57 | 129.35 | 123.11 |
| 2 | J | 374 | VAL | CA-C-N | -5.57 | 113.14 | 121.83 |
| 2 | J | 374 | VAL | C-N-CA | -5.57 | 113.14 | 121.83 |
| 2 | S | 182 | ALA | CA-C-N | -5.57 | 113.20 | 120.44 |
| 2 | S | 182 | ALA | C-N-CA | -5.57 | 113.20 | 120.44 |
| 2 | S | 228 | SER | CA-C-O | -5.57 | 114.94 | 120.90 |
| 2 | H | 238 | HIS | ND1-CE1-NE2 | -5.57 | 102.83 | 108.40 |
| 2 | H | 45 | GLN | OE1-CD-NE2 | 5.57 | 128.17 | 122.60 |
| 2 | H | 209 | GLN | OE1-CD-NE2 | 5.57 | 128.17 | 122.60 |
| 3 | D | 71 | VAL | N-CA-C | -5.56 | 105.10 | 110.72 |
| 2 | J | 312 | ARG | CA-C-O | -5.56 | 114.98 | 120.82 |
| 3 | L | 25 | GLN | O-C-N | 5.56 | 127.80 | 122.07 |
| 3 | E | 79 | ARG | CA-C-N | 5.56 | 127.67 | 120.44 |
| 3 | E | 79 | ARG | C-N-CA | 5.56 | 127.67 | 120.44 |
| 2 | G | 62 | SER | O-C-N | 5.56 | 128.93 | 122.09 |
| 3 | O | 75 | VAL | N-CA-C | -5.56 | 103.99 | 111.44 |
| 1 | F | 302 | PHE | CA-C-N | 5.56 | 130.83 | 122.99 |
| 1 | F | 302 | PHE | C-N-CA | 5.56 | 130.83 | 122.99 |
| 2 | G | 387 | MET | CA-C-O | -5.56 | 113.28 | 118.73 |
| 2 | C | 417 | ALA | N-CA-C | -5.56 | 105.14 | 111.14 |
| 2 | G | 114 | THR | CA-C-N | 5.56 | 127.73 | 120.28 |
| 2 | G | 114 | THR | C-N-CA | 5.56 | 127.73 | 120.28 |
| 2 | G | 116 | ILE | N-CA-C | 5.56 | 115.69 | 110.30 |
| 2 | G | 73 | LEU | CD1-CG-CD2 | 5.56 | 123.03 | 110.80 |
| 2 | Q | 156 | GLN | OE1-CD-NE2 | -5.56 | 117.04 | 122.60 |
| 2 | H | 197 | LEU | N-CA-CB | -5.55 | 101.58 | 109.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 31 | PRO | N-CA-CB | -5.55 | 98.75 | 103.36 |
| 2 | R | 117 | LEU | N-CA-C | -5.55 | 105.31 | 111.36 |
| 2 | R | 125 | PHE | N-CA-C | 5.55 | 118.85 | 111.75 |
| 2 | G | 165 | TYR | N-CA-C | -5.55 | 100.64 | 109.07 |
| 2 | G | 383 | HIS | CA-C-N | 5.55 | 129.72 | 120.62 |
| 2 | G | 383 | HIS | C-N-CA | 5.55 | 129.72 | 120.62 |
| 2 | R | 212 | GLN | CB-CG-CD | -5.55 | 103.17 | 112.60 |
| 1 | A | 271 | GLN | N-CA-C | -5.54 | 105.15 | 111.14 |
| 2 | I | 244 | ALA | CA-C-O | -5.54 | 115.40 | 120.50 |
| 2 | C | 360 | ARG | CA-C-N | 5.54 | 129.88 | 120.91 |
| 2 | C | 360 | ARG | C-N-CA | 5.54 | 129.88 | 120.91 |
| 2 | I | 427 | CYS | N-CA-C | 5.54 | 117.40 | 111.36 |
| 2 | J | 419 | ALA | CA-C-O | -5.54 | 115.00 | 120.82 |
| 2 | H | 163 | ASN | CA-CB-CG | 5.54 | 118.14 | 112.60 |
| 2 | Q | 417 | ALA | N-CA-C | -5.54 | 105.25 | 111.28 |
| 2 | C | 79 | ARG | CA-C-O | -5.53 | 112.79 | 119.49 |
| 2 | G | 327 | HIS | CE1-NE2-CD2 | -5.53 | 103.47 | 109.00 |
| 2 | H | 268 | ASP | CA-CB-CG | 5.53 | 118.13 | 112.60 |
| 2 | R | 293 | ILE | CB-CA-C | 5.53 | 118.63 | 110.77 |
| 2 | R | 417 | ALA | CA-C-O | -5.53 | 114.56 | 120.42 |
| 2 | C | 119 | SER | CA-C-N | -5.53 | 113.48 | 120.56 |
| 2 | C | 119 | SER | C-N-CA | -5.53 | 113.48 | 120.56 |
| 2 | I | 256 | PHE | CA-CB-CG | -5.53 | 108.27 | 113.80 |
| 2 | Q | 309 | ILE | N-CA-C | -5.53 | 99.72 | 108.90 |
| 2 | G | 212 | GLN | OE1-CD-NE2 | -5.53 | 117.07 | 122.60 |
| 2 | G | 292 | HIS | O-C-N | -5.53 | 116.71 | 122.96 |
| 2 | G | 216 | ASP | N-CA-C | -5.53 | 105.34 | 111.36 |
| 2 | R | 28 | ASP | N-CA-CB | -5.53 | 102.53 | 110.65 |
| 2 | G | 125 | PHE | CA-CB-CG | -5.52 | 108.28 | 113.80 |
| 1 | B | 253 | PHE | CA-C-N | 5.52 | 127.99 | 120.54 |
| 1 | B | 253 | PHE | C-N-CA | 5.52 | 127.99 | 120.54 |
| 2 | I | 367 | ASP | CA-C-N | -5.52 | 113.84 | 122.73 |
| 2 | I | 367 | ASP | C-N-CA | -5.52 | 113.84 | 122.73 |
| 2 | G | 277 | ASN | OD1-CG-ND2 | -5.52 | 117.08 | 122.60 |
| 2 | I | 277 | ASN | CB-CG-ND2 | 5.52 | 124.68 | 116.40 |
| 2 | S | 384 | VAL | CA-C-O | -5.52 | 114.63 | 120.64 |
| 3 | D | 35 | GLU | CB-CG-CD | 5.52 | 121.98 | 112.60 |
| 3 | N | 31 | GLU | O-C-N | 5.52 | 127.98 | 122.08 |
| 2 | J | 298 | HIS | CB-CG-CD2 | -5.51 | 124.03 | 131.20 |
| 2 | S | 206 | ILE | CA-C-O | -5.51 | 114.59 | 121.04 |
| 1 | A | 232 | GLN | N-CA-C | 5.51 | 120.41 | 111.37 |
| 1 | B | 293 | ILE | CA-C-O | 5.51 | 126.20 | 120.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | E | 58 | TRP | CB-CA-C | 5.51 | 118.61 | 111.50 |
| 2 | G | 31 | PRO | CA-C-O | -5.51 | 115.06 | 121.34 |
| 2 | S | 43 | SER | CA-C-O | -5.51 | 114.69 | 120.09 |
| 3 | L | 91 | GLY | O-C-N | 5.51 | 127.90 | 123.49 |
| 2 | S | 249 | GLU | CB-CG-CD | 5.51 | 121.97 | 112.60 |
| 2 | S | 80 | TYR | N-CA-C | -5.51 | 103.96 | 111.56 |
| 3 | E | 88 | ARG | O-C-N | 5.50 | 129.22 | 122.84 |
| 2 | J | 234 | GLU | CB-CG-CD | -5.50 | 103.25 | 112.60 |
| 2 | Q | 39 | ALA | CA-C-N | 5.50 | 130.75 | 122.99 |
| 2 | Q | 39 | ALA | C-N-CA | 5.50 | 130.75 | 122.99 |
| 2 | G | 148 | PHE | N-CA-C | -5.50 | 101.87 | 110.17 |
| 2 | S | 327 | HIS | N-CA-C | -5.50 | 102.14 | 110.28 |
| 2 | C | 147 | THR | N-CA-C | 5.50 | 118.03 | 111.71 |
| 3 | L | 12 | PHE | CA-CB-CG | -5.50 | 108.30 | 113.80 |
| 3 | M | 105 | VAL | N-CA-CB | -5.50 | 105.02 | 112.16 |
| 2 | Q | 173 | THR | N-CA-C | -5.50 | 100.22 | 109.07 |
| 2 | Q | 135 | LEU | CA-C-O | -5.49 | 114.39 | 120.60 |
| 2 | Q | 368 | TRP | N-CA-C | 5.49 | 120.26 | 113.50 |
| 2 | S | 438 | TYR | O-C-N | 5.49 | 127.80 | 122.09 |
| 2 | I | 402 | PHE | CA-CB-CG | 5.49 | 119.29 | 113.80 |
| 3 | L | 106 | HIS | CB-CG-ND1 | -5.49 | 114.46 | 122.70 |
| 2 | J | 220 | PHE | CA-C-O | 5.49 | 126.24 | 120.42 |
| 3 | O | 81 | GLU | N-CA-C | -5.49 | 106.71 | 113.41 |
| 3 | P | 31 | GLU | N-CA-C | 5.49 | 120.43 | 111.37 |
| 1 | T | 237 | LEU | N-CA-C | 5.49 | 118.02 | 111.71 |
| 1 | B | 289 | ARG | N-CA-C | -5.49 | 99.49 | 108.76 |
| 3 | K | 32 | TYR | CA-C-O | -5.49 | 114.78 | 120.92 |
| 3 | M | 18 | LEU | CD1-CG-CD2 | 5.49 | 122.87 | 110.80 |
| 2 | G | 292 | HIS | CB-CG-ND1 | 5.48 | 130.93 | 122.70 |
| 1 | T | 295 | THR | N-CA-C | 5.48 | 117.26 | 111.28 |
| 2 | G | 363 | PHE | CA-C-O | -5.48 | 112.65 | 119.28 |
| 2 | C | 90 | VAL | CB-CA-C | 5.48 | 117.71 | 110.91 |
| 2 | Q | 420 | ASN | N-CA-C | -5.48 | 102.39 | 111.37 |
| 2 | H | 72 | ASP | CB-CA-C | -5.48 | 102.52 | 110.96 |
| 2 | J | 230 | ALA | N-CA-C | 5.48 | 116.93 | 111.07 |
| 2 | J | 400 | LEU | CA-C-O | -5.48 | 114.36 | 120.66 |
| 2 | C | 177 | LYS | O-C-N | 5.47 | 127.94 | 122.08 |
| 3 | N | 87 | ILE | N-CA-C | -5.47 | 100.42 | 108.85 |
| 2 | R | 129 | ALA | N-CA-C | 5.47 | 119.06 | 112.38 |
| 2 | J | 125 | PHE | CA-CB-CG | 5.47 | 119.27 | 113.80 |
| 2 | I | 59 | ALA | O-C-N | 5.47 | 127.70 | 122.07 |
| 2 | I | 422 | VAL | CA-C-O | -5.47 | 115.72 | 121.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 401 | GLN | OE1-CD-NE2 | -5.46 | 117.14 | 122.60 |
| 2 | G | 124 | VAL | CA-C-N | 5.46 | 128.35 | 120.38 |
| 2 | G | 124 | VAL | C-N-CA | 5.46 | 128.35 | 120.38 |
| 3 | N | 99 | GLN | N-CA-C | 5.46 | 117.37 | 108.63 |
| 3 | P | 59 | LYS | CA-C-O | -5.46 | 111.90 | 119.16 |
| 3 | E | 31 | GLU | CA-C-O | -5.46 | 114.63 | 121.02 |
| 2 | Q | 59 | ALA | N-CA-C | 5.46 | 116.91 | 111.07 |
| 2 | G | 147 | THR | CB-CA-C | -5.46 | 100.97 | 110.09 |
| 1 | T | 277 | GLU | N-CA-C | -5.46 | 105.41 | 111.36 |
| 1 | F | 260 | PRO | CB-CA-C | -5.46 | 104.42 | 111.46 |
| 2 | I | 325 | HIS | CE1-NE2-CD2 | 5.45 | 114.45 | 109.00 |
| 2 | I | 386 | HIS | CA-C-O | -5.45 | 112.67 | 119.38 |
| 2 | H | 26 | THR | O-C-N | 5.45 | 126.24 | 121.17 |
| 2 | Q | 80 | TYR | N-CA-C | -5.45 | 102.26 | 110.06 |
| 2 | Q | 170 | LEU | CD1-CG-CD2 | 5.45 | 122.79 | 110.80 |
| 2 | Q | 265 | ILE | O-C-N | 5.45 | 129.00 | 122.95 |
| 2 | Q | 296 | ALA | CA-C-O | -5.45 | 115.19 | 121.19 |
| 2 | S | 227 | LYS | N-CA-CB | 5.45 | 118.22 | 110.16 |
| 1 | B | 252 | ARG | N-CA-CB | 5.45 | 118.12 | 110.12 |
| 2 | H | 30 | THR | O-C-N | 5.44 | 125.94 | 121.31 |
| 2 | H | 174 | ILE | N-CA-CB | 5.44 | 117.20 | 111.00 |
| 2 | H | 248 | GLU | CB-CA-C | -5.44 | 102.34 | 110.88 |
| 2 | H | 294 | HIS | CA-C-O | -5.44 | 114.83 | 121.36 |
| 2 | I | 190 | TYR | N-CA-CB | 5.44 | 118.05 | 109.94 |
| 3 | O | 47 | HIS | CE1-NE2-CD2 | -5.44 | 103.56 | 109.00 |
| 2 | J | 155 | ILE | N-CA-C | -5.44 | 105.31 | 110.42 |
| 3 | N | 33 | MET | CB-CA-C | -5.44 | 101.71 | 110.74 |
| 2 | I | 48 | VAL | CA-C-O | -5.44 | 114.40 | 119.62 |
| 2 | H | 389 | ALA | CA-C-O | -5.43 | 114.79 | 120.55 |
| 2 | H | 125 | PHE | N-CA-C | 5.43 | 118.70 | 111.75 |
| 2 | R | 24 | TYR | CA-C-O | -5.43 | 112.71 | 119.18 |
| 2 | C | 157 | VAL | N-CA-C | -5.43 | 105.32 | 110.42 |
| 2 | C | 241 | ASN | CB-CG-ND2 | -5.43 | 108.26 | 116.40 |
| 2 | R | 56 | ALA | N-CA-C | 5.43 | 116.88 | 111.07 |
| 2 | Q | 416 | GLY | CA-C-N | 5.43 | 127.55 | 120.28 |
| 2 | Q | 416 | GLY | C-N-CA | 5.43 | 127.55 | 120.28 |
| 3 | O | 35 | GLU | CA-C-O | -5.42 | 114.12 | 120.20 |
| 2 | Q | 292 | HIS | CA-C-N | 5.42 | 130.48 | 122.94 |
| 2 | Q | 292 | HIS | C-N-CA | 5.42 | 130.48 | 122.94 |
| 2 | C | 425 | GLU | CA-C-O | 5.42 | 127.03 | 121.07 |
| 2 | C | 175 | LYS | O-C-N | 5.42 | 125.78 | 121.55 |
| 2 | C | 256 | PHE | N-CA-CB | 5.42 | 118.02 | 109.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | G | 302 | ASP | O-C-N | -5.42 | 116.36 | 122.10 |
| 2 | I | 175 | LYS | CA-C-O | -5.42 | 115.08 | 120.66 |
| 2 | Q | 178 | LEU | N-CA-C | -5.42 | 100.89 | 108.96 |
| 2 | S | 286 | ASP | N-CA-C | 5.42 | 117.89 | 111.33 |
| 1 | F | 263 | PRO | CB-CA-C | -5.42 | 104.01 | 111.21 |
| 2 | H | 238 | HIS | CB-CG-ND1 | 5.42 | 130.82 | 122.70 |
| 2 | J | 162 | LEU | CA-C-N | -5.42 | 115.27 | 124.31 |
| 2 | J | 162 | LEU | C-N-CA | -5.42 | 115.27 | 124.31 |
| 2 | R | 401 | GLN | CB-CG-CD | -5.42 | 103.39 | 112.60 |
| 1 | B | 232 | GLN | CB-CG-CD | -5.42 | 103.39 | 112.60 |
| 2 | C | 59 | ALA | N-CA-C | 5.42 | 117.26 | 111.36 |
| 2 | S | 343 | LEU | CD1-CG-CD2 | -5.42 | 98.89 | 110.80 |
| 1 | B | 263 | PRO | CB-CA-C | -5.41 | 104.48 | 111.46 |
| 2 | G | 267 | HIS | CA-C-N | 5.41 | 129.61 | 122.30 |
| 2 | G | 267 | HIS | C-N-CA | 5.41 | 129.61 | 122.30 |
| 2 | G | 393 | ILE | CB-CA-C | 5.41 | 119.69 | 112.22 |
| 2 | I | 438 | TYR | N-CA-C | 5.41 | 120.25 | 111.37 |
| 3 | L | 63 | PHE | CA-C-O | -5.41 | 114.68 | 120.42 |
| 2 | Q | 327 | HIS | ND1-CE1-NE2 | 5.41 | 113.81 | 108.40 |
| 2 | G | 291 | LEU | CA-C-O | 5.41 | 126.17 | 120.33 |
| 2 | H | 249 | GLU | O-C-N | -5.41 | 115.89 | 122.22 |
| 2 | G | 309 | ILE | CA-C-O | 5.41 | 126.73 | 120.67 |
| 3 | N | 24 | ARG | CA-C-N | 5.41 | 127.53 | 120.28 |
| 3 | N | 24 | ARG | C-N-CA | 5.41 | 127.53 | 120.28 |
| 2 | S | 175 | LYS | CA-C-O | -5.41 | 114.35 | 120.46 |
| 3 | L | 35 | GLU | CA-C-N | -5.41 | 114.00 | 122.65 |
| 3 | L | 35 | GLU | C-N-CA | -5.41 | 114.00 | 122.65 |
| 2 | Q | 51 | ASP | N-CA-C | 5.41 | 117.17 | 111.28 |
| 2 | R | 242 | VAL | N-CA-CB | -5.41 | 105.13 | 112.16 |
| 2 | G | 354 | ILE | N-CA-C | -5.41 | 100.05 | 108.81 |
| 2 | G | 243 | THR | N-CA-C | -5.41 | 102.05 | 110.10 |
| 2 | S | 415 | PRO | CA-C-N | -5.40 | 113.98 | 119.98 |
| 2 | S | 415 | PRO | C-N-CA | -5.40 | 113.98 | 119.98 |
| 3 | E | 95 | ILE | N-CA-CB | 5.40 | 116.51 | 110.62 |
| 3 | M | 52 | GLU | CB-CA-C | 5.40 | 119.42 | 110.78 |
| 1 | T | 239 | GLN | N-CA-C | 5.40 | 119.35 | 112.87 |
| 2 | R | 382 | ILE | CA-C-O | -5.40 | 114.74 | 120.14 |
| 3 | M | 57 | MET | O-C-N | -5.40 | 115.91 | 122.82 |
| 2 | R | 62 | SER | CA-C-N | 5.39 | 130.33 | 122.08 |
| 2 | R | 62 | SER | C-N-CA | 5.39 | 130.33 | 122.08 |
| 2 | H | 391 | VAL | CB-CA-C | -5.39 | 104.05 | 111.65 |
| 3 | D | 92 | PHE | CA-CB-CG | 5.39 | 119.19 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Q | 208 | SER | N-CA-C | 5.39 | 118.93 | 111.71 |
| 2 | R | 253 | ARG | N-CA-C | -5.39 | 105.49 | 111.36 |
| 1 | T | 228 | GLU | N-CA-C | -5.39 | 105.31 | 111.07 |
| 3 | N | 72 | LEU | CD1-CG-CD2 | -5.38 | 98.95 | 110.80 |
| 2 | G | 155 | ILE | O-C-N | 5.38 | 127.19 | 121.91 |
| 2 | Q | 253 | ARG | N-CA-CB | 5.38 | 117.81 | 110.01 |
| 2 | S | 24 | TYR | CA-C-O | -5.38 | 114.02 | 120.10 |
| 2 | G | 345 | PHE | CA-C-N | 5.38 | 127.54 | 120.60 |
| 2 | G | 345 | PHE | C-N-CA | 5.38 | 127.54 | 120.60 |
| 2 | I | 21 | LYS | CA-C-O | 5.38 | 126.44 | 120.63 |
| 3 | N | 63 | PHE | CA-CB-CG | -5.38 | 108.42 | 113.80 |
| 2 | H | 120 | ILE | CA-C-O | -5.38 | 115.15 | 120.85 |
| 2 | I | 285 | ARG | N-CA-C | 5.38 | 117.56 | 111.11 |
| 2 | I | 276 | ALA | CA-C-N | -5.38 | 113.45 | 120.44 |
| 2 | I | 276 | ALA | C-N-CA | -5.38 | 113.45 | 120.44 |
| 3 | L | 26 | ILE | N-CA-C | -5.38 | 105.26 | 110.42 |
| 2 | I | 206 | ILE | CB-CG1-CD1 | 5.38 | 125.09 | 113.80 |
| 2 | J | 144 | LEU | N-CA-C | -5.38 | 105.46 | 112.23 |
| 2 | C | 444 | ILE | N-CA-CB | -5.37 | 104.55 | 110.51 |
| 2 | H | 167 | ARG | N-CA-CB | 5.37 | 116.32 | 111.27 |
| 2 | Q | 169 | MET | CA-C-N | -5.37 | 114.47 | 122.74 |
| 2 | Q | 169 | MET | C-N-CA | -5.37 | 114.47 | 122.74 |
| 2 | Q | 401 | GLN | CG-CD-NE2 | -5.37 | 108.34 | 116.40 |
| 2 | S | 73 | LEU | N-CA-CB | -5.37 | 102.22 | 110.44 |
| 2 | H | 442 | GLY | N-CA-C | 5.37 | 119.17 | 112.73 |
| 2 | H | 202 | ASP | N-CA-C | 5.37 | 117.61 | 110.53 |
| 2 | I | 50 | ALA | N-CA-C | 5.37 | 117.13 | 111.28 |
| 2 | R | 197 | LEU | N-CA-CB | -5.37 | 101.72 | 109.83 |
| 3 | L | 19 | PRO | N-CA-CB | -5.37 | 100.18 | 103.19 |
| 2 | G | 318 | LEU | CD1-CG-CD2 | 5.37 | 122.60 | 110.80 |
| 2 | J | 199 | PHE | N-CA-C | -5.37 | 101.14 | 109.14 |
| 2 | Q | 326 | LEU | N-CA-C | 5.37 | 118.14 | 108.48 |
| 2 | G | 324 | ASP | N-CA-C | 5.36 | 117.20 | 111.36 |
| 3 | L | 99 | GLN | N-CA-C | 5.36 | 118.34 | 110.30 |
| 2 | I | 431 | ARG | N-CA-C | -5.36 | 105.54 | 111.71 |
| 2 | R | 89 | PRO | CB-CA-C | 5.36 | 118.09 | 111.23 |
| 3 | D | 9 | GLU | CB-CA-C | -5.36 | 102.09 | 110.94 |
| 2 | H | 147 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 2 | S | 307 | HIS | N-CA-C | -5.36 | 99.87 | 108.55 |
| 1 | T | 293 | ILE | N-CA-CB | 5.36 | 118.81 | 111.41 |
| 2 | J | 385 | TRP | N-CA-C | 5.36 | 117.12 | 111.28 |
| 2 | I | 211 | PHE | CA-C-N | -5.36 | 115.45 | 123.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 211 | PHE | C-N-CA | -5.36 | 115.45 | 123.00 |
| 3 | K | 70 | GLN | OE1-CD-NE2 | -5.36 | 117.24 | 122.60 |
| 3 | N | 47 | HIS | N-CA-C | -5.36 | 101.32 | 108.34 |
| 2 | S | 35 | ASP | CA-C-O | -5.36 | 115.11 | 121.16 |
| 2 | S | 100 | PHE | CA-C-N | 5.36 | 130.39 | 122.94 |
| 2 | S | 100 | PHE | C-N-CA | 5.36 | 130.39 | 122.94 |
| 2 | C | 163 | ASN | CA-CB-CG | 5.36 | 117.95 | 112.60 |
| 2 | Q | 346 | VAL | N-CA-C | 5.36 | 115.98 | 110.36 |
| 1 | T | 252 | ARG | CA-C-O | -5.35 | 114.75 | 120.42 |
| 3 | D | 45 | ASN | OD1-CG-ND2 | 5.35 | 127.95 | 122.60 |
| 2 | G | 221 | VAL | CA-C-N | -5.35 | 113.48 | 120.44 |
| 2 | G | 221 | VAL | C-N-CA | -5.35 | 113.48 | 120.44 |
| 2 | I | 73 | LEU | CD1-CG-CD2 | 5.35 | 122.57 | 110.80 |
| 3 | M | 39 | HIS | CB-CG-ND1 | 5.35 | 130.73 | 122.70 |
| 2 | G | 362 | VAL | N-CA-C | -5.35 | 100.18 | 107.99 |
| 2 | I | 326 | LEU | CA-C-O | -5.35 | 114.12 | 120.43 |
| 2 | J | 294 | HIS | CA-C-O | -5.35 | 115.20 | 121.46 |
| 1 | A | 299 | SER | CA-C-N | -5.35 | 115.62 | 123.00 |
| 1 | A | 299 | SER | C-N-CA | -5.35 | 115.62 | 123.00 |
| 3 | O | 43 | GLU | CA-C-O | -5.35 | 114.86 | 121.06 |
| 2 | S | 427 | CYS | N-CA-C | 5.35 | 117.11 | 111.28 |
| 2 | G | 290 | LEU | N-CA-C | 5.34 | 117.19 | 110.24 |
| 2 | H | 460 | ASP | N-CA-C | 5.34 | 118.59 | 111.75 |
| 1 | T | 301 | VAL | CA-C-O | -5.34 | 114.20 | 118.90 |
| 2 | I | 443 | ASP | CA-C-N | 5.34 | 127.29 | 120.56 |
| 2 | I | 443 | ASP | C-N-CA | 5.34 | 127.29 | 120.56 |
| 2 | H | 197 | LEU | N-CA-C | 5.34 | 117.97 | 109.96 |
| 2 | G | 371 | MET | CA-C-O | -5.34 | 115.01 | 119.76 |
| 2 | Q | 143 | ALA | O-C-N | -5.34 | 116.46 | 122.12 |
| 2 | C | 396 | ASP | CA-CB-CG | -5.34 | 107.26 | 112.60 |
| 1 | F | 247 | HIS | N-CA-C | -5.34 | 101.07 | 109.50 |
| 2 | Q | 310 | HIS | CA-CB-CG | -5.34 | 108.46 | 113.80 |
| 2 | H | 423 | ALA | N-CA-C | -5.33 | 105.47 | 111.28 |
| 2 | I | 227 | LYS | CG-CD-CE | 5.33 | 123.57 | 111.30 |
| 2 | R | 309 | ILE | N-CA-C | -5.33 | 100.80 | 108.53 |
| 2 | C | 22 | LEU | CA-C-O | -5.33 | 112.12 | 119.05 |
| 3 | L | 36 | GLN | CB-CA-C | -5.33 | 101.55 | 110.56 |
| 2 | J | 293 | ILE | CB-CG1-CD1 | 5.33 | 124.99 | 113.80 |
| 2 | G | 239 | TYR | CA-C-O | -5.33 | 114.28 | 120.62 |
| 3 | O | 104 | ILE | O-C-N | 5.32 | 128.76 | 122.69 |
| 2 | S | 253 | ARG | CA-C-N | 5.32 | 127.73 | 120.54 |
| 2 | S | 253 | ARG | C-N-CA | 5.32 | 127.73 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 184 | ASN | CA-CB-CG | -5.32 | 107.28 | 112.60 |
| 2 | C | 356 | ALA | O-C-N | -5.32 | 116.33 | 122.87 |
| 3 | O | 31 | GLU | N-CA-C | -5.32 | 105.38 | 111.07 |
| 2 | R | 342 | THR | CA-CB-OG1 | 5.32 | 117.58 | 109.60 |
| 1 | B | 283 | HIS | CE1-NE2-CD2 | -5.32 | 103.68 | 109.00 |
| 2 | R | 168 | PRO | CB-CA-C | 5.32 | 117.94 | 110.60 |
| 2 | R | 319 | ARG | O-C-N | -5.32 | 116.48 | 122.12 |
| 2 | G | 391 | VAL | O-C-N | -5.32 | 116.70 | 121.91 |
| 2 | R | 116 | ILE | O-C-N | -5.32 | 116.70 | 121.91 |
| 2 | R | 138 | ILE | O-C-N | 5.32 | 128.69 | 123.00 |
| 2 | I | 102 | ALA | CA-C-N | 5.31 | 129.68 | 122.56 |
| 2 | I | 102 | ALA | C-N-CA | 5.31 | 129.68 | 122.56 |
| 2 | J | 291 | LEU | CD1-CG-CD2 | -5.31 | 99.11 | 110.80 |
| 2 | Q | 202 | ASP | N-CA-C | -5.31 | 103.38 | 110.55 |
| 2 | H | 97 | TYR | N-CA-CB | -5.31 | 103.28 | 111.46 |
| 2 | I | 319 | ARG | CA-C-O | -5.31 | 114.10 | 120.10 |
| 2 | Q | 194 | ARG | N-CA-CB | 5.31 | 117.93 | 110.12 |
| 2 | S | 181 | SER | N-CA-C | -5.31 | 103.12 | 110.35 |
| 1 | A | 245 | THR | N-CA-C | -5.31 | 101.00 | 109.23 |
| 3 | M | 45 | ASN | OD1-CG-ND2 | -5.31 | 117.29 | 122.60 |
| 3 | P | 39 | HIS | CA-C-N | 5.31 | 126.13 | 120.13 |
| 3 | P | 39 | HIS | C-N-CA | 5.31 | 126.13 | 120.13 |
| 2 | Q | 96 | SER | CA-C-O | -5.31 | 114.59 | 120.38 |
| 2 | R | 282 | LYS | N-CA-CB | 5.31 | 117.70 | 110.01 |
| 3 | D | 13 | GLU | N-CA-C | 5.31 | 120.07 | 111.37 |
| 2 | I | 139 | ARG | CB-CA-C | -5.30 | 102.71 | 111.51 |
| 2 | S | 255 | GLU | CA-C-O | -5.30 | 114.93 | 120.55 |
| 2 | H | 217 | ARG | CB-CA-C | -5.30 | 101.67 | 110.68 |
| 2 | J | 108 | PHE | N-CA-C | -5.30 | 101.01 | 109.23 |
| 2 | S | 61 | SER | CA-CB-OG | -5.30 | 100.50 | 111.10 |
| 2 | J | 242 | VAL | CB-CA-C | -5.30 | 105.12 | 111.85 |
| 3 | L | 39 | HIS | N-CA-C | -5.30 | 102.50 | 110.24 |
| 3 | M | 57 | MET | CA-C-N | 5.30 | 130.03 | 122.08 |
| 3 | M | 57 | MET | C-N-CA | 5.30 | 130.03 | 122.08 |
| 2 | R | 203 | ASP | N-CA-C | -5.30 | 102.44 | 110.28 |
| 2 | I | 78 | ASP | CA-CB-CG | 5.29 | 117.89 | 112.60 |
| 2 | S | 239 | TYR | CA-C-N | 5.29 | 129.46 | 122.42 |
| 2 | S | 239 | TYR | C-N-CA | 5.29 | 129.46 | 122.42 |
| 2 | C | 214 | TRP | N-CA-C | -5.29 | 105.20 | 110.97 |
| 2 | S | 206 | ILE | CA-C-N | -5.29 | 114.02 | 122.17 |
| 2 | S | 206 | ILE | C-N-CA | -5.29 | 114.02 | 122.17 |
| 2 | H | 33 | ASP | CA-CB-CG | -5.29 | 107.31 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 354 | ILE | CA-CB-CG1 | 5.29 | 119.40 | 110.40 |
| 2 | H | 461 | LEU | CD1-CG-CD2 | 5.29 | 122.44 | 110.80 |
| 2 | G | 100 | PHE | CA-C-N | -5.29 | 115.64 | 122.99 |
| 2 | G | 100 | PHE | C-N-CA | -5.29 | 115.64 | 122.99 |
| 2 | G | 398 | SER | CA-C-N | -5.29 | 115.10 | 122.71 |
| 2 | G | 398 | SER | C-N-CA | -5.29 | 115.10 | 122.71 |
| 2 | I | 353 | HIS | O-C-N | 5.28 | 129.49 | 123.31 |
| 2 | R | 189 | VAL | CB-CA-C | 5.28 | 118.64 | 111.88 |
| 2 | R | 230 | ALA | CA-C-N | 5.28 | 127.31 | 120.44 |
| 2 | R | 230 | ALA | C-N-CA | 5.28 | 127.31 | 120.44 |
| 2 | R | 205 | ASN | CA-C-O | -5.28 | 113.90 | 119.97 |
| 2 | R | 343 | LEU | N-CA-CB | 5.28 | 118.07 | 110.20 |
| 2 | S | 294 | HIS | CB-CG-ND1 | 5.28 | 130.62 | 122.70 |
| 3 | E | 42 | ILE | CA-C-O | -5.28 | 114.85 | 120.39 |
| 2 | H | 286 | ASP | CA-C-O | 5.28 | 125.87 | 119.38 |
| 3 | E | 25 | GLN | CA-C-N | 5.28 | 127.21 | 120.56 |
| 3 | E | 25 | GLN | C-N-CA | 5.28 | 127.21 | 120.56 |
| 2 | G | 401 | GLN | N-CA-C | -5.28 | 100.43 | 109.24 |
| 2 | H | 368 | TRP | CA-C-N | -5.28 | 114.75 | 122.40 |
| 2 | H | 368 | TRP | C-N-CA | -5.28 | 114.75 | 122.40 |
| 2 | J | 355 | GLU | N-CA-C | -5.28 | 102.94 | 110.59 |
| 3 | K | 30 | ILE | CA-C-O | -5.28 | 115.46 | 120.95 |
| 2 | R | 120 | ILE | N-CA-C | -5.28 | 104.82 | 110.36 |
| 2 | S | 294 | HIS | ND1-CG-CD2 | -5.28 | 100.82 | 106.10 |
| 2 | Q | 164 | LYS | CG-CD-CE | 5.28 | 123.43 | 111.30 |
| 2 | C | 115 | ASN | N-CA-CB | 5.27 | 117.87 | 110.12 |
| 2 | G | 154 | GLY | N-CA-C | 5.27 | 119.32 | 112.68 |
| 2 | I | 238 | HIS | ND1-CE1-NE2 | -5.27 | 103.13 | 108.40 |
| 2 | C | 461 | LEU | CD1-CG-CD2 | 5.27 | 122.39 | 110.80 |
| 2 | R | 144 | LEU | N-CA-CB | 5.27 | 118.45 | 110.28 |
| 1 | B | 250 | LYS | CB-CA-C | -5.27 | 101.94 | 110.79 |
| 2 | C | 292 | HIS | CA-CB-CG | 5.27 | 119.07 | 113.80 |
| 2 | G | 326 | LEU | CA-C-N | 5.27 | 128.35 | 120.87 |
| 2 | G | 326 | LEU | C-N-CA | 5.27 | 128.35 | 120.87 |
| 2 | R | 397 | ASP | N-CA-CB | -5.27 | 103.00 | 110.58 |
| 2 | S | 375 | LEU | N-CA-CB | 5.27 | 117.40 | 110.29 |
| 2 | C | 280 | LEU | O-C-N | -5.27 | 116.15 | 122.15 |
| 2 | I | 44 | PRO | O-C-N | -5.27 | 116.48 | 123.01 |
| 3 | K | 97 | GLN | CA-C-O | -5.27 | 114.45 | 120.98 |
| 3 | L | 79 | ARG | CB-CA-C | -5.26 | 101.90 | 110.85 |
| 2 | Q | 400 | LEU | CA-C-N | -5.26 | 113.54 | 121.86 |
| 2 | Q | 400 | LEU | C-N-CA | -5.26 | 113.54 | 121.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 220 | PHE | N-CA-CB | 5.26 | 117.64 | 110.01 |
| 2 | I | 233 | GLY | CA-C-N | 5.26 | 130.19 | 122.77 |
| 2 | I | 233 | GLY | C-N-CA | 5.26 | 130.19 | 122.77 |
| 2 | S | 48 | VAL | CA-C-O | -5.26 | 116.05 | 119.15 |
| 2 | S | 222 | ALA | CA-C-O | -5.26 | 115.30 | 120.82 |
| 2 | S | 297 | MET | N-CA-C | 5.26 | 118.69 | 111.54 |
| 2 | I | 298 | HIS | N-CA-C | -5.26 | 105.72 | 111.82 |
| 3 | L | 10 | ARG | CA-C-O | -5.26 | 115.12 | 120.80 |
| 3 | N | 63 | PHE | CA-C-O | 5.26 | 126.18 | 120.55 |
| 2 | G | 385 | TRP | N-CA-C | 5.26 | 119.45 | 113.19 |
| 2 | H | 157 | VAL | CA-C-O | -5.26 | 115.48 | 120.95 |
| 3 | N | 44 | PHE | CA-CB-CG | 5.26 | 119.06 | 113.80 |
| 2 | Q | 153 | HIS | CB-CG-ND1 | -5.26 | 114.81 | 122.70 |
| 2 | C | 120 | ILE | O-C-N | 5.25 | 127.36 | 121.90 |
| 2 | C | 401 | GLN | CB-CG-CD | -5.25 | 103.67 | 112.60 |
| 2 | C | 401 | GLN | N-CA-C | -5.25 | 102.28 | 110.42 |
| 2 | I | 277 | ASN | CA-CB-CG | 5.25 | 117.85 | 112.60 |
| 2 | Q | 459 | LEU | CD1-CG-CD2 | 5.25 | 122.36 | 110.80 |
| 2 | S | 200 | THR | CB-CA-C | 5.25 | 119.71 | 110.36 |
| 2 | I | 194 | ARG | N-CA-C | -5.25 | 105.67 | 111.71 |
| 2 | G | 206 | ILE | CB-CA-C | 5.25 | 117.07 | 111.35 |
| 3 | P | 77 | GLU | N-CA-C | 5.25 | 117.41 | 111.11 |
| 2 | R | 159 | ARG | N-CA-CB | 5.25 | 117.83 | 110.12 |
| 2 | S | 446 | ARG | CA-C-O | -5.25 | 114.86 | 120.42 |
| 2 | G | 301 | ILE | O-C-N | -5.25 | 116.01 | 122.57 |
| 2 | H | 154 | GLY | N-CA-C | 5.25 | 121.78 | 112.02 |
| 2 | J | 42 | PHE | N-CA-C | -5.25 | 101.39 | 109.52 |
| 2 | C | 149 | GLN | N-CA-C | 5.25 | 118.94 | 112.54 |
| 2 | J | 118 | THR | CA-C-O | -5.25 | 115.31 | 120.82 |
| 1 | B | 247 | HIS | N-CA-C | -5.24 | 101.10 | 109.23 |
| 2 | R | 119 | SER | CA-C-O | -5.24 | 113.61 | 120.00 |
| 3 | M | 64 | ASP | CB-CA-C | -5.24 | 104.56 | 111.74 |
| 3 | M | 79 | ARG | N-CA-CB | 5.24 | 117.82 | 110.12 |
| 3 | D | 70 | GLN | OE1-CD-NE2 | 5.24 | 127.84 | 122.60 |
| 2 | R | 369 | ALA | N-CA-C | -5.24 | 104.21 | 111.28 |
| 3 | K | 95 | ILE | N-CA-C | -5.23 | 105.61 | 110.53 |
| 2 | R | 384 | VAL | CA-C-O | -5.23 | 114.94 | 120.64 |
| 2 | C | 363 | PHE | CA-CB-CG | -5.23 | 108.57 | 113.80 |
| 2 | C | 117 | LEU | O-C-N | -5.23 | 116.58 | 122.12 |
| 3 | K | 67 | SER | N-CA-C | 5.23 | 116.99 | 109.04 |
| 3 | K | 97 | GLN | N-CA-C | -5.23 | 104.91 | 111.92 |
| 2 | Q | 101 | ILE | CA-C-O | -5.23 | 115.01 | 120.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 208 | SER | N-CA-C | 5.23 | 118.72 | 111.71 |
| 2 | C | 342 | THR | CB-CA-C | 5.23 | 119.09 | 110.88 |
| 2 | C | 359 | SER | CA-CB-OG | 5.23 | 121.56 | 111.10 |
| 2 | G | 97 | TYR | N-CA-C | -5.23 | 101.12 | 109.07 |
| 2 | H | 210 | PRO | CB-CA-C | -5.23 | 103.55 | 112.64 |
| 3 | N | 26 | ILE | N-CA-C | -5.23 | 105.29 | 110.62 |
| 2 | Q | 60 | GLU | CB-CG-CD | 5.23 | 121.48 | 112.60 |
| 2 | I | 205 | ASN | CA-CB-CG | -5.22 | 107.38 | 112.60 |
| 3 | K | 15 | PHE | N-CA-C | 5.22 | 121.66 | 113.72 |
| 2 | G | 399 | VAL | N-CA-C | -5.22 | 100.72 | 108.45 |
| 3 | K | 40 | PRO | CB-CA-C | -5.22 | 104.39 | 111.12 |
| 2 | R | 288 | GLY | N-CA-C | 5.22 | 122.94 | 114.90 |
| 2 | G | 383 | HIS | ND1-CG-CD2 | -5.22 | 100.88 | 106.10 |
| 2 | H | 145 | VAL | N-CA-C | 5.22 | 120.20 | 109.34 |
| 2 | I | 198 | ASP | CA-C-O | -5.22 | 115.02 | 120.55 |
| 2 | G | 100 | PHE | CA-CB-CG | -5.22 | 108.58 | 113.80 |
| 1 | A | 305 | LEU | CD1-CG-CD2 | 5.22 | 122.28 | 110.80 |
| 2 | C | 238 | HIS | CA-C-N | 5.22 | 130.08 | 122.41 |
| 2 | C | 238 | HIS | C-N-CA | 5.22 | 130.08 | 122.41 |
| 2 | G | 184 | ASN | N-CA-CB | 5.22 | 117.89 | 110.06 |
| 3 | M | 39 | HIS | CA-C-O | -5.22 | 115.38 | 119.66 |
| 2 | R | 347 | ASP | N-CA-C | -5.22 | 105.59 | 111.28 |
| 2 | I | 303 | ARG | O-C-N | 5.21 | 127.65 | 122.12 |
| 2 | I | 23 | THR | N-CA-C | 5.21 | 119.77 | 113.41 |
| 2 | I | 90 | VAL | CA-C-O | -5.21 | 114.82 | 120.71 |
| 1 | F | 279 | CYS | CA-C-N | 5.21 | 127.21 | 120.44 |
| 1 | F | 279 | CYS | C-N-CA | 5.21 | 127.21 | 120.44 |
| 2 | G | 96 | SER | CA-C-O | -5.21 | 114.73 | 120.36 |
| 2 | H | 148 | PHE | CA-CB-CG | -5.21 | 108.59 | 113.80 |
| 2 | J | 314 | LEU | N-CA-CB | -5.21 | 102.46 | 110.01 |
| 2 | C | 376 | PRO | CB-CA-C | -5.21 | 103.41 | 110.60 |
| 2 | I | 147 | THR | N-CA-C | 5.21 | 119.39 | 113.19 |
| 3 | K | 47 | HIS | ND1-CE1-NE2 | 5.21 | 113.61 | 108.40 |
| 1 | B | 276 | LEU | N-CA-C | 5.21 | 116.95 | 111.28 |
| 1 | A | 273 | LEU | CD1-CG-CD2 | -5.20 | 99.35 | 110.80 |
| 2 | I | 59 | ALA | CA-C-N | -5.20 | 113.55 | 120.63 |
| 2 | I | 59 | ALA | C-N-CA | -5.20 | 113.55 | 120.63 |
| 2 | Q | 267 | HIS | ND1-CE1-NE2 | 5.20 | 113.60 | 108.40 |
| 3 | L | 12 | PHE | CA-C-O | -5.20 | 115.88 | 121.45 |
| 3 | P | 12 | PHE | N-CA-CB | -5.20 | 102.62 | 111.31 |
| 2 | R | 43 | SER | CA-C-O | -5.20 | 114.81 | 119.59 |
| 2 | J | 148 | PHE | CA-CB-CG | 5.20 | 119.00 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | M | 21 | LEU | O-C-N | 5.20 | 129.23 | 122.89 |
| 2 | R | 316 | LYS | N-CA-C | -5.20 | 104.68 | 111.02 |
| 1 | B | 287 | TYR | N-CA-C | 5.20 | 118.01 | 110.42 |
| 2 | G | 246 | THR | CA-C-O | 5.20 | 127.09 | 121.06 |
| 1 | T | 279 | CYS | N-CA-C | 5.20 | 116.63 | 111.07 |
| 2 | Q | 207 | ASN | CB-CA-C | -5.19 | 101.85 | 110.37 |
| 2 | R | 302 | ASP | CA-CB-CG | 5.19 | 117.79 | 112.60 |
| 1 | A | 290 | LEU | N-CA-C | -5.19 | 102.37 | 110.42 |
| 3 | O | 26 | ILE | N-CA-C | -5.19 | 105.32 | 110.62 |
| 2 | G | 72 | ASP | O-C-N | -5.19 | 116.62 | 122.12 |
| 3 | M | 103 | PHE | CA-C-N | 5.19 | 127.65 | 120.49 |
| 3 | M | 103 | PHE | C-N-CA | 5.19 | 127.65 | 120.49 |
| 2 | G | 278 | THR | OG1-CB-CG2 | 5.19 | 119.68 | 109.30 |
| 2 | H | 293 | ILE | O-C-N | 5.19 | 128.70 | 123.20 |
| 2 | R | 60 | GLU | CA-C-N | 5.19 | 130.22 | 121.14 |
| 2 | R | 60 | GLU | C-N-CA | 5.19 | 130.22 | 121.14 |
| 1 | B | 228 | GLU | O-C-N | -5.19 | 116.23 | 122.15 |
| 2 | C | 107 | LEU | CD1-CG-CD2 | 5.19 | 122.21 | 110.80 |
| 2 | H | 25 | TYR | CA-C-O | -5.19 | 114.73 | 120.33 |
| 2 | I | 206 | ILE | CA-C-O | -5.19 | 114.15 | 120.69 |
| 3 | N | 101 | VAL | CA-C-O | -5.19 | 114.86 | 120.36 |
| 1 | B | 304 | ALA | CA-C-O | -5.19 | 113.81 | 120.14 |
| 2 | C | 256 | PHE | CA-C-O | 5.19 | 126.45 | 120.90 |
| 2 | G | 209 | GLN | N-CA-C | 5.19 | 121.27 | 109.81 |
| 2 | R | 197 | LEU | N-CA-C | 5.19 | 117.75 | 110.23 |
| 2 | R | 282 | LYS | N-CA-C | 5.19 | 116.62 | 111.07 |
| 3 | O | 19 | PRO | O-C-N | 5.18 | 127.58 | 121.46 |
| 2 | I | 363 | PHE | CA-C-O | -5.18 | 114.01 | 119.97 |
| 2 | Q | 372 | PRO | CA-C-N | 5.18 | 129.03 | 121.05 |
| 2 | Q | 372 | PRO | C-N-CA | 5.18 | 129.03 | 121.05 |
| 3 | P | 71 | VAL | CB-CA-C | -5.18 | 105.07 | 112.22 |
| 2 | C | 118 | THR | OG1-CB-CG2 | 5.18 | 119.66 | 109.30 |
| 2 | S | 201 | LYS | N-CA-C | 5.18 | 117.86 | 109.06 |
| 2 | G | 185 | TYR | CA-C-O | -5.18 | 115.01 | 120.55 |
| 2 | R | 367 | ASP | CA-C-O | -5.18 | 114.71 | 120.66 |
| 2 | S | 367 | ASP | CA-CB-CG | 5.18 | 117.78 | 112.60 |
| 2 | C | 97 | TYR | CA-C-N | 5.17 | 129.65 | 122.77 |
| 2 | C | 97 | TYR | C-N-CA | 5.17 | 129.65 | 122.77 |
| 2 | H | 362 | VAL | N-CA-C | -5.17 | 99.23 | 107.15 |
| 2 | S | 145 | VAL | CB-CA-C | 5.17 | 118.32 | 111.70 |
| 3 | K | 48 | SER | N-CA-C | 5.17 | 116.75 | 107.80 |
| 2 | C | 103 | TYR | CA-C-O | 5.17 | 124.83 | 119.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 209 | GLN | N-CA-C | 5.17 | 117.03 | 109.84 |
| 3 | N | 48 | SER | N-CA-C | 5.17 | 118.48 | 107.67 |
| 2 | S | 287 | ASN | CA-CB-CG | -5.17 | 107.43 | 112.60 |
| 2 | C | 185 | TYR | O-C-N | 5.17 | 127.61 | 122.08 |
| 2 | G | 254 | ALA | N-CA-C | 5.17 | 116.60 | 111.07 |
| 2 | G | 140 | PHE | CA-C-O | -5.17 | 114.80 | 120.17 |
| 3 | E | 89 | VAL | CB-CA-C | -5.17 | 102.99 | 110.63 |
| 2 | H | 301 | ILE | CB-CG1-CD1 | 5.17 | 124.65 | 113.80 |
| 3 | O | 18 | LEU | CD1-CG-CD2 | 5.17 | 122.16 | 110.80 |
| 2 | H | 375 | LEU | N-CA-C | 5.16 | 119.98 | 109.60 |
| 2 | S | 364 | PHE | CA-C-O | -5.16 | 114.76 | 121.73 |
| 2 | Q | 90 | VAL | O-C-N | 5.16 | 128.24 | 122.61 |
| 3 | K | 74 | GLU | N-CA-CB | 5.16 | 117.63 | 109.94 |
| 3 | N | 39 | HIS | CG-CD2-NE2 | 5.16 | 112.36 | 107.20 |
| 3 | P | 91 | GLY | O-C-N | 5.16 | 129.41 | 122.70 |
| 2 | Q | 176 | PRO | N-CD-CG | -5.16 | 97.61 | 103.80 |
| 2 | R | 243 | THR | CA-CB-OG1 | 5.16 | 117.34 | 109.60 |
| 2 | Q | 452 | SER | CA-CB-OG | -5.16 | 100.79 | 111.10 |
| 3 | M | 9 | GLU | CB-CG-CD | 5.15 | 121.36 | 112.60 |
| 2 | C | 209 | GLN | CA-C-O | -5.15 | 114.87 | 120.69 |
| 2 | S | 177 | LYS | CG-CD-CE | 5.15 | 123.15 | 111.30 |
| 3 | K | 86 | TYR | CA-C-O | -5.15 | 115.95 | 121.56 |
| 2 | Q | 461 | LEU | CD1-CG-CD2 | 5.15 | 122.13 | 110.80 |
| 2 | I | 451 | TRP | N-CA-C | 5.15 | 119.55 | 113.16 |
| 2 | J | 36 | LEU | N-CA-C | -5.15 | 100.02 | 108.41 |
| 3 | M | 39 | HIS | ND1-CG-CD2 | -5.15 | 100.95 | 106.10 |
| 2 | G | 401 | GLN | CA-C-O | -5.15 | 114.74 | 120.66 |
| 2 | H | 53 | ALA | N-CA-C | -5.15 | 105.56 | 111.07 |
| 2 | C | 98 | PHE | O-C-N | -5.15 | 117.35 | 123.22 |
| 2 | C | 35 | ASP | CA-CB-CG | 5.14 | 117.74 | 112.60 |
| 2 | I | 379 | SER | O-C-N | 5.14 | 129.37 | 122.73 |
| 2 | I | 139 | ARG | CA-CB-CG | -5.14 | 103.81 | 114.10 |
| 2 | R | 238 | HIS | CB-CG-ND1 | 5.14 | 130.41 | 122.70 |
| 2 | H | 185 | TYR | CA-C-O | -5.14 | 114.54 | 120.24 |
| 2 | J | 185 | TYR | O-C-N | -5.14 | 116.54 | 122.09 |
| 3 | L | 36 | GLN | CG-CD-NE2 | 5.14 | 124.11 | 116.40 |
| 2 | Q | 172 | CYS | CA-C-N | -5.14 | 115.91 | 123.00 |
| 2 | Q | 172 | CYS | C-N-CA | -5.14 | 115.91 | 123.00 |
| 2 | R | 437 | LEU | N-CA-CB | -5.14 | 102.54 | 110.20 |
| 2 | H | 370 | SER | CA-CB-OG | -5.14 | 100.82 | 111.10 |
| 3 | E | 35 | GLU | N-CA-CB | 5.14 | 117.67 | 110.12 |
| 2 | G | 149 | GLN | N-CA-C | -5.14 | 105.31 | 112.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 368 | TRP | N-CA-C | 5.14 | 120.67 | 113.02 |
| 2 | S | 86 | HIS | CB-CA-C | 5.14 | 118.26 | 109.99 |
| 2 | S | 153 | HIS | CB-CG-ND1 | -5.14 | 115.00 | 122.70 |
| 3 | O | 87 | ILE | O-C-N | -5.13 | 117.65 | 123.20 |
| 2 | Q | 279 | THR | CB-CA-C | -5.13 | 102.27 | 110.79 |
| 2 | C | 153 | HIS | CE1-NE2-CD2 | 5.13 | 114.13 | 109.00 |
| 2 | C | 276 | ALA | CA-C-N | 5.13 | 127.11 | 120.44 |
| 2 | C | 276 | ALA | C-N-CA | 5.13 | 127.11 | 120.44 |
| 2 | J | 236 | LYS | CA-C-N | 5.13 | 130.14 | 121.47 |
| 2 | J | 236 | LYS | C-N-CA | 5.13 | 130.14 | 121.47 |
| 3 | M | 94 | ASN | N-CA-C | 5.13 | 116.95 | 111.36 |
| 2 | C | 363 | PHE | N-CA-C | 5.13 | 117.61 | 111.71 |
| 2 | G | 46 | PRO | CB-CA-C | 5.13 | 118.07 | 111.46 |
| 3 | K | 106 | HIS | CG-CD2-NE2 | 5.13 | 112.33 | 107.20 |
| 2 | R | 85 | TYR | CB-CA-C | -5.13 | 101.50 | 110.17 |
| 2 | S | 118 | THR | CB-CA-C | -5.13 | 102.28 | 110.79 |
| 2 | H | 339 | LYS | CA-CB-CG | -5.12 | 103.85 | 114.10 |
| 2 | H | 442 | GLY | CA-C-N | 5.12 | 127.41 | 120.44 |
| 2 | H | 442 | GLY | C-N-CA | 5.12 | 127.41 | 120.44 |
| 2 | I | 448 | ALA | CA-C-N | 5.12 | 126.73 | 120.22 |
| 2 | I | 448 | ALA | C-N-CA | 5.12 | 126.73 | 120.22 |
| 3 | L | 76 | ARG | CB-CG-CD | 5.12 | 123.08 | 111.30 |
| 2 | Q | 353 | HIS | CB-CG-CD2 | -5.12 | 124.54 | 131.20 |
| 2 | R | 40 | PHE | CA-C-O | -5.12 | 115.02 | 120.40 |
| 2 | G | 397 | ASP | N-CA-C | 5.12 | 117.53 | 109.39 |
| 2 | I | 41 | ARG | CB-CA-C | -5.12 | 101.40 | 109.80 |
| 2 | S | 290 | LEU | CA-C-O | -5.12 | 115.98 | 121.56 |
| 2 | C | 36 | LEU | CA-C-O | -5.12 | 114.64 | 120.32 |
| 2 | G | 100 | PHE | O-C-N | 5.12 | 129.06 | 123.22 |
| 2 | J | 347 | ASP | N-CA-C | -5.12 | 105.39 | 111.69 |
| 2 | J | 358 | ARG | N-CA-C | 5.12 | 119.82 | 111.37 |
| 1 | B | 245 | THR | CA-C-O | -5.12 | 115.12 | 121.11 |
| 2 | I | 133 | LEU | CA-C-N | -5.12 | 113.73 | 122.33 |
| 2 | I | 133 | LEU | C-N-CA | -5.12 | 113.73 | 122.33 |
| 2 | I | 177 | LYS | CA-C-O | -5.12 | 113.30 | 119.49 |
| 1 | B | 232 | GLN | O-C-N | 5.12 | 127.41 | 122.09 |
| 1 | T | 257 | SER | N-CA-C | 5.12 | 117.58 | 109.24 |
| 2 | G | 191 | GLU | CA-CB-CG | -5.11 | 103.87 | 114.10 |
| 2 | I | 294 | HIS | CA-CB-CG | 5.11 | 118.91 | 113.80 |
| 2 | J | 202 | ASP | CA-C-O | -5.11 | 116.13 | 121.55 |
| 2 | J | 292 | HIS | ND1-CE1-NE2 | -5.11 | 103.29 | 108.40 |
| 2 | G | 171 | GLY | CA-C-O | -5.11 | 117.12 | 121.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 286 | ASP | CA-CB-CG | 5.11 | 117.71 | 112.60 |
| 2 | J | 109 | GLU | N-CA-C | -5.11 | 102.19 | 110.32 |
| 2 | S | 310 | HIS | CA-C-N | 5.11 | 127.38 | 120.38 |
| 2 | S | 310 | HIS | C-N-CA | 5.11 | 127.38 | 120.38 |
| 2 | S | 204 | GLU | O-C-N | -5.11 | 116.71 | 122.12 |
| 2 | I | 144 | LEU | CA-C-O | -5.10 | 114.33 | 120.10 |
| 2 | H | 350 | ARG | CB-CA-C | -5.10 | 102.00 | 110.37 |
| 2 | Q | 415 | PRO | CA-C-N | 5.10 | 125.60 | 119.94 |
| 2 | Q | 415 | PRO | C-N-CA | 5.10 | 125.60 | 119.94 |
| 1 | A | 246 | GLU | CA-C-O | -5.10 | 114.48 | 120.60 |
| 2 | C | 190 | TYR | CA-C-O | -5.10 | 115.05 | 121.02 |
| 2 | C | 387 | MET | CA-C-O | -5.10 | 113.39 | 118.34 |
| 3 | K | 72 | LEU | N-CA-C | 5.10 | 117.50 | 111.33 |
| 2 | Q | 194 | ARG | CB-CA-C | -5.10 | 102.33 | 110.79 |
| 2 | Q | 205 | ASN | CA-CB-CG | -5.10 | 107.50 | 112.60 |
| 2 | Q | 251 | MET | N-CA-C | 5.10 | 117.23 | 111.11 |
| 2 | R | 115 | ASN | CB-CG-ND2 | -5.10 | 108.75 | 116.40 |
| 2 | S | 371 | MET | O-C-N | 5.10 | 125.64 | 121.31 |
| 1 | T | 250 | LYS | CA-C-N | 5.10 | 127.42 | 120.54 |
| 1 | T | 250 | LYS | C-N-CA | 5.10 | 127.42 | 120.54 |
| 1 | F | 234 | ARG | CA-C-O | -5.10 | 115.47 | 120.82 |
| 2 | H | 429 | GLN | CB-CG-CD | 5.10 | 121.26 | 112.60 |
| 2 | J | 312 | ARG | O-C-N | 5.10 | 127.32 | 122.07 |
| 2 | R | 271 | THR | N-CA-CB | 5.10 | 117.46 | 110.07 |
| 2 | S | 360 | ARG | CA-CB-CG | -5.10 | 103.91 | 114.10 |
| 2 | Q | 233 | GLY | N-CA-C | 5.09 | 122.93 | 113.76 |
| 2 | J | 116 | ILE | O-C-N | -5.09 | 116.58 | 121.83 |
| 2 | I | 158 | GLU | O-C-N | 5.09 | 127.31 | 122.07 |
| 2 | I | 362 | VAL | CA-C-N | 5.09 | 128.05 | 120.31 |
| 2 | I | 362 | VAL | C-N-CA | 5.09 | 128.05 | 120.31 |
| 2 | J | 355 | GLU | CA-C-O | -5.09 | 115.93 | 121.89 |
| 2 | Q | 318 | LEU | CD1-CG-CD2 | 5.09 | 122.00 | 110.80 |
| 2 | S | 206 | ILE | N-CA-CB | 5.09 | 117.46 | 111.66 |
| 2 | H | 112 | SER | CB-CA-C | -5.09 | 102.93 | 110.62 |
| 2 | S | 25 | TYR | CB-CA-C | 5.09 | 119.20 | 110.81 |
| 2 | G | 328 | SER | CA-C-O | -5.09 | 113.80 | 119.34 |
| 2 | H | 108 | PHE | N-CA-C | -5.09 | 101.56 | 109.14 |
| 3 | K | 10 | ARG | O-C-N | 5.08 | 129.12 | 122.87 |
| 2 | J | 438 | TYR | CB-CA-C | 5.08 | 119.00 | 110.92 |
| 3 | K | 35 | GLU | N-CA-CB | 5.08 | 117.59 | 110.12 |
| 2 | R | 235 | ILE | CB-CA-C | 5.08 | 119.88 | 111.59 |
| 2 | S | 128 | LYS | CA-C-O | -5.08 | 112.61 | 119.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | G | 212 | GLN | CG-CD-NE2 | -5.08 | 108.78 | 116.40 |
| 2 | H | 123 | ASN | CA-C-N | 5.08 | 127.69 | 120.53 |
| 2 | H | 123 | ASN | C-N-CA | 5.08 | 127.69 | 120.53 |
| 3 | M | 32 | TYR | N-CA-C | 5.08 | 119.75 | 111.37 |
| 2 | G | 153 | HIS | CB-CG-CD2 | 5.08 | 137.80 | 131.20 |
| 2 | C | 190 | TYR | N-CA-C | 5.08 | 119.69 | 111.37 |
| 3 | K | 103 | PHE | O-C-N | -5.08 | 117.69 | 123.48 |
| 1 | T | 260 | PRO | CB-CA-C | -5.08 | 104.30 | 110.95 |
| 2 | C | 85 | TYR | N-CA-CB | -5.07 | 102.95 | 110.61 |
| 2 | G | 234 | GLU | N-CA-C | 5.07 | 118.08 | 109.76 |
| 2 | G | 310 | HIS | CE1-NE2-CD2 | -5.07 | 103.93 | 109.00 |
| 2 | H | 209 | GLN | O-C-N | 5.07 | 125.54 | 121.38 |
| 3 | K | 45 | ASN | CB-CG-ND2 | 5.07 | 124.01 | 116.40 |
| 3 | K | 81 | GLU | N-CA-C | -5.07 | 106.25 | 112.90 |
| 2 | Q | 299 | ALA | CA-C-N | 5.07 | 127.41 | 120.46 |
| 2 | Q | 299 | ALA | C-N-CA | 5.07 | 127.41 | 120.46 |
| 2 | S | 238 | HIS | CB-CG-ND1 | 5.07 | 130.31 | 122.70 |
| 2 | G | 173 | THR | N-CA-C | -5.07 | 102.01 | 110.17 |
| 2 | I | 229 | GLN | CG-CD-NE2 | -5.07 | 108.80 | 116.40 |
| 2 | J | 292 | HIS | CE1-NE2-CD2 | 5.07 | 114.07 | 109.00 |
| 2 | R | 74 | LEU | CD1-CG-CD2 | 5.07 | 121.95 | 110.80 |
| 2 | H | 91 | GLN | O-C-N | -5.07 | 116.67 | 122.95 |
| 2 | J | 327 | HIS | ND1-CG-CD2 | -5.07 | 101.03 | 106.10 |
| 2 | H | 139 | ARG | CB-CA-C | -5.06 | 102.68 | 110.78 |
| 2 | R | 271 | THR | N-CA-C | -5.06 | 105.67 | 111.14 |
| 2 | H | 149 | GLN | N-CA-C | 5.06 | 118.92 | 112.34 |
| 2 | R | 148 | PHE | CA-C-N | 5.06 | 127.48 | 120.29 |
| 2 | R | 148 | PHE | C-N-CA | 5.06 | 127.48 | 120.29 |
| 2 | I | 438 | TYR | N-CA-CB | 5.06 | 118.32 | 109.72 |
| 2 | Q | 102 | ALA | CA-C-O | -5.06 | 115.24 | 120.70 |
| 2 | Q | 272 | ALA | N-CA-C | 5.06 | 118.55 | 112.38 |
| 2 | R | 39 | ALA | N-CA-C | 5.06 | 117.00 | 108.96 |
| 2 | R | 373 | GLY | O-C-N | 5.06 | 127.80 | 122.59 |
| 2 | S | 251 | MET | CA-C-O | -5.06 | 115.69 | 121.00 |
| 3 | M | 107 | ARG | CA-CB-CG | -5.06 | 103.99 | 114.10 |
| 1 | T | 261 | CYS | CA-C-O | 5.06 | 127.72 | 121.60 |
| 2 | R | 327 | HIS | CA-C-O | -5.05 | 115.50 | 121.16 |
| 2 | C | 443 | ASP | CA-CB-CG | 5.05 | 117.65 | 112.60 |
| 2 | H | 211 | PHE | O-C-N | -5.05 | 115.66 | 122.43 |
| 2 | I | 166 | GLY | N-CA-C | 5.05 | 122.58 | 115.30 |
| 3 | O | 16 | SER | CA-CB-OG | -5.05 | 100.99 | 111.10 |
| 2 | C | 356 | ALA | CA-C-O | 5.05 | 126.75 | 121.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 342 | THR | N-CA-C | -5.05 | 104.86 | 111.02 |
| 2 | J | 194 | ARG | N-CA-C | 5.05 | 117.52 | 111.71 |
| 3 | P | 42 | ILE | CA-C-O | -5.05 | 115.12 | 120.53 |
| 2 | G | 44 | PRO | N-CA-C | 5.05 | 119.24 | 111.21 |
| 3 | O | 47 | HIS | CG-CD2-NE2 | 5.05 | 112.25 | 107.20 |
| 3 | N | 46 | GLU | CA-C-N | -5.05 | 114.11 | 122.39 |
| 3 | N | 46 | GLU | C-N-CA | -5.05 | 114.11 | 122.39 |
| 3 | O | 18 | LEU | CA-C-N | -5.05 | 115.18 | 120.38 |
| 3 | O | 18 | LEU | C-N-CA | -5.05 | 115.18 | 120.38 |
| 3 | D | 35 | GLU | O-C-N | 5.04 | 127.47 | 122.12 |
| 3 | M | 31 | GLU | CA-C-O | -5.04 | 115.52 | 121.07 |
| 2 | Q | 346 | VAL | O-C-N | -5.04 | 116.89 | 121.94 |
| 2 | S | 183 | LYS | CA-C-O | 5.04 | 126.12 | 120.82 |
| 2 | G | 37 | LEU | N-CA-C | -5.04 | 101.65 | 109.72 |
| 3 | P | 23 | ASP | CA-C-N | -5.04 | 113.89 | 120.44 |
| 3 | P | 23 | ASP | C-N-CA | -5.04 | 113.89 | 120.44 |
| 2 | I | 68 | THR | CA-C-N | 5.04 | 128.72 | 121.96 |
| 2 | I | 68 | THR | C-N-CA | 5.04 | 128.72 | 121.96 |
| 2 | Q | 363 | PHE | CA-C-N | -5.04 | 113.53 | 122.20 |
| 2 | Q | 363 | PHE | C-N-CA | -5.04 | 113.53 | 122.20 |
| 2 | R | 307 | HIS | CE1-NE2-CD2 | -5.04 | 103.96 | 109.00 |
| 2 | C | 153 | HIS | ND1-CE1-NE2 | -5.04 | 103.36 | 108.40 |
| 3 | N | 39 | HIS | CA-C-O | -5.04 | 114.88 | 119.62 |
| 2 | Q | 217 | ARG | CB-CG-CD | 5.04 | 122.89 | 111.30 |
| 2 | H | 458 | ALA | CA-C-O | -5.04 | 115.16 | 120.55 |
| 2 | R | 223 | ASP | CA-CB-CG | 5.04 | 117.64 | 112.60 |
| 2 | S | 98 | PHE | CA-C-O | -5.04 | 114.95 | 120.69 |
| 2 | I | 326 | LEU | O-C-N | 5.04 | 129.22 | 123.48 |
| 2 | H | 451 | TRP | N-CA-C | 5.04 | 119.27 | 113.18 |
| 3 | K | 72 | LEU | O-C-N | 5.04 | 127.46 | 122.12 |
| 3 | M | 29 | GLN | O-C-N | 5.04 | 127.89 | 122.15 |
| 2 | R | 326 | LEU | CA-C-N | -5.04 | 113.72 | 120.87 |
| 2 | R | 326 | LEU | C-N-CA | -5.04 | 113.72 | 120.87 |
| 3 | D | 19 | PRO | CA-C-O | -5.03 | 113.26 | 120.56 |
| 1 | A | 276 | LEU | CD1-CG-CD2 | -5.03 | 99.73 | 110.80 |
| 1 | B | 273 | LEU | CD1-CG-CD2 | -5.03 | 99.73 | 110.80 |
| 2 | I | 366 | GLN | CA-C-O | -5.03 | 115.22 | 121.11 |
| 3 | L | 39 | HIS | CA-C-O | -5.03 | 115.46 | 120.64 |
| 2 | Q | 223 | ASP | CA-CB-CG | -5.03 | 107.57 | 112.60 |
| 2 | H | 168 | PRO | N-CA-C | -5.03 | 103.38 | 111.77 |
| 2 | J | 432 | ASN | CA-CB-CG | -5.03 | 107.57 | 112.60 |
| 3 | M | 66 | LYS | CA-C-O | -5.03 | 112.78 | 119.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 221 | VAL | N-CA-C | 5.02 | 115.74 | 110.62 |
| 2 | Q | 179 | GLY | CA-C-N | -5.02 | 113.87 | 121.05 |
| 2 | Q | 179 | GLY | C-N-CA | -5.02 | 113.87 | 121.05 |
| 2 | J | 269 | PHE | CA-C-O | -5.02 | 115.21 | 120.63 |
| 3 | N | 97 | GLN | N-CA-CB | -5.02 | 104.36 | 111.84 |
| 2 | C | 220 | PHE | N-CA-CB | 5.02 | 117.29 | 110.01 |
| 2 | G | 393 | ILE | N-CA-C | 5.02 | 115.79 | 110.72 |
| 2 | H | 300 | VAL | CA-C-O | -5.02 | 115.73 | 120.95 |
| 3 | M | 106 | HIS | CB-CG-CD2 | 5.02 | 137.72 | 131.20 |
| 2 | R | 153 | HIS | CB-CG-ND1 | -5.02 | 115.17 | 122.70 |
| 2 | S | 134 | ARG | CB-CA-C | 5.02 | 118.75 | 111.82 |
| 1 | A | 256 | SER | N-CA-CB | -5.02 | 104.81 | 112.28 |
| 2 | I | 136 | GLU | CA-C-O | -5.02 | 114.49 | 120.56 |
| 3 | L | 51 | GLU | CA-C-N | -5.02 | 115.88 | 122.85 |
| 3 | L | 51 | GLU | C-N-CA | -5.02 | 115.88 | 122.85 |
| 3 | M | 39 | HIS | N-CA-C | -5.02 | 103.45 | 109.72 |
| 2 | Q | 208 | SER | O-C-N | 5.02 | 128.43 | 122.21 |
| 2 | Q | 367 | ASP | CA-CB-CG | 5.02 | 117.62 | 112.60 |
| 2 | R | 184 | ASN | OD1-CG-ND2 | -5.02 | 117.58 | 122.60 |
| 2 | R | 270 | LEU | N-CA-CB | -5.02 | 102.73 | 110.16 |
| 2 | J | 345 | PHE | N-CA-C | 5.02 | 117.64 | 111.82 |
| 3 | L | 25 | GLN | CA-C-O | -5.02 | 115.55 | 120.82 |
| 2 | Q | 207 | ASN | OD1-CG-ND2 | -5.02 | 117.58 | 122.60 |
| 2 | I | 353 | HIS | CA-CB-CG | -5.01 | 108.78 | 113.80 |
| 2 | I | 388 | PRO | CB-CA-C | -5.01 | 104.35 | 112.62 |
| 2 | I | 329 | GLY | CA-C-O | -5.01 | 118.56 | 122.52 |
| 2 | H | 307 | HIS | ND1-CE1-NE2 | 5.01 | 113.41 | 108.40 |
| 3 | K | 16 | SER | O-C-N | -5.01 | 116.36 | 122.22 |
| 3 | P | 71 | VAL | CA-C-O | -5.01 | 115.54 | 120.85 |
| 2 | S | 207 | ASN | CB-CA-C | -5.01 | 102.94 | 111.26 |
| 2 | H | 162 | LEU | CA-C-N | 5.01 | 129.66 | 122.40 |
| 2 | H | 162 | LEU | C-N-CA | 5.01 | 129.66 | 122.40 |
| 2 | C | 106 | ASP | N-CA-CB | 5.01 | 117.48 | 110.12 |
| 2 | Q | 283 | TRP | O-C-N | 5.01 | 127.43 | 122.12 |
| 3 | E | 105 | VAL | CB-CA-C | 5.00 | 116.03 | 110.62 |
| 2 | I | 179 | GLY | CA-C-O | -5.00 | 115.21 | 119.56 |
| 2 | J | 118 | THR | N-CA-C | -5.00 | 105.72 | 111.07 |
| 2 | Q | 161 | LEU | O-C-N | 5.00 | 127.30 | 122.09 |
| 3 | D | 50 | PRO | N-CA-C | 5.00 | 121.21 | 113.75 |
| 2 | J | 147 | THR | N-CA-C | 5.00 | 118.15 | 111.75 |
| 2 | S | 384 | VAL | N-CA-CB | -5.00 | 102.69 | 110.54 |
| 2 | I | 277 | ASN | N-CA-C | 5.00 | 116.42 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | N | 37 | GLY | CA-C-O | -5.00 | 113.46 | 119.06 |

There are no chirality outliers.

All (332) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 228 | GLU | Sidechain |
| 1 | A | 239 | GLN | Sidechain |
| 1 | A | 275 | GLU | Sidechain |
| 1 | A | 278 | ASN | Sidechain |
| 1 | A | 284 | GLU | Sidechain |
| 1 | A | 294 | ASP | Sidechain |
| 1 | A | 300 | ARG | Sidechain |
| 1 | A | 303 | GLU | Sidechain |
| 1 | A | 307 | GLN | Sidechain |
| 1 | B | 228 | GLU | Sidechain |
| 1 | B | 259 | GLN | Sidechain |
| 1 | B | 271 | GLN | Sidechain |
| 1 | B | 278 | ASN | Sidechain |
| 1 | B | 284 | GLU | Sidechain |
| 1 | B | 300 | ARG | Sidechain |
| 1 | B | 303 | GLU | Sidechain |
| 2 | C | 106 | ASP | Sidechain |
| 2 | C | 115 | ASN | Sidechain |
| 2 | C | 139 | ARG | Sidechain |
| 2 | C | 148 | PHE | Sidechain |
| 2 | C | 153 | HIS | Sidechain |
| 2 | C | 185 | TYR | Sidechain |
| 2 | C | 205 | ASN | Sidechain |
| 2 | C | 207 | ASN | Sidechain |
| 2 | C | 223 | ASP | Sidechain |
| 2 | C | 229 | GLN | Sidechain |
| 2 | C | 238 | HIS | Sidechain |
| 2 | C | 241 | ASN | Sidechain |
| 2 | C | 248 | GLU | Sidechain |
| 2 | C | 253 | ARG | Sidechain |
| 2 | C | 256 | PHE | Sidechain |
| 2 | C | 287 | ASN | Sidechain |
| 2 | C | 29 | TYR | Sidechain |
| 2 | C | 302 | ASP | Sidechain |
| 2 | C | 338 | ASP | Sidechain |
| 2 | C | 353 | HIS | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | C | 357 | ASP | Sidechain |
| 2 | C | 363 | PHE | Sidechain |
| 2 | C | 367 | ASP | Sidechain |
| 2 | C | 396 | ASP | Sidechain |
| 2 | C | 420 | ASN | Sidechain |
| 2 | C | 440 | GLU | Sidechain |
| 2 | C | 460 | ASP | Sidechain |
| 2 | C | 98 | PHE | Sidechain |
| 3 | D | 49 | ASN | Sidechain |
| 3 | D | 54 | TYR | Sidechain |
| 3 | D | 73 | ASP | Sidechain |
| 3 | D | 84 | ASP | Sidechain |
| 3 | D | 9 | GLU | Sidechain |
| 3 | D | 93 | ASP | Sidechain |
| 3 | E | 54 | TYR | Sidechain |
| 3 | E | 63 | PHE | Sidechain |
| 3 | E | 70 | GLN | Sidechain |
| 3 | E | 79 | ARG | Sidechain |
| 3 | E | 84 | ASP | Sidechain |
| 3 | E | 93 | ASP | Sidechain |
| 3 | E | 99 | GLN | Sidechain |
| 1 | F | 239 | GLN | Sidechain |
| 1 | F | 241 | TYR | Sidechain |
| 1 | F | 271 | GLN | Sidechain |
| 1 | F | 275 | GLU | Sidechain |
| 1 | F | 278 | ASN | Sidechain |
| 1 | F | 284 | GLU | Sidechain |
| 1 | F | 303 | GLU | Sidechain |
| 2 | G | 103 | TYR | Sidechain |
| 2 | G | 127 | PHE | Sidechain |
| 2 | G | 136 | GLU | Sidechain |
| 2 | G | 153 | HIS | Sidechain |
| 2 | G | 156 | GLN | Sidechain |
| 2 | G | 163 | ASN | Sidechain |
| 2 | G | 165 | TYR | Sidechain |
| 2 | G | 190 | TYR | Sidechain |
| 2 | G | 198 | ASP | Sidechain |
| 2 | G | 199 | PHE | Sidechain |
| 2 | G | 203 | ASP | Sidechain |
| 2 | G | 205 | ASN | Sidechain |
| 2 | G | 212 | GLN | Sidechain |
| 2 | G | 216 | ASP | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | G | 217 | ARG | Sidechain |
| 2 | G | 226 | HIS | Sidechain |
| 2 | G | 24 | TYR | Sidechain |
| 2 | G | 241 | ASN | Sidechain |
| 2 | G | 269 | PHE | Sidechain |
| 2 | G | 277 | ASN | Sidechain |
| 2 | G | 29 | TYR | Sidechain |
| 2 | G | 302 | ASP | Sidechain |
| 2 | G | 325 | HIS | Sidechain |
| 2 | G | 383 | HIS | Sidechain |
| 2 | G | 420 | ASN | Sidechain |
| 2 | G | 421 | ARG | Sidechain |
| 2 | G | 438 | TYR | Sidechain |
| 2 | G | 440 | GLU | Sidechain |
| 2 | G | 95 | ASN | Sidechain |
| 2 | G | 98 | PHE | Sidechain |
| 2 | H | 103 | TYR | Sidechain |
| 2 | H | 125 | PHE | Sidechain |
| 2 | H | 163 | ASN | Sidechain |
| 2 | H | 185 | TYR | Sidechain |
| 2 | H | 191 | GLU | Sidechain |
| 2 | H | 205 | ASN | Sidechain |
| 2 | H | 207 | ASN | Sidechain |
| 2 | H | 223 | ASP | Sidechain |
| 2 | H | 226 | HIS | Sidechain |
| 2 | H | 229 | GLN | Sidechain |
| 2 | H | 234 | GLU | Sidechain |
| 2 | H | 239 | TYR | Sidechain |
| 2 | H | 241 | ASN | Sidechain |
| 2 | H | 256 | PHE | Sidechain |
| 2 | H | 287 | ASN | Sidechain |
| 2 | H | 302 | ASP | Sidechain |
| 2 | H | 325 | HIS | Sidechain |
| 2 | H | 363 | PHE | Sidechain |
| 2 | H | 366 | GLN | Sidechain |
| 2 | H | 383 | HIS | Sidechain |
| 2 | H | 394 | PHE | Sidechain |
| 2 | H | 420 | ASN | Sidechain |
| 2 | H | 425 | GLU | Sidechain |
| 2 | H | 432 | ASN | Sidechain |
| 2 | H | 438 | TYR | Sidechain |
| 2 | H | 447 | GLU | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | H | 80 | TYR | Sidechain |
| 2 | H | 95 | ASN | Sidechain |
| 2 | I | 115 | ASN | Sidechain |
| 2 | I | 149 | GLN | Sidechain |
| 2 | I | 163 | ASN | Sidechain |
| 2 | I | 165 | TYR | Sidechain |
| 2 | I | 185 | TYR | Sidechain |
| 2 | I | 190 | TYR | Sidechain |
| 2 | I | 202 | ASP | Sidechain |
| 2 | I | 205 | ASN | Sidechain |
| 2 | I | 211 | PHE | Sidechain |
| 2 | I | 212 | GLN | Sidechain |
| 2 | I | 216 | ASP | Sidechain |
| 2 | I | 220 | PHE | Sidechain |
| 2 | I | 223 | ASP | Sidechain |
| 2 | I | 229 | GLN | Sidechain |
| 2 | I | 234 | GLU | Sidechain |
| 2 | I | 24 | TYR | Sidechain |
| 2 | I | 25 | TYR | Sidechain |
| 2 | I | 256 | PHE | Sidechain |
| 2 | I | 285 | ARG | Sidechain |
| 2 | I | 286 | ASP | Sidechain |
| 2 | I | 294 | HIS | Sidechain |
| 2 | I | 302 | ASP | Sidechain |
| 2 | I | 312 | ARG | Sidechain |
| 2 | I | 357 | ASP | Sidechain |
| 2 | I | 383 | HIS | Sidechain |
| 2 | I | 432 | ASN | Sidechain |
| 2 | I | 436 | ASP | Sidechain |
| 2 | I | 438 | TYR | Sidechain |
| 2 | I | 440 | GLU | Sidechain |
| 2 | I | 447 | GLU | Sidechain |
| 2 | I | 460 | ASP | Sidechain |
| 2 | I | 78 | ASP | Sidechain |
| 2 | I | 95 | ASN | Sidechain |
| 2 | I | 98 | PHE | Sidechain |
| 2 | J | 103 | TYR | Sidechain |
| 2 | J | 106 | ASP | Sidechain |
| 2 | J | 127 | PHE | Sidechain |
| 2 | J | 163 | ASN | Sidechain |
| 2 | J | 165 | TYR | Sidechain |
| 2 | J | 198 | ASP | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | J | 207 | ASN | Sidechain |
| 2 | J | 212 | GLN | Sidechain |
| 2 | J | 238 | HIS | Sidechain |
| 2 | J | 24 | TYR | Sidechain |
| 2 | J | 241 | ASN | Sidechain |
| 2 | J | 248 | GLU | Sidechain |
| 2 | J | 25 | TYR | Sidechain |
| 2 | J | 277 | ASN | Sidechain |
| 2 | J | 287 | ASN | Sidechain |
| 2 | J | 302 | ASP | Sidechain |
| 2 | J | 357 | ASP | Sidechain |
| 2 | J | 363 | PHE | Sidechain |
| 2 | J | 366 | GLN | Sidechain |
| 2 | J | 383 | HIS | Sidechain |
| 2 | J | 386 | HIS | Sidechain |
| 2 | J | 420 | ASN | Sidechain |
| 2 | J | 432 | ASN | Sidechain |
| 2 | J | 438 | TYR | Sidechain |
| 2 | J | 446 | ARG | Sidechain |
| 2 | J | 447 | GLU | Sidechain |
| 2 | J | 95 | ASN | Sidechain |
| 2 | J | 98 | PHE | Sidechain |
| 3 | K | 13 | GLU | Sidechain |
| 3 | K | 23 | ASP | Sidechain |
| 3 | K | 25 | GLN | Sidechain |
| 3 | K | 29 | GLN | Sidechain |
| 3 | K | 39 | HIS | Sidechain |
| 3 | K | 54 | TYR | Sidechain |
| 3 | K | 70 | GLN | Sidechain |
| 3 | K | 84 | ASP | Sidechain |
| 3 | K | 9 | GLU | Sidechain |
| 3 | K | 97 | GLN | Sidechain |
| 3 | L | 45 | ASN | Sidechain |
| 3 | L | 49 | ASN | Sidechain |
| 3 | L | 97 | GLN | Sidechain |
| 3 | M | 23 | ASP | Sidechain |
| 3 | M | 25 | GLN | Sidechain |
| 3 | M | 29 | GLN | Sidechain |
| 3 | M | 39 | HIS | Sidechain |
| 3 | M | 49 | ASN | Sidechain |
| 3 | M | 52 | GLU | Sidechain |
| 3 | M | 53 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | M | 84 | ASP | Sidechain |
| 3 | M | 9 | GLU | Sidechain |
| 3 | M | 97 | GLN | Sidechain |
| 3 | M | 99 | GLN | Sidechain |
| 3 | N | 17 | TYR | Sidechain |
| 3 | N | 23 | ASP | Sidechain |
| 3 | N | 39 | HIS | Sidechain |
| 3 | N | 53 | PHE | Sidechain |
| 3 | N | 9 | GLU | Sidechain |
| 3 | N | 92 | PHE | Sidechain |
| 3 | N | 93 | ASP | Sidechain |
| 3 | N | 97 | GLN | Sidechain |
| 3 | O | 12 | PHE | Sidechain |
| 3 | O | 13 | GLU | Sidechain |
| 3 | O | 23 | ASP | Sidechain |
| 3 | O | 36 | GLN | Sidechain |
| 3 | O | 54 | TYR | Sidechain |
| 3 | O | 82 | TYR | Sidechain |
| 3 | O | 84 | ASP | Sidechain |
| 3 | O | 9 | GLU | Sidechain |
| 3 | O | 97 | GLN | Sidechain |
| 3 | P | 17 | TYR | Sidechain |
| 3 | P | 23 | ASP | Sidechain |
| 3 | P | 32 | TYR | Sidechain |
| 3 | P | 53 | PHE | Sidechain |
| 3 | P | 86 | TYR | Sidechain |
| 3 | P | 92 | PHE | Sidechain |
| 3 | P | 93 | ASP | Sidechain |
| 3 | P | 97 | GLN | Sidechain |
| 2 | Q | 110 | GLU | Sidechain |
| 2 | Q | 127 | PHE | Sidechain |
| 2 | Q | 136 | GLU | Sidechain |
| 2 | Q | 137 | ASP | Sidechain |
| 2 | Q | 153 | HIS | Sidechain |
| 2 | Q | 163 | ASN | Sidechain |
| 2 | Q | 165 | TYR | Sidechain |
| 2 | Q | 185 | TYR | Sidechain |
| 2 | Q | 190 | TYR | Sidechain |
| 2 | Q | 205 | ASN | Sidechain |
| 2 | Q | 207 | ASN | Sidechain |
| 2 | Q | 209 | GLN | Sidechain |
| 2 | Q | 212 | GLN | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | Q | 226 | HIS | Sidechain |
| 2 | Q | 229 | GLN | Sidechain |
| 2 | Q | 234 | GLU | Sidechain |
| 2 | Q | 24 | TYR | Sidechain |
| 2 | Q | 241 | ASN | Sidechain |
| 2 | Q | 25 | TYR | Sidechain |
| 2 | Q | 253 | ARG | Sidechain |
| 2 | Q | 259 | GLU | Sidechain |
| 2 | Q | 268 | ASP | Sidechain |
| 2 | Q | 277 | ASN | Sidechain |
| 2 | Q | 302 | ASP | Sidechain |
| 2 | Q | 307 | HIS | Sidechain |
| 2 | Q | 324 | ASP | Sidechain |
| 2 | Q | 338 | ASP | Sidechain |
| 2 | Q | 357 | ASP | Sidechain |
| 2 | Q | 401 | GLN | Sidechain |
| 2 | Q | 436 | ASP | Sidechain |
| 2 | Q | 438 | TYR | Sidechain |
| 2 | Q | 446 | ARG | Sidechain |
| 2 | Q | 447 | GLU | Sidechain |
| 2 | Q | 60 | GLU | Sidechain |
| 2 | Q | 95 | ASN | Sidechain |
| 2 | R | 216 | ASP | Sidechain |
| 2 | R | 229 | GLN | Sidechain |
| 2 | R | 239 | TYR | Sidechain |
| 2 | R | 302 | ASP | Sidechain |
| 2 | R | 324 | ASP | Sidechain |
| 2 | R | 325 | HIS | Sidechain |
| 2 | R | 327 | HIS | Sidechain |
| 2 | R | 33 | ASP | Sidechain |
| 2 | R | 338 | ASP | Sidechain |
| 2 | R | 383 | HIS | Sidechain |
| 2 | R | 397 | ASP | Sidechain |
| 2 | R | 440 | GLU | Sidechain |
| 2 | R | 72 | ASP | Sidechain |
| 2 | R | 88 | GLU | Sidechain |
| 2 | R | 95 | ASN | Sidechain |
| 2 | R | 97 | TYR | Sidechain |
| 2 | R | 98 | PHE | Sidechain |
| 2 | S | 103 | TYR | Sidechain |
| 2 | S | 115 | ASN | Sidechain |
| 2 | S | 127 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | S | 136 | GLU | Sidechain |
| 2 | S | 139 | ARG | Sidechain |
| 2 | S | 153 | HIS | Sidechain |
| 2 | S | 158 | GLU | Sidechain |
| 2 | S | 163 | ASN | Sidechain |
| 2 | S | 165 | TYR | Sidechain |
| 2 | S | 185 | TYR | Sidechain |
| 2 | S | 205 | ASN | Sidechain |
| 2 | S | 209 | GLN | Sidechain |
| 2 | S | 211 | PHE | Sidechain |
| 2 | S | 212 | GLN | Sidechain |
| 2 | S | 217 | ARG | Sidechain |
| 2 | S | 223 | ASP | Sidechain |
| 2 | S | 229 | GLN | Sidechain |
| 2 | S | 241 | ASN | Sidechain |
| 2 | S | 25 | TYR | Sidechain |
| 2 | S | 256 | PHE | Sidechain |
| 2 | S | 286 | ASP | Sidechain |
| 2 | S | 302 | ASP | Sidechain |
| 2 | S | 304 | GLN | Sidechain |
| 2 | S | 306 | ASN | Sidechain |
| 2 | S | 324 | ASP | Sidechain |
| 2 | S | 325 | HIS | Sidechain |
| 2 | S | 35 | ASP | Sidechain |
| 2 | S | 352 | ASP | Sidechain |
| 2 | S | 357 | ASP | Sidechain |
| 2 | S | 367 | ASP | Sidechain |
| 2 | S | 383 | HIS | Sidechain |
| 2 | S | 432 | ASN | Sidechain |
| 2 | S | 436 | ASP | Sidechain |
| 2 | S | 438 | TYR | Sidechain |
| 2 | S | 440 | GLU | Sidechain |
| 2 | S | 447 | GLU | Sidechain |
| 2 | S | 78 | ASP | Sidechain |
| 2 | S | 85 | TYR | Sidechain |
| 2 | S | 86 | HIS | Sidechain |
| 2 | S | 98 | PHE | Sidechain |
| 1 | T | 239 | GLN | Sidechain |
| 1 | T | 275 | GLU | Sidechain |
| 1 | T | 278 | ASN | Sidechain |
| 1 | T | 283 | HIS | Sidechain |
| 1 | T | 284 | GLU | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | T | 294 | ASP | Sidechain |
| 1 | T | 307 | GLN | Sidechain |

## 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 | 697 | 0 | 684 | 2 | 0 |
| 1 | B | 697 | 0 | 684 | 1 | 0 |
| 1 | F | 697 | 0 | 684 | 2 | 0 |
| 1 | T | 697 | 0 | 684 | 0 | 0 |
| 2 | C | 3333 | 0 | 3256 | 4 | 0 |
| 2 | G | 3333 | 0 | 3256 | 4 | 0 |
| 2 | H | 3333 | 0 | 3256 | 7 | 0 |
| 2 | I | 3333 | 0 | 3256 | 4 | 0 |
| 2 | J | 3333 | 0 | 3256 | 7 | 0 |
| 2 | Q | 3333 | 0 | 3256 | 3 | 0 |
| 2 | R | 3333 | 0 | 3256 | 1 | 0 |
| 2 | S | 3333 | 0 | 3256 | 4 | 0 |
| 3 | D | 857 | 0 | 810 | 0 | 0 |
| 3 | E | 857 | 0 | 810 | 1 | 0 |
| 3 | K | 857 | 0 | 810 | 0 | 0 |
| 3 | L | 857 | 0 | 810 | 1 | 0 |
| 3 | M | 857 | 0 | 810 | 0 | 0 |
| 3 | N | 857 | 0 | 810 | 0 | 0 |
| 3 | O | 857 | 0 | 810 | 0 | 0 |
| 3 | P | 857 | 0 | 810 | 0 | 0 |
| All | All | 36308 | 0 | 35264 | 36 | 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 0.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:169:MET:HE1 | 2:C:375:LEU:HD13 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:318:LEU:HD12 | 2:G:321:SER:OG | 1.91 | 0.71 |
| 2:Q:348:LEU:HD23 | 2:Q:354:ILE:HG21 | 1.77 | 0.66 |
| 2:C:167:ARG:HH11 | 2:C:425:GLU:HG3 | 1.60 | 0.66 |
| 1:F:300:ARG:HE | 2:I:30:THR:HB | 1.72 | 0.55 |
| 2:C:436:ASP:N | 2:C:440:GLU:OE2 | 2.41 | 0.54 |
| 2:R:169:MET:HE1 | 2:R:375:LEU:HD13 | 1.90 | 0.53 |
| 2:H:436:ASP:N | 2:H:440:GLU:OE1 | 2.44 | 0.50 |
| 2:H:142:VAL:HG13 | 2:H:369:ALA:HB2 | 1.95 | 0.49 |
| 2:H:264:ILE:HB | 2:H:290:LEU:HB2 | 1.96 | 0.48 |
| 2:H:431:ARG:HE | 2:H:437:LEU:HD11 | 1.79 | 0.47 |
| 2:S:397:ASP:N | 2:S:397:ASP:OD1 | 2.46 | 0.47 |
| 2:S:436:ASP:N | 2:S:440:GLU:OE2 | 2.48 | 0.47 |
| 1:B:300:ARG:HE | 2:J:30:THR:HG22 | 1.79 | 0.47 |
| 2:I:319:ARG:HH11 | 2:I:349:MET:HA | 1.80 | 0.46 |
| 1:A:300:ARG:HE | 2:Q:30:THR:HB | 1.80 | 0.46 |
| 2:I:253:ARG:HH11 | 2:I:253:ARG:HG3 | 1.81 | 0.46 |
| 2:S:253:ARG:HG3 | 2:S:253:ARG:HH11 | 1.82 | 0.45 |
| 3:E:79:ARG:HE | 3:E:106:HIS:HB2 | 1.82 | 0.44 |
| 3:L:10:ARG:HE | 2:S:232:THR:C | 2.25 | 0.43 |
| 2:G:319:ARG:HH11 | 2:G:349:MET:HA | 1.84 | 0.43 |
| 2:H:214:TRP:CE3 | 2:H:215:ARG:HA | 2.55 | 0.42 |
| 2:Q:319:ARG:HH11 | 2:Q:349:MET:HA | 1.84 | 0.41 |
| 2:J:234:GLU:HB2 | 2:J:236:LYS:NZ | 2.35 | 0.41 |
| 2:J:27:PRO:HA | 2:J:85:TYR:O | 2.20 | 0.41 |
| 1:A:289:ARG:HG3 | 1:A:305:LEU:HA | 2.02 | 0.41 |
| 2:G:357:ASP:HB3 | 2:G:360:ARG:HE | 1.86 | 0.41 |
| 2:J:82:GLY:C | 2:J:101:ILE:HD11 | 2.46 | 0.41 |
| 2:C:205:ASN:OD1 | 2:G:118:THR:HG22 | 2.20 | 0.41 |
| 2:H:96:SER:C | 2:H:97:TYR:CG | 2.99 | 0.41 |
| 2:H:84:CYS:HA | 2:H:101:ILE:HA | 2.03 | 0.40 |
| 2:J:268:ASP:OD1 | 2:J:268:ASP:N | 2.51 | 0.40 |
| 1:F:264:ILE:HA | 1:F:275:GLU:OE1 | 2.22 | 0.40 |
| 2:I:204:GLU:HG2 | 2:I:205:ASN:N | 2.37 | 0.40 |
| 2:J:295:ARG:O | 2:J:295:ARG:HG3 | 2.21 | 0.40 |
| 2:J:357:ASP:N | 2:J:362:VAL:O | 2.55 | 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 PDB entries followed by that with respect to all EM entries.

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 | 84/86 (98%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 1 | B | 84/86 (98%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | F | 84/86 (98%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 1 | T | 84/86 (98%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 2 | C | 418/442 (95%) | 415 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | G | 418/442 (95%) | 415 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | H | 418/442 (95%) | 413 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | I | 418/442 (95%) | 414 (99%) | 4 (1%) | 0 | 100 | 100 |
| 2 | J | 418/442 (95%) | 414 (99%) | 4 (1%) | 0 | 100 | 100 |
| 2 | Q | 418/442 (95%) | 413 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | R | 418/442 (95%) | 415 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | S | 418/442 (95%) | 415 (99%) | 3 (1%) | 0 | 100 | 100 |
| 3 | D | 99/101 (98%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 3 | E | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | K | 99/101 (98%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 3 | L | 99/101 (98%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 3 | M | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | N | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | O | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | P | 99/101 (98%) | 99 (100%) | 0 | 0 | 100 | 100 |
| All | All | 4472/4688 (95%) | 4436 (99%) | 36 (1%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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 | 79/79 (100%) | 79 (100%) | 0 | 100 100 |
| 1 | B | 79/79 (100%) | 79 (100%) | 0 | 100 100 |
| 1 | F | 79/79 (100%) | 79 (100%) | 0 | 100 100 |
| 1 | T | 79/79 (100%) | 79 (100%) | 0 | 100 100 |
| 2 | C | 347/358 (97%) | 346 (100%) | 1 (0%) | 91 96 |
| 2 | G | 347/358 (97%) | 347 (100%) | 0 | 100 100 |
| 2 | H | 347/358 (97%) | 347 (100%) | 0 | 100 100 |
| 2 | I | 347/358 (97%) | 347 (100%) | 0 | 100 100 |
| 2 | J | 347/358 (97%) | 345 (99%) | 2 (1%) | 84 91 |
| 2 | Q | 347/358 (97%) | 347 (100%) | 0 | 100 100 |
| 2 | R | 347/358 (97%) | 346 (100%) | 1 (0%) | 91 96 |
| 2 | S | 347/358 (97%) | 347 (100%) | 0 | 100 100 |
| 3 | D | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | E | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | K | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | L | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | M | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | N | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | O | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| 3 | P | 95/95 (100%) | 95 (100%) | 0 | 100 100 |
| All | All | 3852/3940 (98%) | 3848 (100%) | 4 (0%) | 92 97 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 167 | ARG |
| 2 | J | 200 | THR |
| 2 | J | 285 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | R | 294 | HIS |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 247 | HIS |
| 2 | C | 366 | GLN |
| 2 | C | 383 | HIS |
| 3 | D | 47 | HIS |
| 3 | E | 47 | HIS |
| 3 | E | 70 | GLN |
| 3 | E | 99 | GLN |
| 2 | G | 294 | HIS |
| 2 | H | 241 | ASN |
| 2 | H | 307 | HIS |
| 2 | I | 184 | ASN |
| 2 | J | 184 | ASN |
| 2 | J | 429 | GLN |
| 3 | L | 69 | GLN |
| 3 | M | 69 | GLN |
| 3 | M | 70 | GLN |
| 3 | N | 69 | GLN |
| 3 | O | 47 | HIS |
| 3 | P | 47 | HIS |
| 2 | Q | 149 | GLN |
| 2 | Q | 163 | ASN |
| 2 | R | 91 | GLN |
| 2 | R | 267 | HIS |
| 2 | R | 353 | HIS |
| 2 | R | 383 | HIS |
| 2 | S | 207 | ASN |
| 2 | S | 226 | HIS |
| 2 | S | 229 | GLN |
| 2 | S | 241 | ASN |
| 2 | S | 267 | HIS |
| 2 | S | 277 | ASN |
| 2 | S | 383 | HIS |
| 2 | S | 386 | HIS |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

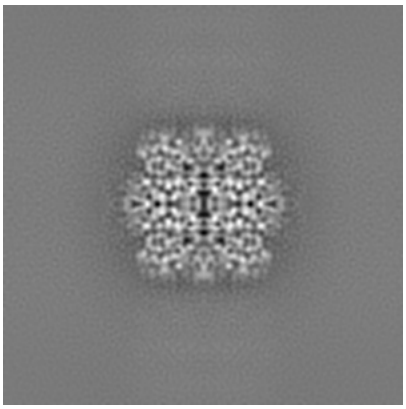
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50836. These allow visual inspection of the internal detail of the map and identification of artifacts.

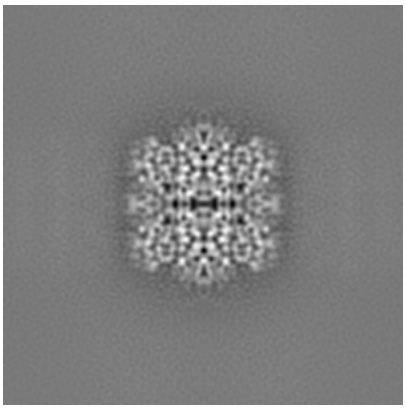
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

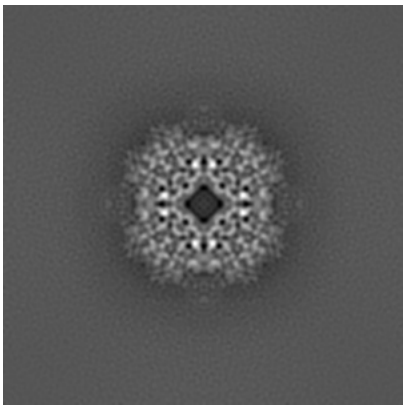
### 6.1.1 Primary map



X

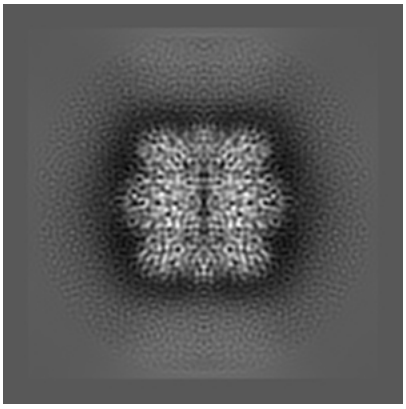


Y

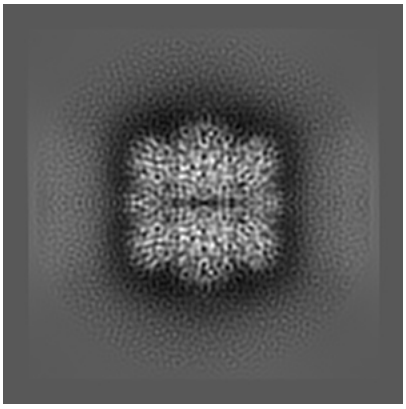


Z

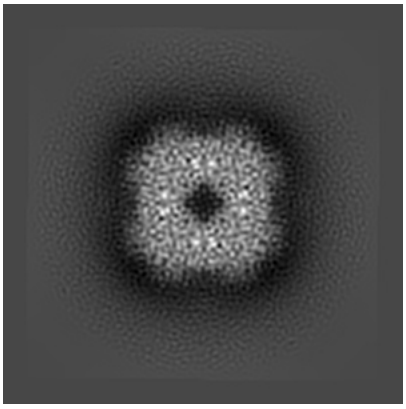
### 6.1.2 Raw map



X



Y

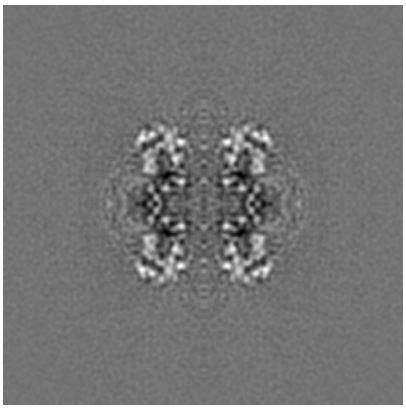


Z

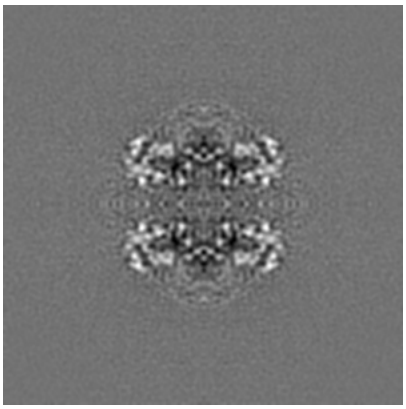
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

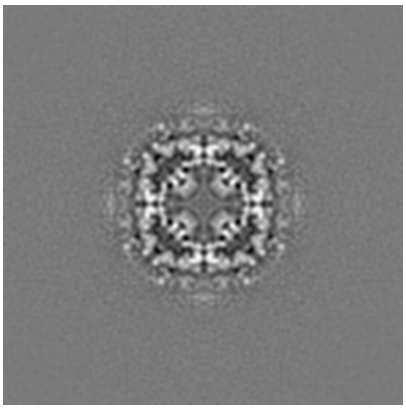
### 6.2.1 Primary map



X Index: 102

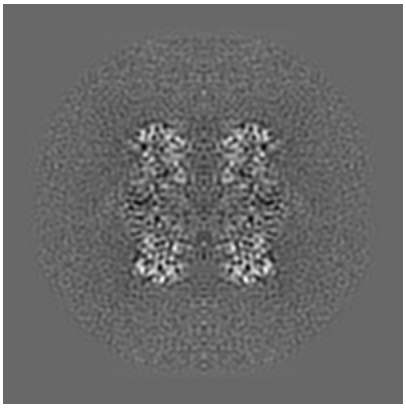


Y Index: 102

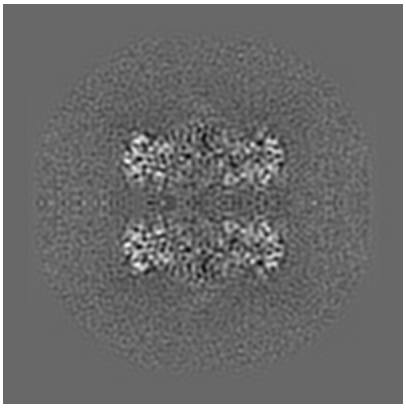


Z Index: 102

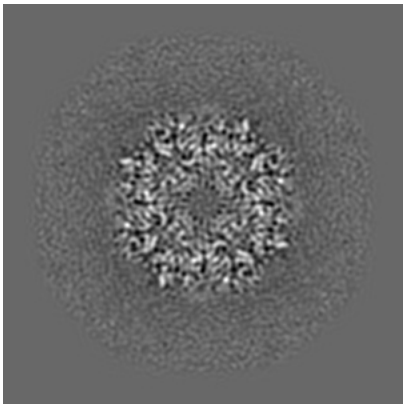
### 6.2.2 Raw map



X Index: 102



Y Index: 102

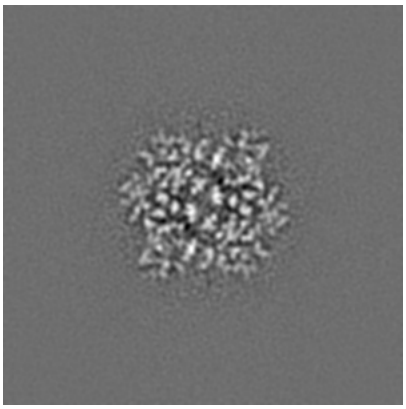


Z Index: 102

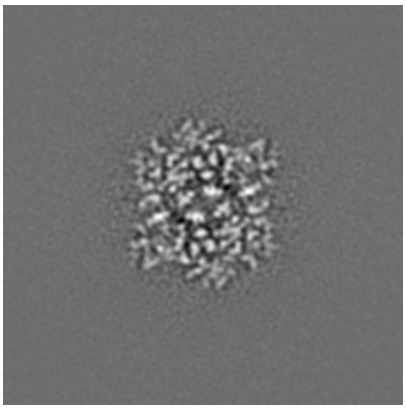
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

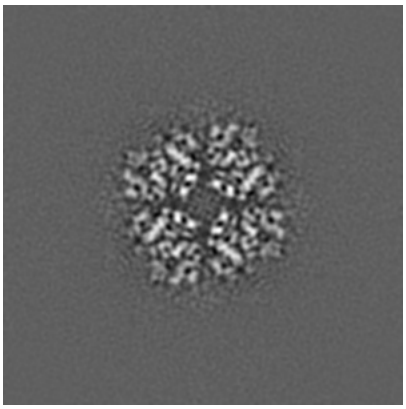
### 6.3.1 Primary map



X Index: 113

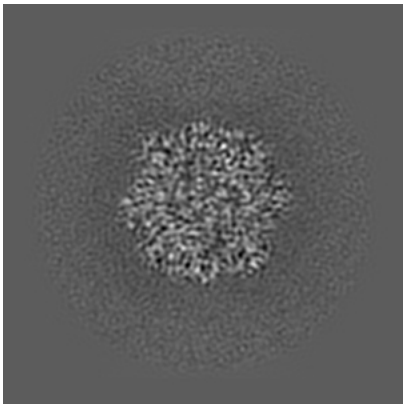


Y Index: 91

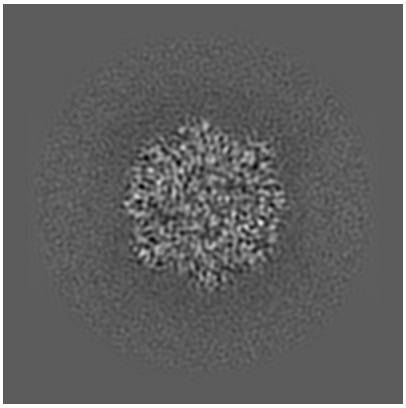


Z Index: 97

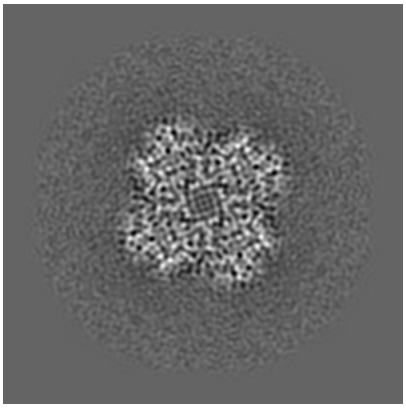
### 6.3.2 Raw map



X Index: 80



Y Index: 80

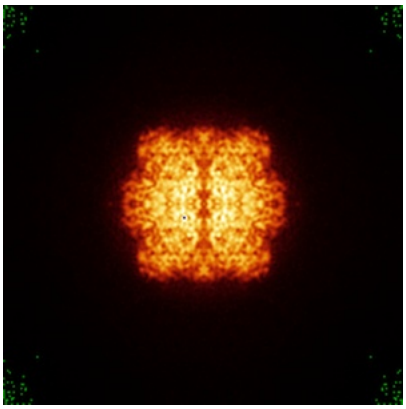


Z Index: 113

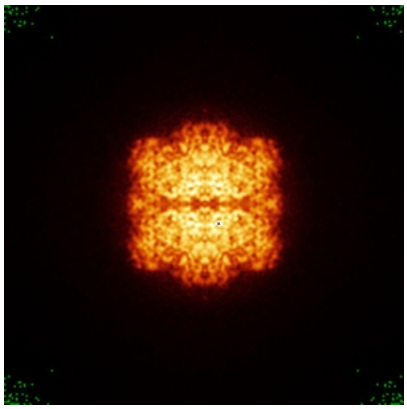
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

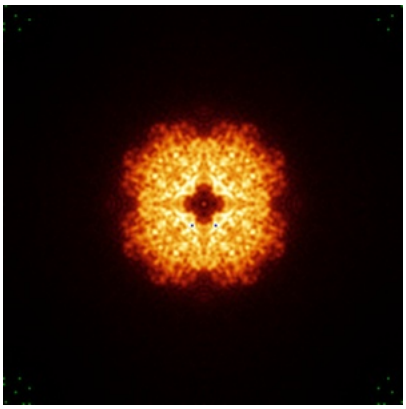
### 6.4.1 Primary map



X

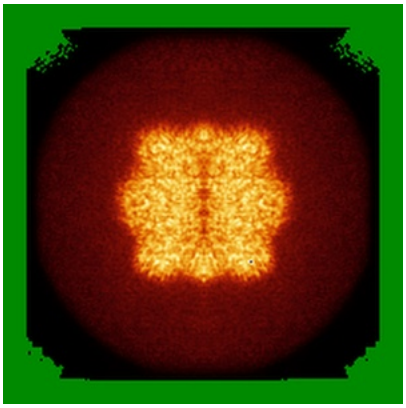


Y

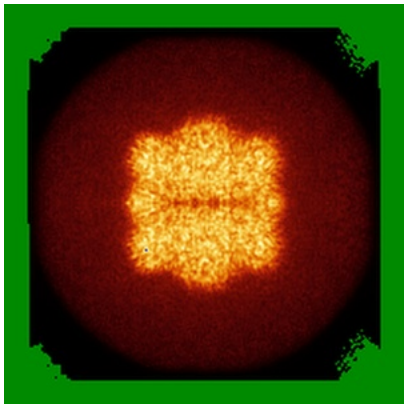


Z

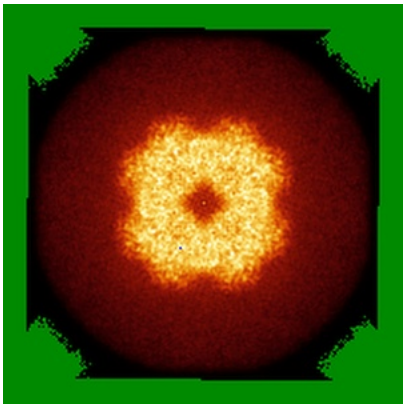
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

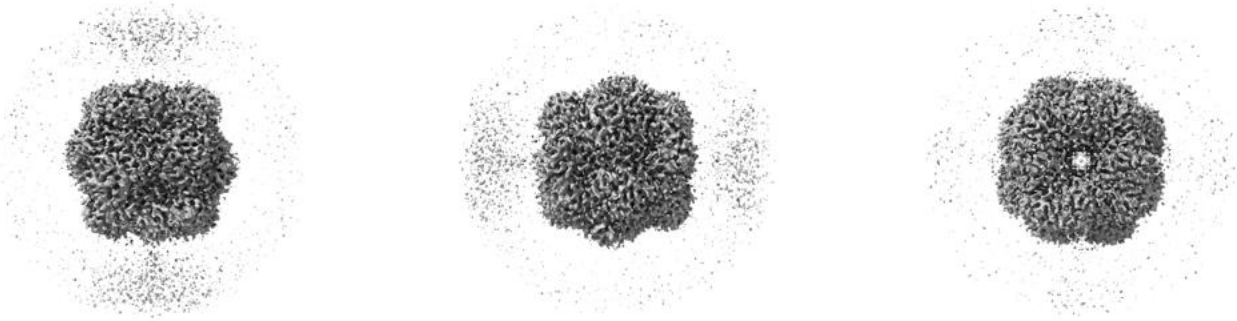
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.311. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

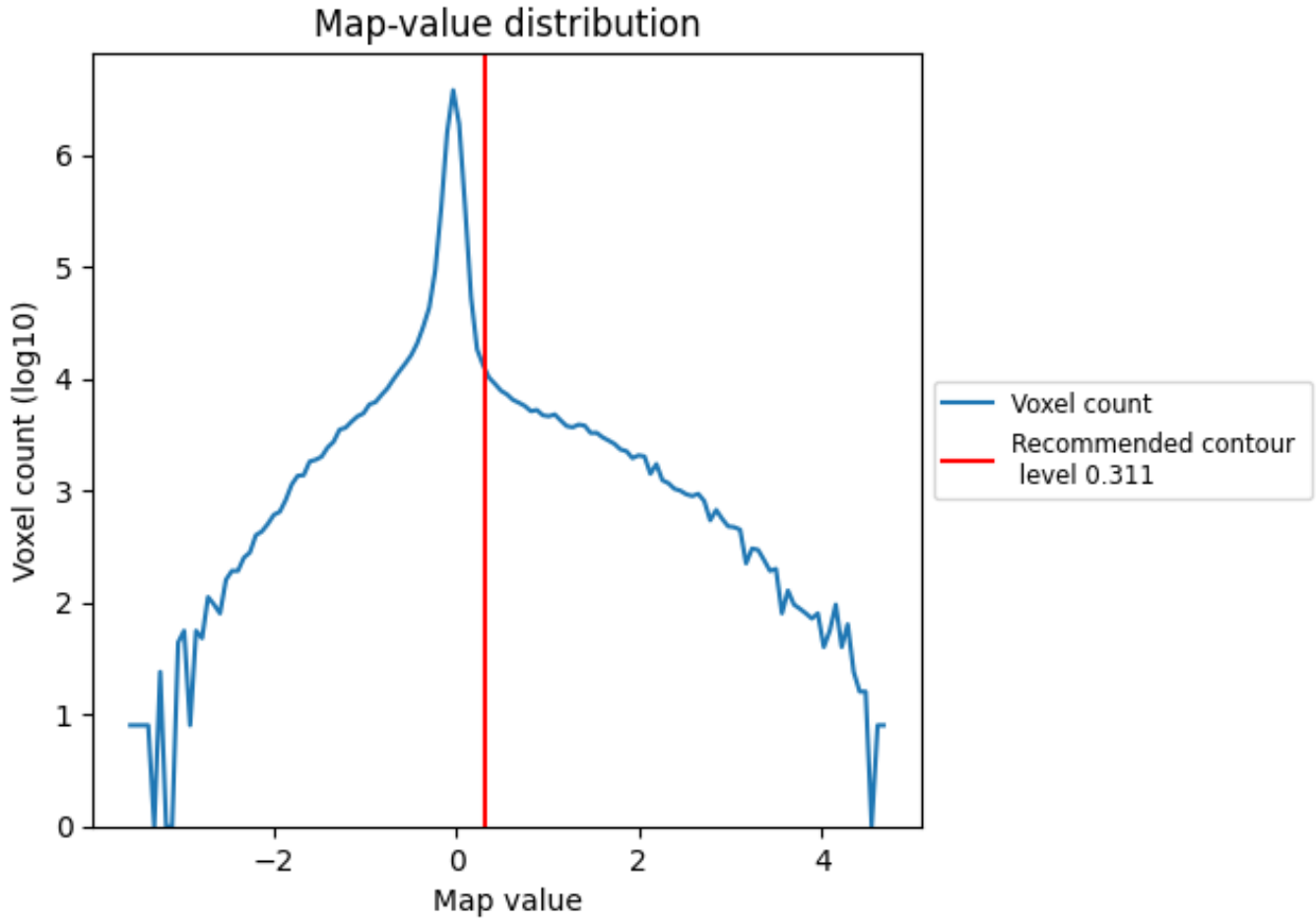
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

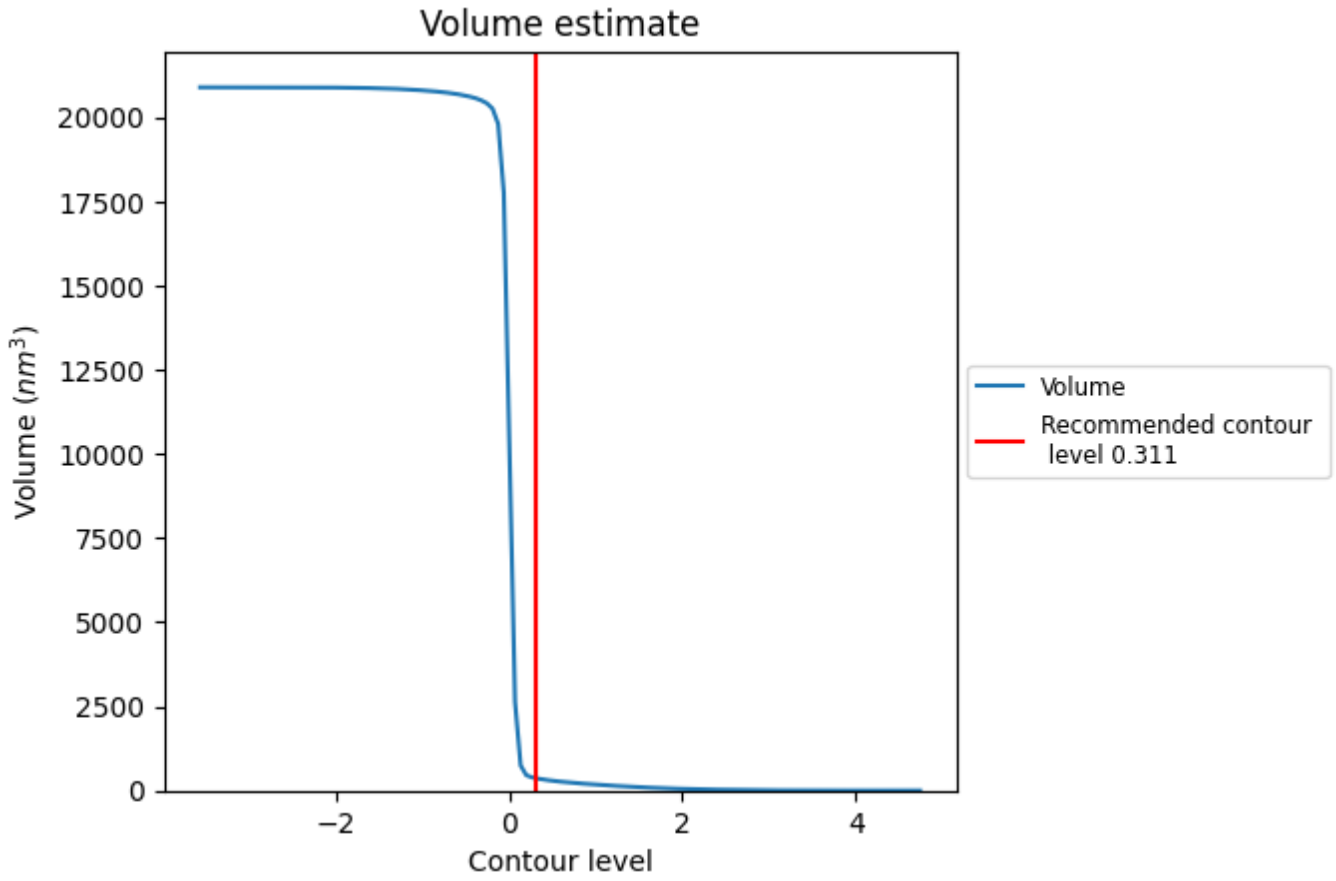
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

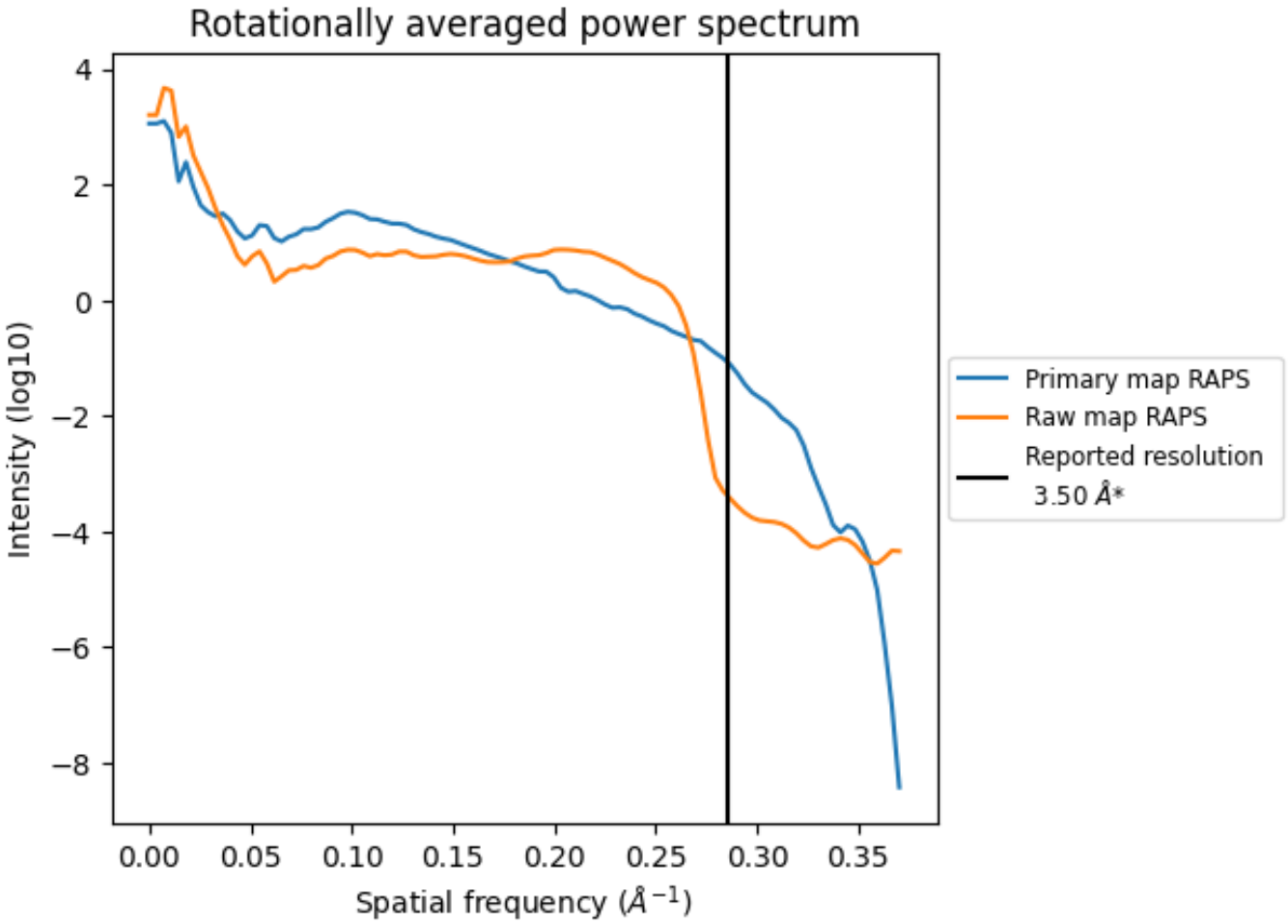
## 7.2 Volume estimate




The volume at the recommended contour level is 365 $nm^3$; this corresponds to an approximate mass of 330 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

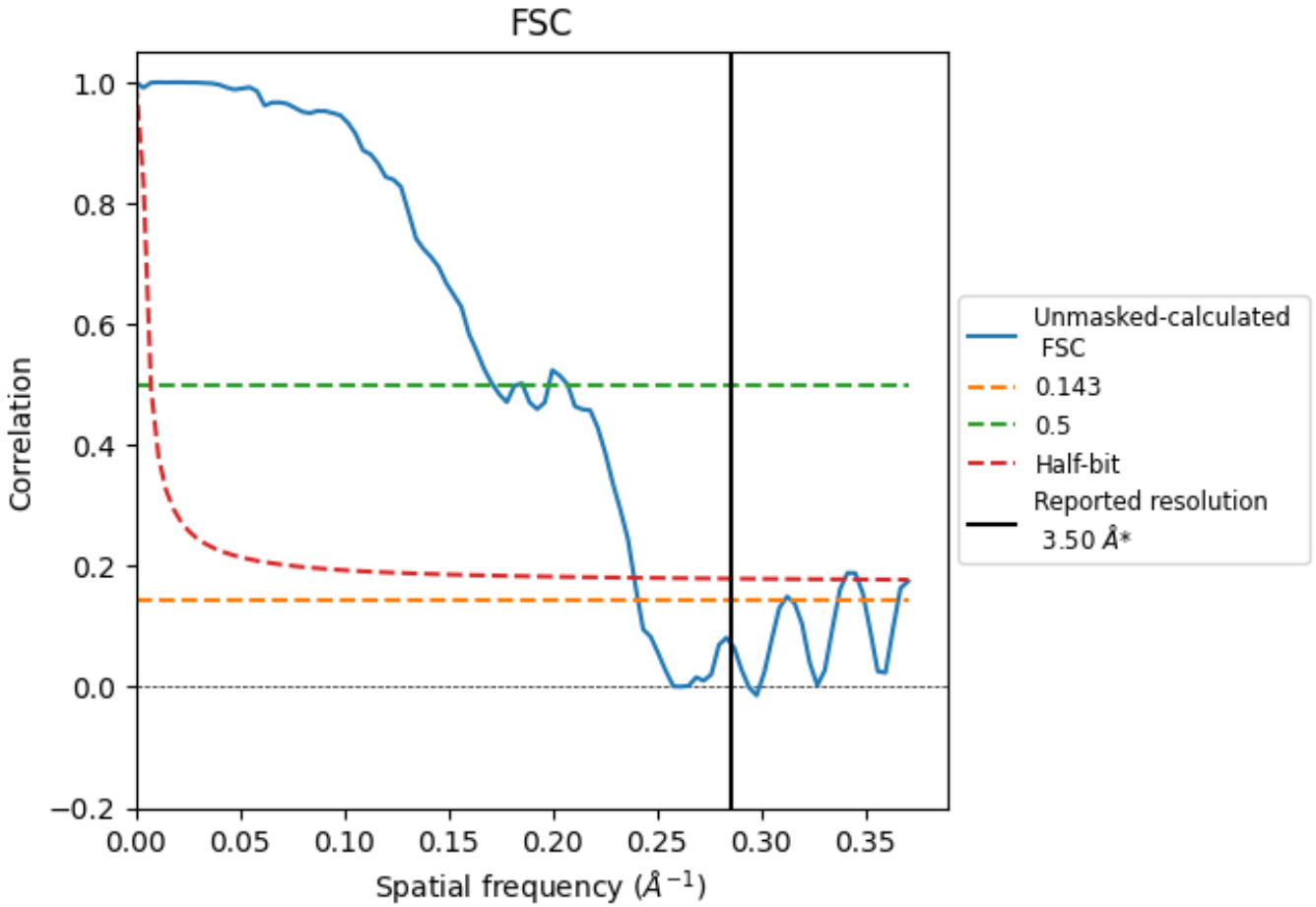



*Reported resolution corresponds to spatial frequency of 0.286 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.286 Å$^{-1}$

## 8.2 Resolution estimates (i)

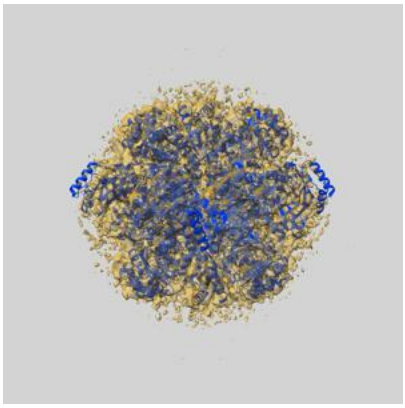
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.50 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 4.15 | 5.84 | 4.19 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.5 by more than 10 %

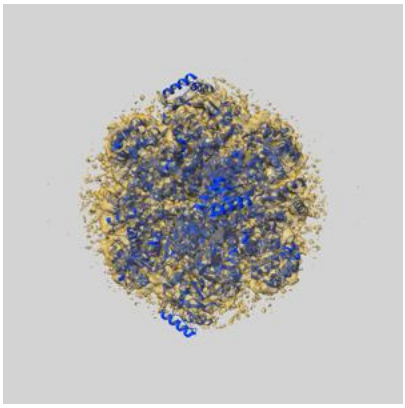
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50836 and PDB model 9FWV. Per-residue inclusion information can be found in section 3 on page 6.

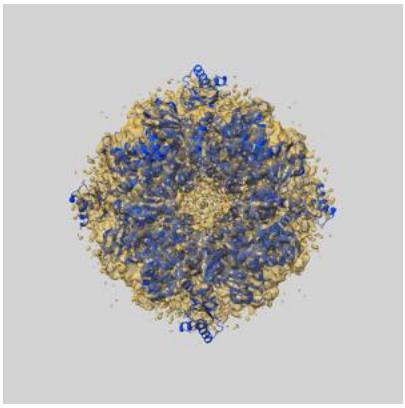
## 9.1 Map-model overlay



X



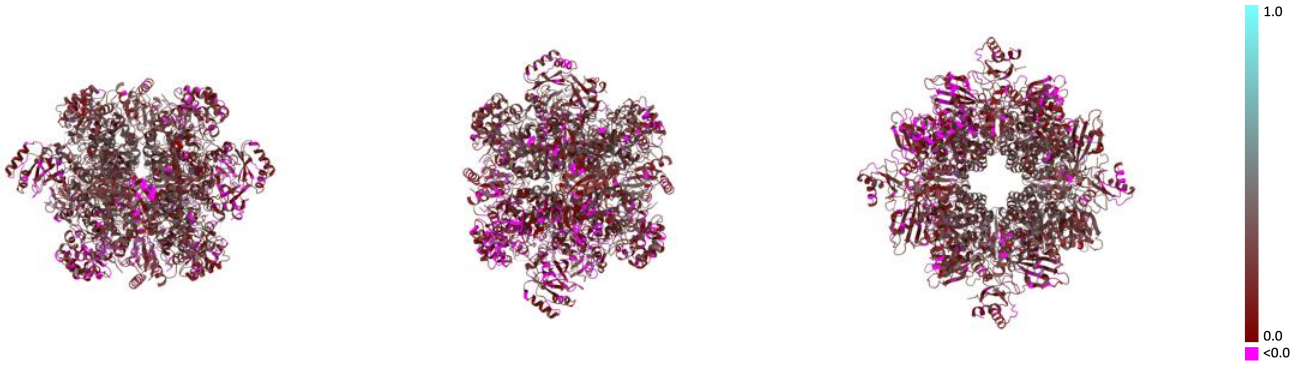
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.311 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

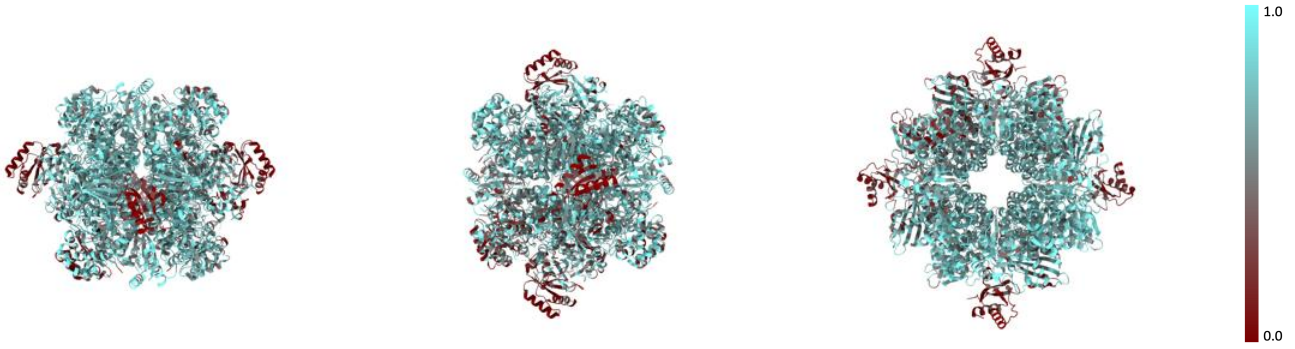
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

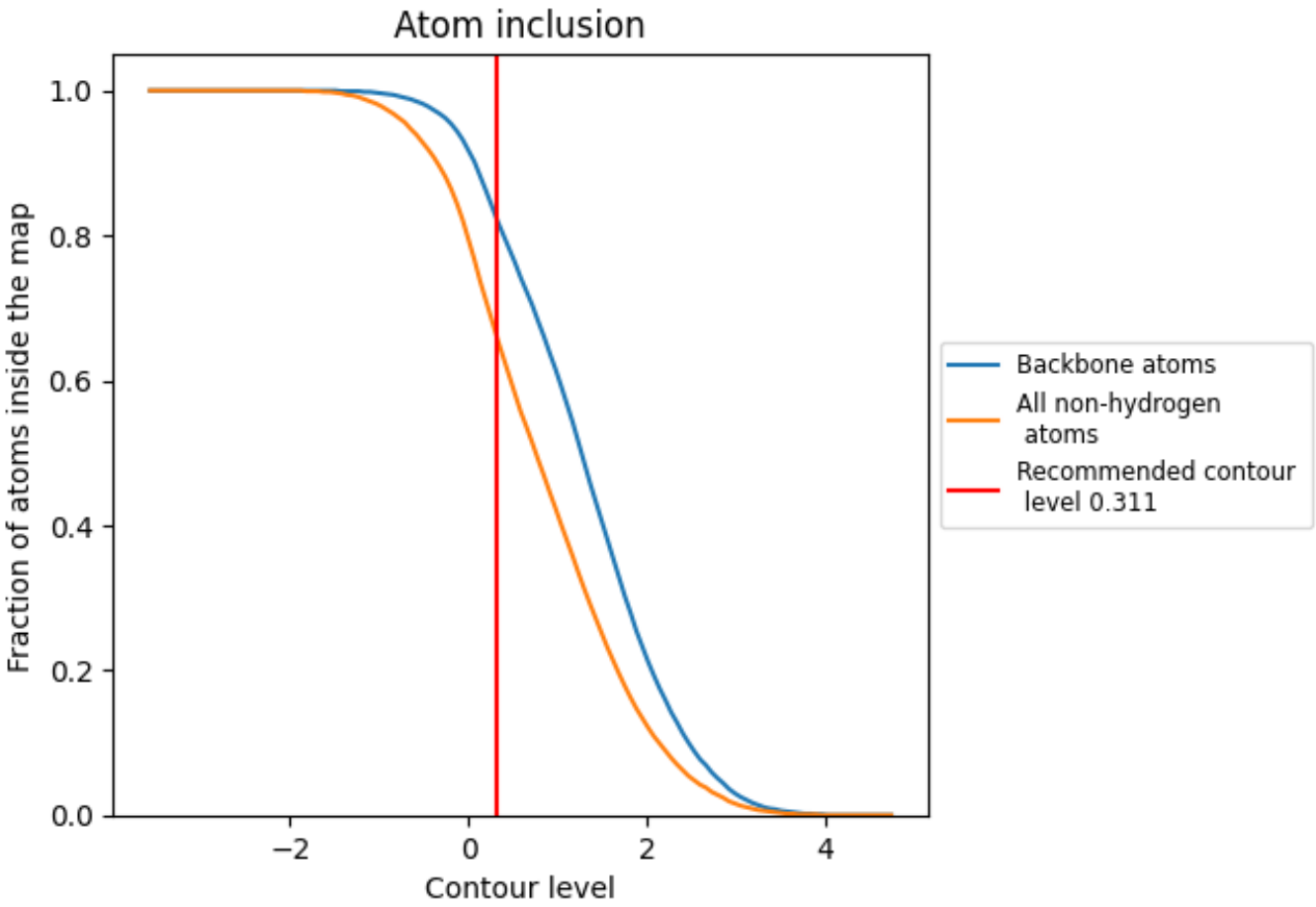
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.311).

## 9.4 Atom inclusion (i)




At the recommended contour level, 82% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.311) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6630 | 0.2120 |
| A | 0.1840 | 0.1660 |
| B | 0.1720 | 0.1580 |
| C | 0.7540 | 0.2740 |
| D | 0.7850 | 0.2800 |
| E | 0.7730 | 0.2360 |
| F | 0.1560 | 0.1590 |
| G | 0.7150 | 0.2190 |
| H | 0.6740 | 0.1950 |
| I | 0.7270 | 0.2400 |
| J | 0.6410 | 0.1490 |
| K | 0.7260 | 0.2190 |
| L | 0.7750 | 0.2730 |
| M | 0.7540 | 0.2180 |
| N | 0.4710 | 0.0300 |
| O | 0.5670 | 0.0980 |
| P | 0.6660 | 0.1630 |
| Q | 0.6310 | 0.1570 |
| R | 0.7710 | 0.2940 |
| S | 0.7480 | 0.2590 |
| T | 0.1620 | 0.1430 |