



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:36 AM EDT

PDB ID : 1K8Z
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
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Deposited on : 2001-10-26
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.23.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

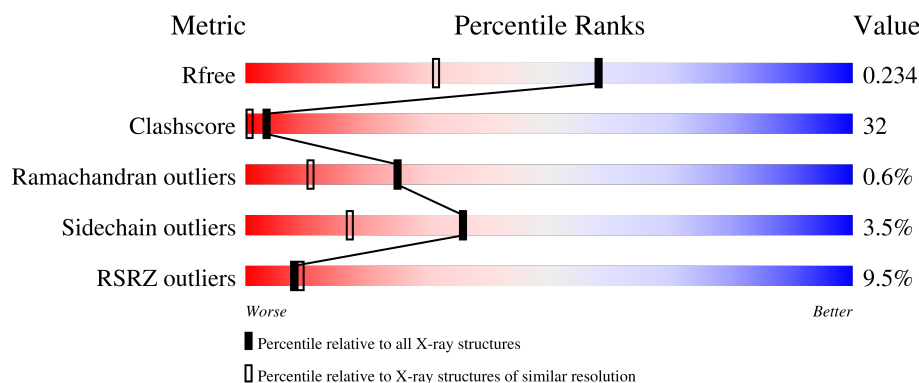
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 4298 (1.70-1.70) |
| Clashscore | 141614 | 4695 (1.70-1.70) |
| Ramachandran outliers | 138981 | 4610 (1.70-1.70) |
| Sidechain outliers | 138945 | 4610 (1.70-1.70) |
| RSRZ outliers | 127900 | 4222 (1.70-1.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 268 | |
| 2 | B | 396 | |

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5352 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRYPTOPHAN SYNTHASE ALPHA CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 257 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 1955 | 1248 | 334 | 365 | 8 | | | |

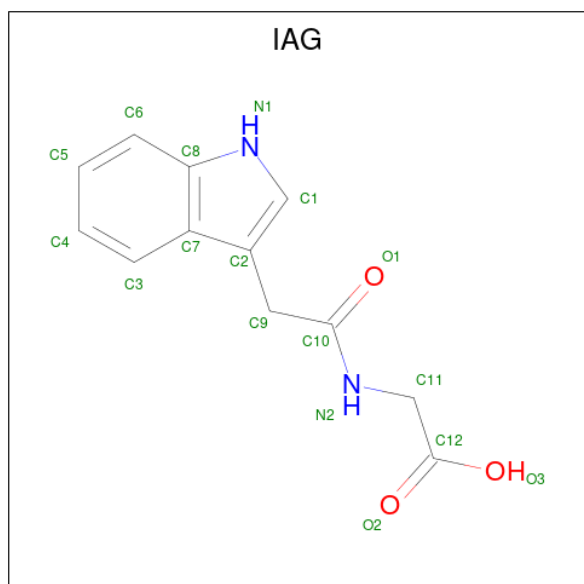
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 394 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2987 | 1877 | 527 | 564 | 19 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 34 | SER | ARG | cloning artifact | UNP P0A2K1 |
| B | 178 | PRO | SER | engineered mutation | UNP P0A2K1 |

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (three-letter code: IAG) (formula: C₁₂H₁₂N₂O₃).

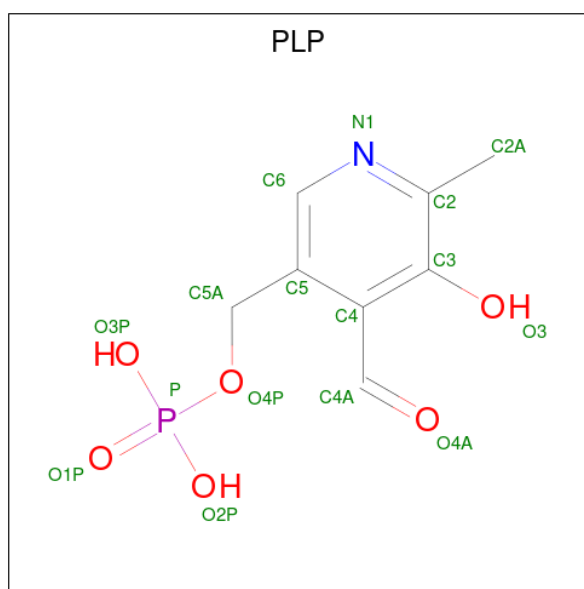


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 17 | 12 | 2 | 3 | | |

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | B | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 5 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 15 | 8 | 1 | 5 | 1 | | |

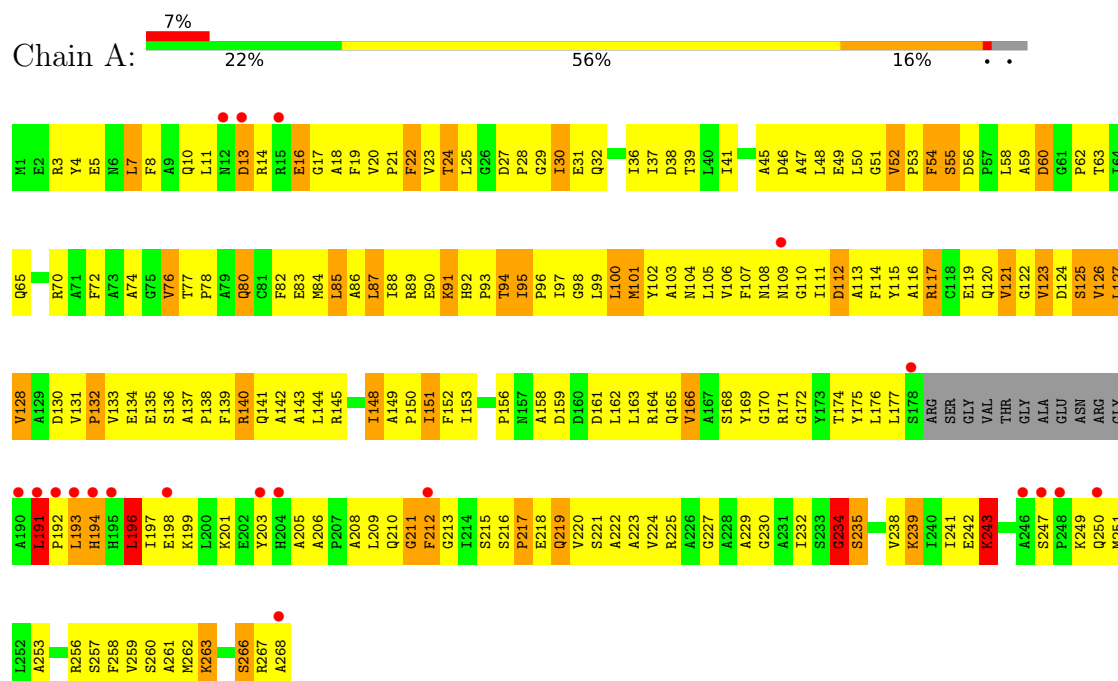
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6 | A | 129 | Total | O | 0 | 0 |
| | | | 129 | 129 | | |
| 6 | B | 248 | Total | O | 0 | 0 |
| | | | 248 | 248 | | |

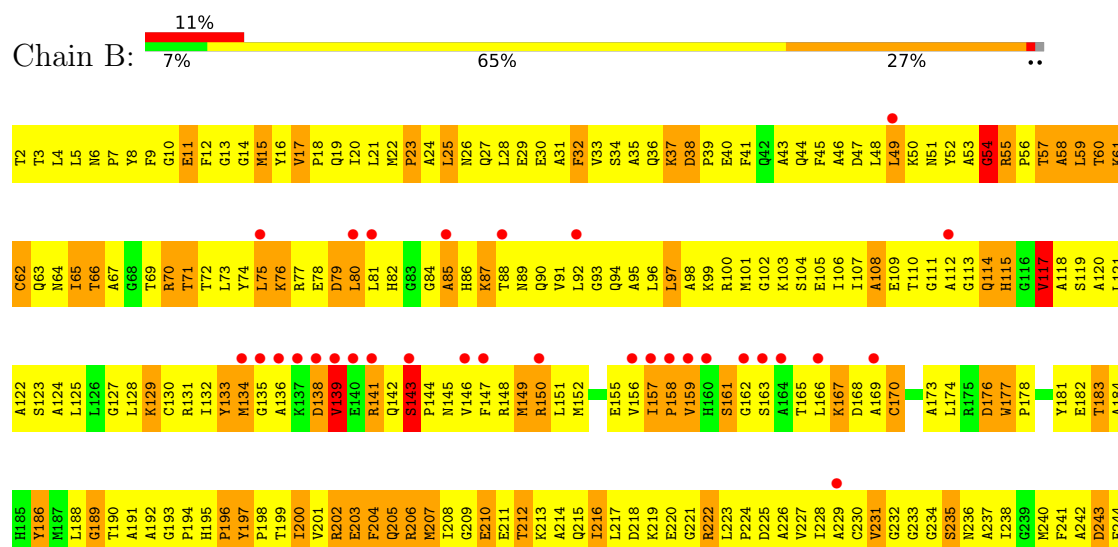
3 Residue-property plots [i](#)

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

• Molecule 1: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



| | | |
|------|------|------|
| I245 | D305 | Q365 |
| N246 | F306 | F366 |
| D247 | P307 | E367 |
| T248 | S308 | K368 |
| S249 | Y309 | E369 |
| V250 | Q310 | Q370 |
| G251 | P311 | L371 |
| L252 | Q312 | L372 |
| I253 | H313 | V373 |
| G254 | A314 | V374 |
| V255 | Y315 | N375 |
| E256 | L316 | L376 |
| P257 | N317 | S377 |
| G258 | S318 | G378 |
| G259 | I319 | R379 |
| H260 | G320 | G380 |
| Q261 | R321 | D381 |
| I262 | A322 | K382 |
| E263 | D323 | D383 |
| T264 | Y324 | T384 |
| G265 | V325 | F385 |
| E266 | S326 | T386 |
| H267 | I327 | V387 |
| Q268 | T328 | H388 |
| A269 | D329 | D389 |
| P270 | D330 | T390 |
| L271 | E331 | L391 |
| K272 | A332 | K392 |
| H273 | L333 | A393 |
| Q274 | F334 | R394 |
| R275 | A335 | G395 |
| V276 | F336 | GLU |
| G277 | K337 | ILE |
| I278 | T338 | |
| Y279 | L339 | |
| F280 | C340 | |
| G281 | R341 | |
| M282 | H342 | |
| K283 | E343 | |
| A284 | G344 | |
| P285 | I345 | |
| M286 | L346 | |
| M287 | P347 | |
| Q288 | A348 | |
| T289 | L349 | |
| A290 | E350 | |
| D291 | S351 | |
| Q292 | S352 | |
| Q293 | H353 | |
| I294 | A354 | |
| E295 | L355 | |
| E296 | A356 | |
| Y298 | H357 | |
| S297 | A358 | |
| S299 | L359 | |
| I300 | K360 | |
| S301 | H361 | |
| A302 | R362 | |
| G303 | R363 | |
| L304 | E364 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 184.42Å 61.03Å 67.53Å 90.00° 94.69° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 1.70 43.36 – 1.70 | Depositor EDS |
| % Data completeness (in resolution range) | 96.4 (20.00-1.70) 96.4 (43.36-1.70) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.06 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.92 (at 1.70Å) | Xtriage |
| Refinement program | CNS, REFMAC | Depositor |
| R, R_{free} | 0.209 , 0.265 0.188 , 0.234 | Depositor DCC |
| R_{free} test set | 4065 reflections (5.12%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 20.8 | Xtriage |
| Anisotropy | 0.592 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.37 , 56.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 5352 | wwPDB-VP |
| Average B, all atoms (Å ²) | 25.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IAG, PLP

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 3.32 | 245/2004 (12.2%) | 2.86 | 199/2722 (7.3%) |
| 2 | B | 4.35 | 703/3052 (23.0%) | 4.01 | 646/4123 (15.7%) |
| All | All | 3.97 | 948/5056 (18.8%) | 3.60 | 845/6845 (12.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 2 | B | 0 | 1 |
| All | All | 0 | 2 |

All (948) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 315 | TYR | CE2-CZ | 24.33 | 1.70 | 1.38 |
| 2 | B | 30 | GLU | CD-OE2 | 20.54 | 1.48 | 1.25 |
| 2 | B | 8 | TYR | CE1-CZ | 19.55 | 1.64 | 1.38 |
| 2 | B | 291 | ASP | CB-CG | -17.49 | 1.15 | 1.51 |
| 2 | B | 16 | TYR | CE2-CZ | 16.98 | 1.60 | 1.38 |
| 2 | B | 286 | MET | CB-CG | 16.45 | 2.04 | 1.51 |
| 2 | B | 256 | GLU | CG-CD | 16.42 | 1.76 | 1.51 |
| 2 | B | 45 | PHE | CE1-CZ | 15.99 | 1.67 | 1.37 |
| 2 | B | 324 | TYR | CE1-CZ | 15.56 | 1.58 | 1.38 |
| 2 | B | 204 | PHE | CD1-CE1 | 15.06 | 1.69 | 1.39 |
| 2 | B | 78 | GLU | CD-OE1 | 14.48 | 1.41 | 1.25 |
| 2 | B | 202 | ARG | NE-CZ | 14.39 | 1.51 | 1.33 |
| 2 | B | 235 | SER | CA-CB | 14.39 | 1.74 | 1.52 |
| 2 | B | 280 | PHE | CD2-CE2 | 14.14 | 1.67 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 373 | VAL | CB-CG1 | 13.92 | 1.82 | 1.52 |
| 2 | B | 257 | PRO | N-CD | 13.83 | 1.67 | 1.47 |
| 2 | B | 295 | GLU | CG-CD | 13.72 | 1.72 | 1.51 |
| 2 | B | 123 | SER | CB-OG | 13.61 | 1.59 | 1.42 |
| 2 | B | 77 | ARG | NE-CZ | 13.47 | 1.50 | 1.33 |
| 2 | B | 78 | GLU | CD-OE2 | -13.36 | 1.10 | 1.25 |
| 2 | B | 12 | PHE | CD1-CE1 | 13.36 | 1.66 | 1.39 |
| 1 | A | 212 | PHE | CD1-CE1 | 13.31 | 1.65 | 1.39 |
| 1 | A | 101 | MET | CG-SD | -13.23 | 1.46 | 1.81 |
| 2 | B | 72 | THR | CA-CB | -13.22 | 1.19 | 1.53 |
| 2 | B | 352 | SER | CB-OG | 12.97 | 1.59 | 1.42 |
| 1 | A | 82 | PHE | CD1-CE1 | -12.94 | 1.13 | 1.39 |
| 2 | B | 6 | ASN | C-O | 12.86 | 1.47 | 1.23 |
| 1 | A | 212 | PHE | CD2-CE2 | 12.84 | 1.65 | 1.39 |
| 2 | B | 61 | LYS | N-CA | 12.81 | 1.72 | 1.46 |
| 2 | B | 139 | VAL | CB-CG2 | 12.70 | 1.79 | 1.52 |
| 2 | B | 11 | GLU | CD-OE2 | 12.65 | 1.39 | 1.25 |
| 2 | B | 205 | GLN | CG-CD | 12.58 | 1.79 | 1.51 |
| 2 | B | 231 | VAL | CB-CG1 | 12.47 | 1.79 | 1.52 |
| 2 | B | 32 | PHE | CG-CD1 | 12.47 | 1.57 | 1.38 |
| 1 | A | 125 | SER | CA-CB | 12.46 | 1.71 | 1.52 |
| 2 | B | 233 | GLY | C-N | 12.46 | 1.55 | 1.33 |
| 2 | B | 108 | ALA | CA-CB | 12.42 | 1.78 | 1.52 |
| 2 | B | 29 | GLU | CD-OE2 | 12.39 | 1.39 | 1.25 |
| 2 | B | 196 | PRO | CA-C | 12.38 | 1.77 | 1.52 |
| 2 | B | 254 | GLY | C-O | 12.37 | 1.43 | 1.23 |
| 2 | B | 231 | VAL | C-N | 12.36 | 1.55 | 1.33 |
| 2 | B | 59 | LEU | N-CA | 12.34 | 1.71 | 1.46 |
| 2 | B | 252 | LEU | C-O | 12.27 | 1.46 | 1.23 |
| 1 | A | 117 | ARG | CG-CD | 12.25 | 1.82 | 1.51 |
| 2 | B | 255 | VAL | CA-CB | 12.16 | 1.80 | 1.54 |
| 2 | B | 135 | GLY | C-O | 12.11 | 1.43 | 1.23 |
| 2 | B | 268 | GLY | CA-C | -12.09 | 1.32 | 1.51 |
| 2 | B | 9 | PHE | CD2-CE2 | 11.86 | 1.62 | 1.39 |
| 1 | A | 13 | ASP | CB-CG | 11.84 | 1.76 | 1.51 |
| 1 | A | 210 | GLN | C-N | 11.82 | 1.54 | 1.33 |
| 2 | B | 319 | ILE | C-O | 11.72 | 1.45 | 1.23 |
| 2 | B | 61 | LYS | CB-CG | 11.70 | 1.84 | 1.52 |
| 1 | A | 166 | VAL | CB-CG2 | 11.54 | 1.77 | 1.52 |
| 2 | B | 205 | GLN | C-O | 11.52 | 1.45 | 1.23 |
| 2 | B | 211 | GLU | CD-OE2 | 11.20 | 1.38 | 1.25 |
| 2 | B | 30 | GLU | CG-CD | 11.14 | 1.68 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 98 | GLY | CA-C | 11.05 | 1.69 | 1.51 |
| 2 | B | 55 | ARG | CZ-NH2 | 11.05 | 1.47 | 1.33 |
| 2 | B | 58 | ALA | CA-CB | 11.02 | 1.75 | 1.52 |
| 2 | B | 314 | ALA | C-O | 11.01 | 1.44 | 1.23 |
| 2 | B | 243 | ASP | N-CA | -10.99 | 1.24 | 1.46 |
| 2 | B | 16 | TYR | CG-CD1 | 10.96 | 1.53 | 1.39 |
| 2 | B | 70 | ARG | CA-C | 10.93 | 1.81 | 1.52 |
| 1 | A | 219 | GLN | CB-CG | 10.91 | 1.82 | 1.52 |
| 2 | B | 12 | PHE | CD2-CE2 | 10.81 | 1.60 | 1.39 |
| 2 | B | 394 | ARG | CZ-NH1 | 10.80 | 1.47 | 1.33 |
| 1 | A | 126 | VAL | CB-CG1 | 10.77 | 1.75 | 1.52 |
| 2 | B | 286 | MET | CA-CB | 10.76 | 1.77 | 1.53 |
| 2 | B | 296 | GLU | CB-CG | 10.76 | 1.72 | 1.52 |
| 1 | A | 97 | ILE | C-N | 10.73 | 1.52 | 1.33 |
| 2 | B | 353 | HIS | CA-CB | 10.73 | 1.77 | 1.53 |
| 2 | B | 51 | ASN | CA-C | -10.72 | 1.25 | 1.52 |
| 1 | A | 151 | ILE | CA-CB | -10.60 | 1.30 | 1.54 |
| 2 | B | 282 | MET | CA-CB | 10.58 | 1.77 | 1.53 |
| 1 | A | 52 | VAL | CB-CG1 | 10.54 | 1.75 | 1.52 |
| 2 | B | 308 | SER | C-O | 10.54 | 1.43 | 1.23 |
| 1 | A | 169 | TYR | CG-CD2 | 10.50 | 1.52 | 1.39 |
| 2 | B | 76 | LYS | CD-CE | 10.47 | 1.77 | 1.51 |
| 1 | A | 143 | ALA | CA-CB | 10.46 | 1.74 | 1.52 |
| 2 | B | 196 | PRO | N-CD | 10.44 | 1.62 | 1.47 |
| 2 | B | 40 | GLU | CG-CD | 10.40 | 1.67 | 1.51 |
| 2 | B | 343 | GLU | CD-OE2 | 10.37 | 1.37 | 1.25 |
| 2 | B | 321 | ARG | C-O | 10.35 | 1.43 | 1.23 |
| 2 | B | 141 | ARG | C-O | 10.31 | 1.43 | 1.23 |
| 2 | B | 95 | ALA | C-O | 10.30 | 1.43 | 1.23 |
| 1 | A | 31 | GLU | CD-OE2 | 10.29 | 1.36 | 1.25 |
| 2 | B | 373 | VAL | C-O | 10.27 | 1.42 | 1.23 |
| 2 | B | 120 | ALA | CA-CB | -10.26 | 1.30 | 1.52 |
| 2 | B | 149 | MET | CG-SD | 10.26 | 2.07 | 1.81 |
| 2 | B | 367 | GLU | C-O | 10.25 | 1.42 | 1.23 |
| 1 | A | 145 | ARG | CZ-NH2 | 10.16 | 1.46 | 1.33 |
| 1 | A | 123 | VAL | CA-CB | 10.16 | 1.76 | 1.54 |
| 1 | A | 65 | GLN | CG-CD | 10.14 | 1.74 | 1.51 |
| 2 | B | 138 | ASP | C-O | 10.14 | 1.42 | 1.23 |
| 2 | B | 324 | TYR | CG-CD2 | 10.13 | 1.52 | 1.39 |
| 2 | B | 93 | GLY | C-O | 10.09 | 1.39 | 1.23 |
| 2 | B | 207 | MET | C-O | 10.09 | 1.42 | 1.23 |
| 2 | B | 17 | VAL | CB-CG1 | 10.08 | 1.74 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 297 | SER | CA-CB | -10.02 | 1.38 | 1.52 |
| 1 | A | 107 | PHE | CE1-CZ | 10.02 | 1.56 | 1.37 |
| 2 | B | 360 | LYS | C-O | 9.99 | 1.42 | 1.23 |
| 2 | B | 356 | ALA | CA-CB | -9.97 | 1.31 | 1.52 |
| 2 | B | 36 | GLN | CG-CD | 9.96 | 1.74 | 1.51 |
| 2 | B | 95 | ALA | CA-CB | 9.89 | 1.73 | 1.52 |
| 1 | A | 140 | ARG | CG-CD | 9.85 | 1.76 | 1.51 |
| 2 | B | 31 | ALA | N-CA | 9.81 | 1.66 | 1.46 |
| 2 | B | 117 | VAL | CA-CB | 9.78 | 1.75 | 1.54 |
| 1 | A | 158 | ALA | CA-CB | 9.75 | 1.73 | 1.52 |
| 2 | B | 78 | GLU | C-O | 9.74 | 1.41 | 1.23 |
| 2 | B | 279 | TYR | CE2-CZ | 9.74 | 1.51 | 1.38 |
| 2 | B | 181 | TYR | CD1-CE1 | 9.72 | 1.53 | 1.39 |
| 2 | B | 303 | GLY | N-CA | -9.69 | 1.31 | 1.46 |
| 2 | B | 289 | THR | CB-OG1 | 9.68 | 1.62 | 1.43 |
| 1 | A | 97 | ILE | N-CA | 9.67 | 1.65 | 1.46 |
| 2 | B | 85 | ALA | N-CA | 9.62 | 1.65 | 1.46 |
| 2 | B | 79 | ASP | CG-OD2 | 9.60 | 1.47 | 1.25 |
| 2 | B | 59 | LEU | CA-C | 9.57 | 1.77 | 1.52 |
| 2 | B | 29 | GLU | C-N | 9.54 | 1.55 | 1.34 |
| 1 | A | 20 | VAL | CB-CG1 | 9.53 | 1.72 | 1.52 |
| 2 | B | 260 | HIS | CA-CB | -9.51 | 1.33 | 1.53 |
| 2 | B | 328 | THR | CA-C | 9.49 | 1.77 | 1.52 |
| 2 | B | 203 | GLU | CA-C | 9.44 | 1.77 | 1.52 |
| 2 | B | 204 | PHE | CB-CG | 9.41 | 1.67 | 1.51 |
| 2 | B | 182 | GLU | CG-CD | 9.38 | 1.66 | 1.51 |
| 2 | B | 208 | ILE | CA-CB | -9.38 | 1.33 | 1.54 |
| 2 | B | 311 | PRO | N-CD | 9.36 | 1.60 | 1.47 |
| 2 | B | 194 | PRO | CA-C | -9.35 | 1.34 | 1.52 |
| 2 | B | 52 | TYR | CB-CG | -9.33 | 1.37 | 1.51 |
| 2 | B | 315 | TYR | CB-CG | -9.32 | 1.37 | 1.51 |
| 2 | B | 305 | ASP | CG-OD1 | 9.26 | 1.46 | 1.25 |
| 1 | A | 169 | TYR | CE2-CZ | -9.25 | 1.26 | 1.38 |
| 2 | B | 30 | GLU | CA-CB | 9.25 | 1.74 | 1.53 |
| 2 | B | 232 | GLY | CA-C | 9.23 | 1.66 | 1.51 |
| 1 | A | 203 | TYR | CE2-CZ | -9.22 | 1.26 | 1.38 |
| 2 | B | 361 | MET | SD-CE | -9.22 | 1.26 | 1.77 |
| 2 | B | 117 | VAL | CB-CG1 | 9.21 | 1.72 | 1.52 |
| 2 | B | 55 | ARG | CG-CD | 9.20 | 1.75 | 1.51 |
| 2 | B | 204 | PHE | CD2-CE2 | 9.19 | 1.57 | 1.39 |
| 1 | A | 74 | ALA | CA-CB | 9.17 | 1.71 | 1.52 |
| 1 | A | 170 | GLY | C-O | 9.17 | 1.38 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 7 | PRO | CA-C | 9.16 | 1.71 | 1.52 |
| 2 | B | 195 | HIS | N-CA | -9.13 | 1.28 | 1.46 |
| 2 | B | 22 | MET | SD-CE | -9.12 | 1.26 | 1.77 |
| 2 | B | 52 | TYR | CZ-OH | -9.11 | 1.22 | 1.37 |
| 2 | B | 6 | ASN | CA-C | -9.09 | 1.29 | 1.52 |
| 2 | B | 351 | SER | CA-C | 9.05 | 1.76 | 1.52 |
| 2 | B | 340 | CYS | CA-CB | -9.05 | 1.34 | 1.53 |
| 2 | B | 182 | GLU | CD-OE2 | 9.00 | 1.35 | 1.25 |
| 2 | B | 360 | LYS | CB-CG | -8.99 | 1.28 | 1.52 |
| 2 | B | 310 | GLY | C-O | 8.98 | 1.38 | 1.23 |
| 1 | A | 121 | VAL | N-CA | -8.97 | 1.28 | 1.46 |
| 2 | B | 197 | TYR | CA-CB | -8.96 | 1.34 | 1.53 |
| 2 | B | 367 | GLU | CG-CD | -8.87 | 1.38 | 1.51 |
| 2 | B | 52 | TYR | N-CA | -8.87 | 1.28 | 1.46 |
| 2 | B | 316 | LEU | C-O | 8.86 | 1.40 | 1.23 |
| 2 | B | 340 | CYS | CB-SG | 8.86 | 1.97 | 1.82 |
| 2 | B | 376 | LEU | CG-CD2 | 8.86 | 1.84 | 1.51 |
| 2 | B | 252 | LEU | CA-C | -8.84 | 1.29 | 1.52 |
| 2 | B | 276 | VAL | CA-CB | -8.83 | 1.36 | 1.54 |
| 2 | B | 362 | MET | SD-CE | -8.82 | 1.28 | 1.77 |
| 2 | B | 199 | THR | N-CA | -8.80 | 1.28 | 1.46 |
| 2 | B | 167 | LYS | CE-NZ | 8.79 | 1.71 | 1.49 |
| 2 | B | 159 | VAL | CB-CG1 | 8.76 | 1.71 | 1.52 |
| 1 | A | 229 | ALA | CA-C | -8.76 | 1.30 | 1.52 |
| 2 | B | 296 | GLU | CD-OE2 | 8.75 | 1.35 | 1.25 |
| 2 | B | 368 | LYS | CA-C | 8.75 | 1.75 | 1.52 |
| 2 | B | 227 | VAL | C-O | 8.73 | 1.40 | 1.23 |
| 1 | A | 140 | ARG | NE-CZ | -8.71 | 1.21 | 1.33 |
| 2 | B | 212 | THR | N-CA | 8.70 | 1.63 | 1.46 |
| 2 | B | 151 | LEU | C-O | 8.69 | 1.39 | 1.23 |
| 1 | A | 54 | PHE | CA-C | 8.68 | 1.75 | 1.52 |
| 1 | A | 140 | ARG | CB-CG | -8.67 | 1.29 | 1.52 |
| 2 | B | 245 | ILE | C-O | 8.66 | 1.39 | 1.23 |
| 2 | B | 362 | MET | C-O | 8.66 | 1.39 | 1.23 |
| 2 | B | 315 | TYR | CE1-CZ | -8.65 | 1.27 | 1.38 |
| 2 | B | 214 | ALA | CA-CB | 8.64 | 1.70 | 1.52 |
| 2 | B | 215 | GLN | N-CA | 8.64 | 1.63 | 1.46 |
| 2 | B | 263 | GLU | CG-CD | 8.63 | 1.64 | 1.51 |
| 2 | B | 244 | PHE | CB-CG | 8.62 | 1.66 | 1.51 |
| 2 | B | 255 | VAL | N-CA | -8.62 | 1.29 | 1.46 |
| 1 | A | 169 | TYR | CG-CD1 | -8.62 | 1.27 | 1.39 |
| 1 | A | 152 | PHE | CA-CB | -8.61 | 1.35 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 230 | GLY | CA-C | 8.60 | 1.65 | 1.51 |
| 1 | A | 139 | PHE | CB-CG | 8.59 | 1.66 | 1.51 |
| 2 | B | 117 | VAL | CA-C | -8.58 | 1.30 | 1.52 |
| 2 | B | 106 | ILE | CA-C | -8.58 | 1.30 | 1.52 |
| 2 | B | 325 | VAL | CA-CB | 8.57 | 1.72 | 1.54 |
| 2 | B | 165 | THR | C-O | 8.56 | 1.39 | 1.23 |
| 1 | A | 136 | SER | CA-CB | 8.54 | 1.65 | 1.52 |
| 2 | B | 284 | ALA | C-N | 8.52 | 1.50 | 1.34 |
| 1 | A | 107 | PHE | CG-CD1 | -8.51 | 1.25 | 1.38 |
| 2 | B | 177 | TRP | CD2-CE3 | 8.50 | 1.53 | 1.40 |
| 1 | A | 135 | GLU | CD-OE2 | 8.48 | 1.34 | 1.25 |
| 2 | B | 82 | HIS | CG-CD2 | 8.48 | 1.50 | 1.35 |
| 2 | B | 53 | ALA | CA-CB | 8.47 | 1.70 | 1.52 |
| 1 | A | 212 | PHE | CE2-CZ | 8.47 | 1.53 | 1.37 |
| 2 | B | 225 | ASP | CG-OD2 | 8.45 | 1.44 | 1.25 |
| 2 | B | 374 | VAL | CB-CG2 | 8.44 | 1.70 | 1.52 |
| 1 | A | 221 | SER | CA-CB | 8.44 | 1.65 | 1.52 |
| 2 | B | 304 | LEU | CG-CD1 | 8.43 | 1.83 | 1.51 |
| 1 | A | 112 | ASP | CB-CG | -8.43 | 1.34 | 1.51 |
| 1 | A | 120 | GLN | CG-CD | 8.43 | 1.70 | 1.51 |
| 2 | B | 280 | PHE | C-N | 8.43 | 1.48 | 1.33 |
| 2 | B | 203 | GLU | N-CA | -8.41 | 1.29 | 1.46 |
| 1 | A | 102 | TYR | CD2-CE2 | 8.40 | 1.51 | 1.39 |
| 2 | B | 19 | GLN | CA-CB | 8.38 | 1.72 | 1.53 |
| 1 | A | 94 | THR | CA-CB | 8.38 | 1.75 | 1.53 |
| 1 | A | 102 | TYR | CA-CB | 8.36 | 1.72 | 1.53 |
| 1 | A | 24 | THR | CA-CB | 8.35 | 1.75 | 1.53 |
| 2 | B | 341 | ARG | CZ-NH1 | 8.35 | 1.44 | 1.33 |
| 2 | B | 189 | GLY | N-CA | 8.35 | 1.58 | 1.46 |
| 2 | B | 30 | GLU | CD-OE1 | 8.34 | 1.34 | 1.25 |
| 2 | B | 324 | TYR | C-O | 8.33 | 1.39 | 1.23 |
| 2 | B | 221 | GLY | CA-C | 8.31 | 1.65 | 1.51 |
| 2 | B | 282 | MET | CG-SD | 8.31 | 2.02 | 1.81 |
| 2 | B | 223 | LEU | C-O | 8.30 | 1.39 | 1.23 |
| 2 | B | 8 | TYR | CG-CD2 | 8.28 | 1.50 | 1.39 |
| 2 | B | 10 | GLY | C-O | 8.27 | 1.36 | 1.23 |
| 2 | B | 302 | ALA | CA-CB | 8.27 | 1.69 | 1.52 |
| 2 | B | 52 | TYR | CG-CD2 | 8.26 | 1.49 | 1.39 |
| 2 | B | 211 | GLU | CB-CG | 8.24 | 1.67 | 1.52 |
| 2 | B | 27 | GLN | CA-C | 8.24 | 1.74 | 1.52 |
| 2 | B | 49 | LEU | C-O | 8.24 | 1.39 | 1.23 |
| 2 | B | 337 | LYS | C-O | 8.24 | 1.39 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 145 | ARG | C-O | 8.21 | 1.39 | 1.23 |
| 2 | B | 10 | GLY | CA-C | -8.20 | 1.38 | 1.51 |
| 2 | B | 285 | PRO | CA-C | -8.20 | 1.36 | 1.52 |
| 2 | B | 119 | SER | CA-CB | 8.20 | 1.65 | 1.52 |
| 2 | B | 282 | MET | SD-CE | -8.20 | 1.31 | 1.77 |
| 1 | A | 21 | PRO | CA-CB | -8.19 | 1.37 | 1.53 |
| 2 | B | 230 | CYS | CB-SG | 8.19 | 1.96 | 1.82 |
| 1 | A | 83 | GLU | CG-CD | 8.18 | 1.64 | 1.51 |
| 1 | A | 116 | ALA | CA-CB | 8.16 | 1.69 | 1.52 |
| 2 | B | 241 | PHE | CG-CD1 | 8.16 | 1.50 | 1.38 |
| 2 | B | 150 | ARG | CB-CG | 8.16 | 1.74 | 1.52 |
| 2 | B | 131 | ARG | CZ-NH2 | 8.15 | 1.43 | 1.33 |
| 2 | B | 256 | GLU | C-O | 8.14 | 1.38 | 1.23 |
| 2 | B | 323 | ASP | C-O | 8.13 | 1.38 | 1.23 |
| 2 | B | 67 | ALA | CA-CB | 8.12 | 1.69 | 1.52 |
| 2 | B | 262 | ILE | CA-CB | -8.12 | 1.36 | 1.54 |
| 1 | A | 134 | GLU | CG-CD | 8.11 | 1.64 | 1.51 |
| 2 | B | 367 | GLU | CD-OE2 | 8.10 | 1.34 | 1.25 |
| 1 | A | 96 | PRO | CA-CB | -8.10 | 1.37 | 1.53 |
| 2 | B | 77 | ARG | CB-CG | 8.07 | 1.74 | 1.52 |
| 2 | B | 40 | GLU | CD-OE1 | 8.06 | 1.34 | 1.25 |
| 2 | B | 341 | ARG | N-CA | 8.06 | 1.62 | 1.46 |
| 2 | B | 123 | SER | CA-CB | -8.05 | 1.40 | 1.52 |
| 2 | B | 118 | ALA | N-CA | -8.04 | 1.30 | 1.46 |
| 2 | B | 13 | GLY | CA-C | 8.03 | 1.64 | 1.51 |
| 2 | B | 351 | SER | CA-CB | 8.03 | 1.65 | 1.52 |
| 2 | B | 109 | GLU | CA-CB | 8.02 | 1.71 | 1.53 |
| 2 | B | 21 | LEU | CA-C | -8.00 | 1.32 | 1.52 |
| 2 | B | 245 | ILE | N-CA | 8.00 | 1.62 | 1.46 |
| 1 | A | 127 | LEU | CA-C | 8.00 | 1.73 | 1.52 |
| 1 | A | 137 | ALA | CA-CB | -7.99 | 1.35 | 1.52 |
| 1 | A | 138 | PRO | CA-CB | 7.99 | 1.69 | 1.53 |
| 2 | B | 369 | GLU | CA-CB | -7.98 | 1.36 | 1.53 |
| 2 | B | 227 | VAL | N-CA | 7.98 | 1.62 | 1.46 |
| 2 | B | 256 | GLU | CD-OE2 | 7.98 | 1.34 | 1.25 |
| 1 | A | 169 | TYR | CA-CB | 7.97 | 1.71 | 1.53 |
| 2 | B | 306 | PHE | CE1-CZ | 7.97 | 1.52 | 1.37 |
| 2 | B | 287 | MET | CB-CG | 7.97 | 1.76 | 1.51 |
| 2 | B | 334 | GLU | CD-OE2 | 7.96 | 1.34 | 1.25 |
| 1 | A | 115 | TYR | CG-CD2 | 7.96 | 1.49 | 1.39 |
| 1 | A | 119 | GLU | CB-CG | 7.96 | 1.67 | 1.52 |
| 2 | B | 24 | ALA | N-CA | 7.96 | 1.62 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 269 | ALA | CA-CB | 7.95 | 1.69 | 1.52 |
| 1 | A | 84 | MET | C-O | 7.95 | 1.38 | 1.23 |
| 2 | B | 76 | LYS | CA-CB | 7.95 | 1.71 | 1.53 |
| 2 | B | 86 | HIS | CA-C | 7.95 | 1.73 | 1.52 |
| 2 | B | 335 | ALA | CA-C | 7.94 | 1.73 | 1.52 |
| 1 | A | 227 | GLY | CA-C | 7.93 | 1.64 | 1.51 |
| 2 | B | 9 | PHE | CD1-CE1 | 7.92 | 1.55 | 1.39 |
| 1 | A | 51 | GLY | N-CA | 7.91 | 1.57 | 1.46 |
| 2 | B | 82 | HIS | C-O | 7.91 | 1.38 | 1.23 |
| 1 | A | 121 | VAL | CA-CB | 7.89 | 1.71 | 1.54 |
| 2 | B | 37 | LYS | CD-CE | 7.89 | 1.71 | 1.51 |
| 1 | A | 5 | GLU | N-CA | 7.87 | 1.62 | 1.46 |
| 2 | B | 238 | ILE | CA-CB | 7.87 | 1.73 | 1.54 |
| 1 | A | 145 | ARG | CD-NE | 7.86 | 1.59 | 1.46 |
| 2 | B | 362 | MET | CG-SD | 7.86 | 2.01 | 1.81 |
| 2 | B | 363 | ARG | CB-CG | 7.86 | 1.73 | 1.52 |
| 2 | B | 336 | PHE | CD1-CE1 | 7.86 | 1.54 | 1.39 |
| 2 | B | 49 | LEU | CG-CD2 | 7.86 | 1.80 | 1.51 |
| 2 | B | 380 | GLY | N-CA | -7.86 | 1.34 | 1.46 |
| 2 | B | 374 | VAL | N-CA | -7.85 | 1.30 | 1.46 |
| 2 | B | 52 | TYR | CG-CD1 | 7.83 | 1.49 | 1.39 |
| 2 | B | 339 | LEU | CG-CD2 | 7.83 | 1.80 | 1.51 |
| 2 | B | 128 | LEU | CA-C | -7.81 | 1.32 | 1.52 |
| 2 | B | 63 | GLN | CG-CD | 7.81 | 1.69 | 1.51 |
| 2 | B | 152 | MET | SD-CE | -7.80 | 1.34 | 1.77 |
| 1 | A | 206 | ALA | CA-CB | 7.79 | 1.68 | 1.52 |
| 2 | B | 50 | LYS | CA-CB | -7.77 | 1.36 | 1.53 |
| 2 | B | 314 | ALA | N-CA | 7.76 | 1.61 | 1.46 |
| 2 | B | 228 | ILE | CA-CB | 7.75 | 1.72 | 1.54 |
| 2 | B | 194 | PRO | C-O | 7.75 | 1.38 | 1.23 |
| 2 | B | 317 | ASN | CG-OD1 | 7.74 | 1.41 | 1.24 |
| 1 | A | 126 | VAL | N-CA | 7.74 | 1.61 | 1.46 |
| 2 | B | 59 | LEU | CA-CB | -7.74 | 1.35 | 1.53 |
| 1 | A | 52 | VAL | CA-C | 7.73 | 1.73 | 1.52 |
| 2 | B | 12 | PHE | CE2-CZ | -7.73 | 1.22 | 1.37 |
| 1 | A | 8 | PHE | CD2-CE2 | 7.72 | 1.54 | 1.39 |
| 1 | A | 101 | MET | CB-CG | 7.72 | 1.76 | 1.51 |
| 2 | B | 353 | HIS | C-O | 7.71 | 1.38 | 1.23 |
| 2 | B | 385 | PHE | CB-CG | -7.71 | 1.38 | 1.51 |
| 2 | B | 91 | VAL | CB-CG1 | 7.70 | 1.69 | 1.52 |
| 2 | B | 26 | ASN | CA-CB | 7.69 | 1.73 | 1.53 |
| 2 | B | 263 | GLU | CD-OE2 | 7.68 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 202 | ARG | CG-CD | 7.68 | 1.71 | 1.51 |
| 2 | B | 266 | GLU | C-O | 7.68 | 1.38 | 1.23 |
| 2 | B | 51 | ASN | C-O | 7.67 | 1.38 | 1.23 |
| 2 | B | 148 | ARG | CB-CG | 7.67 | 1.73 | 1.52 |
| 2 | B | 281 | GLY | N-CA | -7.64 | 1.34 | 1.46 |
| 2 | B | 143 | SER | CA-CB | -7.63 | 1.41 | 1.52 |
| 2 | B | 225 | ASP | N-CA | 7.60 | 1.61 | 1.46 |
| 2 | B | 369 | GLU | CD-OE2 | 7.60 | 1.34 | 1.25 |
| 2 | B | 25 | LEU | CA-C | -7.59 | 1.33 | 1.52 |
| 2 | B | 308 | SER | CA-CB | 7.59 | 1.64 | 1.52 |
| 2 | B | 349 | LEU | CA-CB | -7.58 | 1.36 | 1.53 |
| 1 | A | 139 | PHE | CD1-CE1 | 7.58 | 1.54 | 1.39 |
| 2 | B | 258 | GLY | CA-C | -7.57 | 1.39 | 1.51 |
| 1 | A | 152 | PHE | CD2-CE2 | 7.55 | 1.54 | 1.39 |
| 2 | B | 254 | GLY | CA-C | -7.55 | 1.39 | 1.51 |
| 2 | B | 375 | ASN | C-N | 7.55 | 1.51 | 1.34 |
| 2 | B | 149 | MET | CA-CB | 7.54 | 1.70 | 1.53 |
| 1 | A | 16 | GLU | CD-OE1 | 7.54 | 1.33 | 1.25 |
| 2 | B | 366 | PRO | CA-C | -7.54 | 1.37 | 1.52 |
| 1 | A | 138 | PRO | CA-C | -7.53 | 1.37 | 1.52 |
| 2 | B | 114 | GLN | CB-CG | 7.53 | 1.72 | 1.52 |
| 2 | B | 270 | PRO | CA-CB | 7.51 | 1.68 | 1.53 |
| 2 | B | 343 | GLU | C-N | -7.51 | 1.19 | 1.33 |
| 2 | B | 241 | PHE | CE2-CZ | 7.51 | 1.51 | 1.37 |
| 2 | B | 212 | THR | CB-CG2 | 7.50 | 1.77 | 1.52 |
| 2 | B | 71 | THR | CB-CG2 | 7.49 | 1.77 | 1.52 |
| 2 | B | 257 | PRO | N-CA | -7.49 | 1.34 | 1.47 |
| 2 | B | 32 | PHE | N-CA | 7.49 | 1.61 | 1.46 |
| 2 | B | 8 | TYR | CD1-CE1 | -7.49 | 1.28 | 1.39 |
| 2 | B | 80 | LEU | N-CA | 7.49 | 1.61 | 1.46 |
| 2 | B | 155 | GLU | CD-OE1 | 7.48 | 1.33 | 1.25 |
| 2 | B | 260 | HIS | CB-CG | 7.48 | 1.63 | 1.50 |
| 2 | B | 323 | ASP | CA-CB | 7.46 | 1.70 | 1.53 |
| 2 | B | 12 | PHE | CB-CG | 7.45 | 1.64 | 1.51 |
| 2 | B | 19 | GLN | CA-C | 7.44 | 1.72 | 1.52 |
| 2 | B | 311 | PRO | C-O | 7.43 | 1.38 | 1.23 |
| 1 | A | 107 | PHE | CG-CD2 | 7.42 | 1.49 | 1.38 |
| 1 | A | 175 | TYR | CE1-CZ | -7.42 | 1.28 | 1.38 |
| 2 | B | 299 | SER | CB-OG | 7.40 | 1.51 | 1.42 |
| 2 | B | 373 | VAL | CB-CG2 | -7.40 | 1.37 | 1.52 |
| 2 | B | 74 | TYR | CE2-CZ | 7.40 | 1.48 | 1.38 |
| 2 | B | 280 | PHE | CA-C | -7.38 | 1.33 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 103 | ALA | CA-CB | -7.36 | 1.36 | 1.52 |
| 2 | B | 319 | ILE | CB-CG2 | 7.36 | 1.75 | 1.52 |
| 2 | B | 120 | ALA | C-O | 7.35 | 1.37 | 1.23 |
| 2 | B | 104 | SER | C-O | 7.34 | 1.37 | 1.23 |
| 2 | B | 105 | GLU | CA-C | 7.34 | 1.72 | 1.52 |
| 2 | B | 201 | VAL | CA-CB | -7.34 | 1.39 | 1.54 |
| 2 | B | 353 | HIS | CA-C | -7.33 | 1.33 | 1.52 |
| 1 | A | 17 | GLY | N-CA | 7.32 | 1.57 | 1.46 |
| 1 | A | 95 | ILE | C-O | 7.32 | 1.37 | 1.23 |
| 2 | B | 207 | MET | CA-CB | 7.32 | 1.70 | 1.53 |
| 2 | B | 186 | TYR | CE1-CZ | -7.32 | 1.29 | 1.38 |
| 2 | B | 63 | GLN | C-O | 7.32 | 1.37 | 1.23 |
| 2 | B | 242 | ALA | CA-CB | 7.30 | 1.67 | 1.52 |
| 2 | B | 219 | LYS | CD-CE | 7.29 | 1.69 | 1.51 |
| 2 | B | 281 | GLY | CA-C | -7.29 | 1.40 | 1.51 |
| 2 | B | 237 | ALA | CA-CB | 7.29 | 1.67 | 1.52 |
| 2 | B | 20 | ILE | N-CA | 7.29 | 1.60 | 1.46 |
| 2 | B | 177 | TRP | CZ3-CH2 | -7.29 | 1.28 | 1.40 |
| 1 | A | 54 | PHE | CA-CB | -7.28 | 1.38 | 1.53 |
| 2 | B | 369 | GLU | C-O | 7.27 | 1.37 | 1.23 |
| 1 | A | 257 | SER | CB-OG | -7.24 | 1.32 | 1.42 |
| 2 | B | 106 | ILE | C-N | 7.23 | 1.50 | 1.34 |
| 2 | B | 76 | LYS | C-N | 7.22 | 1.50 | 1.34 |
| 2 | B | 190 | THR | CB-OG1 | 7.22 | 1.57 | 1.43 |
| 1 | A | 7 | LEU | CG-CD2 | 7.21 | 1.78 | 1.51 |
| 2 | B | 345 | ILE | C-O | 7.21 | 1.37 | 1.23 |
| 2 | B | 73 | LEU | CA-CB | -7.21 | 1.37 | 1.53 |
| 1 | A | 222 | ALA | CA-CB | 7.21 | 1.67 | 1.52 |
| 2 | B | 6 | ASN | C-N | -7.20 | 1.20 | 1.34 |
| 2 | B | 11 | GLU | CG-CD | 7.20 | 1.62 | 1.51 |
| 2 | B | 134 | MET | C-O | 7.20 | 1.37 | 1.23 |
| 2 | B | 335 | ALA | N-CA | -7.19 | 1.31 | 1.46 |
| 2 | B | 219 | LYS | CG-CD | -7.19 | 1.28 | 1.52 |
| 2 | B | 394 | ARG | CZ-NH2 | 7.18 | 1.42 | 1.33 |
| 2 | B | 322 | ALA | CA-CB | 7.18 | 1.67 | 1.52 |
| 2 | B | 71 | THR | CA-CB | -7.18 | 1.34 | 1.53 |
| 2 | B | 9 | PHE | CA-C | 7.17 | 1.71 | 1.52 |
| 2 | B | 241 | PHE | C-N | 7.17 | 1.50 | 1.34 |
| 1 | A | 104 | ASN | N-CA | 7.16 | 1.60 | 1.46 |
| 1 | A | 108 | ASN | CG-OD1 | -7.15 | 1.08 | 1.24 |
| 1 | A | 161 | ASP | CG-OD1 | 7.15 | 1.41 | 1.25 |
| 1 | A | 211 | GLY | CA-C | 7.14 | 1.63 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 37 | LYS | CE-NZ | 7.14 | 1.67 | 1.49 |
| 2 | B | 44 | GLN | CG-CD | 7.14 | 1.67 | 1.51 |
| 1 | A | 149 | ALA | C-N | -7.13 | 1.20 | 1.34 |
| 2 | B | 227 | VAL | CB-CG2 | 7.13 | 1.67 | 1.52 |
| 1 | A | 140 | ARG | C-O | 7.12 | 1.36 | 1.23 |
| 1 | A | 82 | PHE | CE1-CZ | 7.12 | 1.50 | 1.37 |
| 1 | A | 16 | GLU | C-N | 7.12 | 1.45 | 1.33 |
| 2 | B | 3 | THR | CA-C | -7.12 | 1.34 | 1.52 |
| 2 | B | 44 | GLN | N-CA | -7.10 | 1.32 | 1.46 |
| 2 | B | 244 | PHE | CD1-CE1 | 7.10 | 1.53 | 1.39 |
| 2 | B | 336 | PHE | CA-C | 7.10 | 1.71 | 1.52 |
| 1 | A | 5 | GLU | CD-OE1 | 7.09 | 1.33 | 1.25 |
| 2 | B | 291 | ASP | CA-CB | 7.08 | 1.69 | 1.53 |
| 1 | A | 128 | VAL | N-CA | 7.07 | 1.60 | 1.46 |
| 2 | B | 253 | ILE | CA-CB | 7.07 | 1.71 | 1.54 |
| 2 | B | 247 | ASP | N-CA | 7.07 | 1.60 | 1.46 |
| 2 | B | 287 | MET | SD-CE | -7.06 | 1.38 | 1.77 |
| 2 | B | 103 | LYS | N-CA | -7.06 | 1.32 | 1.46 |
| 2 | B | 255 | VAL | C-O | 7.06 | 1.36 | 1.23 |
| 2 | B | 229 | ALA | CA-C | -7.06 | 1.34 | 1.52 |
| 2 | B | 87 | LYS | CA-CB | -7.04 | 1.38 | 1.53 |
| 2 | B | 315 | TYR | CZ-OH | -7.04 | 1.25 | 1.37 |
| 2 | B | 311 | PRO | CA-C | -7.04 | 1.38 | 1.52 |
| 2 | B | 198 | PRO | C-O | 7.03 | 1.37 | 1.23 |
| 2 | B | 203 | GLU | CB-CG | 7.03 | 1.65 | 1.52 |
| 2 | B | 90 | GLN | CD-OE1 | 7.02 | 1.39 | 1.24 |
| 2 | B | 260 | HIS | C-O | 7.02 | 1.36 | 1.23 |
| 2 | B | 283 | LYS | CE-NZ | 7.01 | 1.66 | 1.49 |
| 2 | B | 66 | THR | CB-CG2 | 7.01 | 1.75 | 1.52 |
| 2 | B | 285 | PRO | C-O | 7.00 | 1.37 | 1.23 |
| 1 | A | 38 | ASP | N-CA | 7.00 | 1.60 | 1.46 |
| 2 | B | 279 | TYR | CD1-CE1 | 7.00 | 1.49 | 1.39 |
| 2 | B | 326 | SER | CA-CB | -6.98 | 1.42 | 1.52 |
| 2 | B | 176 | ASP | CA-CB | 6.98 | 1.69 | 1.53 |
| 2 | B | 155 | GLU | CG-CD | 6.97 | 1.62 | 1.51 |
| 1 | A | 125 | SER | CA-C | 6.97 | 1.71 | 1.52 |
| 2 | B | 384 | ILE | CA-CB | 6.97 | 1.70 | 1.54 |
| 2 | B | 372 | LEU | CA-CB | -6.97 | 1.37 | 1.53 |
| 1 | A | 205 | ALA | CA-CB | 6.96 | 1.67 | 1.52 |
| 2 | B | 258 | GLY | C-N | 6.96 | 1.45 | 1.33 |
| 2 | B | 313 | HIS | N-CA | 6.96 | 1.60 | 1.46 |
| 2 | B | 80 | LEU | CB-CG | 6.95 | 1.72 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 39 | PRO | C-O | 6.95 | 1.37 | 1.23 |
| 1 | A | 86 | ALA | CA-CB | 6.95 | 1.67 | 1.52 |
| 2 | B | 24 | ALA | CA-CB | -6.95 | 1.37 | 1.52 |
| 2 | B | 32 | PHE | CE1-CZ | 6.93 | 1.50 | 1.37 |
| 2 | B | 211 | GLU | CA-C | 6.93 | 1.71 | 1.52 |
| 2 | B | 234 | GLY | C-N | 6.92 | 1.50 | 1.34 |
| 2 | B | 53 | ALA | CA-C | 6.92 | 1.71 | 1.52 |
| 2 | B | 117 | VAL | CB-CG2 | -6.91 | 1.38 | 1.52 |
| 2 | B | 177 | TRP | CE3-CZ3 | -6.90 | 1.26 | 1.38 |
| 2 | B | 339 | LEU | CA-CB | 6.90 | 1.69 | 1.53 |
| 2 | B | 264 | THR | CB-CG2 | 6.90 | 1.75 | 1.52 |
| 2 | B | 37 | LYS | CG-CD | 6.88 | 1.75 | 1.52 |
| 2 | B | 364 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 2 | B | 215 | GLN | CB-CG | 6.86 | 1.71 | 1.52 |
| 1 | A | 171 | ARG | CA-C | -6.85 | 1.35 | 1.52 |
| 2 | B | 390 | ILE | CA-C | -6.85 | 1.35 | 1.52 |
| 2 | B | 309 | VAL | CA-CB | 6.83 | 1.69 | 1.54 |
| 2 | B | 329 | ASP | CA-CB | -6.83 | 1.39 | 1.53 |
| 2 | B | 338 | THR | CA-CB | 6.83 | 1.71 | 1.53 |
| 2 | B | 120 | ALA | N-CA | 6.83 | 1.60 | 1.46 |
| 1 | A | 70 | ARG | NE-CZ | -6.83 | 1.24 | 1.33 |
| 2 | B | 100 | ARG | CA-C | 6.83 | 1.70 | 1.52 |
| 2 | B | 184 | ALA | CA-CB | -6.82 | 1.38 | 1.52 |
| 2 | B | 317 | ASN | CA-CB | -6.82 | 1.35 | 1.53 |
| 2 | B | 133 | TYR | CD2-CE2 | 6.81 | 1.49 | 1.39 |
| 2 | B | 29 | GLU | N-CA | -6.81 | 1.32 | 1.46 |
| 2 | B | 218 | ASP | CB-CG | 6.80 | 1.66 | 1.51 |
| 2 | B | 84 | GLY | N-CA | 6.79 | 1.56 | 1.46 |
| 2 | B | 183 | THR | CB-CG2 | 6.78 | 1.74 | 1.52 |
| 1 | A | 136 | SER | CB-OG | -6.78 | 1.33 | 1.42 |
| 2 | B | 203 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | A | 39 | THR | C-O | 6.76 | 1.36 | 1.23 |
| 2 | B | 278 | ILE | CA-CB | 6.75 | 1.70 | 1.54 |
| 1 | A | 212 | PHE | CB-CG | 6.74 | 1.62 | 1.51 |
| 2 | B | 281 | GLY | C-N | 6.74 | 1.49 | 1.34 |
| 2 | B | 8 | TYR | CB-CG | -6.74 | 1.41 | 1.51 |
| 2 | B | 210 | GLU | CD-OE1 | 6.74 | 1.33 | 1.25 |
| 1 | A | 165 | GLN | CA-C | -6.74 | 1.35 | 1.52 |
| 2 | B | 56 | PRO | C-O | 6.73 | 1.36 | 1.23 |
| 2 | B | 261 | GLY | CA-C | 6.72 | 1.62 | 1.51 |
| 1 | A | 120 | GLN | CA-C | -6.72 | 1.35 | 1.52 |
| 2 | B | 215 | GLN | CA-CB | -6.71 | 1.39 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 285 | PRO | CG-CD | 6.71 | 1.72 | 1.50 |
| 2 | B | 231 | VAL | N-CA | 6.70 | 1.59 | 1.46 |
| 2 | B | 229 | ALA | C-O | 6.69 | 1.36 | 1.23 |
| 2 | B | 256 | GLU | CA-CB | 6.69 | 1.68 | 1.53 |
| 2 | B | 55 | ARG | CA-C | -6.69 | 1.35 | 1.52 |
| 2 | B | 328 | THR | CB-OG1 | 6.68 | 1.56 | 1.43 |
| 2 | B | 192 | ALA | N-CA | 6.68 | 1.59 | 1.46 |
| 2 | B | 29 | GLU | CA-C | -6.67 | 1.35 | 1.52 |
| 1 | A | 213 | GLY | CA-C | 6.66 | 1.62 | 1.51 |
| 2 | B | 34 | SER | CA-CB | 6.66 | 1.62 | 1.52 |
| 2 | B | 129 | LYS | CG-CD | 6.66 | 1.75 | 1.52 |
| 2 | B | 131 | ARG | CG-CD | 6.65 | 1.68 | 1.51 |
| 1 | A | 116 | ALA | CA-C | -6.65 | 1.35 | 1.52 |
| 2 | B | 41 | PHE | CG-CD2 | 6.64 | 1.48 | 1.38 |
| 2 | B | 379 | ARG | CA-C | -6.64 | 1.35 | 1.52 |
| 1 | A | 126 | VAL | C-N | 6.64 | 1.49 | 1.34 |
| 2 | B | 60 | THR | CB-OG1 | 6.64 | 1.56 | 1.43 |
| 2 | B | 321 | ARG | NE-CZ | 6.63 | 1.41 | 1.33 |
| 2 | B | 367 | GLU | N-CA | -6.63 | 1.33 | 1.46 |
| 2 | B | 20 | ILE | CA-CB | -6.61 | 1.39 | 1.54 |
| 2 | B | 65 | ILE | N-CA | 6.61 | 1.59 | 1.46 |
| 1 | A | 139 | PHE | CA-C | 6.61 | 1.70 | 1.52 |
| 2 | B | 220 | GLU | N-CA | 6.61 | 1.59 | 1.46 |
| 2 | B | 369 | GLU | CB-CG | 6.61 | 1.64 | 1.52 |
| 2 | B | 333 | LEU | CA-CB | -6.60 | 1.38 | 1.53 |
| 1 | A | 152 | PHE | CE1-CZ | 6.59 | 1.49 | 1.37 |
| 1 | A | 232 | ILE | C-N | -6.59 | 1.18 | 1.34 |
| 2 | B | 380 | GLY | C-O | -6.56 | 1.13 | 1.23 |
| 2 | B | 231 | VAL | CB-CG2 | -6.56 | 1.39 | 1.52 |
| 2 | B | 55 | ARG | CD-NE | 6.55 | 1.57 | 1.46 |
| 2 | B | 362 | MET | C-N | -6.55 | 1.19 | 1.34 |
| 2 | B | 110 | THR | CA-CB | 6.55 | 1.70 | 1.53 |
| 2 | B | 283 | LYS | CA-C | 6.55 | 1.70 | 1.52 |
| 2 | B | 293 | GLN | CA-CB | -6.54 | 1.39 | 1.53 |
| 1 | A | 139 | PHE | N-CA | -6.54 | 1.33 | 1.46 |
| 1 | A | 55 | SER | N-CA | 6.54 | 1.59 | 1.46 |
| 1 | A | 142 | ALA | CA-CB | 6.54 | 1.66 | 1.52 |
| 2 | B | 157 | ILE | C-N | -6.53 | 1.21 | 1.34 |
| 2 | B | 376 | LEU | CA-CB | 6.50 | 1.68 | 1.53 |
| 2 | B | 238 | ILE | CB-CG2 | 6.50 | 1.73 | 1.52 |
| 2 | B | 23 | PRO | CA-C | 6.50 | 1.65 | 1.52 |
| 2 | B | 93 | GLY | CA-C | 6.49 | 1.62 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 94 | GLN | CA-CB | -6.49 | 1.39 | 1.53 |
| 2 | B | 265 | GLY | C-O | 6.49 | 1.34 | 1.23 |
| 1 | A | 104 | ASN | CB-CG | 6.49 | 1.66 | 1.51 |
| 1 | A | 141 | GLN | C-O | 6.48 | 1.35 | 1.23 |
| 2 | B | 368 | LYS | C-N | -6.48 | 1.19 | 1.34 |
| 1 | A | 136 | SER | CA-C | 6.48 | 1.69 | 1.52 |
| 2 | B | 218 | ASP | C-O | 6.48 | 1.35 | 1.23 |
| 1 | A | 120 | GLN | CA-CB | 6.47 | 1.68 | 1.53 |
| 1 | A | 203 | TYR | CG-CD2 | 6.47 | 1.47 | 1.39 |
| 1 | A | 5 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 2 | B | 198 | PRO | CG-CD | 6.46 | 1.72 | 1.50 |
| 2 | B | 133 | TYR | CA-CB | 6.46 | 1.68 | 1.53 |
| 1 | A | 220 | VAL | CB-CG2 | 6.45 | 1.66 | 1.52 |
| 1 | A | 130 | ASP | CA-C | -6.44 | 1.36 | 1.52 |
| 2 | B | 363 | ARG | CZ-NH2 | 6.44 | 1.41 | 1.33 |
| 2 | B | 106 | ILE | CB-CG2 | 6.44 | 1.72 | 1.52 |
| 2 | B | 347 | PRO | CA-C | -6.44 | 1.40 | 1.52 |
| 1 | A | 217 | PRO | CA-C | -6.43 | 1.40 | 1.52 |
| 2 | B | 327 | ILE | N-CA | 6.43 | 1.59 | 1.46 |
| 2 | B | 256 | GLU | C-N | -6.42 | 1.22 | 1.34 |
| 2 | B | 94 | GLN | CB-CG | 6.41 | 1.69 | 1.52 |
| 2 | B | 105 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 2 | B | 38 | ASP | CB-CG | 6.41 | 1.65 | 1.51 |
| 2 | B | 371 | LEU | C-O | 6.41 | 1.35 | 1.23 |
| 1 | A | 10 | GLN | N-CA | -6.40 | 1.33 | 1.46 |
| 1 | A | 218 | GLU | CD-OE1 | 6.40 | 1.32 | 1.25 |
| 2 | B | 360 | LYS | CG-CD | 6.40 | 1.74 | 1.52 |
| 1 | A | 259 | VAL | CA-CB | 6.40 | 1.68 | 1.54 |
| 1 | A | 223 | ALA | CA-CB | 6.39 | 1.65 | 1.52 |
| 2 | B | 121 | LEU | CG-CD1 | -6.39 | 1.28 | 1.51 |
| 1 | A | 105 | LEU | CA-CB | -6.38 | 1.39 | 1.53 |
| 1 | A | 203 | TYR | CE1-CZ | 6.38 | 1.46 | 1.38 |
| 1 | A | 262 | MET | SD-CE | -6.38 | 1.42 | 1.77 |
| 2 | B | 36 | GLN | CA-CB | 6.37 | 1.68 | 1.53 |
| 2 | B | 298 | TYR | CD2-CE2 | 6.37 | 1.49 | 1.39 |
| 2 | B | 241 | PHE | CB-CG | -6.37 | 1.40 | 1.51 |
| 2 | B | 295 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 2 | B | 316 | LEU | CA-CB | 6.36 | 1.68 | 1.53 |
| 2 | B | 333 | LEU | CG-CD2 | 6.33 | 1.75 | 1.51 |
| 2 | B | 59 | LEU | CB-CG | 6.33 | 1.71 | 1.52 |
| 2 | B | 130 | CYS | CA-C | -6.33 | 1.36 | 1.52 |
| 2 | B | 385 | PHE | CE2-CZ | 6.33 | 1.49 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 149 | ALA | CA-CB | 6.32 | 1.65 | 1.52 |
| 2 | B | 58 | ALA | CA-C | 6.32 | 1.69 | 1.52 |
| 2 | B | 100 | ARG | N-CA | -6.32 | 1.33 | 1.46 |
| 2 | B | 25 | LEU | CG-CD2 | 6.31 | 1.75 | 1.51 |
| 2 | B | 70 | ARG | N-CA | -6.31 | 1.33 | 1.46 |
| 1 | A | 72 | PHE | CE1-CZ | 6.31 | 1.49 | 1.37 |
| 1 | A | 113 | ALA | CA-CB | 6.31 | 1.65 | 1.52 |
| 2 | B | 82 | HIS | CA-CB | 6.31 | 1.67 | 1.53 |
| 1 | A | 110 | GLY | CA-C | 6.30 | 1.61 | 1.51 |
| 1 | A | 11 | LEU | CA-CB | 6.30 | 1.68 | 1.53 |
| 2 | B | 192 | ALA | CA-C | 6.30 | 1.69 | 1.52 |
| 2 | B | 372 | LEU | CB-CG | 6.29 | 1.70 | 1.52 |
| 1 | A | 162 | LEU | N-CA | -6.29 | 1.33 | 1.46 |
| 1 | A | 53 | PRO | CG-CD | 6.28 | 1.71 | 1.50 |
| 2 | B | 352 | SER | N-CA | 6.28 | 1.58 | 1.46 |
| 2 | B | 48 | LEU | CA-C | 6.28 | 1.69 | 1.52 |
| 2 | B | 53 | ALA | C-N | -6.27 | 1.21 | 1.33 |
| 2 | B | 234 | GLY | CA-C | -6.27 | 1.41 | 1.51 |
| 2 | B | 279 | TYR | CG-CD1 | 6.27 | 1.47 | 1.39 |
| 2 | B | 69 | THR | CB-OG1 | 6.26 | 1.55 | 1.43 |
| 2 | B | 147 | PHE | CE1-CZ | 6.26 | 1.49 | 1.37 |
| 2 | B | 324 | TYR | CD2-CE2 | -6.26 | 1.29 | 1.39 |
| 2 | B | 157 | ILE | CA-CB | 6.26 | 1.69 | 1.54 |
| 2 | B | 199 | THR | CB-OG1 | 6.26 | 1.55 | 1.43 |
| 1 | A | 18 | ALA | CA-C | 6.25 | 1.69 | 1.52 |
| 1 | A | 201 | LYS | CE-NZ | 6.24 | 1.64 | 1.49 |
| 2 | B | 209 | GLY | CA-C | -6.24 | 1.41 | 1.51 |
| 1 | A | 235 | SER | CB-OG | -6.24 | 1.34 | 1.42 |
| 1 | A | 37 | ILE | CA-C | 6.23 | 1.69 | 1.52 |
| 1 | A | 92 | HIS | C-O | 6.23 | 1.35 | 1.23 |
| 2 | B | 276 | VAL | C-N | 6.23 | 1.44 | 1.33 |
| 1 | A | 22 | PHE | CD1-CE1 | 6.23 | 1.51 | 1.39 |
| 2 | B | 228 | ILE | N-CA | -6.22 | 1.33 | 1.46 |
| 2 | B | 375 | ASN | N-CA | 6.22 | 1.58 | 1.46 |
| 2 | B | 192 | ALA | CA-CB | -6.21 | 1.39 | 1.52 |
| 2 | B | 340 | CYS | N-CA | 6.21 | 1.58 | 1.46 |
| 1 | A | 87 | LEU | CG-CD1 | 6.21 | 1.74 | 1.51 |
| 2 | B | 237 | ALA | C-N | 6.20 | 1.48 | 1.34 |
| 1 | A | 31 | GLU | CG-CD | 6.19 | 1.61 | 1.51 |
| 1 | A | 266 | SER | CA-CB | 6.19 | 1.62 | 1.52 |
| 2 | B | 60 | THR | CA-CB | -6.19 | 1.37 | 1.53 |
| 1 | A | 62 | PRO | N-CD | 6.18 | 1.56 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 208 | ALA | CA-C | -6.18 | 1.36 | 1.52 |
| 2 | B | 182 | GLU | CA-C | 6.18 | 1.69 | 1.52 |
| 2 | B | 157 | ILE | N-CA | 6.18 | 1.58 | 1.46 |
| 1 | A | 102 | TYR | CD1-CE1 | 6.17 | 1.48 | 1.39 |
| 1 | A | 253 | ALA | CA-CB | -6.17 | 1.39 | 1.52 |
| 2 | B | 315 | TYR | CD2-CE2 | 6.17 | 1.48 | 1.39 |
| 2 | B | 359 | LEU | N-CA | 6.17 | 1.58 | 1.46 |
| 2 | B | 65 | ILE | C-N | -6.17 | 1.19 | 1.34 |
| 2 | B | 243 | ASP | CA-C | 6.16 | 1.69 | 1.52 |
| 2 | B | 332 | ALA | C-N | -6.16 | 1.19 | 1.34 |
| 2 | B | 368 | LYS | CB-CG | 6.16 | 1.69 | 1.52 |
| 2 | B | 220 | GLU | CG-CD | 6.16 | 1.61 | 1.51 |
| 2 | B | 321 | ARG | C-N | -6.15 | 1.20 | 1.34 |
| 1 | A | 166 | VAL | CA-C | 6.14 | 1.69 | 1.52 |
| 2 | B | 40 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 2 | B | 130 | CYS | C-N | 6.14 | 1.48 | 1.34 |
| 2 | B | 6 | ASN | CA-CB | 6.13 | 1.69 | 1.53 |
| 2 | B | 298 | TYR | CE1-CZ | 6.12 | 1.46 | 1.38 |
| 2 | B | 61 | LYS | CA-C | -6.12 | 1.37 | 1.52 |
| 2 | B | 243 | ASP | CG-OD1 | 6.12 | 1.39 | 1.25 |
| 2 | B | 35 | ALA | N-CA | 6.11 | 1.58 | 1.46 |
| 2 | B | 23 | PRO | CB-CG | 6.11 | 1.80 | 1.50 |
| 1 | A | 139 | PHE | CD2-CE2 | 6.11 | 1.51 | 1.39 |
| 2 | B | 207 | MET | CA-C | 6.11 | 1.68 | 1.52 |
| 2 | B | 230 | CYS | N-CA | -6.11 | 1.34 | 1.46 |
| 2 | B | 309 | VAL | N-CA | -6.11 | 1.34 | 1.46 |
| 2 | B | 355 | LEU | CB-CG | 6.10 | 1.70 | 1.52 |
| 2 | B | 245 | ILE | CB-CG2 | 6.10 | 1.71 | 1.52 |
| 2 | B | 201 | VAL | CB-CG1 | 6.09 | 1.65 | 1.52 |
| 2 | B | 186 | TYR | CZ-OH | 6.09 | 1.48 | 1.37 |
| 1 | A | 104 | ASN | CA-CB | 6.08 | 1.69 | 1.53 |
| 2 | B | 323 | ASP | CA-C | -6.08 | 1.37 | 1.52 |
| 1 | A | 261 | ALA | C-O | 6.08 | 1.34 | 1.23 |
| 1 | A | 249 | LYS | CD-CE | 6.07 | 1.66 | 1.51 |
| 2 | B | 47 | ASP | C-O | 6.07 | 1.34 | 1.23 |
| 2 | B | 373 | VAL | N-CA | 6.07 | 1.58 | 1.46 |
| 2 | B | 138 | ASP | CA-CB | -6.06 | 1.40 | 1.53 |
| 2 | B | 242 | ALA | CA-C | -6.06 | 1.37 | 1.52 |
| 1 | A | 135 | GLU | CG-CD | 6.06 | 1.61 | 1.51 |
| 2 | B | 100 | ARG | CZ-NH2 | -6.06 | 1.25 | 1.33 |
| 2 | B | 7 | PRO | N-CA | -6.05 | 1.36 | 1.47 |
| 1 | A | 29 | GLY | CA-C | 6.05 | 1.61 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1 | A | 109 | ASN | CG-OD1 | 6.05 | 1.37 | 1.24 |
| 1 | A | 85 | LEU | CA-CB | -6.05 | 1.39 | 1.53 |
| 2 | B | 56 | PRO | CA-C | -6.05 | 1.40 | 1.52 |
| 2 | B | 206[A] | ARG | CA-C | 6.05 | 1.68 | 1.52 |
| 2 | B | 206[B] | ARG | CA-C | 6.05 | 1.68 | 1.52 |
| 2 | B | 85 | ALA | C-O | 6.05 | 1.34 | 1.23 |
| 1 | A | 107 | PHE | CB-CG | -6.05 | 1.41 | 1.51 |
| 2 | B | 317 | ASN | N-CA | 6.05 | 1.58 | 1.46 |
| 2 | B | 97 | LEU | CG-CD1 | 6.04 | 1.74 | 1.51 |
| 2 | B | 33 | VAL | CA-CB | 6.04 | 1.67 | 1.54 |
| 2 | B | 69 | THR | CA-C | -6.04 | 1.37 | 1.52 |
| 1 | A | 268 | ALA | C-O | 6.04 | 1.34 | 1.23 |
| 2 | B | 119 | SER | CA-C | 6.04 | 1.68 | 1.52 |
| 2 | B | 262 | ILE | N-CA | 6.03 | 1.58 | 1.46 |
| 2 | B | 294 | ILE | CB-CG1 | 6.03 | 1.71 | 1.54 |
| 2 | B | 371 | LEU | N-CA | 6.03 | 1.58 | 1.46 |
| 1 | A | 143 | ALA | C-O | 6.02 | 1.34 | 1.23 |
| 2 | B | 71 | THR | N-CA | 6.02 | 1.58 | 1.46 |
| 2 | B | 318 | SER | N-CA | 6.02 | 1.58 | 1.46 |
| 2 | B | 60 | THR | N-CA | 6.02 | 1.58 | 1.46 |
| 2 | B | 161 | SER | CB-OG | 6.01 | 1.50 | 1.42 |
| 2 | B | 17 | VAL | CA-C | 6.01 | 1.68 | 1.52 |
| 2 | B | 200 | ILE | CB-CG2 | 6.01 | 1.71 | 1.52 |
| 2 | B | 235 | SER | C-O | -6.01 | 1.11 | 1.23 |
| 2 | B | 100 | ARG | CB-CG | -6.00 | 1.36 | 1.52 |
| 2 | B | 152 | MET | CA-C | 6.00 | 1.68 | 1.52 |
| 2 | B | 193 | GLY | C-N | 5.99 | 1.45 | 1.34 |
| 2 | B | 350 | GLU | CA-CB | 5.99 | 1.67 | 1.53 |
| 1 | A | 144 | LEU | C-O | 5.99 | 1.34 | 1.23 |
| 2 | B | 63 | GLN | N-CA | 5.99 | 1.58 | 1.46 |
| 1 | A | 77 | THR | CA-C | 5.99 | 1.68 | 1.52 |
| 2 | B | 86 | HIS | CA-CB | 5.98 | 1.67 | 1.53 |
| 1 | A | 224 | VAL | CB-CG2 | 5.98 | 1.65 | 1.52 |
| 2 | B | 45 | PHE | C-O | 5.97 | 1.34 | 1.23 |
| 2 | B | 210 | GLU | N-CA | -5.97 | 1.34 | 1.46 |
| 1 | A | 89 | ARG | C-O | 5.96 | 1.34 | 1.23 |
| 2 | B | 195 | HIS | CB-CG | -5.96 | 1.39 | 1.50 |
| 1 | A | 171 | ARG | CZ-NH2 | -5.95 | 1.25 | 1.33 |
| 1 | A | 102 | TYR | CG-CD2 | -5.94 | 1.31 | 1.39 |
| 2 | B | 238 | ILE | N-CA | -5.94 | 1.34 | 1.46 |
| 2 | B | 312 | GLN | CD-NE2 | -5.94 | 1.18 | 1.32 |
| 1 | A | 230 | GLY | N-CA | -5.93 | 1.37 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 156 | VAL | CB-CG1 | -5.92 | 1.40 | 1.52 |
| 2 | B | 43 | ALA | CA-CB | -5.91 | 1.40 | 1.52 |
| 2 | B | 365 | GLN | CD-NE2 | 5.91 | 1.47 | 1.32 |
| 1 | A | 96 | PRO | CA-C | 5.90 | 1.64 | 1.52 |
| 2 | B | 208 | ILE | C-O | 5.90 | 1.34 | 1.23 |
| 2 | B | 55 | ARG | C-O | 5.89 | 1.34 | 1.23 |
| 2 | B | 202 | ARG | CD-NE | -5.89 | 1.36 | 1.46 |
| 2 | B | 236 | ASN | C-O | -5.89 | 1.12 | 1.23 |
| 2 | B | 336 | PHE | CD2-CE2 | 5.89 | 1.51 | 1.39 |
| 2 | B | 368 | LYS | CD-CE | 5.88 | 1.66 | 1.51 |
| 2 | B | 188 | LEU | CG-CD1 | 5.88 | 1.73 | 1.51 |
| 2 | B | 264 | THR | C-N | -5.88 | 1.22 | 1.33 |
| 1 | A | 45 | ALA | CA-CB | 5.87 | 1.64 | 1.52 |
| 1 | A | 70 | ARG | CG-CD | 5.87 | 1.66 | 1.51 |
| 2 | B | 71 | THR | CA-C | 5.87 | 1.68 | 1.52 |
| 1 | A | 83 | GLU | CA-CB | 5.86 | 1.66 | 1.53 |
| 1 | A | 7 | LEU | CA-CB | 5.85 | 1.67 | 1.53 |
| 2 | B | 315 | TYR | CG-CD1 | 5.85 | 1.46 | 1.39 |
| 2 | B | 356 | ALA | N-CA | 5.85 | 1.58 | 1.46 |
| 1 | A | 50 | LEU | CA-C | 5.84 | 1.68 | 1.52 |
| 1 | A | 90 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 2 | B | 201 | VAL | N-CA | 5.83 | 1.58 | 1.46 |
| 2 | B | 123 | SER | N-CA | 5.83 | 1.58 | 1.46 |
| 1 | A | 238 | VAL | CB-CG1 | 5.82 | 1.65 | 1.52 |
| 2 | B | 146 | VAL | CB-CG2 | 5.82 | 1.65 | 1.52 |
| 1 | A | 117 | ARG | N-CA | -5.81 | 1.34 | 1.46 |
| 2 | B | 319 | ILE | CB-CG1 | 5.81 | 1.70 | 1.54 |
| 2 | B | 388 | HIS | C-O | -5.80 | 1.12 | 1.23 |
| 2 | B | 208 | ILE | N-CA | 5.79 | 1.57 | 1.46 |
| 2 | B | 331 | GLU | N-CA | -5.79 | 1.34 | 1.46 |
| 2 | B | 99 | LYS | CD-CE | 5.78 | 1.65 | 1.51 |
| 2 | B | 121 | LEU | C-N | 5.78 | 1.47 | 1.34 |
| 1 | A | 250 | GLN | CG-CD | 5.77 | 1.64 | 1.51 |
| 2 | B | 106 | ILE | N-CA | 5.77 | 1.57 | 1.46 |
| 2 | B | 362 | MET | CA-CB | 5.77 | 1.66 | 1.53 |
| 2 | B | 55 | ARG | CZ-NH1 | -5.76 | 1.25 | 1.33 |
| 2 | B | 216 | ILE | CA-C | -5.75 | 1.38 | 1.52 |
| 2 | B | 260 | HIS | CA-C | -5.75 | 1.38 | 1.52 |
| 2 | B | 110 | THR | CB-CG2 | -5.74 | 1.33 | 1.52 |
| 2 | B | 57 | THR | C-N | 5.74 | 1.47 | 1.34 |
| 1 | A | 131 | VAL | CB-CG2 | 5.73 | 1.64 | 1.52 |
| 2 | B | 146 | VAL | C-O | 5.73 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2 | B | 287 | MET | CG-SD | 5.73 | 1.96 | 1.81 |
| 2 | B | 69 | THR | CB-CG2 | -5.73 | 1.33 | 1.52 |
| 2 | B | 271 | LEU | C-O | 5.73 | 1.34 | 1.23 |
| 1 | A | 145 | ARG | NE-CZ | -5.72 | 1.25 | 1.33 |
| 2 | B | 222 | ARG | N-CA | 5.72 | 1.57 | 1.46 |
| 1 | A | 53 | PRO | N-CA | 5.72 | 1.56 | 1.47 |
| 2 | B | 374 | VAL | CB-CG1 | -5.72 | 1.40 | 1.52 |
| 2 | B | 139 | VAL | CA-C | -5.72 | 1.38 | 1.52 |
| 2 | B | 298 | TYR | CD1-CE1 | 5.72 | 1.48 | 1.39 |
| 1 | A | 168 | SER | CA-CB | -5.71 | 1.44 | 1.52 |
| 2 | B | 274 | GLY | N-CA | 5.71 | 1.54 | 1.46 |
| 2 | B | 28 | LEU | CB-CG | 5.71 | 1.69 | 1.52 |
| 2 | B | 121 | LEU | C-O | 5.70 | 1.34 | 1.23 |
| 2 | B | 268 | GLY | C-N | 5.70 | 1.47 | 1.34 |
| 2 | B | 354 | ALA | CA-C | 5.70 | 1.67 | 1.52 |
| 2 | B | 215 | GLN | CA-C | 5.69 | 1.67 | 1.52 |
| 1 | A | 213 | GLY | N-CA | 5.69 | 1.54 | 1.46 |
| 2 | B | 188 | LEU | CG-CD2 | 5.68 | 1.72 | 1.51 |
| 2 | B | 231 | VAL | CA-C | -5.67 | 1.38 | 1.52 |
| 2 | B | 376 | LEU | N-CA | -5.66 | 1.35 | 1.46 |
| 1 | A | 210 | GLN | CA-C | -5.66 | 1.38 | 1.52 |
| 2 | B | 252 | LEU | CB-CG | -5.66 | 1.36 | 1.52 |
| 2 | B | 165 | THR | CA-CB | 5.65 | 1.68 | 1.53 |
| 2 | B | 61 | LYS | CE-NZ | 5.64 | 1.63 | 1.49 |
| 2 | B | 270 | PRO | CA-C | -5.64 | 1.41 | 1.52 |
| 2 | B | 312 | GLN | N-CA | -5.64 | 1.35 | 1.46 |
| 1 | A | 131 | VAL | CA-CB | 5.63 | 1.66 | 1.54 |
| 1 | A | 152 | PHE | CB-CG | 5.63 | 1.60 | 1.51 |
| 2 | B | 190 | THR | N-CA | 5.63 | 1.57 | 1.46 |
| 2 | B | 18 | PRO | C-N | 5.62 | 1.47 | 1.34 |
| 2 | B | 13 | GLY | N-CA | 5.62 | 1.54 | 1.46 |
| 2 | B | 122 | ALA | CA-C | 5.62 | 1.67 | 1.52 |
| 1 | A | 142 | ALA | N-CA | -5.62 | 1.35 | 1.46 |
| 2 | B | 279 | TYR | CZ-OH | 5.61 | 1.47 | 1.37 |
| 2 | B | 136 | ALA | N-CA | 5.61 | 1.57 | 1.46 |
| 1 | A | 171 | ARG | NE-CZ | -5.61 | 1.25 | 1.33 |
| 2 | B | 32 | PHE | CB-CG | 5.60 | 1.60 | 1.51 |
| 2 | B | 297 | SER | CA-C | 5.60 | 1.67 | 1.52 |
| 2 | B | 197 | TYR | CB-CG | 5.60 | 1.60 | 1.51 |
| 2 | B | 78 | GLU | CA-CB | 5.60 | 1.66 | 1.53 |
| 2 | B | 170 | CYS | CB-SG | 5.59 | 1.91 | 1.82 |
| 2 | B | 206[A] | ARG | CB-CG | -5.59 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 2 | B | 206[B] | ARG | CB-CG | -5.59 | 1.37 | 1.52 |
| 2 | B | 55 | ARG | C-N | 5.59 | 1.44 | 1.34 |
| 2 | B | 46 | ALA | CA-C | 5.58 | 1.67 | 1.52 |
| 2 | B | 361 | MET | CA-C | 5.57 | 1.67 | 1.52 |
| 2 | B | 186 | TYR | CE2-CZ | -5.57 | 1.31 | 1.38 |
| 2 | B | 322 | ALA | C-O | 5.57 | 1.33 | 1.23 |
| 2 | B | 297 | SER | CB-OG | -5.56 | 1.35 | 1.42 |
| 1 | A | 259 | VAL | CB-CG2 | 5.56 | 1.64 | 1.52 |
| 1 | A | 133 | VAL | CA-CB | 5.55 | 1.66 | 1.54 |
| 1 | A | 141 | GLN | CA-C | -5.55 | 1.38 | 1.52 |
| 1 | A | 128 | VAL | CB-CG2 | 5.53 | 1.64 | 1.52 |
| 1 | A | 119 | GLU | CA-CB | -5.53 | 1.41 | 1.53 |
| 2 | B | 359 | LEU | CB-CG | 5.53 | 1.68 | 1.52 |
| 2 | B | 279 | TYR | CA-C | 5.52 | 1.67 | 1.52 |
| 2 | B | 363 | ARG | CD-NE | 5.52 | 1.55 | 1.46 |
| 2 | B | 121 | LEU | CG-CD2 | 5.51 | 1.72 | 1.51 |
| 2 | B | 225 | ASP | C-O | 5.50 | 1.33 | 1.23 |
| 2 | B | 288 | GLN | CG-CD | 5.50 | 1.63 | 1.51 |
| 2 | B | 334 | GLU | CA-CB | 5.50 | 1.66 | 1.53 |
| 2 | B | 342 | HIS | N-CA | -5.50 | 1.35 | 1.46 |
| 2 | B | 276 | VAL | N-CA | 5.48 | 1.57 | 1.46 |
| 2 | B | 91 | VAL | N-CA | 5.48 | 1.57 | 1.46 |
| 2 | B | 252 | LEU | CG-CD1 | 5.48 | 1.72 | 1.51 |
| 2 | B | 85 | ALA | CA-CB | -5.47 | 1.41 | 1.52 |
| 1 | A | 136 | SER | C-N | -5.47 | 1.21 | 1.34 |
| 2 | B | 163 | SER | CB-OG | 5.46 | 1.49 | 1.42 |
| 2 | B | 363 | ARG | CA-CB | -5.46 | 1.42 | 1.53 |
| 1 | A | 99 | LEU | N-CA | 5.46 | 1.57 | 1.46 |
| 1 | A | 106 | VAL | CA-CB | 5.46 | 1.66 | 1.54 |
| 2 | B | 216 | ILE | CB-CG1 | 5.46 | 1.69 | 1.54 |
| 2 | B | 236 | ASN | CB-CG | 5.46 | 1.63 | 1.51 |
| 2 | B | 113 | GLY | CA-C | -5.45 | 1.43 | 1.51 |
| 1 | A | 48 | LEU | CG-CD2 | 5.45 | 1.72 | 1.51 |
| 2 | B | 366 | PRO | C-O | 5.44 | 1.34 | 1.23 |
| 1 | A | 45 | ALA | C-O | 5.44 | 1.33 | 1.23 |
| 1 | A | 174 | THR | C-O | 5.43 | 1.33 | 1.23 |
| 2 | B | 12 | PHE | CG-CD1 | -5.43 | 1.30 | 1.38 |
| 2 | B | 98 | ALA | CA-CB | -5.43 | 1.41 | 1.52 |
| 1 | A | 5 | GLU | CG-CD | 5.42 | 1.60 | 1.51 |
| 1 | A | 54 | PHE | CE1-CZ | -5.42 | 1.27 | 1.37 |
| 2 | B | 65 | ILE | CA-CB | 5.42 | 1.67 | 1.54 |
| 1 | A | 47 | ALA | N-CA | 5.42 | 1.57 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 360 | LYS | CE-NZ | 5.42 | 1.62 | 1.49 |
| 2 | B | 10 | GLY | N-CA | 5.42 | 1.54 | 1.46 |
| 2 | B | 371 | LEU | CA-CB | -5.41 | 1.41 | 1.53 |
| 2 | B | 343 | GLU | CA-C | 5.41 | 1.67 | 1.52 |
| 2 | B | 63 | GLN | CB-CG | -5.41 | 1.38 | 1.52 |
| 2 | B | 73 | LEU | CA-C | 5.40 | 1.67 | 1.52 |
| 1 | A | 199 | LYS | C-O | 5.40 | 1.33 | 1.23 |
| 2 | B | 213 | LYS | CE-NZ | 5.40 | 1.62 | 1.49 |
| 2 | B | 15 | MET | C-O | 5.40 | 1.33 | 1.23 |
| 2 | B | 86 | HIS | CG-CD2 | 5.39 | 1.45 | 1.35 |
| 2 | B | 102 | GLY | CA-C | -5.38 | 1.43 | 1.51 |
| 2 | B | 46 | ALA | CA-CB | -5.37 | 1.41 | 1.52 |
| 2 | B | 272 | LYS | N-CA | 5.37 | 1.57 | 1.46 |
| 2 | B | 17 | VAL | C-N | -5.37 | 1.24 | 1.34 |
| 2 | B | 12 | PHE | CE1-CZ | -5.37 | 1.27 | 1.37 |
| 2 | B | 14 | GLY | C-O | 5.37 | 1.32 | 1.23 |
| 1 | A | 234 | GLY | N-CA | 5.37 | 1.54 | 1.46 |
| 2 | B | 115 | HIS | C-N | -5.36 | 1.23 | 1.33 |
| 2 | B | 59 | LEU | CG-CD2 | -5.36 | 1.32 | 1.51 |
| 2 | B | 312 | GLN | CA-C | 5.36 | 1.66 | 1.52 |
| 2 | B | 81 | LEU | CA-CB | 5.35 | 1.66 | 1.53 |
| 2 | B | 125 | LEU | N-CA | -5.35 | 1.35 | 1.46 |
| 2 | B | 310 | GLY | CA-C | 5.35 | 1.60 | 1.51 |
| 1 | A | 172 | GLY | N-CA | -5.34 | 1.38 | 1.46 |
| 1 | A | 239 | LYS | CG-CD | 5.34 | 1.70 | 1.52 |
| 2 | B | 49 | LEU | CA-C | 5.34 | 1.66 | 1.52 |
| 2 | B | 360 | LYS | CA-C | -5.34 | 1.39 | 1.52 |
| 1 | A | 134 | GLU | CD-OE1 | 5.32 | 1.31 | 1.25 |
| 1 | A | 220 | VAL | CA-C | 5.32 | 1.66 | 1.52 |
| 2 | B | 251 | GLY | C-O | 5.32 | 1.32 | 1.23 |
| 1 | A | 99 | LEU | C-N | 5.32 | 1.46 | 1.34 |
| 2 | B | 311 | PRO | CG-CD | 5.32 | 1.68 | 1.50 |
| 2 | B | 389 | ASP | CB-CG | 5.32 | 1.62 | 1.51 |
| 2 | B | 16 | TYR | CG-CD2 | -5.31 | 1.32 | 1.39 |
| 2 | B | 79 | ASP | CA-CB | 5.31 | 1.65 | 1.53 |
| 1 | A | 20 | VAL | CA-CB | -5.31 | 1.43 | 1.54 |
| 1 | A | 256 | ARG | CZ-NH2 | 5.31 | 1.40 | 1.33 |
| 2 | B | 339 | LEU | CA-C | 5.31 | 1.66 | 1.52 |
| 2 | B | 166 | LEU | CG-CD1 | 5.31 | 1.71 | 1.51 |
| 1 | A | 176 | LEU | CG-CD2 | 5.29 | 1.71 | 1.51 |
| 2 | B | 231 | VAL | CA-CB | 5.29 | 1.65 | 1.54 |
| 1 | A | 95 | ILE | N-CA | 5.29 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 345 | ILE | CB-CG2 | 5.29 | 1.69 | 1.52 |
| 1 | A | 111 | ILE | C-O | 5.26 | 1.33 | 1.23 |
| 2 | B | 330 | ASP | CA-C | -5.26 | 1.39 | 1.52 |
| 2 | B | 232 | GLY | N-CA | -5.25 | 1.38 | 1.46 |
| 1 | A | 20 | VAL | C-N | -5.25 | 1.24 | 1.34 |
| 2 | B | 376 | LEU | CG-CD1 | 5.24 | 1.71 | 1.51 |
| 1 | A | 14 | ARG | C-O | -5.24 | 1.13 | 1.23 |
| 2 | B | 330 | ASP | C-O | 5.23 | 1.33 | 1.23 |
| 1 | A | 112 | ASP | CA-C | -5.23 | 1.39 | 1.52 |
| 2 | B | 79 | ASP | CA-C | 5.23 | 1.66 | 1.52 |
| 2 | B | 347 | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 2 | B | 72 | THR | C-O | 5.23 | 1.33 | 1.23 |
| 1 | A | 130 | ASP | CG-OD1 | 5.23 | 1.37 | 1.25 |
| 2 | B | 216 | ILE | N-CA | 5.22 | 1.56 | 1.46 |
| 2 | B | 244 | PHE | CE1-CZ | 5.22 | 1.47 | 1.37 |
| 2 | B | 214 | ALA | C-N | -5.22 | 1.22 | 1.34 |
| 1 | A | 219 | GLN | CA-CB | 5.22 | 1.65 | 1.53 |
| 1 | A | 114 | PHE | N-CA | -5.21 | 1.35 | 1.46 |
| 2 | B | 63 | GLN | CD-OE1 | 5.21 | 1.35 | 1.24 |
| 1 | A | 3 | ARG | CB-CG | 5.21 | 1.66 | 1.52 |
| 2 | B | 38 | ASP | C-N | -5.20 | 1.24 | 1.34 |
| 2 | B | 12 | PHE | CA-C | 5.20 | 1.66 | 1.52 |
| 2 | B | 348 | ALA | C-O | 5.20 | 1.33 | 1.23 |
| 2 | B | 132 | ILE | CA-CB | -5.19 | 1.43 | 1.54 |
| 2 | B | 230 | CYS | CA-C | 5.19 | 1.66 | 1.52 |
| 2 | B | 277 | GLY | CA-C | 5.19 | 1.60 | 1.51 |
| 1 | A | 124 | ASP | CG-OD2 | -5.19 | 1.13 | 1.25 |
| 1 | A | 258 | PHE | CB-CG | -5.19 | 1.42 | 1.51 |
| 2 | B | 347 | PRO | C-N | 5.18 | 1.46 | 1.34 |
| 2 | B | 379 | ARG | CZ-NH2 | -5.18 | 1.26 | 1.33 |
| 2 | B | 221 | GLY | N-CA | -5.18 | 1.38 | 1.46 |
| 2 | B | 234 | GLY | N-CA | -5.17 | 1.38 | 1.46 |
| 2 | B | 59 | LEU | C-N | -5.17 | 1.22 | 1.34 |
| 1 | A | 60 | ASP | CG-OD1 | 5.16 | 1.37 | 1.25 |
| 2 | B | 125 | LEU | CA-C | 5.16 | 1.66 | 1.52 |
| 1 | A | 25 | LEU | CB-CG | 5.16 | 1.67 | 1.52 |
| 1 | A | 261 | ALA | CA-C | -5.15 | 1.39 | 1.52 |
| 2 | B | 41 | PHE | CD2-CE2 | 5.15 | 1.49 | 1.39 |
| 2 | B | 319 | ILE | C-N | -5.15 | 1.23 | 1.33 |
| 1 | A | 77 | THR | C-N | -5.15 | 1.24 | 1.34 |
| 2 | B | 57 | THR | CA-C | 5.14 | 1.66 | 1.52 |
| 2 | B | 86 | HIS | C-N | -5.14 | 1.22 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 320 | GLY | C-N | 5.14 | 1.45 | 1.34 |
| 2 | B | 333 | LEU | N-CA | 5.14 | 1.56 | 1.46 |
| 2 | B | 5 | LEU | CA-CB | 5.14 | 1.65 | 1.53 |
| 2 | B | 168 | ASP | CA-CB | -5.14 | 1.42 | 1.53 |
| 2 | B | 188 | LEU | CA-C | 5.13 | 1.66 | 1.52 |
| 2 | B | 207 | MET | N-CA | -5.13 | 1.36 | 1.46 |
| 2 | B | 215 | GLN | CG-CD | -5.13 | 1.39 | 1.51 |
| 1 | A | 59 | ALA | CA-CB | -5.13 | 1.41 | 1.52 |
| 2 | B | 236 | ASN | CA-CB | 5.13 | 1.66 | 1.53 |
| 2 | B | 360 | LYS | N-CA | 5.13 | 1.56 | 1.46 |
| 2 | B | 89 | ASN | N-CA | -5.11 | 1.36 | 1.46 |
| 1 | A | 209 | LEU | C-O | 5.11 | 1.33 | 1.23 |
| 2 | B | 294 | ILE | CA-CB | -5.11 | 1.43 | 1.54 |
| 2 | B | 60 | THR | CA-C | 5.10 | 1.66 | 1.52 |
| 2 | B | 253 | ILE | N-CA | -5.10 | 1.36 | 1.46 |
| 2 | B | 381 | ASP | CA-CB | 5.10 | 1.65 | 1.53 |
| 2 | B | 148 | ARG | CZ-NH2 | 5.09 | 1.39 | 1.33 |
| 1 | A | 249 | LYS | CG-CD | 5.09 | 1.69 | 1.52 |
| 1 | A | 132 | PRO | C-O | 5.09 | 1.33 | 1.23 |
| 2 | B | 353 | HIS | CB-CG | -5.09 | 1.40 | 1.50 |
| 2 | B | 284 | ALA | N-CA | 5.08 | 1.56 | 1.46 |
| 1 | A | 169 | TYR | CD1-CE1 | 5.08 | 1.47 | 1.39 |
| 2 | B | 348 | ALA | C-N | -5.08 | 1.22 | 1.34 |
| 1 | A | 114 | PHE | CG-CD2 | 5.07 | 1.46 | 1.38 |
| 2 | B | 287 | MET | CA-CB | 5.07 | 1.65 | 1.53 |
| 2 | B | 387 | VAL | CA-CB | -5.07 | 1.44 | 1.54 |
| 2 | B | 59 | LEU | C-O | 5.07 | 1.32 | 1.23 |
| 2 | B | 138 | ASP | CA-C | 5.07 | 1.66 | 1.52 |
| 1 | A | 137 | ALA | N-CA | 5.06 | 1.56 | 1.46 |
| 1 | A | 170 | GLY | N-CA | -5.06 | 1.38 | 1.46 |
| 2 | B | 152 | MET | CB-CG | 5.06 | 1.67 | 1.51 |
| 2 | B | 266 | GLU | CD-OE1 | -5.06 | 1.20 | 1.25 |
| 2 | B | 127 | GLY | CA-C | 5.06 | 1.59 | 1.51 |
| 1 | A | 263 | LYS | CE-NZ | -5.05 | 1.36 | 1.49 |
| 2 | B | 145 | ASN | C-O | 5.05 | 1.32 | 1.23 |
| 2 | B | 357 | HIS | CB-CG | 5.05 | 1.59 | 1.50 |
| 2 | B | 37 | LYS | CA-C | 5.05 | 1.66 | 1.52 |
| 1 | A | 32 | GLN | CB-CG | 5.04 | 1.66 | 1.52 |
| 1 | A | 141 | GLN | N-CA | 5.04 | 1.56 | 1.46 |
| 2 | B | 100 | ARG | CZ-NH1 | -5.04 | 1.26 | 1.33 |
| 2 | B | 219 | LYS | CE-NZ | 5.04 | 1.61 | 1.49 |
| 2 | B | 87 | LYS | N-CA | 5.04 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 171 | ARG | CA-CB | 5.03 | 1.65 | 1.53 |
| 1 | A | 102 | TYR | C-O | 5.03 | 1.32 | 1.23 |
| 2 | B | 233 | GLY | CA-C | -5.02 | 1.43 | 1.51 |
| 2 | B | 89 | ASN | CG-ND2 | 5.02 | 1.45 | 1.32 |
| 1 | A | 218 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 2 | B | 267 | HIS | CB-CG | 5.01 | 1.59 | 1.50 |
| 2 | B | 271 | LEU | CG-CD2 | 5.01 | 1.70 | 1.51 |
| 2 | B | 78 | GLU | N-CA | 5.01 | 1.56 | 1.46 |
| 1 | A | 31 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |
| 2 | B | 213 | LYS | C-N | 5.00 | 1.45 | 1.34 |

All (845) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | B | 55 | ARG | NE-CZ-NH1 | 35.94 | 138.27 | 120.30 |
| 2 | B | 291 | ASP | CB-CG-OD1 | -34.65 | 87.12 | 118.30 |
| 2 | B | 55 | ARG | NE-CZ-NH2 | -29.76 | 105.42 | 120.30 |
| 1 | A | 140 | ARG | NE-CZ-NH1 | -28.07 | 106.26 | 120.30 |
| 2 | B | 222 | ARG | NE-CZ-NH2 | -26.74 | 106.93 | 120.30 |
| 2 | B | 222 | ARG | NE-CZ-NH1 | 25.71 | 133.16 | 120.30 |
| 2 | B | 100 | ARG | NE-CZ-NH1 | 25.32 | 132.96 | 120.30 |
| 1 | A | 225 | ARG | NE-CZ-NH1 | 19.90 | 130.25 | 120.30 |
| 2 | B | 204 | PHE | CB-CG-CD2 | -19.72 | 107.00 | 120.80 |
| 2 | B | 9 | PHE | CB-CG-CD2 | -19.33 | 107.27 | 120.80 |
| 2 | B | 324 | TYR | CZ-CE2-CD2 | 19.21 | 137.09 | 119.80 |
| 2 | B | 315 | TYR | CB-CG-CD2 | 18.96 | 132.38 | 121.00 |
| 2 | B | 394 | ARG | NE-CZ-NH1 | -18.89 | 110.85 | 120.30 |
| 2 | B | 202 | ARG | NE-CZ-NH1 | -18.74 | 110.93 | 120.30 |
| 2 | B | 291 | ASP | CB-CG-OD2 | 18.69 | 135.12 | 118.30 |
| 2 | B | 52 | TYR | CB-CG-CD1 | 18.61 | 132.17 | 121.00 |
| 2 | B | 379 | ARG | CD-NE-CZ | -18.61 | 97.55 | 123.60 |
| 1 | A | 107 | PHE | CB-CG-CD1 | 18.13 | 133.49 | 120.80 |
| 2 | B | 79 | ASP | CB-CG-OD1 | 17.58 | 134.12 | 118.30 |
| 2 | B | 315 | TYR | CD1-CE1-CZ | 17.57 | 135.61 | 119.80 |
| 2 | B | 286 | MET | CA-CB-CG | 17.38 | 142.85 | 113.30 |
| 2 | B | 330 | ASP | CB-CG-OD1 | 17.04 | 133.64 | 118.30 |
| 2 | B | 204 | PHE | CD1-CE1-CZ | -16.95 | 99.76 | 120.10 |
| 2 | B | 321 | ARG | NE-CZ-NH2 | -16.39 | 112.11 | 120.30 |
| 1 | A | 225 | ARG | NE-CZ-NH2 | -16.24 | 112.18 | 120.30 |
| 1 | A | 140 | ARG | NE-CZ-NH2 | 16.11 | 128.35 | 120.30 |
| 2 | B | 368 | LYS | O-C-N | 16.03 | 148.35 | 122.70 |
| 2 | B | 339 | LEU | CB-CG-CD1 | 15.71 | 137.70 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | B | 97 | LEU | CB-CG-CD2 | 15.60 | 137.51 | 111.00 |
| 2 | B | 323 | ASP | CB-CG-OD2 | 15.37 | 132.13 | 118.30 |
| 2 | B | 324 | TYR | CG-CD1-CE1 | 15.12 | 133.40 | 121.30 |
| 2 | B | 255 | VAL | CG1-CB-CG2 | 14.96 | 134.84 | 110.90 |
| 2 | B | 70 | ARG | O-C-N | 14.54 | 145.97 | 122.70 |
| 2 | B | 334 | GLU | OE1-CD-OE2 | -14.51 | 105.89 | 123.30 |
| 2 | B | 353 | HIS | O-C-N | -14.44 | 99.59 | 122.70 |
| 2 | B | 243 | ASP | CB-CG-OD2 | 14.38 | 131.25 | 118.30 |
| 2 | B | 47 | ASP | CB-CG-OD2 | 14.27 | 131.14 | 118.30 |
| 2 | B | 8 | TYR | CG-CD1-CE1 | 14.16 | 132.62 | 121.30 |
| 2 | B | 328 | THR | O-C-N | 14.15 | 145.34 | 122.70 |
| 2 | B | 316 | LEU | CB-CG-CD2 | 13.74 | 134.36 | 111.00 |
| 2 | B | 52 | TYR | CD1-CG-CD2 | -13.38 | 103.18 | 117.90 |
| 2 | B | 304 | LEU | CB-CG-CD2 | 13.33 | 133.66 | 111.00 |
| 2 | B | 348 | ALA | O-C-N | 13.27 | 143.92 | 122.70 |
| 1 | A | 127 | LEU | O-C-N | 13.16 | 143.75 | 122.70 |
| 2 | B | 204 | PHE | CE1-CZ-CE2 | 13.05 | 143.50 | 120.00 |
| 2 | B | 32 | PHE | CB-CG-CD1 | -13.03 | 111.68 | 120.80 |
| 1 | A | 107 | PHE | CB-CG-CD2 | -12.96 | 111.73 | 120.80 |
| 2 | B | 351 | SER | O-C-N | 12.92 | 143.37 | 122.70 |
| 2 | B | 23 | PRO | O-C-N | 12.73 | 143.07 | 122.70 |
| 2 | B | 297 | SER | N-CA-CB | -12.68 | 91.48 | 110.50 |
| 2 | B | 196 | PRO | O-C-N | 12.57 | 142.81 | 122.70 |
| 2 | B | 47 | ASP | CB-CG-OD1 | -12.54 | 107.01 | 118.30 |
| 1 | A | 125 | SER | O-C-N | 12.52 | 142.73 | 122.70 |
| 2 | B | 54 | GLY | O-C-N | -12.52 | 102.68 | 122.70 |
| 2 | B | 86 | HIS | O-C-N | 12.45 | 142.62 | 122.70 |
| 2 | B | 375 | ASN | O-C-N | -12.40 | 102.85 | 122.70 |
| 1 | A | 107 | PHE | CG-CD1-CE1 | 12.37 | 134.40 | 120.80 |
| 1 | A | 169 | TYR | CB-CG-CD1 | 12.26 | 128.36 | 121.00 |
| 2 | B | 305 | ASP | CB-CG-OD1 | 11.99 | 129.09 | 118.30 |
| 1 | A | 124 | ASP | CB-CG-OD2 | 11.90 | 129.01 | 118.30 |
| 2 | B | 203 | GLU | O-C-N | 11.90 | 141.74 | 122.70 |
| 1 | A | 100 | LEU | CB-CG-CD2 | 11.74 | 130.96 | 111.00 |
| 2 | B | 316 | LEU | CB-CG-CD1 | -11.71 | 91.09 | 111.00 |
| 2 | B | 204 | PHE | CG-CD2-CE2 | -11.65 | 107.98 | 120.80 |
| 1 | A | 56 | ASP | CB-CG-OD2 | 11.63 | 128.77 | 118.30 |
| 2 | B | 8 | TYR | CZ-CE2-CD2 | 11.61 | 130.25 | 119.80 |
| 2 | B | 59 | LEU | O-C-N | 11.55 | 141.18 | 122.70 |
| 2 | B | 252 | LEU | O-C-N | -11.50 | 104.29 | 122.70 |
| 1 | A | 139 | PHE | CB-CG-CD1 | -11.44 | 112.80 | 120.80 |
| 2 | B | 12 | PHE | CG-CD2-CE2 | -11.42 | 108.24 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | B | 29 | GLU | O-C-N | -11.40 | 104.46 | 122.70 |
| 2 | B | 321 | ARG | CA-C-O | -11.38 | 96.20 | 120.10 |
| 2 | B | 324 | TYR | CD1-CE1-CZ | -11.38 | 109.56 | 119.80 |
| 2 | B | 243 | ASP | O-C-N | 11.36 | 140.88 | 122.70 |
| 2 | B | 204 | PHE | CD1-CG-CD2 | 11.33 | 133.03 | 118.30 |
| 2 | B | 363 | ARG | NE-CZ-NH1 | 11.26 | 125.93 | 120.30 |
| 2 | B | 183 | THR | CA-CB-CG2 | -11.19 | 96.73 | 112.40 |
| 2 | B | 339 | LEU | O-C-N | 11.18 | 140.58 | 122.70 |
| 2 | B | 18 | PRO | O-C-N | -11.01 | 105.09 | 122.70 |
| 2 | B | 261 | GLY | O-C-N | 11.00 | 140.30 | 122.70 |
| 2 | B | 7 | PRO | O-C-N | 10.99 | 140.29 | 122.70 |
| 2 | B | 272 | LYS | CB-CG-CD | 10.98 | 140.16 | 111.60 |
| 2 | B | 375 | ASN | CA-C-O | 10.92 | 143.04 | 120.10 |
| 2 | B | 225 | ASP | CB-CG-OD1 | 10.91 | 128.12 | 118.30 |
| 2 | B | 119 | SER | N-CA-CB | -10.86 | 94.21 | 110.50 |
| 1 | A | 47 | ALA | N-CA-CB | 10.85 | 125.29 | 110.10 |
| 2 | B | 105 | GLU | O-C-N | 10.85 | 140.06 | 122.70 |
| 2 | B | 186 | TYR | CZ-CE2-CD2 | 10.85 | 129.56 | 119.80 |
| 2 | B | 263 | GLU | OE1-CD-OE2 | 10.85 | 136.31 | 123.30 |
| 2 | B | 60 | THR | O-C-N | 10.82 | 140.01 | 122.70 |
| 2 | B | 254 | GLY | O-C-N | -10.79 | 105.43 | 122.70 |
| 1 | A | 139 | PHE | CD1-CG-CD2 | 10.79 | 132.33 | 118.30 |
| 2 | B | 263 | GLU | CG-CD-OE2 | -10.76 | 96.79 | 118.30 |
| 2 | B | 354 | ALA | N-CA-CB | 10.75 | 125.15 | 110.10 |
| 2 | B | 211 | GLU | OE1-CD-OE2 | -10.71 | 110.45 | 123.30 |
| 1 | A | 11 | LEU | CB-CG-CD2 | 10.68 | 129.16 | 111.00 |
| 2 | B | 152 | MET | CG-SD-CE | -10.63 | 83.18 | 100.20 |
| 2 | B | 315 | TYR | CE1-CZ-OH | 10.61 | 148.74 | 120.10 |
| 1 | A | 171 | ARG | NE-CZ-NH1 | 10.59 | 125.59 | 120.30 |
| 2 | B | 372 | LEU | N-CA-CB | 10.59 | 131.57 | 110.40 |
| 2 | B | 315 | TYR | CG-CD2-CE2 | 10.56 | 129.75 | 121.30 |
| 2 | B | 19 | GLN | O-C-N | 10.52 | 139.53 | 122.70 |
| 2 | B | 12 | PHE | CD1-CE1-CZ | -10.49 | 107.52 | 120.10 |
| 2 | B | 9 | PHE | O-C-N | 10.40 | 140.88 | 123.20 |
| 2 | B | 360 | LYS | O-C-N | -10.38 | 106.09 | 122.70 |
| 2 | B | 341 | ARG | NE-CZ-NH2 | -10.30 | 115.15 | 120.30 |
| 2 | B | 379 | ARG | NE-CZ-NH2 | 10.27 | 125.44 | 120.30 |
| 2 | B | 15 | MET | CB-CG-SD | 10.22 | 143.07 | 112.40 |
| 2 | B | 52 | TYR | CG-CD1-CE1 | 10.21 | 129.47 | 121.30 |
| 2 | B | 333 | LEU | CB-CG-CD2 | -10.19 | 93.68 | 111.00 |
| 2 | B | 97 | LEU | CA-CB-CG | -10.18 | 91.89 | 115.30 |
| 2 | B | 106 | ILE | O-C-N | -10.17 | 106.43 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | B | 12 | PHE | CD1-CG-CD2 | 10.15 | 131.50 | 118.30 |
| 2 | B | 316 | LEU | CA-C-O | -10.14 | 98.81 | 120.10 |
| 2 | B | 347 | PRO | CA-C-O | 10.12 | 144.48 | 120.20 |
| 2 | B | 58 | ALA | N-CA-CB | -10.00 | 96.10 | 110.10 |
| 2 | B | 194 | PRO | O-C-N | -10.00 | 106.70 | 122.70 |
| 2 | B | 74 | TYR | CZ-CE2-CD2 | 9.98 | 128.78 | 119.80 |
| 2 | B | 341 | ARG | O-C-N | -9.95 | 106.78 | 122.70 |
| 2 | B | 106 | ILE | CA-C-O | 9.93 | 140.94 | 120.10 |
| 2 | B | 30 | GLU | O-C-N | 9.87 | 138.49 | 122.70 |
| 2 | B | 122 | ALA | O-C-N | 9.86 | 138.48 | 122.70 |
| 2 | B | 29 | GLU | CA-C-O | 9.86 | 140.81 | 120.10 |
| 2 | B | 394 | ARG | NH1-CZ-NH2 | 9.83 | 130.21 | 119.40 |
| 2 | B | 233 | GLY | O-C-N | -9.83 | 106.50 | 123.20 |
| 1 | A | 7 | LEU | CB-CG-CD2 | -9.82 | 94.30 | 111.00 |
| 2 | B | 212 | THR | CA-CB-OG1 | 9.80 | 129.58 | 109.00 |
| 2 | B | 6 | ASN | CA-C-N | 9.79 | 144.51 | 117.10 |
| 1 | A | 163 | LEU | CB-CG-CD2 | 9.78 | 127.63 | 111.00 |
| 2 | B | 376 | LEU | CB-CG-CD2 | -9.78 | 94.37 | 111.00 |
| 2 | B | 370 | GLN | CA-CB-CG | 9.77 | 134.90 | 113.40 |
| 2 | B | 12 | PHE | CB-CG-CD1 | -9.76 | 113.97 | 120.80 |
| 2 | B | 49 | LEU | CA-C-O | -9.72 | 99.68 | 120.10 |
| 2 | B | 226 | ALA | N-CA-CB | 9.65 | 123.61 | 110.10 |
| 2 | B | 336 | PHE | O-C-N | 9.65 | 138.14 | 122.70 |
| 2 | B | 3 | THR | O-C-N | -9.64 | 107.27 | 122.70 |
| 2 | B | 77 | ARG | NE-CZ-NH1 | -9.62 | 115.49 | 120.30 |
| 2 | B | 17 | VAL | CA-CB-CG2 | 9.62 | 125.33 | 110.90 |
| 2 | B | 91 | VAL | CA-CB-CG1 | 9.62 | 125.33 | 110.90 |
| 2 | B | 98 | ALA | N-CA-CB | 9.59 | 123.53 | 110.10 |
| 2 | B | 9 | PHE | CD1-CG-CD2 | 9.59 | 130.76 | 118.30 |
| 1 | A | 191 | LEU | N-CA-C | 9.53 | 136.72 | 111.00 |
| 2 | B | 213 | LYS | CD-CE-NZ | -9.50 | 89.84 | 111.70 |
| 1 | A | 196 | LEU | CB-CG-CD1 | 9.45 | 127.06 | 111.00 |
| 2 | B | 12 | PHE | CB-CG-CD2 | -9.43 | 114.20 | 120.80 |
| 2 | B | 368 | LYS | CA-C-O | -9.42 | 100.31 | 120.10 |
| 2 | B | 93 | GLY | CA-C-O | -9.42 | 103.64 | 120.60 |
| 2 | B | 319 | ILE | CG1-CB-CG2 | -9.36 | 90.82 | 111.40 |
| 2 | B | 258 | GLY | CA-C-O | 9.35 | 137.43 | 120.60 |
| 2 | B | 21 | LEU | O-C-N | -9.33 | 107.77 | 122.70 |
| 2 | B | 244 | PHE | CB-CG-CD2 | -9.31 | 114.28 | 120.80 |
| 2 | B | 74 | TYR | CG-CD1-CE1 | 9.27 | 128.72 | 121.30 |
| 2 | B | 128 | LEU | O-C-N | -9.24 | 107.91 | 122.70 |
| 1 | A | 97 | ILE | O-C-N | -9.21 | 107.53 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 2 | B | 6 | ASN | CA-C-O | -9.20 | 100.78 | 120.10 |
| 2 | B | 78 | GLU | O-C-N | -9.19 | 108.00 | 122.70 |
| 2 | B | 79 | ASP | O-C-N | 9.19 | 137.40 | 122.70 |
| 2 | B | 12 | PHE | CE1-CZ-CE2 | 9.16 | 136.49 | 120.00 |
| 2 | B | 18 | PRO | CA-C-O | 9.14 | 142.14 | 120.20 |
| 2 | B | 230 | CYS | O-C-N | 9.13 | 137.32 | 122.70 |
| 2 | B | 215 | GLN | CG-CD-OE1 | 9.13 | 139.86 | 121.60 |
| 2 | B | 314 | ALA | O-C-N | -9.13 | 108.09 | 122.70 |
| 2 | B | 347 | PRO | O-C-N | -9.12 | 108.10 | 122.70 |
| 1 | A | 13 | ASP | CB-CG-OD1 | 9.12 | 126.51 | 118.30 |
| 2 | B | 373 | VAL | CA-CB-CG2 | 9.12 | 124.58 | 110.90 |
| 2 | B | 284 | ALA | CA-C-O | 9.10 | 139.21 | 120.10 |
| 2 | B | 286 | MET | CB-CG-SD | -9.08 | 85.15 | 112.40 |
| 2 | B | 374 | VAL | CA-CB-CG1 | 9.07 | 124.51 | 110.90 |
| 2 | B | 202 | ARG | NH1-CZ-NH2 | 9.07 | 129.38 | 119.40 |
| 1 | A | 145 | ARG | NE-CZ-NH2 | -9.07 | 115.77 | 120.30 |
| 2 | B | 69 | THR | CA-CB-CG2 | 9.04 | 125.06 | 112.40 |
| 2 | B | 243 | ASP | OD1-CG-OD2 | -9.03 | 106.15 | 123.30 |
| 1 | A | 4 | TYR | CB-CG-CD2 | -9.01 | 115.59 | 121.00 |
| 2 | B | 281 | GLY | CA-C-O | 9.00 | 136.81 | 120.60 |
| 2 | B | 55 | ARG | O-C-N | -9.00 | 104.00 | 121.10 |
| 1 | A | 145 | ARG | NE-CZ-NH1 | 9.00 | 124.80 | 120.30 |
| 2 | B | 150 | ARG | NE-CZ-NH2 | -8.94 | 115.83 | 120.30 |
| 2 | B | 202 | ARG | O-C-N | -8.95 | 108.39 | 122.70 |
| 2 | B | 206[A] | ARG | NE-CZ-NH2 | -8.92 | 115.84 | 120.30 |
| 2 | B | 206[B] | ARG | NE-CZ-NH2 | -8.92 | 115.84 | 120.30 |
| 1 | A | 148 | ILE | CG1-CB-CG2 | -8.92 | 91.78 | 111.40 |
| 2 | B | 9 | PHE | CA-C-N | -8.91 | 98.38 | 116.20 |
| 1 | A | 139 | PHE | CE1-CZ-CE2 | 8.88 | 135.99 | 120.00 |
| 2 | B | 336 | PHE | CG-CD2-CE2 | -8.88 | 111.03 | 120.80 |
| 2 | B | 308 | SER | CA-C-N | 8.85 | 136.66 | 117.20 |
| 2 | B | 298 | TYR | CA-CB-CG | -8.84 | 96.61 | 113.40 |
| 1 | A | 46 | ASP | CB-CG-OD2 | 8.83 | 126.25 | 118.30 |
| 2 | B | 33 | VAL | CG1-CB-CG2 | 8.83 | 125.03 | 110.90 |
| 2 | B | 360 | LYS | CA-C-N | 8.82 | 136.61 | 117.20 |
| 2 | B | 32 | PHE | CG-CD1-CE1 | -8.82 | 111.10 | 120.80 |
| 2 | B | 133 | TYR | CZ-CE2-CD2 | -8.81 | 111.88 | 119.80 |
| 2 | B | 211 | GLU | CG-CD-OE1 | 8.80 | 135.90 | 118.30 |
| 2 | B | 295 | GLU | CG-CD-OE2 | 8.77 | 135.84 | 118.30 |
| 2 | B | 203 | GLU | CA-C-O | -8.76 | 101.71 | 120.10 |
| 2 | B | 311 | PRO | O-C-N | -8.75 | 108.71 | 122.70 |
| 2 | B | 117 | VAL | O-C-N | -8.74 | 108.71 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 24 | THR | CA-CB-CG2 | -8.74 | 100.17 | 112.40 |
| 2 | B | 59 | LEU | CA-C-O | -8.71 | 101.80 | 120.10 |
| 2 | B | 379 | ARG | O-C-N | -8.71 | 108.39 | 123.20 |
| 2 | B | 380 | GLY | N-CA-C | 8.70 | 134.86 | 113.10 |
| 2 | B | 62 | CYS | CA-CB-SG | -8.70 | 98.34 | 114.00 |
| 1 | A | 3 | ARG | NE-CZ-NH1 | 8.68 | 124.64 | 120.30 |
| 1 | A | 141 | GLN | O-C-N | -8.66 | 108.85 | 122.70 |
| 2 | B | 241 | PHE | CA-C-O | 8.64 | 138.25 | 120.10 |
| 1 | A | 7 | LEU | CB-CG-CD1 | 8.64 | 125.69 | 111.00 |
| 1 | A | 100 | LEU | CB-CG-CD1 | -8.63 | 96.33 | 111.00 |
| 2 | B | 99 | LYS | CD-CE-NZ | -8.57 | 91.99 | 111.70 |
| 2 | B | 269 | ALA | CB-CA-C | -8.56 | 97.25 | 110.10 |
| 2 | B | 105 | GLU | N-CA-CB | 8.56 | 126.00 | 110.60 |
| 2 | B | 66 | THR | CA-CB-OG1 | 8.55 | 126.96 | 109.00 |
| 2 | B | 379 | ARG | NE-CZ-NH1 | -8.55 | 116.03 | 120.30 |
| 1 | A | 121 | VAL | C-N-CA | -8.51 | 104.43 | 122.30 |
| 2 | B | 324 | TYR | CG-CD2-CE2 | -8.51 | 114.49 | 121.30 |
| 2 | B | 368 | LYS | CD-CE-NZ | -8.49 | 92.17 | 111.70 |
| 1 | A | 139 | PHE | CB-CG-CD2 | -8.47 | 114.87 | 120.80 |
| 2 | B | 282 | MET | O-C-N | 8.46 | 136.23 | 122.70 |
| 2 | B | 231 | VAL | O-C-N | -8.46 | 108.82 | 123.20 |
| 2 | B | 45 | PHE | CD1-CE1-CZ | -8.45 | 109.96 | 120.10 |
| 1 | A | 163 | LEU | CB-CG-CD1 | -8.45 | 96.64 | 111.00 |
| 1 | A | 96 | PRO | N-CA-CB | 8.44 | 113.43 | 103.30 |
| 1 | A | 139 | PHE | O-C-N | 8.43 | 136.18 | 122.70 |
| 2 | B | 193 | GLY | O-C-N | -8.42 | 105.10 | 121.10 |
| 1 | A | 176 | LEU | CB-CG-CD2 | -8.41 | 96.71 | 111.00 |
| 2 | B | 326 | SER | N-CA-CB | 8.39 | 123.08 | 110.50 |
| 2 | B | 12 | PHE | O-C-N | 8.38 | 137.46 | 123.20 |
| 2 | B | 350 | GLU | O-C-N | -8.37 | 109.31 | 122.70 |
| 2 | B | 6 | ASN | N-CA-C | 8.37 | 133.59 | 111.00 |
| 2 | B | 193 | GLY | CA-C-O | 8.35 | 135.64 | 120.60 |
| 1 | A | 4 | TYR | CD1-CE1-CZ | -8.33 | 112.30 | 119.80 |
| 2 | B | 103 | LYS | CD-CE-NZ | -8.33 | 92.55 | 111.70 |
| 2 | B | 17 | VAL | O-C-N | 8.31 | 136.90 | 121.10 |
| 2 | B | 315 | TYR | CZ-CE2-CD2 | -8.30 | 112.33 | 119.80 |
| 2 | B | 264 | THR | CA-CB-CG2 | -8.30 | 100.78 | 112.40 |
| 2 | B | 373 | VAL | CA-CB-CG1 | -8.27 | 98.50 | 110.90 |
| 2 | B | 59 | LEU | CB-CG-CD2 | -8.26 | 96.95 | 111.00 |
| 2 | B | 331 | GLU | N-CA-CB | 8.26 | 125.47 | 110.60 |
| 2 | B | 61 | LYS | N-CA-CB | -8.21 | 95.82 | 110.60 |
| 2 | B | 41 | PHE | CB-CG-CD2 | 8.20 | 126.54 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 124 | ASP | CB-CG-OD1 | -8.15 | 110.96 | 118.30 |
| 2 | B | 76 | LYS | CA-C-O | 8.14 | 137.19 | 120.10 |
| 2 | B | 56 | PRO | O-C-N | -8.13 | 109.69 | 122.70 |
| 1 | A | 175 | TYR | CD1-CE1-CZ | 8.13 | 127.11 | 119.80 |
| 2 | B | 275 | ARG | NE-CZ-NH2 | -8.13 | 116.24 | 120.30 |
| 1 | A | 153 | ILE | CA-C-O | 8.12 | 137.16 | 120.10 |
| 2 | B | 371 | LEU | CB-CG-CD1 | -8.13 | 97.19 | 111.00 |
| 2 | B | 345 | ILE | CA-CB-CG1 | 8.12 | 126.43 | 111.00 |
| 2 | B | 73 | LEU | CB-CG-CD1 | -8.11 | 97.22 | 111.00 |
| 1 | A | 48 | LEU | CA-C-O | 8.10 | 137.12 | 120.10 |
| 2 | B | 8 | TYR | CB-CG-CD1 | 8.09 | 125.85 | 121.00 |
| 2 | B | 315 | TYR | CB-CG-CD1 | -8.08 | 116.15 | 121.00 |
| 2 | B | 370 | GLN | O-C-N | 8.08 | 135.63 | 122.70 |
| 2 | B | 86 | HIS | CA-C-O | -8.07 | 103.14 | 120.10 |
| 2 | B | 327 | ILE | O-C-N | -8.06 | 109.80 | 122.70 |
| 2 | B | 242 | ALA | O-C-N | -8.04 | 109.84 | 122.70 |
| 2 | B | 355 | LEU | CB-CG-CD2 | -8.02 | 97.37 | 111.00 |
| 2 | B | 271 | LEU | N-CA-CB | 8.01 | 126.42 | 110.40 |
| 2 | B | 280 | PHE | O-C-N | -8.01 | 109.58 | 123.20 |
| 2 | B | 100 | ARG | NH1-CZ-NH2 | -8.00 | 110.60 | 119.40 |
| 2 | B | 372 | LEU | CB-CG-CD2 | -7.99 | 97.41 | 111.00 |
| 2 | B | 231 | VAL | CA-CB-CG1 | -7.99 | 98.92 | 110.90 |
| 1 | A | 41 | ILE | CG1-CB-CG2 | -7.97 | 93.86 | 111.40 |
| 2 | B | 67 | ALA | O-C-N | 7.97 | 136.75 | 123.20 |
| 2 | B | 9 | PHE | CG-CD2-CE2 | -7.96 | 112.04 | 120.80 |
| 2 | B | 305 | ASP | CB-CG-OD2 | -7.96 | 111.14 | 118.30 |
| 1 | A | 139 | PHE | CD1-CE1-CZ | -7.95 | 110.56 | 120.10 |
| 2 | B | 380 | GLY | CA-C-O | 7.93 | 134.87 | 120.60 |
| 2 | B | 59 | LEU | CA-CB-CG | -7.91 | 97.12 | 115.30 |
| 2 | B | 376 | LEU | CA-CB-CG | -7.90 | 97.14 | 115.30 |
| 2 | B | 56 | PRO | C-N-CA | 7.89 | 141.43 | 121.70 |
| 2 | B | 49 | LEU | O-C-N | 7.89 | 135.32 | 122.70 |
| 2 | B | 161 | SER | CB-CA-C | -7.88 | 95.12 | 110.10 |
| 2 | B | 251 | GLY | CA-C-O | -7.87 | 106.44 | 120.60 |
| 2 | B | 331 | GLU | OE1-CD-OE2 | -7.85 | 113.88 | 123.30 |
| 2 | B | 15 | MET | CA-CB-CG | 7.84 | 126.63 | 113.30 |
| 2 | B | 336 | PHE | CB-CG-CD2 | -7.84 | 115.31 | 120.80 |
| 2 | B | 119 | SER | O-C-N | 7.82 | 135.22 | 122.70 |
| 1 | A | 11 | LEU | CA-CB-CG | -7.82 | 97.31 | 115.30 |
| 2 | B | 357 | HIS | O-C-N | -7.79 | 110.24 | 122.70 |
| 2 | B | 181 | TYR | CB-CG-CD1 | -7.79 | 116.33 | 121.00 |
| 2 | B | 52 | TYR | CZ-CE2-CD2 | 7.78 | 126.81 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 348 | ALA | CA-C-O | -7.78 | 103.75 | 120.10 |
| 2 | B | 69 | THR | O-C-N | -7.78 | 110.25 | 122.70 |
| 2 | B | 100 | ARG | CD-NE-CZ | 7.78 | 134.49 | 123.60 |
| 2 | B | 100 | ARG | NE-CZ-NH2 | -7.76 | 116.42 | 120.30 |
| 1 | A | 76 | VAL | CA-CB-CG2 | -7.74 | 99.29 | 110.90 |
| 2 | B | 330 | ASP | OD1-CG-OD2 | -7.73 | 108.61 | 123.30 |
| 2 | B | 343 | GLU | OE1-CD-OE2 | -7.72 | 114.03 | 123.30 |
| 2 | B | 6 | ASN | N-CA-CB | -7.71 | 96.72 | 110.60 |
| 2 | B | 236 | ASN | O-C-N | 7.70 | 135.02 | 122.70 |
| 2 | B | 5 | LEU | CA-C-O | 7.70 | 136.26 | 120.10 |
| 2 | B | 70 | ARG | CA-C-O | -7.70 | 103.94 | 120.10 |
| 2 | B | 332 | ALA | O-C-N | 7.69 | 135.01 | 122.70 |
| 2 | B | 91 | VAL | CA-CB-CG2 | -7.69 | 99.36 | 110.90 |
| 2 | B | 361 | MET | CG-SD-CE | 7.69 | 112.50 | 100.20 |
| 1 | A | 121 | VAL | O-C-N | 7.68 | 136.26 | 123.20 |
| 1 | A | 139 | PHE | CG-CD2-CE2 | -7.68 | 112.36 | 120.80 |
| 2 | B | 78 | GLU | CG-CD-OE1 | -7.67 | 102.95 | 118.30 |
| 2 | B | 328 | THR | CA-C-O | -7.67 | 104.00 | 120.10 |
| 2 | B | 71 | THR | O-C-N | 7.66 | 134.95 | 122.70 |
| 2 | B | 275 | ARG | O-C-N | 7.66 | 134.95 | 122.70 |
| 1 | A | 136 | SER | O-C-N | 7.64 | 134.93 | 122.70 |
| 2 | B | 203 | GLU | OE1-CD-OE2 | -7.63 | 114.14 | 123.30 |
| 2 | B | 264 | THR | O-C-N | 7.63 | 136.18 | 123.20 |
| 2 | B | 57 | THR | C-N-CA | -7.61 | 102.67 | 121.70 |
| 2 | B | 291 | ASP | OD1-CG-OD2 | 7.61 | 137.75 | 123.30 |
| 2 | B | 373 | VAL | O-C-N | -7.59 | 110.56 | 122.70 |
| 1 | A | 140 | ARG | CD-NE-CZ | -7.58 | 112.98 | 123.60 |
| 1 | A | 134 | GLU | CG-CD-OE1 | 7.57 | 133.43 | 118.30 |
| 2 | B | 228 | ILE | CA-CB-CG1 | -7.56 | 96.64 | 111.00 |
| 2 | B | 57 | THR | N-CA-CB | 7.56 | 124.66 | 110.30 |
| 2 | B | 323 | ASP | OD1-CG-OD2 | -7.55 | 108.94 | 123.30 |
| 2 | B | 194 | PRO | CA-C-N | 7.54 | 133.78 | 117.20 |
| 2 | B | 281 | GLY | N-CA-C | 7.54 | 131.94 | 113.10 |
| 2 | B | 343 | GLU | CG-CD-OE1 | 7.52 | 133.34 | 118.30 |
| 2 | B | 58 | ALA | O-C-N | 7.50 | 134.70 | 122.70 |
| 2 | B | 295 | GLU | OE1-CD-OE2 | -7.50 | 114.30 | 123.30 |
| 2 | B | 32 | PHE | O-C-N | -7.49 | 110.72 | 122.70 |
| 2 | B | 194 | PRO | CA-N-CD | 7.49 | 122.18 | 111.70 |
| 2 | B | 41 | PHE | CG-CD2-CE2 | 7.48 | 129.03 | 120.80 |
| 2 | B | 367 | GLU | N-CA-C | 7.48 | 131.19 | 111.00 |
| 1 | A | 98 | GLY | O-C-N | 7.47 | 134.66 | 122.70 |
| 2 | B | 121 | LEU | O-C-N | -7.45 | 110.77 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 210 | GLN | CA-C-O | 7.45 | 135.74 | 120.10 |
| 2 | B | 314 | ALA | CA-C-N | 7.45 | 133.58 | 117.20 |
| 2 | B | 339 | LEU | CA-C-O | -7.44 | 104.47 | 120.10 |
| 2 | B | 343 | GLU | O-C-N | 7.44 | 135.85 | 123.20 |
| 1 | A | 114 | PHE | CG-CD1-CE1 | 7.44 | 128.98 | 120.80 |
| 2 | B | 282 | MET | CA-CB-CG | -7.43 | 100.67 | 113.30 |
| 2 | B | 362 | MET | CA-CB-CG | -7.42 | 100.69 | 113.30 |
| 2 | B | 353 | HIS | C-N-CA | 7.42 | 140.24 | 121.70 |
| 1 | A | 131 | VAL | CA-CB-CG2 | -7.36 | 99.87 | 110.90 |
| 2 | B | 321 | ARG | CA-C-N | 7.34 | 133.34 | 117.20 |
| 1 | A | 100 | LEU | O-C-N | 7.33 | 134.43 | 122.70 |
| 1 | A | 197 | ILE | CG1-CB-CG2 | -7.33 | 95.28 | 111.40 |
| 1 | A | 142 | ALA | CB-CA-C | -7.32 | 99.12 | 110.10 |
| 2 | B | 186 | TYR | CG-CD2-CE2 | -7.32 | 115.45 | 121.30 |
| 2 | B | 81 | LEU | CB-CG-CD1 | 7.31 | 123.42 | 111.00 |
| 2 | B | 159 | VAL | CA-CB-CG1 | 7.31 | 121.86 | 110.90 |
| 2 | B | 78 | GLU | CG-CD-OE2 | 7.30 | 132.91 | 118.30 |
| 2 | B | 335 | ALA | O-C-N | 7.28 | 134.35 | 122.70 |
| 2 | B | 361 | MET | CA-CB-CG | -7.28 | 100.92 | 113.30 |
| 2 | B | 207 | MET | CB-CG-SD | 7.28 | 134.24 | 112.40 |
| 2 | B | 221 | GLY | O-C-N | 7.28 | 134.34 | 122.70 |
| 2 | B | 207 | MET | CG-SD-CE | -7.27 | 88.57 | 100.20 |
| 2 | B | 258 | GLY | O-C-N | -7.24 | 110.89 | 123.20 |
| 2 | B | 353 | HIS | CA-C-N | 7.24 | 133.13 | 117.20 |
| 2 | B | 51 | ASN | O-C-N | -7.24 | 111.12 | 122.70 |
| 2 | B | 188 | LEU | C-N-CA | -7.24 | 107.11 | 122.30 |
| 2 | B | 207 | MET | CA-C-O | -7.24 | 104.91 | 120.10 |
| 2 | B | 252 | LEU | CA-C-N | 7.23 | 133.10 | 117.20 |
| 1 | A | 259 | VAL | CA-CB-CG2 | -7.22 | 100.07 | 110.90 |
| 2 | B | 90 | GLN | CG-CD-OE1 | -7.22 | 107.16 | 121.60 |
| 2 | B | 200 | ILE | O-C-N | 7.19 | 134.21 | 122.70 |
| 2 | B | 358 | ALA | O-C-N | 7.17 | 134.17 | 122.70 |
| 2 | B | 287 | MET | CG-SD-CE | 7.17 | 111.67 | 100.20 |
| 2 | B | 45 | PHE | CZ-CE2-CD2 | 7.16 | 128.69 | 120.10 |
| 2 | B | 71 | THR | CA-C-O | -7.16 | 105.08 | 120.10 |
| 2 | B | 196 | PRO | CA-CB-CG | -7.15 | 90.41 | 104.00 |
| 1 | A | 159 | ASP | CB-CG-OD2 | 7.12 | 124.71 | 118.30 |
| 2 | B | 32 | PHE | CB-CG-CD2 | 7.10 | 125.77 | 120.80 |
| 1 | A | 148 | ILE | CB-CA-C | -7.09 | 97.41 | 111.60 |
| 2 | B | 158 | PRO | CB-CA-C | -7.09 | 94.28 | 112.00 |
| 2 | B | 231 | VAL | CA-C-O | 7.09 | 134.99 | 120.10 |
| 2 | B | 360 | LYS | C-N-CA | 7.08 | 139.40 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 2 | B | 381 | ASP | CB-CG-OD2 | 7.07 | 124.66 | 118.30 |
| 2 | B | 92 | LEU | CB-CG-CD1 | -7.06 | 98.99 | 111.00 |
| 2 | B | 52 | TYR | CE1-CZ-CE2 | -7.06 | 108.51 | 119.80 |
| 1 | A | 114 | PHE | CB-CG-CD2 | -7.06 | 115.86 | 120.80 |
| 1 | A | 131 | VAL | CG1-CB-CG2 | -7.05 | 99.61 | 110.90 |
| 2 | B | 52 | TYR | CD1-CE1-CZ | 7.05 | 126.14 | 119.80 |
| 2 | B | 373 | VAL | CA-C-N | 7.02 | 132.65 | 117.20 |
| 1 | A | 219 | GLN | CG-CD-OE1 | -7.02 | 107.57 | 121.60 |
| 2 | B | 271 | LEU | CA-CB-CG | 7.01 | 131.43 | 115.30 |
| 2 | B | 71 | THR | CA-CB-CG2 | -7.01 | 102.59 | 112.40 |
| 2 | B | 75 | LEU | N-CA-CB | 7.00 | 124.41 | 110.40 |
| 1 | A | 169 | TYR | CZ-CE2-CD2 | 6.98 | 126.08 | 119.80 |
| 2 | B | 77 | ARG | NH1-CZ-NH2 | 6.96 | 127.06 | 119.40 |
| 2 | B | 85 | ALA | O-C-N | -6.96 | 111.56 | 122.70 |
| 2 | B | 337 | LYS | O-C-N | -6.96 | 111.56 | 122.70 |
| 1 | A | 18 | ALA | N-CA-CB | -6.92 | 100.41 | 110.10 |
| 2 | B | 28 | LEU | CB-CG-CD1 | -6.91 | 99.25 | 111.00 |
| 1 | A | 63 | THR | CA-CB-CG2 | -6.91 | 102.73 | 112.40 |
| 2 | B | 195 | HIS | CG-ND1-CE1 | 6.91 | 117.87 | 108.20 |
| 1 | A | 37 | ILE | CG1-CB-CG2 | -6.89 | 96.23 | 111.40 |
| 1 | A | 93 | PRO | N-CD-CG | -6.89 | 92.86 | 103.20 |
| 2 | B | 27 | GLN | O-C-N | 6.89 | 133.72 | 122.70 |
| 2 | B | 182 | GLU | CG-CD-OE2 | 6.88 | 132.05 | 118.30 |
| 1 | A | 114 | PHE | CB-CG-CD1 | 6.86 | 125.60 | 120.80 |
| 2 | B | 149 | MET | CA-CB-CG | -6.86 | 101.64 | 113.30 |
| 1 | A | 143 | ALA | CB-CA-C | -6.85 | 99.83 | 110.10 |
| 2 | B | 315 | TYR | CE1-CZ-CE2 | -6.84 | 108.86 | 119.80 |
| 2 | B | 205 | GLN | CG-CD-OE1 | -6.84 | 107.92 | 121.60 |
| 1 | A | 140 | ARG | CG-CD-NE | -6.83 | 97.45 | 111.80 |
| 2 | B | 38 | ASP | CB-CG-OD1 | -6.83 | 112.16 | 118.30 |
| 2 | B | 222 | ARG | CD-NE-CZ | 6.81 | 133.13 | 123.60 |
| 2 | B | 248 | THR | CA-CB-CG2 | -6.79 | 102.89 | 112.40 |
| 1 | A | 229 | ALA | N-CA-C | 6.79 | 129.32 | 111.00 |
| 2 | B | 9 | PHE | C-N-CA | -6.77 | 108.08 | 122.30 |
| 2 | B | 206[A] | ARG | CD-NE-CZ | 6.77 | 133.07 | 123.60 |
| 2 | B | 206[B] | ARG | CD-NE-CZ | 6.77 | 133.07 | 123.60 |
| 1 | A | 91 | LYS | CD-CE-NZ | -6.74 | 96.21 | 111.70 |
| 2 | B | 316 | LEU | CA-CB-CG | -6.71 | 99.86 | 115.30 |
| 1 | A | 63 | THR | OG1-CB-CG2 | -6.71 | 94.56 | 110.00 |
| 2 | B | 351 | SER | CA-C-O | -6.71 | 106.01 | 120.10 |
| 2 | B | 45 | PHE | CA-C-O | -6.70 | 106.02 | 120.10 |
| 2 | B | 285 | PRO | CA-C-N | 6.70 | 131.95 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | A | 138 | PRO | O-C-N | -6.70 | 111.98 | 122.70 |
| 2 | B | 198 | PRO | O-C-N | -6.69 | 112.00 | 122.70 |
| 2 | B | 5 | LEU | CB-CG-CD1 | -6.68 | 99.64 | 111.00 |
| 2 | B | 45 | PHE | O-C-N | 6.68 | 133.39 | 122.70 |
| 1 | A | 175 | TYR | CG-CD2-CE2 | 6.68 | 126.64 | 121.30 |
| 2 | B | 241 | PHE | N-CA-C | 6.66 | 128.98 | 111.00 |
| 2 | B | 270 | PRO | O-C-N | -6.66 | 112.05 | 122.70 |
| 1 | A | 136 | SER | CA-C-O | -6.65 | 106.13 | 120.10 |
| 1 | A | 52 | VAL | CG1-CB-CG2 | -6.63 | 100.29 | 110.90 |
| 2 | B | 85 | ALA | CB-CA-C | 6.63 | 120.04 | 110.10 |
| 1 | A | 116 | ALA | O-C-N | -6.63 | 112.10 | 122.70 |
| 2 | B | 30 | GLU | CG-CD-OE2 | 6.62 | 131.53 | 118.30 |
| 2 | B | 227 | VAL | O-C-N | -6.59 | 112.15 | 122.70 |
| 2 | B | 214 | ALA | O-C-N | 6.59 | 133.25 | 122.70 |
| 2 | B | 361 | MET | N-CA-CB | 6.58 | 122.45 | 110.60 |
| 1 | A | 145 | ARG | O-C-N | -6.58 | 112.17 | 122.70 |
| 2 | B | 324 | TYR | CB-CG-CD1 | 6.58 | 124.94 | 121.00 |
| 1 | A | 4 | TYR | CB-CA-C | -6.57 | 97.26 | 110.40 |
| 2 | B | 315 | TYR | OH-CZ-CE2 | -6.57 | 102.37 | 120.10 |
| 2 | B | 196 | PRO | N-CD-CG | -6.55 | 93.37 | 103.20 |
| 2 | B | 324 | TYR | OH-CZ-CE2 | 6.55 | 137.78 | 120.10 |
| 2 | B | 134 | MET | C-N-CA | -6.53 | 108.59 | 122.30 |
| 2 | B | 196 | PRO | CA-C-O | -6.53 | 104.53 | 120.20 |
| 2 | B | 371 | LEU | CB-CG-CD2 | 6.53 | 122.10 | 111.00 |
| 2 | B | 114 | GLN | N-CA-CB | 6.53 | 122.35 | 110.60 |
| 2 | B | 77 | ARG | CG-CD-NE | 6.52 | 125.50 | 111.80 |
| 1 | A | 145 | ARG | CA-C-N | 6.52 | 131.54 | 117.20 |
| 1 | A | 107 | PHE | CE1-CZ-CE2 | -6.51 | 108.28 | 120.00 |
| 2 | B | 12 | PHE | C-N-CA | -6.51 | 108.62 | 122.30 |
| 2 | B | 82 | HIS | C-N-CA | 6.51 | 135.98 | 122.30 |
| 2 | B | 90 | GLN | OE1-CD-NE2 | 6.50 | 136.86 | 121.90 |
| 1 | A | 175 | TYR | CG-CD1-CE1 | -6.50 | 116.10 | 121.30 |
| 2 | B | 64 | ASN | N-CA-CB | 6.50 | 122.30 | 110.60 |
| 2 | B | 377 | SER | N-CA-CB | -6.50 | 100.75 | 110.50 |
| 2 | B | 94 | GLN | CA-CB-CG | -6.49 | 99.12 | 113.40 |
| 2 | B | 364 | GLU | CA-CB-CG | 6.49 | 127.67 | 113.40 |
| 2 | B | 357 | HIS | CB-CG-ND1 | -6.49 | 106.98 | 123.20 |
| 1 | A | 49[A] | GLU | C-N-CA | -6.47 | 105.52 | 121.70 |
| 1 | A | 49[B] | GLU | C-N-CA | -6.47 | 105.52 | 121.70 |
| 1 | A | 142 | ALA | O-C-N | -6.47 | 112.35 | 122.70 |
| 2 | B | 362 | MET | CA-C-O | -6.46 | 106.52 | 120.10 |
| 2 | B | 201 | VAL | CG1-CB-CG2 | -6.46 | 100.57 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 23 | VAL | N-CA-CB | 6.46 | 125.70 | 111.50 |
| 2 | B | 183 | THR | CA-CB-OG1 | 6.45 | 122.55 | 109.00 |
| 2 | B | 242 | ALA | N-CA-C | 6.45 | 128.40 | 111.00 |
| 2 | B | 283 | LYS | O-C-N | 6.44 | 133.01 | 122.70 |
| 2 | B | 129 | LYS | CD-CE-NZ | 6.41 | 126.44 | 111.70 |
| 2 | B | 234 | GLY | N-CA-C | 6.41 | 129.11 | 113.10 |
| 2 | B | 325 | VAL | O-C-N | -6.40 | 112.45 | 122.70 |
| 1 | A | 144 | LEU | CB-CG-CD1 | -6.40 | 100.11 | 111.00 |
| 1 | A | 219 | GLN | O-C-N | 6.39 | 132.93 | 122.70 |
| 2 | B | 256 | GLU | CA-C-N | 6.39 | 134.98 | 117.10 |
| 1 | A | 48 | LEU | CA-C-N | -6.36 | 103.22 | 117.20 |
| 2 | B | 290 | ALA | C-N-CA | 6.36 | 137.59 | 121.70 |
| 2 | B | 284 | ALA | O-C-N | -6.35 | 109.03 | 121.10 |
| 2 | B | 245 | ILE | CA-C-N | 6.35 | 131.16 | 117.20 |
| 2 | B | 7 | PRO | CA-C-N | -6.33 | 103.26 | 117.20 |
| 1 | A | 126 | VAL | CA-C-O | 6.32 | 133.37 | 120.10 |
| 1 | A | 107 | PHE | CZ-CE2-CD2 | 6.32 | 127.68 | 120.10 |
| 2 | B | 320 | GLY | O-C-N | -6.31 | 112.60 | 122.70 |
| 2 | B | 283 | LYS | CD-CE-NZ | -6.30 | 97.21 | 111.70 |
| 1 | A | 97 | ILE | CA-C-O | 6.29 | 133.32 | 120.10 |
| 2 | B | 236 | ASN | CA-C-N | -6.29 | 103.35 | 117.20 |
| 2 | B | 370 | GLN | CB-CG-CD | 6.28 | 127.94 | 111.60 |
| 2 | B | 356 | ALA | CB-CA-C | 6.28 | 119.52 | 110.10 |
| 1 | A | 47 | ALA | N-CA-C | -6.28 | 94.05 | 111.00 |
| 2 | B | 203 | GLU | CB-CA-C | -6.28 | 97.85 | 110.40 |
| 2 | B | 296 | GLU | CA-CB-CG | 6.28 | 127.21 | 113.40 |
| 1 | A | 80 | GLN | O-C-N | 6.27 | 132.74 | 122.70 |
| 1 | A | 92 | HIS | O-C-N | -6.27 | 109.18 | 121.10 |
| 2 | B | 306 | PHE | CG-CD2-CE2 | 6.27 | 127.70 | 120.80 |
| 2 | B | 23 | PRO | CA-C-O | -6.27 | 105.16 | 120.20 |
| 1 | A | 96 | PRO | O-C-N | 6.26 | 132.72 | 122.70 |
| 2 | B | 96 | LEU | N-CA-CB | 6.26 | 122.92 | 110.40 |
| 2 | B | 78 | GLU | N-CA-CB | -6.25 | 99.34 | 110.60 |
| 2 | B | 53 | ALA | O-C-N | 6.25 | 133.83 | 123.20 |
| 2 | B | 206[A] | ARG | N-CA-CB | 6.25 | 121.84 | 110.60 |
| 2 | B | 206[B] | ARG | N-CA-CB | 6.25 | 121.84 | 110.60 |
| 2 | B | 205 | GLN | O-C-N | -6.24 | 112.71 | 122.70 |
| 2 | B | 61 | LYS | CB-CA-C | 6.24 | 122.88 | 110.40 |
| 2 | B | 166 | LEU | CB-CG-CD2 | 6.24 | 121.61 | 111.00 |
| 2 | B | 244 | PHE | CD1-CG-CD2 | 6.24 | 126.41 | 118.30 |
| 2 | B | 228 | ILE | CG1-CB-CG2 | 6.24 | 125.12 | 111.40 |
| 1 | A | 20 | VAL | CG1-CB-CG2 | -6.23 | 100.94 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 2 | B | 327 | ILE | CA-CB-CG1 | 6.22 | 122.83 | 111.00 |
| 2 | B | 240 | MET | C-N-CA | -6.22 | 106.14 | 121.70 |
| 2 | B | 206[A] | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 2 | B | 206[B] | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 2 | B | 30 | GLU | OE1-CD-OE2 | -6.21 | 115.85 | 123.30 |
| 2 | B | 97 | LEU | CB-CG-CD1 | -6.20 | 100.45 | 111.00 |
| 2 | B | 271 | LEU | CB-CG-CD1 | 6.20 | 121.54 | 111.00 |
| 2 | B | 312 | GLN | O-C-N | 6.20 | 132.62 | 122.70 |
| 1 | A | 171 | ARG | CD-NE-CZ | 6.20 | 132.28 | 123.60 |
| 2 | B | 332 | ALA | CA-C-O | -6.20 | 107.08 | 120.10 |
| 2 | B | 339 | LEU | CA-CB-CG | -6.20 | 101.05 | 115.30 |
| 1 | A | 4 | TYR | CB-CG-CD1 | 6.19 | 124.71 | 121.00 |
| 1 | A | 194 | HIS | CB-CA-C | 6.19 | 122.78 | 110.40 |
| 2 | B | 79 | ASP | OD1-CG-OD2 | -6.19 | 111.54 | 123.30 |
| 2 | B | 243 | ASP | CA-C-N | -6.18 | 103.59 | 117.20 |
| 1 | A | 150 | PRO | N-CD-CG | 6.18 | 112.47 | 103.20 |
| 2 | B | 5 | LEU | CB-CG-CD2 | 6.18 | 121.50 | 111.00 |
| 2 | B | 141 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 2 | B | 124 | ALA | O-C-N | -6.17 | 112.83 | 122.70 |
| 2 | B | 197 | TYR | CB-CG-CD2 | -6.17 | 117.30 | 121.00 |
| 2 | B | 97 | LEU | CB-CA-C | -6.16 | 98.49 | 110.20 |
| 2 | B | 200 | ILE | CA-CB-CG1 | -6.16 | 99.29 | 111.00 |
| 2 | B | 9 | PHE | CD1-CE1-CZ | -6.16 | 112.71 | 120.10 |
| 2 | B | 9 | PHE | CE1-CZ-CE2 | 6.16 | 131.09 | 120.00 |
| 2 | B | 316 | LEU | N-CA-CB | -6.16 | 98.08 | 110.40 |
| 2 | B | 16 | TYR | CB-CG-CD2 | 6.16 | 124.69 | 121.00 |
| 2 | B | 278 | ILE | CA-C-O | 6.15 | 133.02 | 120.10 |
| 2 | B | 67 | ALA | N-CA-CB | -6.14 | 101.50 | 110.10 |
| 1 | A | 164 | ARG | NE-CZ-NH2 | -6.14 | 117.23 | 120.30 |
| 2 | B | 298 | TYR | N-CA-C | -6.13 | 94.45 | 111.00 |
| 2 | B | 16 | TYR | CD1-CE1-CZ | 6.12 | 125.31 | 119.80 |
| 1 | A | 162 | LEU | CB-CG-CD2 | 6.12 | 121.40 | 111.00 |
| 1 | A | 210 | GLN | O-C-N | -6.12 | 112.80 | 123.20 |
| 2 | B | 375 | ASN | CB-CA-C | -6.12 | 98.17 | 110.40 |
| 1 | A | 105 | LEU | N-CA-CB | 6.11 | 122.61 | 110.40 |
| 2 | B | 226 | ALA | CB-CA-C | -6.11 | 100.94 | 110.10 |
| 1 | A | 96 | PRO | CA-C-N | -6.11 | 103.77 | 117.20 |
| 2 | B | 280 | PHE | N-CA-CB | -6.11 | 99.61 | 110.60 |
| 2 | B | 109 | GLU | OE1-CD-OE2 | -6.10 | 115.97 | 123.30 |
| 1 | A | 128 | VAL | O-C-N | 6.10 | 132.46 | 122.70 |
| 2 | B | 229 | ALA | CA-C-N | 6.09 | 130.60 | 117.20 |
| 1 | A | 139 | PHE | CG-CD1-CE1 | -6.08 | 114.11 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 45 | PHE | CG-CD2-CE2 | -6.08 | 114.11 | 120.80 |
| 1 | A | 230 | GLY | O-C-N | 6.08 | 132.42 | 122.70 |
| 2 | B | 207 | MET | O-C-N | 6.07 | 132.42 | 122.70 |
| 2 | B | 285 | PRO | CA-N-CD | 6.07 | 120.20 | 111.70 |
| 2 | B | 169 | ALA | N-CA-C | 6.05 | 127.34 | 111.00 |
| 2 | B | 28 | LEU | CB-CA-C | 6.04 | 121.69 | 110.20 |
| 2 | B | 159 | VAL | CG1-CB-CG2 | -6.03 | 101.25 | 110.90 |
| 2 | B | 306 | PHE | N-CA-C | -6.03 | 94.72 | 111.00 |
| 2 | B | 250 | VAL | CG1-CB-CG2 | 6.03 | 120.54 | 110.90 |
| 2 | B | 149 | MET | O-C-N | 6.02 | 132.34 | 122.70 |
| 2 | B | 8 | TYR | CD1-CE1-CZ | -6.02 | 114.38 | 119.80 |
| 2 | B | 81 | LEU | N-CA-CB | -6.02 | 98.36 | 110.40 |
| 2 | B | 245 | ILE | O-C-N | -6.01 | 113.08 | 122.70 |
| 2 | B | 264 | THR | CA-C-O | -6.01 | 107.47 | 120.10 |
| 2 | B | 41 | PHE | CD1-CG-CD2 | -6.00 | 110.51 | 118.30 |
| 2 | B | 223 | LEU | CB-CG-CD2 | -5.99 | 100.82 | 111.00 |
| 2 | B | 52 | TYR | C-N-CA | -5.98 | 106.75 | 121.70 |
| 2 | B | 177 | TRP | CE3-CZ3-CH2 | 5.98 | 127.78 | 121.20 |
| 2 | B | 30 | GLU | CB-CG-CD | 5.97 | 130.33 | 114.20 |
| 1 | A | 77 | THR | CB-CA-C | -5.97 | 95.48 | 111.60 |
| 2 | B | 287 | MET | CB-CA-C | -5.97 | 98.46 | 110.40 |
| 2 | B | 188 | LEU | CA-CB-CG | -5.96 | 101.58 | 115.30 |
| 2 | B | 234 | GLY | C-N-CA | -5.96 | 106.79 | 121.70 |
| 2 | B | 82 | HIS | CA-C-O | -5.94 | 107.62 | 120.10 |
| 1 | A | 205 | ALA | O-C-N | -5.94 | 113.20 | 122.70 |
| 2 | B | 241 | PHE | CB-CG-CD1 | 5.94 | 124.95 | 120.80 |
| 1 | A | 161 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 2 | B | 337 | LYS | CA-C-N | 5.93 | 130.25 | 117.20 |
| 2 | B | 316 | LEU | CA-C-N | 5.93 | 130.25 | 117.20 |
| 1 | A | 120 | GLN | N-CA-C | 5.92 | 126.98 | 111.00 |
| 2 | B | 103 | LYS | O-C-N | 5.92 | 132.17 | 122.70 |
| 1 | A | 251 | MET | CG-SD-CE | 5.91 | 109.66 | 100.20 |
| 2 | B | 79 | ASP | CA-C-O | -5.91 | 107.69 | 120.10 |
| 2 | B | 93 | GLY | O-C-N | 5.90 | 132.14 | 122.70 |
| 2 | B | 315 | TYR | CD1-CG-CD2 | -5.89 | 111.42 | 117.90 |
| 1 | A | 121 | VAL | CG1-CB-CG2 | 5.89 | 120.33 | 110.90 |
| 1 | A | 256 | ARG | NE-CZ-NH1 | -5.89 | 117.35 | 120.30 |
| 2 | B | 262 | ILE | O-C-N | -5.89 | 113.27 | 122.70 |
| 2 | B | 308 | SER | O-C-N | -5.89 | 113.27 | 122.70 |
| 2 | B | 256 | GLU | CB-CG-CD | -5.89 | 98.30 | 114.20 |
| 1 | A | 52 | VAL | O-C-N | 5.88 | 132.27 | 121.10 |
| 1 | A | 88 | ILE | CA-CB-CG1 | -5.87 | 99.85 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 262 | ILE | CA-CB-CG1 | 5.86 | 122.14 | 111.00 |
| 2 | B | 65 | ILE | CA-CB-CG1 | -5.85 | 99.89 | 111.00 |
| 2 | B | 298 | TYR | CD1-CE1-CZ | -5.83 | 114.55 | 119.80 |
| 2 | B | 26 | ASN | O-C-N | 5.83 | 132.03 | 122.70 |
| 2 | B | 181 | TYR | CD1-CG-CD2 | 5.83 | 124.31 | 117.90 |
| 2 | B | 338 | THR | CA-CB-OG1 | -5.83 | 96.76 | 109.00 |
| 1 | A | 127 | LEU | CB-CG-CD2 | 5.83 | 120.91 | 111.00 |
| 1 | A | 163 | LEU | O-C-N | 5.83 | 132.02 | 122.70 |
| 2 | B | 51 | ASN | N-CA-CB | -5.83 | 100.12 | 110.60 |
| 2 | B | 77 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |
| 2 | B | 194 | PRO | C-N-CA | 5.82 | 136.25 | 121.70 |
| 2 | B | 59 | LEU | N-CA-CB | -5.81 | 98.79 | 110.40 |
| 2 | B | 308 | SER | C-N-CA | 5.81 | 136.22 | 121.70 |
| 2 | B | 278 | ILE | CA-CB-CG2 | -5.80 | 99.30 | 110.90 |
| 1 | A | 241 | ILE | CG1-CB-CG2 | -5.80 | 98.64 | 111.40 |
| 2 | B | 267 | HIS | CA-C-O | -5.79 | 107.93 | 120.10 |
| 1 | A | 153 | ILE | O-C-N | -5.79 | 113.43 | 122.70 |
| 2 | B | 133 | TYR | CE1-CZ-CE2 | 5.79 | 129.07 | 119.80 |
| 2 | B | 13 | GLY | O-C-N | 5.79 | 133.04 | 123.20 |
| 2 | B | 341 | ARG | CA-C-N | 5.79 | 129.93 | 117.20 |
| 1 | A | 11 | LEU | CB-CG-CD1 | -5.77 | 101.20 | 111.00 |
| 2 | B | 19 | GLN | CA-C-N | -5.77 | 104.52 | 117.20 |
| 2 | B | 257 | PRO | N-CA-CB | 5.77 | 110.22 | 103.30 |
| 1 | A | 7 | LEU | CB-CA-C | -5.76 | 99.25 | 110.20 |
| 2 | B | 304 | LEU | CA-CB-CG | -5.76 | 102.05 | 115.30 |
| 2 | B | 123 | SER | CA-CB-OG | -5.76 | 95.65 | 111.20 |
| 1 | A | 19 | PHE | CZ-CE2-CD2 | -5.74 | 113.21 | 120.10 |
| 2 | B | 47 | ASP | O-C-N | -5.73 | 113.53 | 122.70 |
| 2 | B | 17 | VAL | CB-CA-C | -5.73 | 100.52 | 111.40 |
| 2 | B | 336 | PHE | CD1-CG-CD2 | 5.73 | 125.75 | 118.30 |
| 1 | A | 171 | ARG | O-C-N | -5.72 | 113.47 | 123.20 |
| 1 | A | 115 | TYR | CB-CG-CD1 | -5.72 | 117.57 | 121.00 |
| 2 | B | 202 | ARG | CA-C-O | 5.72 | 132.11 | 120.10 |
| 2 | B | 41 | PHE | CZ-CE2-CD2 | -5.71 | 113.24 | 120.10 |
| 2 | B | 374 | VAL | CG1-CB-CG2 | -5.71 | 101.76 | 110.90 |
| 1 | A | 112 | ASP | O-C-N | -5.71 | 113.56 | 122.70 |
| 2 | B | 106 | ILE | C-N-CA | 5.71 | 135.98 | 121.70 |
| 2 | B | 328 | THR | N-CA-CB | 5.71 | 121.15 | 110.30 |
| 1 | A | 243 | LYS | N-CA-C | 5.71 | 126.41 | 111.00 |
| 2 | B | 255 | VAL | O-C-N | -5.71 | 113.57 | 122.70 |
| 2 | B | 198 | PRO | CA-C-N | 5.71 | 129.75 | 117.20 |
| 2 | B | 51 | ASN | N-CA-C | 5.70 | 126.39 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 188 | LEU | O-C-N | 5.70 | 132.89 | 123.20 |
| 2 | B | 6 | ASN | C-N-CD | -5.70 | 108.07 | 120.60 |
| 2 | B | 231 | VAL | CA-CB-CG2 | 5.69 | 119.44 | 110.90 |
| 2 | B | 151 | LEU | O-C-N | -5.69 | 113.60 | 122.70 |
| 2 | B | 52 | TYR | CB-CG-CD2 | 5.68 | 124.41 | 121.00 |
| 2 | B | 224 | PRO | N-CA-CB | 5.68 | 110.12 | 103.30 |
| 1 | A | 121 | VAL | CA-C-O | -5.68 | 108.17 | 120.10 |
| 2 | B | 212 | THR | CA-CB-CG2 | -5.68 | 104.45 | 112.40 |
| 1 | A | 262 | MET | CG-SD-CE | 5.67 | 109.27 | 100.20 |
| 2 | B | 233 | GLY | CA-C-O | 5.67 | 130.80 | 120.60 |
| 2 | B | 238 | ILE | CB-CG1-CD1 | -5.67 | 98.03 | 113.90 |
| 2 | B | 372 | LEU | CD1-CG-CD2 | 5.67 | 127.49 | 110.50 |
| 1 | A | 126 | VAL | CG1-CB-CG2 | -5.66 | 101.84 | 110.90 |
| 2 | B | 336 | PHE | CD1-CE1-CZ | -5.66 | 113.31 | 120.10 |
| 1 | A | 134 | GLU | O-C-N | 5.66 | 131.75 | 122.70 |
| 2 | B | 28 | LEU | O-C-N | -5.66 | 113.65 | 122.70 |
| 2 | B | 45 | PHE | CB-CG-CD2 | -5.66 | 116.84 | 120.80 |
| 2 | B | 256 | GLU | CA-C-O | -5.66 | 108.22 | 120.10 |
| 2 | B | 262 | ILE | CG1-CB-CG2 | -5.66 | 98.96 | 111.40 |
| 1 | A | 39 | THR | CA-CB-CG2 | -5.65 | 104.49 | 112.40 |
| 2 | B | 321 | ARG | N-CA-C | -5.65 | 95.74 | 111.00 |
| 2 | B | 209 | GLY | O-C-N | -5.65 | 113.67 | 122.70 |
| 2 | B | 4 | LEU | CB-CG-CD2 | -5.64 | 101.41 | 111.00 |
| 1 | A | 266 | SER | CB-CA-C | -5.64 | 99.39 | 110.10 |
| 2 | B | 355 | LEU | CA-C-O | -5.63 | 108.27 | 120.10 |
| 1 | A | 116 | ALA | N-CA-C | 5.62 | 126.19 | 111.00 |
| 2 | B | 322 | ALA | N-CA-CB | -5.62 | 102.23 | 110.10 |
| 2 | B | 200 | ILE | CB-CG1-CD1 | -5.62 | 98.17 | 113.90 |
| 1 | A | 114 | PHE | CG-CD2-CE2 | -5.60 | 114.64 | 120.80 |
| 2 | B | 212 | THR | O-C-N | -5.60 | 113.74 | 122.70 |
| 2 | B | 387 | VAL | CA-CB-CG1 | 5.60 | 119.30 | 110.90 |
| 2 | B | 132 | ILE | CA-CB-CG1 | -5.60 | 100.37 | 111.00 |
| 2 | B | 365 | GLN | CA-CB-CG | -5.59 | 101.09 | 113.40 |
| 2 | B | 89 | ASN | O-C-N | 5.58 | 131.63 | 122.70 |
| 2 | B | 70 | ARG | NE-CZ-NH2 | 5.58 | 123.09 | 120.30 |
| 1 | A | 123 | VAL | CG1-CB-CG2 | 5.57 | 119.82 | 110.90 |
| 1 | A | 3 | ARG | NH1-CZ-NH2 | -5.57 | 113.28 | 119.40 |
| 1 | A | 48 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 2 | B | 57 | THR | CA-C-N | -5.57 | 104.95 | 117.20 |
| 2 | B | 334 | GLU | O-C-N | -5.55 | 113.81 | 122.70 |
| 2 | B | 288 | GLN | CG-CD-OE1 | -5.55 | 110.50 | 121.60 |
| 2 | B | 70 | ARG | CG-CD-NE | 5.55 | 123.45 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 215 | GLN | CA-CB-CG | -5.55 | 101.19 | 113.40 |
| 2 | B | 349 | LEU | CB-CG-CD1 | 5.54 | 120.42 | 111.00 |
| 2 | B | 355 | LEU | O-C-N | 5.54 | 131.57 | 122.70 |
| 2 | B | 236 | ASN | C-N-CA | -5.54 | 107.86 | 121.70 |
| 1 | A | 134 | GLU | CG-CD-OE2 | -5.53 | 107.23 | 118.30 |
| 1 | A | 56 | ASP | CB-CG-OD1 | -5.53 | 113.32 | 118.30 |
| 2 | B | 287 | MET | CA-CB-CG | 5.53 | 122.70 | 113.30 |
| 1 | A | 144 | LEU | CB-CA-C | 5.53 | 120.70 | 110.20 |
| 2 | B | 107 | ILE | O-C-N | 5.52 | 131.54 | 122.70 |
| 2 | B | 267 | HIS | O-C-N | 5.52 | 132.59 | 123.20 |
| 2 | B | 228 | ILE | CA-CB-CG2 | 5.52 | 121.93 | 110.90 |
| 2 | B | 67 | ALA | CA-C-N | -5.51 | 105.17 | 116.20 |
| 1 | A | 126 | VAL | N-CA-CB | -5.51 | 99.38 | 111.50 |
| 2 | B | 3 | THR | CA-CB-CG2 | 5.51 | 120.11 | 112.40 |
| 2 | B | 321 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | A | 220 | VAL | CA-CB-CG2 | 5.50 | 119.15 | 110.90 |
| 2 | B | 106 | ILE | CB-CG1-CD1 | 5.50 | 129.29 | 113.90 |
| 2 | B | 122 | ALA | CA-C-O | -5.50 | 108.56 | 120.10 |
| 1 | A | 60 | ASP | CB-CG-OD1 | -5.49 | 113.36 | 118.30 |
| 1 | A | 169 | TYR | CB-CG-CD2 | -5.49 | 117.71 | 121.00 |
| 2 | B | 40 | GLU | O-C-N | -5.49 | 113.92 | 122.70 |
| 2 | B | 43 | ALA | CB-CA-C | 5.49 | 118.33 | 110.10 |
| 2 | B | 256 | GLU | N-CA-C | 5.49 | 125.83 | 111.00 |
| 2 | B | 48 | LEU | CB-CG-CD2 | -5.48 | 101.68 | 111.00 |
| 2 | B | 321 | ARG | CB-CA-C | -5.48 | 99.43 | 110.40 |
| 1 | A | 117 | ARG | NE-CZ-NH2 | -5.48 | 117.56 | 120.30 |
| 1 | A | 95 | ILE | CB-CG1-CD1 | -5.48 | 98.56 | 113.90 |
| 2 | B | 17 | VAL | CA-CB-CG1 | -5.48 | 102.68 | 110.90 |
| 2 | B | 217 | LEU | N-CA-CB | 5.47 | 121.35 | 110.40 |
| 2 | B | 281 | GLY | CA-C-N | -5.47 | 105.16 | 117.20 |
| 1 | A | 140 | ARG | CB-CA-C | 5.47 | 121.34 | 110.40 |
| 2 | B | 55 | ARG | CD-NE-CZ | -5.47 | 115.94 | 123.60 |
| 2 | B | 65 | ILE | N-CA-CB | -5.47 | 98.22 | 110.80 |
| 2 | B | 117 | VAL | N-CA-C | 5.46 | 125.74 | 111.00 |
| 1 | A | 127 | LEU | N-CA-CB | -5.45 | 99.50 | 110.40 |
| 2 | B | 59 | LEU | CB-CA-C | 5.45 | 120.55 | 110.20 |
| 1 | A | 140 | ARG | NH1-CZ-NH2 | 5.44 | 125.38 | 119.40 |
| 1 | A | 107 | PHE | O-C-N | 5.43 | 131.39 | 122.70 |
| 2 | B | 232 | GLY | N-CA-C | -5.43 | 99.52 | 113.10 |
| 2 | B | 22 | MET | N-CA-CB | 5.43 | 120.37 | 110.60 |
| 2 | B | 47 | ASP | CA-C-N | 5.42 | 129.12 | 117.20 |
| 1 | A | 260 | SER | CA-CB-OG | -5.41 | 96.59 | 111.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 2 | THR | OG1-CB-CG2 | -5.41 | 97.57 | 110.00 |
| 2 | B | 317 | ASN | CB-CG-OD1 | -5.40 | 110.80 | 121.60 |
| 1 | A | 169 | TYR | N-CA-C | 5.39 | 125.56 | 111.00 |
| 1 | A | 117 | ARG | NE-CZ-NH1 | -5.39 | 117.60 | 120.30 |
| 2 | B | 15 | MET | CG-SD-CE | -5.39 | 91.57 | 100.20 |
| 2 | B | 246 | ASN | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 2 | B | 379 | ARG | CA-C-O | 5.37 | 131.38 | 120.10 |
| 2 | B | 104 | SER | O-C-N | -5.37 | 114.12 | 122.70 |
| 2 | B | 52 | TYR | CG-CD2-CE2 | 5.36 | 125.59 | 121.30 |
| 2 | B | 291 | ASP | N-CA-CB | -5.36 | 100.95 | 110.60 |
| 2 | B | 275 | ARG | N-CA-CB | -5.35 | 100.97 | 110.60 |
| 2 | B | 99 | LYS | CB-CG-CD | -5.34 | 97.70 | 111.60 |
| 2 | B | 368 | LYS | CG-CD-CE | -5.34 | 95.87 | 111.90 |
| 2 | B | 247 | ASP | CA-C-N | -5.34 | 105.45 | 117.20 |
| 2 | B | 285 | PRO | CA-C-O | -5.33 | 107.40 | 120.20 |
| 2 | B | 191 | ALA | N-CA-CB | 5.32 | 117.55 | 110.10 |
| 2 | B | 205 | GLN | OE1-CD-NE2 | 5.32 | 134.14 | 121.90 |
| 2 | B | 168 | ASP | C-N-CA | -5.32 | 108.40 | 121.70 |
| 2 | B | 199 | THR | O-C-N | 5.32 | 131.21 | 122.70 |
| 2 | B | 61 | LYS | CA-CB-CG | -5.32 | 101.70 | 113.40 |
| 2 | B | 73 | LEU | O-C-N | 5.32 | 131.21 | 122.70 |
| 1 | A | 149 | ALA | N-CA-CB | -5.31 | 102.66 | 110.10 |
| 2 | B | 360 | LYS | CD-CE-NZ | 5.31 | 123.92 | 111.70 |
| 2 | B | 236 | ASN | CB-CG-OD1 | -5.31 | 110.98 | 121.60 |
| 1 | A | 123 | VAL | CA-C-O | 5.31 | 131.24 | 120.10 |
| 2 | B | 391 | LEU | CA-CB-CG | -5.31 | 103.10 | 115.30 |
| 2 | B | 76 | LYS | C-N-CA | -5.30 | 108.46 | 121.70 |
| 2 | B | 211 | GLU | CB-CA-C | -5.29 | 99.81 | 110.40 |
| 1 | A | 134 | GLU | CA-C-O | -5.29 | 108.99 | 120.10 |
| 2 | B | 162 | GLY | N-CA-C | -5.29 | 99.88 | 113.10 |
| 2 | B | 223 | LEU | CB-CG-CD1 | -5.28 | 102.02 | 111.00 |
| 1 | A | 127 | LEU | CA-C-N | -5.28 | 105.58 | 117.20 |
| 1 | A | 176 | LEU | N-CA-C | -5.28 | 96.74 | 111.00 |
| 1 | A | 27 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | A | 232 | ILE | CA-CB-CG2 | -5.28 | 100.35 | 110.90 |
| 2 | B | 342 | HIS | N-CA-C | 5.27 | 125.24 | 111.00 |
| 1 | A | 150 | PRO | O-C-N | 5.27 | 131.13 | 122.70 |
| 2 | B | 101 | MET | CA-CB-CG | -5.27 | 104.34 | 113.30 |
| 2 | B | 268 | GLY | O-C-N | -5.27 | 114.27 | 122.70 |
| 1 | A | 101 | MET | CA-CB-CG | -5.26 | 104.36 | 113.30 |
| 2 | B | 51 | ASN | CA-C-N | 5.26 | 128.77 | 117.20 |
| 2 | B | 183 | THR | CB-CA-C | -5.26 | 97.40 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 94 | THR | O-C-N | 5.26 | 131.11 | 122.70 |
| 2 | B | 283 | LYS | CG-CD-CE | -5.26 | 96.13 | 111.90 |
| 1 | A | 219 | GLN | N-CA-C | 5.25 | 125.19 | 111.00 |
| 1 | A | 171 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 2 | B | 43 | ALA | O-C-N | -5.25 | 114.30 | 122.70 |
| 1 | A | 222 | ALA | C-N-CA | -5.24 | 108.59 | 121.70 |
| 2 | B | 383 | ASP | CB-CG-OD1 | -5.24 | 113.58 | 118.30 |
| 1 | A | 122 | GLY | N-CA-C | 5.24 | 126.19 | 113.10 |
| 2 | B | 13 | GLY | CA-C-N | -5.23 | 105.73 | 116.20 |
| 2 | B | 250 | VAL | C-N-CA | 5.23 | 133.29 | 122.30 |
| 1 | A | 126 | VAL | CB-CA-C | -5.23 | 101.47 | 111.40 |
| 2 | B | 366 | PRO | O-C-N | -5.22 | 114.35 | 122.70 |
| 2 | B | 49 | LEU | N-CA-CB | -5.21 | 99.97 | 110.40 |
| 2 | B | 21 | LEU | CA-C-O | 5.21 | 131.05 | 120.10 |
| 1 | A | 221 | SER | O-C-N | -5.21 | 114.36 | 122.70 |
| 2 | B | 312 | GLN | N-CA-CB | 5.21 | 119.98 | 110.60 |
| 2 | B | 249 | SER | N-CA-CB | -5.21 | 102.69 | 110.50 |
| 2 | B | 65 | ILE | CG1-CB-CG2 | -5.20 | 99.96 | 111.40 |
| 2 | B | 345 | ILE | O-C-N | -5.20 | 114.38 | 122.70 |
| 2 | B | 335 | ALA | CA-C-O | -5.19 | 109.20 | 120.10 |
| 2 | B | 25 | LEU | O-C-N | -5.19 | 114.40 | 122.70 |
| 2 | B | 309 | VAL | CA-CB-CG1 | -5.18 | 103.12 | 110.90 |
| 2 | B | 334 | GLU | CG-CD-OE2 | 5.18 | 128.66 | 118.30 |
| 2 | B | 222 | ARG | O-C-N | -5.18 | 114.41 | 122.70 |
| 1 | A | 106 | VAL | CG1-CB-CG2 | 5.18 | 119.19 | 110.90 |
| 2 | B | 292 | GLY | CA-C-N | 5.18 | 128.59 | 117.20 |
| 1 | A | 36 | ILE | CA-CB-CG1 | -5.17 | 101.17 | 111.00 |
| 2 | B | 244 | PHE | C-N-CA | -5.17 | 108.77 | 121.70 |
| 2 | B | 152 | MET | O-C-N | 5.17 | 131.99 | 123.20 |
| 1 | A | 117 | ARG | CD-NE-CZ | 5.17 | 130.83 | 123.60 |
| 2 | B | 188 | LEU | N-CA-CB | -5.17 | 100.07 | 110.40 |
| 1 | A | 149 | ALA | O-C-N | 5.16 | 130.91 | 121.10 |
| 1 | A | 257 | SER | CB-CA-C | -5.16 | 100.30 | 110.10 |
| 2 | B | 241 | PHE | CB-CA-C | -5.16 | 100.09 | 110.40 |
| 2 | B | 118 | ALA | C-N-CA | -5.16 | 108.81 | 121.70 |
| 1 | A | 263 | LYS | O-C-N | 5.15 | 130.94 | 122.70 |
| 2 | B | 316 | LEU | O-C-N | 5.15 | 130.94 | 122.70 |
| 1 | A | 101 | MET | CG-SD-CE | -5.15 | 91.97 | 100.20 |
| 1 | A | 218 | GLU | C-N-CA | -5.14 | 108.85 | 121.70 |
| 2 | B | 7 | PRO | N-CD-CG | -5.14 | 95.49 | 103.20 |
| 2 | B | 197 | TYR | CG-CD1-CE1 | -5.14 | 117.19 | 121.30 |
| 2 | B | 235 | SER | C-N-CA | -5.14 | 108.86 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 2 | B | 324 | TYR | CD1-CG-CD2 | -5.13 | 112.25 | 117.90 |
| 2 | B | 212 | THR | OG1-CB-CG2 | -5.13 | 98.20 | 110.00 |
| 1 | A | 121 | VAL | CB-CA-C | -5.13 | 101.66 | 111.40 |
| 2 | B | 110 | THR | C-N-CA | -5.13 | 111.53 | 122.30 |
| 2 | B | 59 | LEU | N-CA-C | -5.13 | 97.16 | 111.00 |
| 2 | B | 380 | GLY | CA-C-N | -5.13 | 105.92 | 117.20 |
| 2 | B | 34 | SER | O-C-N | 5.12 | 130.90 | 122.70 |
| 2 | B | 74 | TYR | CE1-CZ-CE2 | -5.12 | 111.61 | 119.80 |
| 2 | B | 11 | GLU | CG-CD-OE2 | 5.12 | 128.54 | 118.30 |
| 2 | B | 8 | TYR | CE1-CZ-CE2 | -5.12 | 111.61 | 119.80 |
| 1 | A | 127 | LEU | CA-C-O | -5.12 | 109.36 | 120.10 |
| 1 | A | 196 | LEU | CA-CB-CG | 5.12 | 127.06 | 115.30 |
| 2 | B | 314 | ALA | CB-CA-C | 5.11 | 117.77 | 110.10 |
| 2 | B | 210 | GLU | C-N-CA | -5.11 | 108.94 | 121.70 |
| 2 | B | 3 | THR | CA-C-O | 5.10 | 130.81 | 120.10 |
| 2 | B | 7 | PRO | C-N-CA | -5.10 | 108.95 | 121.70 |
| 2 | B | 223 | LEU | N-CA-C | 5.10 | 124.77 | 111.00 |
| 2 | B | 254 | GLY | CA-C-O | 5.10 | 129.78 | 120.60 |
| 2 | B | 367 | GLU | CG-CD-OE2 | 5.10 | 128.50 | 118.30 |
| 2 | B | 283 | LYS | CA-CB-CG | -5.10 | 102.19 | 113.40 |
| 2 | B | 74 | TYR | CB-CG-CD2 | 5.09 | 124.06 | 121.00 |
| 2 | B | 208 | ILE | CA-CB-CG1 | 5.09 | 120.68 | 111.00 |
| 2 | B | 206[A] | ARG | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 2 | B | 206[B] | ARG | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 2 | B | 350 | GLU | N-CA-CB | 5.09 | 119.76 | 110.60 |
| 1 | A | 125 | SER | CA-C-N | -5.09 | 106.01 | 117.20 |
| 2 | B | 252 | LEU | C-N-CA | 5.09 | 134.41 | 121.70 |
| 2 | B | 53 | ALA | C-N-CA | -5.08 | 111.62 | 122.30 |
| 1 | A | 126 | VAL | CA-CB-CG1 | -5.08 | 103.28 | 110.90 |
| 2 | B | 39 | PRO | N-CD-CG | -5.08 | 95.58 | 103.20 |
| 2 | B | 280 | PHE | CZ-CE2-CD2 | -5.08 | 114.01 | 120.10 |
| 2 | B | 330 | ASP | N-CA-C | 5.08 | 124.71 | 111.00 |
| 2 | B | 23 | PRO | CA-CB-CG | -5.07 | 94.37 | 104.00 |
| 2 | B | 225 | ASP | CA-C-N | 5.07 | 128.35 | 117.20 |
| 1 | A | 89 | ARG | CG-CD-NE | -5.07 | 101.16 | 111.80 |
| 1 | A | 175 | TYR | CZ-CE2-CD2 | -5.06 | 115.24 | 119.80 |
| 2 | B | 76 | LYS | CA-C-N | -5.06 | 106.06 | 117.20 |
| 2 | B | 270 | PRO | CA-C-N | 5.06 | 128.33 | 117.20 |
| 2 | B | 220 | GLU | CA-CB-CG | 5.06 | 124.53 | 113.40 |
| 1 | A | 176 | LEU | CA-C-N | -5.05 | 106.09 | 117.20 |
| 2 | B | 88 | THR | O-C-N | -5.05 | 114.62 | 122.70 |
| 2 | B | 56 | PRO | N-CD-CG | 5.05 | 110.77 | 103.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 197 | TYR | CD1-CG-CD2 | 5.05 | 123.45 | 117.90 |
| 2 | B | 248 | THR | CA-C-O | -5.05 | 109.50 | 120.10 |
| 1 | A | 126 | VAL | CA-CB-CG2 | -5.04 | 103.33 | 110.90 |
| 2 | B | 102 | GLY | N-CA-C | 5.04 | 125.70 | 113.10 |
| 2 | B | 261 | GLY | CA-C-O | -5.04 | 111.53 | 120.60 |
| 2 | B | 157 | ILE | CG1-CB-CG2 | -5.03 | 100.33 | 111.40 |
| 2 | B | 261 | GLY | C-N-CA | -5.03 | 109.12 | 121.70 |
| 2 | B | 385 | PHE | CB-CA-C | -5.03 | 100.34 | 110.40 |
| 1 | A | 151 | ILE | CA-CB-CG1 | 5.03 | 120.56 | 111.00 |
| 1 | A | 130 | ASP | O-C-N | -5.03 | 114.66 | 122.70 |
| 1 | A | 28 | PRO | N-CD-CG | 5.02 | 110.74 | 103.20 |
| 2 | B | 221 | GLY | C-N-CA | -5.02 | 109.15 | 121.70 |
| 2 | B | 283 | LYS | CA-C-N | -5.02 | 106.16 | 117.20 |
| 2 | B | 66 | THR | OG1-CB-CG2 | -5.02 | 98.46 | 110.00 |
| 2 | B | 382 | LYS | CD-CE-NZ | -5.02 | 100.16 | 111.70 |
| 2 | B | 368 | LYS | CA-CB-CG | -5.01 | 102.38 | 113.40 |
| 2 | B | 235 | SER | O-C-N | 5.01 | 130.71 | 122.70 |
| 2 | B | 61 | LYS | CA-C-N | 5.01 | 128.22 | 117.20 |
| 2 | B | 391 | LEU | CB-CG-CD1 | 5.01 | 119.51 | 111.00 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 267 | ARG | Peptide |
| 2 | B | 54 | GLY | Mainchain |

5.2 Too-close contacts ⓘ

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 | 1955 | 0 | 1959 | 85 | 0 |
| 2 | B | 2987 | 0 | 2961 | 236 | 0 |
| 3 | A | 17 | 0 | 11 | 1 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 15 | 0 | 7 | 1 | 0 |
| 6 | A | 129 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | B | 248 | 0 | 0 | 2 | 0 |
| All | All | 5352 | 0 | 4938 | 319 | 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 32.

All (319) 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:B:235:SER:CA | 2:B:235:SER:CB | 1.74 | 1.64 |
| 2:B:278:ILE:CG1 | 2:B:278:ILE:CD1 | 1.74 | 1.64 |
| 2:B:129:LYS:CD | 2:B:129:LYS:CG | 1.75 | 1.63 |
| 1:A:52:VAL:CB | 1:A:52:VAL:CG1 | 1.75 | 1.63 |
| 1:A:126:VAL:CB | 1:A:126:VAL:CG1 | 1.75 | 1.63 |
| 2:B:71:THR:CB | 2:B:71:THR:CG2 | 1.77 | 1.63 |
| 2:B:37:LYS:CD | 2:B:37:LYS:CG | 1.75 | 1.62 |
| 1:A:87:LEU:CG | 1:A:87:LEU:CD1 | 1.74 | 1.61 |
| 2:B:58:ALA:CA | 2:B:58:ALA:CB | 1.75 | 1.61 |
| 2:B:183:THR:CB | 2:B:183:THR:CG2 | 1.74 | 1.61 |
| 1:A:140:ARG:CD | 1:A:140:ARG:CG | 1.76 | 1.60 |
| 2:B:231:VAL:CB | 2:B:231:VAL:CG1 | 1.79 | 1.60 |
| 2:B:117:VAL:CA | 2:B:117:VAL:CB | 1.75 | 1.59 |
| 2:B:66:THR:CB | 2:B:66:THR:CG2 | 1.75 | 1.58 |
| 2:B:212:THR:CB | 2:B:212:THR:CG2 | 1.77 | 1.58 |
| 2:B:25:LEU:CD2 | 2:B:25:LEU:CG | 1.75 | 1.58 |
| 2:B:319:ILE:CB | 2:B:319:ILE:CG2 | 1.75 | 1.58 |
| 2:B:353:HIS:CB | 2:B:353:HIS:CA | 1.77 | 1.58 |
| 2:B:49:LEU:CD2 | 2:B:49:LEU:CG | 1.80 | 1.57 |
| 2:B:286:MET:CA | 2:B:286:MET:CB | 1.77 | 1.57 |
| 2:B:55:ARG:CD | 2:B:55:ARG:CG | 1.75 | 1.57 |
| 2:B:333:LEU:CD2 | 2:B:333:LEU:CG | 1.75 | 1.57 |
| 1:A:94:THR:CB | 1:A:94:THR:CA | 1.75 | 1.57 |
| 2:B:282:MET:CB | 2:B:282:MET:CA | 1.77 | 1.57 |
| 2:B:76:LYS:CE | 2:B:76:LYS:CD | 1.77 | 1.57 |
| 2:B:287:MET:CG | 2:B:287:MET:CB | 1.76 | 1.57 |
| 1:A:101:MET:CG | 1:A:101:MET:CB | 1.76 | 1.56 |
| 2:B:61:LYS:CG | 2:B:61:LYS:CB | 1.84 | 1.56 |
| 2:B:339:LEU:CD2 | 2:B:339:LEU:CG | 1.80 | 1.56 |
| 2:B:150:ARG:CG | 2:B:150:ARG:CB | 1.74 | 1.56 |
| 2:B:264:THR:CB | 2:B:264:THR:CG2 | 1.75 | 1.56 |
| 1:A:123:VAL:CB | 1:A:123:VAL:CA | 1.76 | 1.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:166:VAL:CG2 | 1:A:166:VAL:CB | 1.77 | 1.55 |
| 2:B:139:VAL:CB | 2:B:139:VAL:CG2 | 1.79 | 1.55 |
| 1:A:7:LEU:CD2 | 1:A:7:LEU:CG | 1.78 | 1.54 |
| 1:A:54:PHE:C | 1:A:54:PHE:CA | 1.75 | 1.54 |
| 1:A:219:GLN:CG | 1:A:219:GLN:CB | 1.82 | 1.54 |
| 2:B:59:LEU:N | 2:B:59:LEU:CA | 1.71 | 1.54 |
| 2:B:108:ALA:CB | 2:B:108:ALA:CA | 1.78 | 1.54 |
| 2:B:373:VAL:CB | 2:B:373:VAL:CG1 | 1.82 | 1.53 |
| 1:A:13:ASP:CG | 1:A:13:ASP:CB | 1.76 | 1.53 |
| 2:B:351:SER:CA | 2:B:351:SER:C | 1.76 | 1.53 |
| 2:B:23:PRO:CG | 2:B:23:PRO:CB | 1.80 | 1.53 |
| 1:A:117:ARG:CG | 1:A:117:ARG:CD | 1.82 | 1.52 |
| 1:A:24:THR:CB | 1:A:24:THR:CA | 1.75 | 1.52 |
| 2:B:304:LEU:CD1 | 2:B:304:LEU:CG | 1.83 | 1.52 |
| 2:B:255:VAL:CA | 2:B:255:VAL:CB | 1.80 | 1.52 |
| 2:B:256:GLU:CG | 2:B:256:GLU:CD | 1.76 | 1.51 |
| 2:B:59:LEU:CA | 2:B:59:LEU:C | 1.77 | 1.50 |
| 2:B:203:GLU:CA | 2:B:203:GLU:C | 1.77 | 1.50 |
| 2:B:196:PRO:C | 2:B:196:PRO:CA | 1.77 | 1.50 |
| 2:B:205:GLN:CD | 2:B:205:GLN:CG | 1.80 | 1.50 |
| 2:B:61:LYS:N | 2:B:61:LYS:CA | 1.72 | 1.50 |
| 2:B:368:LYS:C | 2:B:368:LYS:CA | 1.75 | 1.50 |
| 2:B:167:LYS:CE | 2:B:167:LYS:NZ | 1.71 | 1.50 |
| 2:B:376:LEU:CG | 2:B:376:LEU:CD2 | 1.84 | 1.49 |
| 2:B:362:MET:SD | 2:B:362:MET:CG | 2.01 | 1.49 |
| 2:B:328:THR:C | 2:B:328:THR:CA | 1.77 | 1.49 |
| 2:B:15:MET:CE | 2:B:15:MET:SD | 2.02 | 1.47 |
| 2:B:70:ARG:C | 2:B:70:ARG:CA | 1.81 | 1.47 |
| 2:B:282:MET:CG | 2:B:282:MET:SD | 2.02 | 1.45 |
| 2:B:149:MET:SD | 2:B:149:MET:CG | 2.07 | 1.40 |
| 2:B:286:MET:CB | 2:B:286:MET:CG | 2.04 | 1.35 |
| 1:A:191:LEU:HD12 | 1:A:192:PRO:CD | 1.85 | 1.06 |
| 1:A:191:LEU:CD1 | 1:A:192:PRO:HD2 | 1.86 | 1.04 |
| 1:A:243:LYS:HD2 | 1:A:243:LYS:N | 1.74 | 1.03 |
| 2:B:134:MET:CE | 2:B:139:VAL:HG22 | 1.89 | 1.02 |
| 2:B:134:MET:HE3 | 2:B:139:VAL:HG22 | 1.40 | 1.02 |
| 1:A:194:HIS:O | 1:A:198:GLU:HG2 | 1.63 | 0.98 |
| 2:B:376:LEU:CD2 | 2:B:376:LEU:CB | 2.43 | 0.97 |
| 2:B:183:THR:CG2 | 2:B:183:THR:CA | 2.41 | 0.97 |
| 2:B:71:THR:CG2 | 2:B:71:THR:CA | 2.44 | 0.95 |
| 2:B:333:LEU:CD2 | 2:B:333:LEU:CB | 2.46 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:LEU:CD2 | 1:A:7:LEU:CB | 2.46 | 0.94 |
| 1:A:243:LYS:HD2 | 1:A:243:LYS:H | 1.27 | 0.94 |
| 2:B:282:MET:CG | 2:B:282:MET:CE | 2.47 | 0.93 |
| 1:A:126:VAL:CG1 | 1:A:126:VAL:CG2 | 2.47 | 0.92 |
| 2:B:282:MET:CA | 2:B:282:MET:CG | 2.46 | 0.92 |
| 2:B:319:ILE:CG2 | 2:B:319:ILE:CG1 | 2.46 | 0.92 |
| 2:B:59:LEU:N | 2:B:59:LEU:CB | 2.33 | 0.90 |
| 2:B:333:LEU:CD2 | 2:B:333:LEU:CD1 | 2.50 | 0.89 |
| 1:A:24:THR:CA | 1:A:24:THR:CG2 | 2.49 | 0.89 |
| 2:B:61:LYS:CB | 2:B:61:LYS:N | 2.36 | 0.88 |
| 2:B:25:LEU:CD2 | 2:B:25:LEU:CD1 | 2.52 | 0.87 |
| 1:A:215:SER:H | 1:A:219:GLN:HE22 | 1.17 | 0.86 |
| 2:B:373:VAL:CG1 | 2:B:373:VAL:CG2 | 2.54 | 0.86 |
| 1:A:52:VAL:CG1 | 1:A:52:VAL:CG2 | 2.54 | 0.86 |
| 2:B:373:VAL:CG1 | 2:B:373:VAL:CA | 2.53 | 0.86 |
| 1:A:140:ARG:CD | 1:A:140:ARG:CB | 2.54 | 0.84 |
| 1:A:54:PHE:C | 1:A:54:PHE:CB | 2.46 | 0.84 |
| 1:A:215:SER:H | 1:A:219:GLN:NE2 | 1.74 | 0.84 |
| 2:B:297:SER:HB3 | 2:B:305:ASP:OD1 | 1.78 | 0.84 |
| 2:B:304:LEU:CD1 | 2:B:304:LEU:CD2 | 2.54 | 0.84 |
| 1:A:156:PRO:O | 1:A:191:LEU:HB3 | 1.78 | 0.84 |
| 2:B:339:LEU:CD2 | 2:B:339:LEU:CD1 | 2.56 | 0.84 |
| 1:A:140:ARG:CG | 1:A:140:ARG:NE | 2.40 | 0.83 |
| 2:B:112:ALA:HB2 | 2:B:302:ALA:HB1 | 1.60 | 0.83 |
| 2:B:282:MET:CB | 2:B:282:MET:SD | 2.66 | 0.83 |
| 2:B:55:ARG:CD | 2:B:55:ARG:CB | 2.57 | 0.83 |
| 2:B:61:LYS:CG | 2:B:61:LYS:CA | 2.56 | 0.83 |
| 2:B:286:MET:CB | 2:B:286:MET:SD | 2.66 | 0.83 |
| 2:B:256:GLU:CD | 2:B:256:GLU:CB | 2.47 | 0.82 |
| 2:B:212:THR:CG2 | 2:B:212:THR:CA | 2.57 | 0.82 |
| 2:B:255:VAL:CA | 2:B:255:VAL:CG1 | 2.58 | 0.82 |
| 2:B:222:ARG:NH2 | 6:B:736:HOH:O | 2.13 | 0.81 |
| 1:A:7:LEU:CD2 | 1:A:7:LEU:CD1 | 2.58 | 0.81 |
| 1:A:191:LEU:HD12 | 1:A:192:PRO:HD2 | 0.91 | 0.81 |
| 2:B:58:ALA:CB | 2:B:58:ALA:N | 2.45 | 0.80 |
| 2:B:368:LYS:CA | 2:B:369:GLU:N | 2.44 | 0.80 |
| 1:A:123:VAL:CA | 1:A:123:VAL:CG1 | 2.59 | 0.80 |
| 2:B:362:MET:CG | 2:B:362:MET:CE | 2.59 | 0.79 |
| 2:B:264:THR:CG2 | 2:B:264:THR:CA | 2.60 | 0.79 |
| 1:A:94:THR:CB | 1:A:94:THR:C | 2.51 | 0.79 |
| 1:A:87:LEU:CD1 | 1:A:87:LEU:CD2 | 2.61 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:368:LYS:CA | 2:B:368:LYS:O | 2.32 | 0.78 |
| 1:A:126:VAL:CG1 | 1:A:126:VAL:CA | 2.62 | 0.78 |
| 2:B:362:MET:SD | 2:B:362:MET:CB | 2.71 | 0.78 |
| 1:A:52:VAL:CG1 | 1:A:52:VAL:CA | 2.62 | 0.78 |
| 2:B:66:THR:CG2 | 2:B:66:THR:CA | 2.62 | 0.78 |
| 2:B:353:HIS:CA | 2:B:353:HIS:CG | 2.66 | 0.78 |
| 2:B:231:VAL:CG1 | 2:B:231:VAL:CA | 2.62 | 0.77 |
| 2:B:203:GLU:C | 2:B:203:GLU:CB | 2.53 | 0.77 |
| 2:B:339:LEU:CD2 | 2:B:339:LEU:CB | 2.61 | 0.77 |
| 2:B:231:VAL:CG1 | 2:B:231:VAL:CG2 | 2.60 | 0.77 |
| 2:B:353:HIS:CB | 2:B:353:HIS:C | 2.53 | 0.77 |
| 1:A:239:LYS:O | 1:A:243:LYS:HD3 | 1.85 | 0.77 |
| 2:B:287:MET:HG3 | 2:B:307:PRO:CB | 2.16 | 0.75 |
| 2:B:60:THR:C | 2:B:61:LYS:CA | 2.53 | 0.74 |
| 2:B:351:SER:CA | 2:B:352:SER:N | 2.48 | 0.74 |
| 1:A:101:MET:CG | 1:A:101:MET:CA | 2.64 | 0.74 |
| 1:A:239:LYS:O | 1:A:243:LYS:CD | 2.36 | 0.74 |
| 2:B:70:ARG:CA | 2:B:71:THR:N | 2.49 | 0.74 |
| 2:B:76:LYS:CE | 2:B:76:LYS:CG | 2.64 | 0.74 |
| 1:A:94:THR:CA | 1:A:94:THR:CG2 | 2.64 | 0.73 |
| 2:B:117:VAL:CA | 2:B:117:VAL:CG2 | 2.64 | 0.73 |
| 2:B:255:VAL:CA | 2:B:255:VAL:CG2 | 2.67 | 0.73 |
| 2:B:328:THR:C | 2:B:328:THR:CB | 2.57 | 0.73 |
| 2:B:15:MET:CE | 2:B:15:MET:CG | 2.66 | 0.73 |
| 2:B:49:LEU:CD2 | 2:B:49:LEU:CD1 | 2.66 | 0.73 |
| 2:B:203:GLU:C | 2:B:203:GLU:N | 2.39 | 0.73 |
| 1:A:123:VAL:CB | 1:A:123:VAL:N | 2.53 | 0.72 |
| 2:B:139:VAL:CG2 | 2:B:139:VAL:CG1 | 2.64 | 0.72 |
| 2:B:149:MET:SD | 2:B:149:MET:CB | 2.77 | 0.72 |
| 2:B:278:ILE:CD1 | 2:B:278:ILE:CB | 2.66 | 0.72 |
| 2:B:37:LYS:CD | 2:B:37:LYS:CB | 2.68 | 0.72 |
| 2:B:54:GLY:O | 6:B:735:HOH:O | 2.06 | 0.72 |
| 2:B:61:LYS:CB | 2:B:61:LYS:CD | 2.68 | 0.72 |
| 1:A:166:VAL:CG2 | 1:A:166:VAL:CG1 | 2.66 | 0.72 |
| 2:B:376:LEU:CD2 | 2:B:376:LEU:CD1 | 2.68 | 0.72 |
| 2:B:297:SER:C | 2:B:305:ASP:OD1 | 2.28 | 0.71 |
| 2:B:328:THR:CA | 2:B:329:ASP:N | 2.49 | 0.71 |
| 1:A:166:VAL:CG2 | 1:A:166:VAL:CA | 2.68 | 0.71 |
| 1:A:54:PHE:C | 1:A:54:PHE:N | 2.44 | 0.70 |
| 2:B:235:SER:CB | 2:B:235:SER:N | 2.53 | 0.70 |
| 2:B:58:ALA:C | 2:B:59:LEU:CA | 2.59 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:B:212:THR:CG2 | 2:B:212:THR:OG1 | 2.39 | 0.70 |
| 2:B:150:ARG:CG | 2:B:150:ARG:CA | 2.69 | 0.69 |
| 2:B:255:VAL:CB | 2:B:255:VAL:N | 2.52 | 0.69 |
| 2:B:286:MET:CB | 2:B:286:MET:N | 2.55 | 0.69 |
| 2:B:304:LEU:CD1 | 2:B:304:LEU:CB | 2.69 | 0.69 |
| 1:A:24:THR:CA | 1:A:24:THR:OG1 | 2.41 | 0.69 |
| 2:B:134:MET:HE2 | 2:B:139:VAL:HG22 | 1.72 | 0.68 |
| 2:B:196:PRO:CA | 2:B:197:TYR:N | 2.52 | 0.68 |
| 2:B:203:GLU:CA | 2:B:203:GLU:O | 2.41 | 0.67 |
| 2:B:351:SER:CA | 2:B:351:SER:O | 2.38 | 0.67 |
| 2:B:287:MET:CG | 2:B:307:PRO:CB | 2.72 | 0.67 |
| 1:A:24:THR:CB | 1:A:24:THR:C | 2.62 | 0.67 |
| 2:B:70:ARG:CA | 2:B:70:ARG:O | 2.38 | 0.67 |
| 1:A:123:VAL:CA | 1:A:123:VAL:CG2 | 2.70 | 0.67 |
| 2:B:59:LEU:CA | 2:B:59:LEU:O | 2.42 | 0.66 |
| 2:B:386:THR:O | 2:B:390:ILE:HD12 | 1.95 | 0.66 |
| 2:B:206[B]:ARG:NH2 | 2:B:243:ASP:OD1 | 2.28 | 0.66 |
| 2:B:117:VAL:CB | 2:B:117:VAL:N | 2.57 | 0.66 |
| 2:B:235:SER:CB | 2:B:235:SER:C | 2.64 | 0.65 |
| 2:B:328:THR:CA | 2:B:328:THR:O | 2.40 | 0.65 |
| 2:B:11:GLU:HG2 | 2:B:11:GLU:O | 1.94 | 0.65 |
| 1:A:60:ASP:OD1 | 3:A:501:IAG:N1 | 2.29 | 0.65 |
| 2:B:177:TRP:N | 2:B:178:PRO:CD | 2.59 | 0.65 |
| 2:B:353:HIS:CB | 2:B:353:HIS:N | 2.60 | 0.64 |
| 2:B:319:ILE:HD13 | 2:B:319:ILE:HG21 | 1.80 | 0.64 |
| 2:B:143:SER:N | 2:B:144:PRO:CD | 2.61 | 0.64 |
| 2:B:66:THR:CG2 | 2:B:66:THR:OG1 | 2.45 | 0.63 |
| 2:B:255:VAL:CB | 2:B:255:VAL:C | 2.62 | 0.63 |
| 2:B:327:ILE:HG23 | 2:B:331:GLU:HB2 | 1.80 | 0.63 |
| 2:B:282:MET:CB | 2:B:282:MET:C | 2.66 | 0.63 |
| 2:B:206[A]:ARG:HD2 | 2:B:210:GLU:OE2 | 1.99 | 0.63 |
| 2:B:55:ARG:CG | 2:B:55:ARG:NE | 2.63 | 0.62 |
| 2:B:196:PRO:CA | 2:B:196:PRO:O | 2.45 | 0.62 |
| 2:B:287:MET:CG | 2:B:307:PRO:HA | 2.30 | 0.61 |
| 1:A:24:THR:CB | 1:A:24:THR:N | 2.62 | 0.61 |
| 2:B:25:LEU:CD2 | 2:B:25:LEU:CB | 2.69 | 0.60 |
| 2:B:76:LYS:CD | 2:B:76:LYS:NZ | 2.61 | 0.60 |
| 2:B:134:MET:O | 2:B:158:PRO:HA | 2.02 | 0.60 |
| 2:B:287:MET:CB | 2:B:287:MET:SD | 2.88 | 0.60 |
| 1:A:219:GLN:CB | 1:A:219:GLN:CD | 2.67 | 0.59 |
| 1:A:194:HIS:O | 1:A:198:GLU:CG | 2.47 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:58:LEU:C | 1:A:58:LEU:HD12 | 2.23 | 0.59 |
| 2:B:287:MET:CG | 2:B:307:PRO:CA | 2.80 | 0.59 |
| 2:B:286:MET:CB | 2:B:286:MET:C | 2.69 | 0.59 |
| 2:B:264:THR:CG2 | 2:B:264:THR:OG1 | 2.46 | 0.58 |
| 1:A:177:LEU:HD11 | 1:A:212:PHE:CD2 | 2.38 | 0.58 |
| 2:B:70:ARG:C | 2:B:70:ARG:CB | 2.71 | 0.58 |
| 2:B:287:MET:HG3 | 2:B:307:PRO:HB3 | 1.86 | 0.58 |
| 1:A:87:LEU:CD1 | 1:A:87:LEU:CB | 2.78 | 0.58 |
| 1:A:239:LYS:O | 1:A:243:LYS:HD2 | 2.04 | 0.58 |
| 1:A:54:PHE:CA | 1:A:55:SER:N | 2.62 | 0.58 |
| 2:B:112:ALA:CB | 2:B:302:ALA:HB1 | 2.32 | 0.57 |
| 2:B:362:MET:CG | 2:B:362:MET:HE3 | 2.35 | 0.57 |
| 2:B:351:SER:C | 2:B:351:SER:N | 2.51 | 0.57 |
| 1:A:16:GLU:HG3 | 6:A:566:HOH:O | 2.05 | 0.57 |
| 2:B:38:ASP:OD1 | 2:B:38:ASP:C | 2.40 | 0.57 |
| 2:B:59:LEU:CA | 2:B:60:THR:N | 2.56 | 0.57 |
| 2:B:139:VAL:CG2 | 2:B:139:VAL:CA | 2.78 | 0.57 |
| 1:A:117:ARG:CD | 1:A:117:ARG:CB | 2.74 | 0.56 |
| 1:A:211:GLY:O | 1:A:212:PHE:HB2 | 2.04 | 0.56 |
| 2:B:87:LYS:HD2 | 2:B:114:GLN:HG3 | 1.87 | 0.56 |
| 2:B:287:MET:HG3 | 2:B:307:PRO:CA | 2.36 | 0.56 |
| 2:B:117:VAL:CB | 2:B:117:VAL:C | 2.62 | 0.56 |
| 1:A:123:VAL:CB | 1:A:123:VAL:C | 2.68 | 0.55 |
| 2:B:333:LEU:CD2 | 2:B:333:LEU:HB3 | 2.36 | 0.55 |
| 2:B:287:MET:HB2 | 2:B:307:PRO:HB2 | 1.88 | 0.55 |
| 1:A:156:PRO:HA | 1:A:196:LEU:HD21 | 1.89 | 0.55 |
| 2:B:319:ILE:CG2 | 2:B:319:ILE:CD1 | 2.84 | 0.55 |
| 2:B:203:GLU:CA | 2:B:204:PHE:N | 2.58 | 0.55 |
| 2:B:287:MET:HG3 | 2:B:307:PRO:HA | 1.88 | 0.55 |
| 2:B:58:ALA:CB | 2:B:58:ALA:C | 2.73 | 0.54 |
| 1:A:16:GLU:CG | 6:A:566:HOH:O | 2.56 | 0.54 |
| 2:B:134:MET:O | 2:B:159:VAL:N | 2.41 | 0.53 |
| 2:B:297:SER:CB | 2:B:305:ASP:OD1 | 2.53 | 0.53 |
| 2:B:205:GLN:CG | 2:B:205:GLN:OE1 | 2.51 | 0.53 |
| 1:A:234:GLY:O | 1:A:235:SER:C | 2.42 | 0.53 |
| 2:B:129:LYS:CD | 2:B:129:LYS:CB | 2.77 | 0.52 |
| 2:B:59:LEU:N | 2:B:59:LEU:C | 2.61 | 0.52 |
| 2:B:32:PHE:CD1 | 2:B:200:ILE:HG12 | 2.44 | 0.52 |
| 2:B:287:MET:HG2 | 2:B:307:PRO:HA | 1.91 | 0.52 |
| 2:B:255:VAL:CG1 | 2:B:255:VAL:C | 2.78 | 0.51 |
| 2:B:287:MET:HG2 | 2:B:307:PRO:CA | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:286:MET:CA | 2:B:286:MET:HB2 | 2.18 | 0.51 |
| 1:A:125:SER:HB2 | 1:A:151:ILE:HG12 | 1.91 | 0.51 |
| 2:B:111:GLY:O | 2:B:138:ASP:HB3 | 2.10 | 0.51 |
| 2:B:117:VAL:HG23 | 2:B:117:VAL:H | 1.76 | 0.51 |
| 2:B:319:ILE:CG2 | 2:B:319:ILE:CA | 2.78 | 0.51 |
| 1:A:100:LEU:C | 1:A:100:LEU:HD13 | 2.31 | 0.50 |
| 2:B:206[A]:ARG:CD | 2:B:210:GLU:OE2 | 2.57 | 0.50 |
| 1:A:243:LYS:H | 1:A:243:LYS:CD | 2.11 | 0.50 |
| 2:B:143:SER:N | 2:B:144:PRO:HD2 | 2.26 | 0.50 |
| 2:B:85:ALA:HA | 2:B:377:SER:O | 2.10 | 0.50 |
| 2:B:177:TRP:N | 2:B:178:PRO:HD3 | 2.25 | 0.49 |
| 1:A:263:LYS:O | 1:A:266:SER:OG | 2.26 | 0.49 |
| 2:B:129:LYS:CG | 2:B:129:LYS:CE | 2.83 | 0.49 |
| 2:B:297:SER:O | 2:B:305:ASP:OD1 | 2.31 | 0.49 |
| 2:B:150:ARG:CB | 2:B:150:ARG:CD | 2.81 | 0.49 |
| 2:B:142:GLN:C | 2:B:144:PRO:HD2 | 2.33 | 0.48 |
| 2:B:328:THR:C | 2:B:328:THR:N | 2.59 | 0.48 |
| 2:B:319:ILE:CG2 | 2:B:319:ILE:HD13 | 2.40 | 0.48 |
| 1:A:125:SER:HB2 | 1:A:151:ILE:CG1 | 2.44 | 0.48 |
| 1:A:242:GLU:CD | 1:A:243:LYS:HZ1 | 2.18 | 0.47 |
| 2:B:62:CYS:SG | 2:B:75:LEU:HG | 2.54 | 0.47 |
| 2:B:87:LYS:HD2 | 2:B:114:GLN:CG | 2.44 | 0.47 |
| 2:B:286:MET:CA | 2:B:286:MET:HB3 | 2.18 | 0.47 |
| 2:B:87:LYS:NZ | 5:B:502:PLP:O3 | 2.47 | 0.47 |
| 2:B:373:VAL:CG1 | 2:B:373:VAL:C | 2.82 | 0.47 |
| 1:A:148:ILE:HD12 | 1:A:148:ILE:HG23 | 1.54 | 0.47 |
| 2:B:59:LEU:HD12 | 2:B:59:LEU:HA | 1.67 | 0.47 |
| 2:B:115:HIS:CE1 | 2:B:189:GLY:HA2 | 2.50 | 0.47 |
| 2:B:381:ASP:O | 2:B:384:ILE:HG12 | 2.15 | 0.47 |
| 1:A:127:LEU:HD23 | 1:A:128:VAL:N | 2.30 | 0.46 |
| 2:B:203:GLU:N | 2:B:204:PHE:N | 2.64 | 0.46 |
| 1:A:132:PRO:HD3 | 2:B:17:VAL:O | 2.15 | 0.46 |
| 2:B:333:LEU:CD2 | 2:B:333:LEU:HD13 | 2.44 | 0.46 |
| 1:A:76:VAL:HA | 1:A:80:GLN:OE1 | 2.16 | 0.45 |
| 1:A:216:SER:H | 1:A:219:GLN:HE21 | 1.63 | 0.45 |
| 2:B:279:TYR:CG | 2:B:280:PHE:N | 2.83 | 0.45 |
| 2:B:117:VAL:CA | 2:B:117:VAL:CG1 | 2.85 | 0.45 |
| 2:B:362:MET:CE | 2:B:362:MET:CB | 2.91 | 0.45 |
| 2:B:134:MET:HE2 | 2:B:134:MET:HB3 | 1.41 | 0.45 |
| 2:B:255:VAL:CG2 | 2:B:255:VAL:N | 2.78 | 0.45 |
| 2:B:108:ALA:CB | 2:B:108:ALA:C | 2.71 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:112:ALA:HB2 | 2:B:302:ALA:CB | 2.39 | 0.45 |
| 2:B:173:ALA:HB1 | 2:B:186:TYR:CE1 | 2.51 | 0.45 |
| 1:A:123:VAL:CG1 | 1:A:123:VAL:C | 2.86 | 0.44 |
| 2:B:351:SER:N | 2:B:352:SER:N | 2.65 | 0.44 |
| 1:A:91:LYS:NZ | 6:A:626:HOH:O | 2.43 | 0.44 |
| 2:B:287:MET:CG | 2:B:307:PRO:HB2 | 2.47 | 0.44 |
| 2:B:319:ILE:HG21 | 2:B:319:ILE:CD1 | 2.43 | 0.44 |
| 1:A:55:SER:HB3 | 2:B:293:GLN:HB3 | 1.99 | 0.44 |
| 2:B:70:ARG:C | 2:B:70:ARG:N | 2.57 | 0.44 |
| 2:B:264:THR:CG2 | 2:B:264:THR:N | 2.81 | 0.43 |
| 2:B:272:LYS:HD3 | 2:B:324:TYR:HB2 | 2.00 | 0.43 |
| 2:B:287:MET:HG2 | 2:B:307:PRO:O | 2.18 | 0.43 |
| 2:B:205:GLN:CG | 2:B:205:GLN:NE2 | 2.68 | 0.43 |
| 2:B:279:TYR:CD1 | 2:B:280:PHE:N | 2.84 | 0.43 |
| 1:A:95:ILE:HG21 | 1:A:95:ILE:HD13 | 1.64 | 0.43 |
| 2:B:157:ILE:HA | 2:B:158:PRO:HD3 | 1.42 | 0.43 |
| 2:B:117:VAL:CG2 | 2:B:117:VAL:N | 2.82 | 0.43 |
| 2:B:255:VAL:C | 2:B:255:VAL:HG12 | 2.39 | 0.43 |
| 1:A:219:GLN:CG | 1:A:219:GLN:CA | 2.89 | 0.43 |
| 2:B:349:LEU:HD23 | 2:B:349:LEU:HA | 1.90 | 0.43 |
| 1:A:193:LEU:HA | 1:A:193:LEU:HD23 | 1.51 | 0.42 |
| 1:A:22:PHE:CD1 | 1:A:22:PHE:C | 2.92 | 0.42 |
| 1:A:140:ARG:HH11 | 1:A:140:ARG:HD3 | 0.88 | 0.42 |
| 2:B:70:ARG:N | 2:B:71:THR:N | 2.67 | 0.42 |
| 2:B:301:SER:OG | 2:B:350:GLU:HG3 | 2.19 | 0.42 |
| 2:B:80:LEU:HD23 | 2:B:80:LEU:HA | 1.66 | 0.42 |
| 2:B:205:GLN:CD | 2:B:205:GLN:CB | 2.75 | 0.42 |
| 2:B:79:ASP:HB2 | 2:B:379:ARG:HB3 | 2.02 | 0.41 |
| 2:B:97:LEU:HD23 | 2:B:97:LEU:HA | 2.00 | 0.41 |
| 1:A:85:LEU:HD23 | 1:A:85:LEU:HA | 1.95 | 0.41 |
| 2:B:57:THR:OG1 | 2:B:76:LYS:HE3 | 2.19 | 0.41 |
| 2:B:364:GLU:C | 2:B:365:GLN:CG | 2.88 | 0.41 |
| 1:A:216:SER:HA | 1:A:217:PRO:HD3 | 1.91 | 0.41 |
| 2:B:174:LEU:HA | 2:B:174:LEU:HD23 | 1.73 | 0.41 |
| 2:B:300:ILE:HB | 2:B:329:ASP:CG | 2.41 | 0.41 |
| 1:A:30:ILE:HD11 | 1:A:76:VAL:HG22 | 2.03 | 0.41 |
| 2:B:133:TYR:HA | 2:B:157:ILE:O | 2.21 | 0.41 |
| 2:B:167:LYS:O | 2:B:170:CYS:HB2 | 2.21 | 0.41 |
| 2:B:71:THR:CG2 | 2:B:71:THR:OG1 | 2.61 | 0.40 |
| 2:B:202:ARG:HH11 | 2:B:202:ARG:HD3 | 1.48 | 0.40 |
| 2:B:66:THR:HA | 2:B:362:MET:SD | 2.61 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 255/268 (95%) | 250 (98%) | 3 (1%) | 2 (1%) | 19 | 6 |
| 2 | B | 393/396 (99%) | 371 (94%) | 20 (5%) | 2 (0%) | 29 | 13 |
| All | All | 648/664 (98%) | 621 (96%) | 23 (4%) | 4 (1%) | 25 | 11 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 191 | LEU |
| 1 | A | 234 | GLY |
| 2 | B | 117 | VAL |
| 2 | B | 139 | VAL |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 203/208 (98%) | 195 (96%) | 8 (4%) | 32 | 13 |
| 2 | B | 309/310 (100%) | 299 (97%) | 10 (3%) | 39 | 20 |
| All | All | 512/518 (99%) | 494 (96%) | 18 (4%) | 36 | 17 |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 30 | ILE |
| 1 | A | 78 | PRO |
| 1 | A | 112 | ASP |
| 1 | A | 121 | VAL |
| 1 | A | 193 | LEU |
| 1 | A | 196 | LEU |
| 1 | A | 243 | LYS |
| 1 | A | 247 | SER |
| 2 | B | 65 | ILE |
| 2 | B | 141 | ARG |
| 2 | B | 143 | SER |
| 2 | B | 161 | SER |
| 2 | B | 176 | ASP |
| 2 | B | 207 | MET |
| 2 | B | 216 | ILE |
| 2 | B | 297 | SER |
| 2 | B | 347 | PRO |
| 2 | B | 394 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 109 | ASN |
| 1 | A | 219 | GLN |
| 2 | B | 246 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 5 | PLP | B | 502 | 2 | 15,15,16 | 3.62 | 9 (60%) | 20,22,23 | 2.94 | 5 (25%) |
| 3 | IAG | A | 501 | - | 14,18,18 | 1.80 | 4 (28%) | 15,24,24 | 3.67 | 9 (60%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 5 | PLP | B | 502 | 2 | - | 0/6/6/8 | 0/1/1/1 |
| 3 | IAG | A | 501 | - | - | 2/7/9/9 | 0/2/2/2 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | B | 502 | PLP | P-O4P | -6.76 | 1.38 | 1.60 |
| 5 | B | 502 | PLP | C3-C2 | -5.71 | 1.35 | 1.40 |
| 5 | B | 502 | PLP | C2A-C2 | 5.64 | 1.59 | 1.50 |
| 5 | B | 502 | PLP | P-O3P | -4.32 | 1.38 | 1.54 |
| 5 | B | 502 | PLP | C5-C4 | 4.07 | 1.45 | 1.40 |
| 3 | A | 501 | IAG | O1-C10 | 4.07 | 1.31 | 1.23 |
| 5 | B | 502 | PLP | C5A-C5 | 3.94 | 1.61 | 1.50 |
| 3 | A | 501 | IAG | C3-C7 | -3.48 | 1.35 | 1.42 |
| 5 | B | 502 | PLP | O4P-C5A | 3.02 | 1.56 | 1.45 |
| 5 | B | 502 | PLP | C2-N1 | 2.62 | 1.38 | 1.33 |
| 5 | B | 502 | PLP | C3-C4 | -2.20 | 1.35 | 1.40 |
| 3 | A | 501 | IAG | C11-N2 | 2.16 | 1.50 | 1.46 |
| 3 | A | 501 | IAG | C9-C2 | -2.10 | 1.45 | 1.52 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | A | 501 | IAG | C11-N2-C10 | -9.07 | 108.22 | 122.34 |
| 5 | B | 502 | PLP | O4P-C5A-C5 | 8.30 | 125.17 | 109.35 |
| 5 | B | 502 | PLP | O3P-P-O4P | 6.90 | 125.09 | 106.73 |
| 3 | A | 501 | IAG | C6-C8-N1 | 5.28 | 145.41 | 130.80 |
| 3 | A | 501 | IAG | C7-C8-N1 | -4.68 | 97.53 | 107.92 |
| 3 | A | 501 | IAG | C12-C11-N2 | -4.34 | 102.06 | 110.43 |
| 5 | B | 502 | PLP | C4A-C4-C5 | -4.30 | 116.50 | 120.94 |
| 3 | A | 501 | IAG | C4-C5-C6 | -3.98 | 114.86 | 120.44 |
| 3 | A | 501 | IAG | C9-C10-N2 | -3.62 | 111.29 | 116.19 |
| 5 | B | 502 | PLP | O4P-P-O1P | -3.52 | 96.60 | 106.47 |
| 3 | A | 501 | IAG | C5-C6-C8 | 2.72 | 124.00 | 120.08 |
| 3 | A | 501 | IAG | C5-C4-C3 | 2.52 | 123.97 | 120.44 |
| 5 | B | 502 | PLP | C4A-C4-C3 | 2.44 | 124.64 | 120.50 |
| 3 | A | 501 | IAG | C6-C8-C7 | -2.11 | 116.91 | 120.76 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | A | 501 | IAG | O1-C10-C9-C2 |
| 3 | A | 501 | IAG | N2-C10-C9-C2 |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | B | 502 | PLP | 1 | 0 |
| 3 | A | 501 | IAG | 1 | 0 |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2 | B | 6 |
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 65:ILE | C | 66:THR | N | 1.19 |
| 1 | B | 321:ARG | C | 322:ALA | N | 1.19 |
| 1 | B | 332:ALA | C | 333:LEU | N | 1.19 |
| 1 | B | 343:GLU | C | 344:GLY | N | 1.19 |
| 1 | B | 362:MET | C | 363:ARG | N | 1.19 |
| 1 | B | 368:LYS | C | 369:GLU | N | 1.19 |
| 1 | A | 232:ILE | C | 233:SER | N | 1.18 |

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1 | A | 257/268 (95%) | 0.51 | 20 (7%) 13 15 | 13, 26, 48, 78 | 0 |
| 2 | B | 394/396 (99%) | 0.66 | 42 (10%) 6 7 | 11, 19, 42, 73 | 0 |
| All | All | 651/664 (98%) | 0.60 | 62 (9%) 8 9 | 11, 22, 44, 78 | 0 |

All (62) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 268 | ALA | 7.2 |
| 2 | B | 159 | VAL | 6.9 |
| 1 | A | 190 | ALA | 6.4 |
| 2 | B | 385 | PHE | 6.3 |
| 1 | A | 191 | LEU | 5.8 |
| 1 | A | 194 | HIS | 5.2 |
| 2 | B | 164 | ALA | 5.0 |
| 2 | B | 393 | ALA | 4.5 |
| 2 | B | 160 | HIS | 4.5 |
| 2 | B | 395 | GLY | 4.3 |
| 2 | B | 135 | GLY | 4.1 |
| 2 | B | 158 | PRO | 3.9 |
| 2 | B | 394 | ARG | 3.8 |
| 2 | B | 143 | SER | 3.8 |
| 2 | B | 140 | GLU | 3.7 |
| 2 | B | 391 | LEU | 3.7 |
| 2 | B | 112 | ALA | 3.7 |
| 1 | A | 109 | ASN | 3.5 |
| 2 | B | 163 | SER | 3.4 |
| 1 | A | 195 | HIS | 3.3 |
| 2 | B | 138 | ASP | 3.3 |
| 2 | B | 134 | MET | 3.2 |
| 2 | B | 146 | VAL | 3.2 |
| 2 | B | 139 | VAL | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 392 | LYS | 3.1 |
| 1 | A | 15 | ARG | 3.1 |
| 2 | B | 92 | LEU | 3.1 |
| 2 | B | 166 | LEU | 3.1 |
| 2 | B | 137 | LYS | 3.0 |
| 1 | A | 246 | ALA | 3.0 |
| 1 | A | 198 | GLU | 3.0 |
| 2 | B | 141 | ARG | 3.0 |
| 2 | B | 136 | ALA | 3.0 |
| 1 | A | 13 | ASP | 3.0 |
| 2 | B | 81 | LEU | 2.9 |
| 2 | B | 162 | GLY | 2.8 |
| 1 | A | 250 | GLN | 2.8 |
| 1 | A | 247 | SER | 2.7 |
| 2 | B | 390 | ILE | 2.7 |
| 2 | B | 80 | LEU | 2.7 |
| 1 | A | 248 | PRO | 2.7 |
| 2 | B | 147 | PHE | 2.7 |
| 1 | A | 204 | HIS | 2.6 |
| 2 | B | 248 | THR | 2.6 |
| 2 | B | 156 | VAL | 2.5 |
| 2 | B | 325 | VAL | 2.5 |
| 2 | B | 85 | ALA | 2.4 |
| 2 | B | 88 | THR | 2.4 |
| 2 | B | 157 | ILE | 2.4 |
| 2 | B | 150 | ARG | 2.3 |
| 1 | A | 203 | TYR | 2.3 |
| 2 | B | 49 | LEU | 2.3 |
| 1 | A | 193 | LEU | 2.2 |
| 2 | B | 388 | HIS | 2.2 |
| 2 | B | 169 | ALA | 2.2 |
| 2 | B | 306 | PHE | 2.1 |
| 2 | B | 75 | LEU | 2.1 |
| 1 | A | 12 | ASN | 2.1 |
| 1 | A | 212 | PHE | 2.1 |
| 1 | A | 178 | SER | 2.1 |
| 1 | A | 192 | PRO | 2.0 |
| 2 | B | 229 | ALA | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | IAG | A | 501 | 17/17 | 0.84 | 0.15 | 22,35,50,52 | 0 |
| 5 | PLP | B | 502 | 15/16 | 0.98 | 0.12 | 15,18,28,30 | 0 |
| 4 | NA | B | 503 | 1/1 | 0.99 | 0.09 | 17,17,17,17 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.