



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:21 AM UTC

PDB ID : 1K7X / pdb\_00001k7x  
Title : CRYSTAL STRUCTURE OF THE BETA-SER178PRO MUTANT OF TRYPTOPHAN SYNTHASE  
Authors : Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.  
Deposited on : 2001-10-22  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

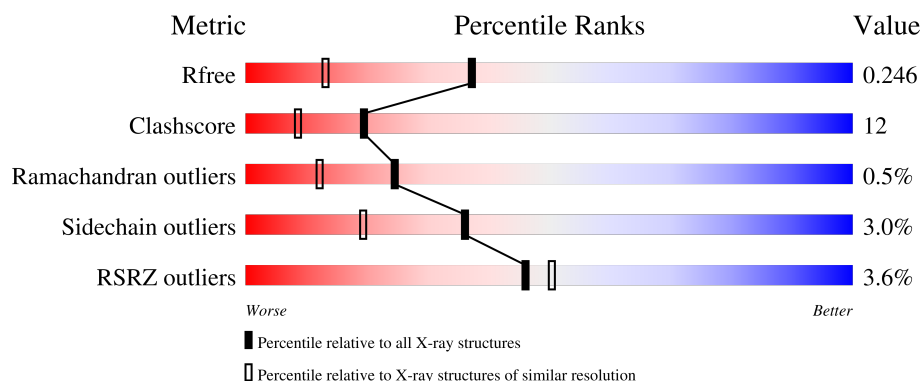
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

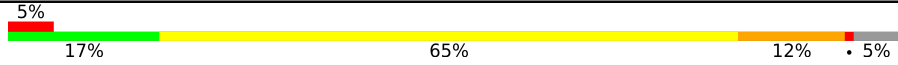
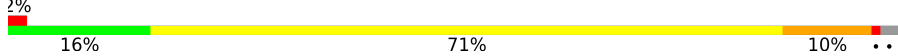
The reported resolution of this entry is 1.70 Å.

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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5551 (1.70-1.70)                                      |
| Clashscore            | 190562                      | 5924 (1.70-1.70)                                      |
| Ramachandran outliers | 187476                      | 5846 (1.70-1.70)                                      |
| Sidechain outliers    | 187428                      | 5846 (1.70-1.70)                                      |
| RSRZ outliers         | 180081                      | 5554 (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  $\geq 3$ , 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

There are 5 unique types of molecules in this entry. The entry contains 5326 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     | 254      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1917  | 1221 | 331 | 357 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 390      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2959  | 1861 | 517 | 561 | 20 |         |         |       |

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 SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | B     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 4   | B     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |

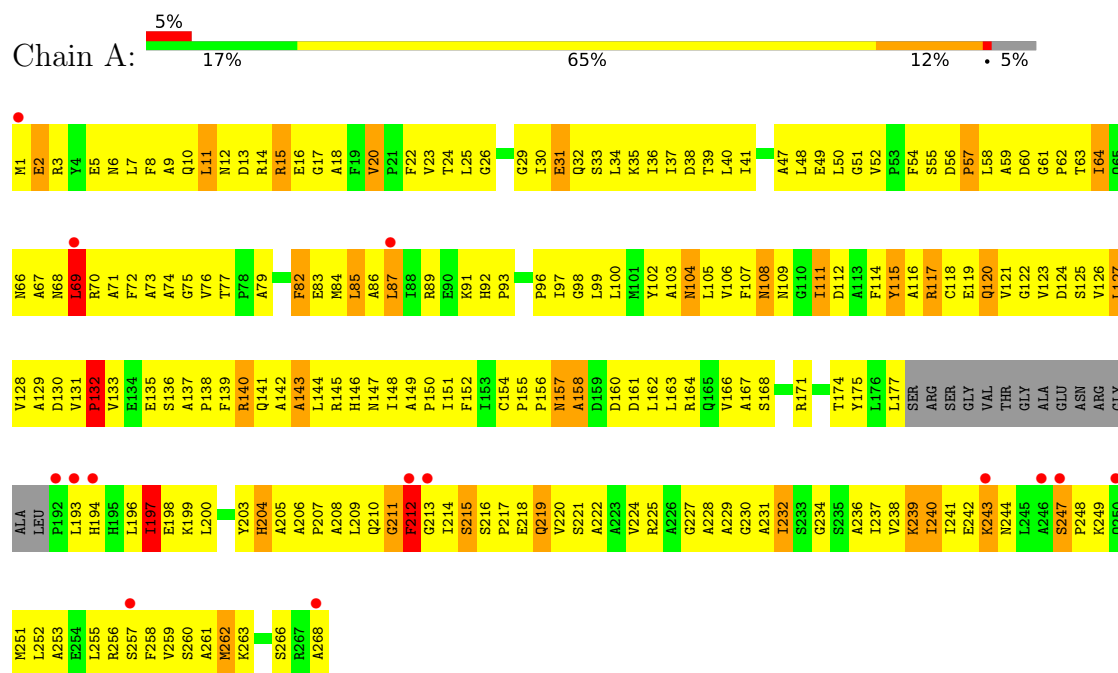
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 139      | Total | O   | 0       | 0       |
|     |       |          | 139   | 139 |         |         |
| 5   | B     | 295      | Total | O   | 0       | 0       |
|     |       |          | 295   | 295 |         |         |

### 3 Residue-property plots

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



|      |      |      |
|------|------|------|
| N375 | Y315 | V255 |
| L376 | L316 | E256 |
| S377 | N317 | P257 |
| G378 | S318 | G258 |
| R379 | I319 | G259 |
| G380 | G320 | H260 |
| D381 | R321 | G261 |
| K382 | A322 | T262 |
| D383 | D323 | E263 |
| I384 | Y324 | T264 |
| F385 | V325 | G265 |
| T386 | S326 | E266 |
| V387 | I327 | H267 |
| H388 | T328 | G268 |
| D389 | D329 | A269 |
| L390 | D330 | P270 |
| L391 | E331 | L271 |
| LYS  | A332 | K272 |
| ALA  | L333 | H273 |
| ARG  | E334 | G274 |
| GLY  | A335 | R275 |
| GLU  | F336 | V276 |
| ILE  | K337 | G277 |
|      | T338 | T278 |
|      | L339 | T279 |
|      | C340 | F280 |
|      | R341 | G281 |
|      | H342 | N282 |
|      | E343 | K283 |
|      | G344 | A284 |
|      | I345 | P285 |
|      | L346 | N286 |
|      | P347 | T287 |
|      | A348 | Q288 |
|      | L349 | T289 |
|      | E350 | A290 |
|      | S351 | D291 |
|      | S352 | G292 |
|      | H353 | Q293 |
|      | A354 | I294 |
|      | L355 | E295 |
|      | A356 | E296 |
|      | H357 | S297 |
|      | A358 | Y298 |
|      | L359 | S299 |
|      | K360 | T300 |
|      | M361 | S301 |
|      | T362 | A302 |
|      | K363 | G303 |
|      | E364 | L304 |
|      | Q365 | D305 |
|      | P366 | F306 |
|      | E367 | P307 |
|      | K368 | S308 |
|      | E369 | V309 |
|      | Q370 | G310 |
|      | L371 | P311 |
|      | L372 | Q312 |
|      | V373 | H313 |
|      | V274 | L314 |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 184.01Å 59.99Å 67.54Å<br>90.00° 94.65° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 1.70<br>20.00 – 1.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.8 (20.00-1.70)<br>96.7 (20.00-1.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.51 (at 1.70Å)                                             | Xtriage          |
| Refinement program                                                      | CNS, REFMAC                                                 | Depositor        |
| R, $R_{free}$                                                           | 0.187 , 0.238<br>0.195 , 0.246                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3973 reflections (5.08%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 16.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.626                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.44 , 53.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 5326                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 21.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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     | 3.27         | 223/1955 (11.4%) | 2.51        | 153/2656 (5.8%) |
| 2   | B     | 3.54         | 435/3035 (14.3%) | 2.71        | 290/4101 (7.1%) |
| All | All   | 3.44         | 658/4990 (13.2%) | 2.64        | 443/6757 (6.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |

All (658) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2   | B     | 152 | MET  | SD-CE | -19.24 | 1.31        | 1.79     |
| 2   | B     | 138 | ASP  | C-O   | 18.56  | 1.46        | 1.24     |
| 1   | A     | 111 | ILE  | CA-CB | 16.62  | 1.75        | 1.54     |
| 1   | A     | 155 | PRO  | CA-C  | 15.53  | 1.66        | 1.52     |
| 2   | B     | 319 | ILE  | C-O   | -14.98 | 1.07        | 1.24     |
| 1   | A     | 84  | MET  | SD-CE | -14.70 | 1.42        | 1.79     |
| 2   | B     | 135 | GLY  | C-O   | 14.48  | 1.38        | 1.23     |
| 2   | B     | 346 | ILE  | N-CA  | 14.30  | 1.57        | 1.46     |
| 2   | B     | 388 | HIS  | N-CA  | 13.96  | 1.63        | 1.46     |
| 1   | A     | 259 | VAL  | CA-CB | 13.86  | 1.71        | 1.54     |
| 1   | A     | 144 | LEU  | C-O   | 13.27  | 1.39        | 1.24     |
| 2   | B     | 302 | ALA  | C-O   | -13.21 | 1.07        | 1.24     |
| 1   | A     | 18  | ALA  | CA-CB | 12.98  | 1.73        | 1.53     |
| 1   | A     | 55  | SER  | N-CA  | 12.85  | 1.62        | 1.46     |
| 2   | B     | 61  | LYS  | N-CA  | 12.69  | 1.61        | 1.46     |
| 2   | B     | 113 | GLY  | C-O   | 12.49  | 1.42        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 148 | ARG  | N-CA   | 12.45  | 1.61        | 1.46     |
| 2   | B     | 101 | MET  | SD-CE  | -12.42 | 1.48        | 1.79     |
| 1   | A     | 79  | ALA  | CA-C   | -12.12 | 1.36        | 1.52     |
| 1   | A     | 57  | PRO  | CA-CB  | 12.11  | 1.69        | 1.53     |
| 2   | B     | 124 | ALA  | CA-CB  | 12.11  | 1.72        | 1.53     |
| 2   | B     | 371 | LEU  | N-CA   | 11.94  | 1.61        | 1.46     |
| 2   | B     | 165 | THR  | N-CA   | 11.75  | 1.61        | 1.46     |
| 2   | B     | 164 | ALA  | C-O    | 11.65  | 1.40        | 1.23     |
| 1   | A     | 119 | GLU  | CA-C   | 11.62  | 1.67        | 1.52     |
| 2   | B     | 70  | ARG  | CA-CB  | 11.62  | 1.69        | 1.53     |
| 2   | B     | 108 | ALA  | CA-CB  | 11.58  | 1.74        | 1.53     |
| 2   | B     | 39  | PRO  | C-O    | 11.40  | 1.38        | 1.24     |
| 1   | A     | 167 | ALA  | CA-C   | -11.40 | 1.38        | 1.52     |
| 2   | B     | 59  | LEU  | N-CA   | 11.39  | 1.60        | 1.46     |
| 2   | B     | 106 | ILE  | N-CA   | 11.15  | 1.59        | 1.46     |
| 2   | B     | 141 | ARG  | C-O    | 10.92  | 1.38        | 1.24     |
| 2   | B     | 346 | ILE  | CA-C   | -10.89 | 1.44        | 1.53     |
| 2   | B     | 283 | LYS  | N-CA   | 10.83  | 1.59        | 1.46     |
| 2   | B     | 238 | ILE  | CA-C   | 10.79  | 1.68        | 1.52     |
| 2   | B     | 330 | ASP  | C-O    | -10.68 | 1.10        | 1.24     |
| 1   | A     | 217 | PRO  | C-O    | 10.62  | 1.37        | 1.24     |
| 2   | B     | 17  | VAL  | CA-CB  | 10.55  | 1.64        | 1.55     |
| 2   | B     | 184 | ALA  | CA-C   | 10.41  | 1.65        | 1.52     |
| 2   | B     | 245 | ILE  | CA-CB  | 10.39  | 1.67        | 1.54     |
| 2   | B     | 76  | LYS  | CA-CB  | 10.34  | 1.68        | 1.53     |
| 1   | A     | 214 | ILE  | N-CA   | -10.30 | 1.33        | 1.46     |
| 1   | A     | 54  | PHE  | CA-C   | 10.25  | 1.64        | 1.52     |
| 2   | B     | 373 | VAL  | N-CA   | 10.23  | 1.58        | 1.46     |
| 1   | A     | 83  | GLU  | N-CA   | 10.22  | 1.58        | 1.46     |
| 2   | B     | 390 | ILE  | CB-CG2 | 10.15  | 1.86        | 1.52     |
| 2   | B     | 98  | ALA  | CA-C   | 10.14  | 1.65        | 1.52     |
| 1   | A     | 141 | GLN  | N-CA   | -10.08 | 1.33        | 1.46     |
| 2   | B     | 100 | ARG  | C-O    | 10.03  | 1.36        | 1.24     |
| 2   | B     | 118 | ALA  | CA-CB  | 9.93   | 1.69        | 1.53     |
| 2   | B     | 294 | ILE  | C-O    | 9.88   | 1.37        | 1.24     |
| 2   | B     | 215 | GLN  | N-CA   | 9.83   | 1.58        | 1.46     |
| 2   | B     | 88  | THR  | N-CA   | 9.82   | 1.58        | 1.46     |
| 2   | B     | 227 | VAL  | CA-C   | 9.79   | 1.64        | 1.52     |
| 1   | A     | 253 | ALA  | CA-C   | -9.73  | 1.40        | 1.52     |
| 1   | A     | 119 | GLU  | C-O    | 9.72   | 1.35        | 1.24     |
| 2   | B     | 172 | GLU  | C-O    | 9.71   | 1.35        | 1.24     |
| 2   | B     | 158 | PRO  | C-O    | 9.65   | 1.34        | 1.23     |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | A     | 227    | GLY  | C-O    | 9.65  | 1.36        | 1.24     |
| 2   | B     | 307    | PRO  | CA-C   | 9.63  | 1.66        | 1.52     |
| 2   | B     | 119    | SER  | CA-C   | 9.55  | 1.65        | 1.52     |
| 2   | B     | 231    | VAL  | CA-C   | 9.53  | 1.64        | 1.52     |
| 1   | A     | 38     | ASP  | N-CA   | 9.43  | 1.58        | 1.46     |
| 2   | B     | 290    | ALA  | CA-C   | 9.42  | 1.65        | 1.52     |
| 2   | B     | 264    | THR  | N-CA   | 9.41  | 1.58        | 1.46     |
| 2   | B     | 143    | SER  | CA-C   | -9.33 | 1.43        | 1.52     |
| 2   | B     | 62     | CYS  | CA-CB  | 9.33  | 1.69        | 1.53     |
| 1   | A     | 47     | ALA  | C-O    | 9.32  | 1.34        | 1.23     |
| 2   | B     | 157    | ILE  | N-CA   | 9.32  | 1.54        | 1.46     |
| 2   | B     | 218    | ASP  | C-O    | 9.30  | 1.34        | 1.24     |
| 2   | B     | 88     | THR  | CA-C   | 9.28  | 1.65        | 1.52     |
| 1   | A     | 209    | LEU  | CA-C   | -9.27 | 1.41        | 1.52     |
| 1   | A     | 6      | ASN  | CA-C   | -9.26 | 1.41        | 1.52     |
| 2   | B     | 72     | THR  | CA-CB  | -9.25 | 1.39        | 1.53     |
| 2   | B     | 59     | LEU  | CA-C   | 9.13  | 1.63        | 1.52     |
| 2   | B     | 27     | GLN  | C-O    | 9.11  | 1.34        | 1.24     |
| 1   | A     | 205    | ALA  | CA-CB  | 9.10  | 1.67        | 1.53     |
| 2   | B     | 285    | PRO  | CA-CB  | 9.08  | 1.66        | 1.53     |
| 1   | A     | 117    | ARG  | CA-C   | 9.05  | 1.64        | 1.52     |
| 2   | B     | 319    | ILE  | CA-CB  | 9.01  | 1.67        | 1.54     |
| 1   | A     | 24     | THR  | CA-CB  | 9.00  | 1.66        | 1.53     |
| 2   | B     | 241    | PHE  | CA-C   | 9.00  | 1.64        | 1.52     |
| 2   | B     | 280    | PHE  | CA-C   | -8.99 | 1.41        | 1.53     |
| 2   | B     | 231    | VAL  | CA-CB  | -8.99 | 1.41        | 1.53     |
| 2   | B     | 63     | GLN  | CG-CD  | 8.98  | 1.74        | 1.52     |
| 2   | B     | 211    | GLU  | CA-C   | 8.96  | 1.64        | 1.52     |
| 2   | B     | 219[A] | LYS  | CA-C   | 8.92  | 1.65        | 1.52     |
| 2   | B     | 219[B] | LYS  | CA-C   | 8.92  | 1.65        | 1.52     |
| 2   | B     | 11     | GLU  | CD-OE2 | 8.85  | 1.42        | 1.25     |
| 2   | B     | 44     | GLN  | CA-C   | 8.82  | 1.64        | 1.52     |
| 2   | B     | 303    | GLY  | C-O    | -8.82 | 1.14        | 1.24     |
| 1   | A     | 262    | MET  | CG-SD  | 8.76  | 2.02        | 1.80     |
| 1   | A     | 140    | ARG  | CG-CD  | 8.76  | 1.78        | 1.52     |
| 2   | B     | 363    | ARG  | CA-C   | 8.72  | 1.64        | 1.52     |
| 1   | A     | 56     | ASP  | N-CA   | 8.68  | 1.56        | 1.46     |
| 1   | A     | 174    | THR  | C-O    | 8.67  | 1.34        | 1.24     |
| 2   | B     | 32     | PHE  | CG-CD1 | 8.67  | 1.57        | 1.38     |
| 2   | B     | 107    | ILE  | CA-CB  | 8.65  | 1.65        | 1.54     |
| 2   | B     | 325    | VAL  | CA-C   | -8.65 | 1.45        | 1.52     |
| 1   | A     | 230    | GLY  | CA-C   | 8.64  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 215 | GLN  | CA-C    | 8.62  | 1.64        | 1.52     |
| 2   | B     | 245 | ILE  | N-CA    | 8.62  | 1.56        | 1.46     |
| 2   | B     | 255 | VAL  | C-O     | 8.58  | 1.33        | 1.24     |
| 2   | B     | 132 | ILE  | C-O     | 8.56  | 1.33        | 1.24     |
| 2   | B     | 189 | GLY  | C-O     | -8.51 | 1.18        | 1.24     |
| 2   | B     | 265 | GLY  | CA-C    | 8.50  | 1.63        | 1.51     |
| 2   | B     | 137 | LYS  | CA-CB   | 8.48  | 1.67        | 1.53     |
| 2   | B     | 41  | PHE  | C-O     | 8.44  | 1.33        | 1.24     |
| 2   | B     | 375 | ASN  | N-CA    | 8.42  | 1.56        | 1.46     |
| 2   | B     | 310 | GLY  | N-CA    | 8.41  | 1.56        | 1.44     |
| 1   | A     | 164 | ARG  | N-CA    | -8.40 | 1.36        | 1.46     |
| 2   | B     | 316 | LEU  | C-O     | 8.40  | 1.34        | 1.24     |
| 2   | B     | 99  | LYS  | N-CA    | 8.39  | 1.56        | 1.46     |
| 2   | B     | 252 | LEU  | N-CA    | 8.38  | 1.56        | 1.46     |
| 2   | B     | 134 | MET  | SD-CE   | 8.34  | 2.00        | 1.79     |
| 1   | A     | 123 | VAL  | CA-CB   | 8.34  | 1.63        | 1.54     |
| 2   | B     | 372 | LEU  | CA-C    | 8.33  | 1.62        | 1.52     |
| 1   | A     | 160 | ASP  | C-O     | 8.32  | 1.34        | 1.24     |
| 2   | B     | 359 | LEU  | CA-C    | 8.31  | 1.63        | 1.52     |
| 2   | B     | 311 | PRO  | N-CD    | 8.30  | 1.59        | 1.47     |
| 1   | A     | 13  | ASP  | CA-C    | 8.28  | 1.64        | 1.52     |
| 2   | B     | 50  | LYS  | C-O     | 8.27  | 1.33        | 1.24     |
| 2   | B     | 204 | PHE  | CD1-CE1 | 8.27  | 1.63        | 1.38     |
| 2   | B     | 171 | ASN  | N-CA    | 8.23  | 1.56        | 1.46     |
| 2   | B     | 209 | GLY  | N-CA    | 8.21  | 1.55        | 1.45     |
| 1   | A     | 109 | ASN  | N-CA    | -8.20 | 1.36        | 1.46     |
| 1   | A     | 93  | PRO  | C-O     | -8.19 | 1.14        | 1.24     |
| 1   | A     | 222 | ALA  | N-CA    | -8.12 | 1.35        | 1.46     |
| 2   | B     | 149 | MET  | CG-SD   | 8.12  | 2.01        | 1.80     |
| 2   | B     | 313 | HIS  | N-CA    | 8.10  | 1.56        | 1.46     |
| 2   | B     | 217 | LEU  | CG-CD2  | 8.09  | 1.79        | 1.52     |
| 1   | A     | 71  | ALA  | C-O     | 8.08  | 1.33        | 1.24     |
| 2   | B     | 3   | THR  | CA-C    | -8.08 | 1.42        | 1.52     |
| 2   | B     | 386 | THR  | C-O     | 8.08  | 1.33        | 1.24     |
| 2   | B     | 32  | PHE  | CA-CB   | 8.06  | 1.65        | 1.53     |
| 1   | A     | 11  | LEU  | N-CA    | -8.05 | 1.36        | 1.46     |
| 2   | B     | 284 | ALA  | N-CA    | 8.05  | 1.53        | 1.46     |
| 1   | A     | 126 | VAL  | C-O     | 8.04  | 1.32        | 1.24     |
| 2   | B     | 35  | ALA  | CA-CB   | 8.04  | 1.65        | 1.53     |
| 1   | A     | 206 | ALA  | CA-C    | -7.98 | 1.43        | 1.53     |
| 1   | A     | 69  | LEU  | N-CA    | 7.92  | 1.55        | 1.46     |
| 1   | A     | 197 | ILE  | CA-CB   | 7.92  | 1.64        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 195 | HIS  | N-CA    | -7.92 | 1.35        | 1.45     |
| 1   | A     | 17  | GLY  | C-O     | 7.91  | 1.35        | 1.23     |
| 1   | A     | 2   | GLU  | N-CA    | 7.89  | 1.56        | 1.46     |
| 1   | A     | 210 | GLN  | C-O     | 7.83  | 1.33        | 1.24     |
| 2   | B     | 124 | ALA  | C-O     | 7.82  | 1.33        | 1.24     |
| 2   | B     | 58  | ALA  | CA-C    | 7.81  | 1.63        | 1.53     |
| 2   | B     | 335 | ALA  | CA-CB   | 7.79  | 1.66        | 1.53     |
| 1   | A     | 106 | VAL  | CA-CB   | 7.74  | 1.65        | 1.54     |
| 1   | A     | 117 | ARG  | CG-CD   | 7.74  | 1.75        | 1.52     |
| 2   | B     | 65  | ILE  | CA-CB   | 7.65  | 1.64        | 1.54     |
| 2   | B     | 252 | LEU  | C-O     | 7.65  | 1.33        | 1.24     |
| 1   | A     | 30  | ILE  | CA-CB   | -7.64 | 1.45        | 1.54     |
| 2   | B     | 368 | LYS  | CA-C    | 7.63  | 1.62        | 1.52     |
| 2   | B     | 40  | GLU  | CA-C    | 7.60  | 1.62        | 1.52     |
| 1   | A     | 129 | ALA  | CA-CB   | 7.58  | 1.65        | 1.53     |
| 1   | A     | 82  | PHE  | CD2-CE2 | 7.55  | 1.61        | 1.38     |
| 1   | A     | 62  | PRO  | CA-C    | 7.51  | 1.63        | 1.52     |
| 2   | B     | 377 | SER  | N-CA    | 7.51  | 1.56        | 1.46     |
| 2   | B     | 14  | GLY  | CA-C    | 7.50  | 1.61        | 1.52     |
| 1   | A     | 18  | ALA  | N-CA    | -7.50 | 1.36        | 1.45     |
| 1   | A     | 33  | SER  | CA-C    | 7.50  | 1.62        | 1.52     |
| 2   | B     | 382 | LYS  | N-CA    | -7.49 | 1.36        | 1.46     |
| 1   | A     | 131 | VAL  | C-O     | 7.49  | 1.33        | 1.24     |
| 2   | B     | 60  | THR  | CA-C    | 7.48  | 1.61        | 1.52     |
| 1   | A     | 232 | ILE  | CA-CB   | 7.47  | 1.63        | 1.54     |
| 1   | A     | 140 | ARG  | CA-C    | -7.45 | 1.43        | 1.52     |
| 2   | B     | 97  | LEU  | CG-CD1  | 7.45  | 1.77        | 1.52     |
| 1   | A     | 23  | VAL  | CA-CB   | 7.44  | 1.66        | 1.55     |
| 1   | A     | 37  | ILE  | CA-CB   | 7.43  | 1.64        | 1.54     |
| 1   | A     | 26  | GLY  | CA-C    | -7.43 | 1.41        | 1.51     |
| 2   | B     | 348 | ALA  | CA-C    | 7.43  | 1.62        | 1.52     |
| 2   | B     | 22  | MET  | SD-CE   | -7.42 | 1.61        | 1.79     |
| 2   | B     | 381 | ASP  | N-CA    | 7.41  | 1.55        | 1.46     |
| 2   | B     | 39  | PRO  | N-CD    | 7.39  | 1.58        | 1.47     |
| 2   | B     | 159 | VAL  | CA-CB   | 7.39  | 1.63        | 1.54     |
| 2   | B     | 223 | LEU  | CA-C    | 7.38  | 1.62        | 1.52     |
| 1   | A     | 137 | ALA  | C-O     | 7.38  | 1.31        | 1.24     |
| 1   | A     | 152 | PHE  | CD1-CE1 | 7.38  | 1.60        | 1.38     |
| 2   | B     | 332 | ALA  | N-CA    | 7.36  | 1.55        | 1.46     |
| 1   | A     | 239 | LYS  | CA-CB   | 7.35  | 1.65        | 1.53     |
| 2   | B     | 282 | MET  | SD-CE   | -7.35 | 1.61        | 1.79     |
| 1   | A     | 108 | ASN  | CA-C    | -7.33 | 1.43        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 73  | ALA  | CA-CB   | -7.32 | 1.41        | 1.53     |
| 2   | B     | 55  | ARG  | CA-C    | -7.31 | 1.44        | 1.53     |
| 2   | B     | 376 | LEU  | CG-CD2  | 7.30  | 1.76        | 1.52     |
| 2   | B     | 353 | HIS  | N-CA    | -7.30 | 1.37        | 1.46     |
| 1   | A     | 104 | ASN  | CA-CB   | 7.29  | 1.65        | 1.53     |
| 2   | B     | 168 | ASP  | CA-C    | -7.29 | 1.43        | 1.52     |
| 2   | B     | 139 | VAL  | CB-CG2  | 7.28  | 1.76        | 1.52     |
| 1   | A     | 86  | ALA  | CA-CB   | 7.28  | 1.64        | 1.53     |
| 2   | B     | 378 | GLY  | N-CA    | 7.27  | 1.53        | 1.45     |
| 1   | A     | 219 | GLN  | CA-C    | -7.26 | 1.42        | 1.52     |
| 1   | A     | 102 | TYR  | CD1-CE1 | 7.25  | 1.60        | 1.38     |
| 1   | A     | 5   | GLU  | N-CA    | 7.25  | 1.55        | 1.46     |
| 1   | A     | 127 | LEU  | CA-CB   | 7.24  | 1.63        | 1.53     |
| 2   | B     | 264 | THR  | CA-C    | -7.24 | 1.42        | 1.52     |
| 2   | B     | 129 | LYS  | CA-C    | 7.24  | 1.61        | 1.52     |
| 1   | A     | 97  | ILE  | C-N     | 7.23  | 1.43        | 1.33     |
| 2   | B     | 321 | ARG  | CA-C    | 7.23  | 1.62        | 1.52     |
| 2   | B     | 339 | LEU  | CB-CG   | 7.23  | 1.68        | 1.53     |
| 2   | B     | 311 | PRO  | N-CA    | -7.23 | 1.37        | 1.47     |
| 1   | A     | 20  | VAL  | CA-C    | -7.22 | 1.45        | 1.52     |
| 1   | A     | 20  | VAL  | CA-CB   | 7.22  | 1.63        | 1.54     |
| 2   | B     | 188 | LEU  | C-O     | 7.21  | 1.32        | 1.23     |
| 1   | A     | 241 | ILE  | CA-C    | -7.20 | 1.44        | 1.52     |
| 1   | A     | 163 | LEU  | CA-C    | -7.20 | 1.43        | 1.52     |
| 2   | B     | 363 | ARG  | CB-CG   | 7.19  | 1.74        | 1.52     |
| 2   | B     | 260 | HIS  | C-O     | 7.19  | 1.33        | 1.24     |
| 2   | B     | 69  | THR  | CA-C    | -7.18 | 1.43        | 1.52     |
| 2   | B     | 339 | LEU  | CA-CB   | 7.16  | 1.64        | 1.53     |
| 2   | B     | 51  | ASN  | C-O     | -7.15 | 1.14        | 1.24     |
| 1   | A     | 104 | ASN  | CA-C    | 7.15  | 1.62        | 1.52     |
| 2   | B     | 255 | VAL  | CA-CB   | 7.14  | 1.63        | 1.54     |
| 2   | B     | 368 | LYS  | N-CA    | 7.14  | 1.54        | 1.46     |
| 1   | A     | 105 | LEU  | C-O     | 7.14  | 1.33        | 1.24     |
| 1   | A     | 118 | CYS  | C-O     | -7.13 | 1.15        | 1.24     |
| 1   | A     | 89  | ARG  | C-O     | 7.12  | 1.32        | 1.24     |
| 2   | B     | 339 | LEU  | CA-C    | 7.11  | 1.61        | 1.52     |
| 2   | B     | 271 | LEU  | C-O     | 7.11  | 1.32        | 1.24     |
| 1   | A     | 142 | ALA  | CA-C    | 7.11  | 1.62        | 1.52     |
| 2   | B     | 8   | TYR  | C-O     | 7.10  | 1.33        | 1.23     |
| 2   | B     | 279 | TYR  | CA-C    | 7.10  | 1.61        | 1.52     |
| 2   | B     | 245 | ILE  | C-O     | 7.09  | 1.32        | 1.24     |
| 2   | B     | 76  | LYS  | N-CA    | 7.08  | 1.55        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 240 | MET  | C-O    | 7.08  | 1.32        | 1.24     |
| 2   | B     | 208 | ILE  | CA-C   | 7.08  | 1.61        | 1.52     |
| 2   | B     | 390 | ILE  | C-O    | 7.06  | 1.32        | 1.24     |
| 2   | B     | 57  | THR  | CA-C   | 7.05  | 1.61        | 1.52     |
| 2   | B     | 311 | PRO  | CA-CB  | 7.05  | 1.64        | 1.53     |
| 2   | B     | 323 | ASP  | N-CA   | -7.05 | 1.37        | 1.45     |
| 2   | B     | 59  | LEU  | C-O    | 7.03  | 1.32        | 1.24     |
| 1   | A     | 64  | ILE  | CB-CG1 | 7.03  | 1.67        | 1.53     |
| 1   | A     | 209 | LEU  | N-CA   | 7.03  | 1.54        | 1.46     |
| 1   | A     | 13  | ASP  | N-CA   | 7.03  | 1.55        | 1.46     |
| 2   | B     | 360 | LYS  | CB-CG  | -7.01 | 1.31        | 1.52     |
| 1   | A     | 83  | GLU  | C-O    | 7.00  | 1.32        | 1.24     |
| 1   | A     | 98  | GLY  | N-CA   | 7.00  | 1.53        | 1.45     |
| 2   | B     | 20  | ILE  | N-CA   | 6.98  | 1.55        | 1.46     |
| 2   | B     | 386 | THR  | CA-C   | -6.97 | 1.43        | 1.52     |
| 1   | A     | 143 | ALA  | CA-CB  | 6.97  | 1.64        | 1.53     |
| 1   | A     | 36  | ILE  | CA-CB  | 6.97  | 1.63        | 1.54     |
| 2   | B     | 139 | VAL  | CA-CB  | 6.97  | 1.63        | 1.54     |
| 2   | B     | 363 | ARG  | NE-CZ  | 6.94  | 1.40        | 1.33     |
| 2   | B     | 336 | PHE  | CA-CB  | 6.94  | 1.64        | 1.53     |
| 1   | A     | 174 | THR  | N-CA   | 6.91  | 1.54        | 1.46     |
| 2   | B     | 232 | GLY  | C-O    | -6.91 | 1.14        | 1.23     |
| 1   | A     | 11  | LEU  | C-O    | 6.90  | 1.32        | 1.24     |
| 2   | B     | 250 | VAL  | CA-CB  | 6.90  | 1.62        | 1.54     |
| 2   | B     | 200 | ILE  | C-O    | 6.89  | 1.31        | 1.24     |
| 2   | B     | 344 | GLY  | CA-C   | -6.89 | 1.42        | 1.51     |
| 2   | B     | 87  | LYS  | CA-C   | 6.89  | 1.62        | 1.52     |
| 1   | A     | 209 | LEU  | CA-CB  | 6.88  | 1.64        | 1.53     |
| 2   | B     | 369 | GLU  | C-N    | 6.88  | 1.42        | 1.33     |
| 2   | B     | 274 | GLY  | CA-C   | -6.88 | 1.44        | 1.51     |
| 2   | B     | 341 | ARG  | CD-NE  | 6.87  | 1.55        | 1.46     |
| 2   | B     | 53  | ALA  | CA-CB  | -6.87 | 1.42        | 1.53     |
| 2   | B     | 6   | ASN  | CA-CB  | 6.87  | 1.66        | 1.53     |
| 2   | B     | 45  | PHE  | CE1-CZ | 6.87  | 1.59        | 1.38     |
| 1   | A     | 215 | SER  | CA-C   | 6.84  | 1.61        | 1.52     |
| 2   | B     | 349 | LEU  | C-O    | 6.81  | 1.32        | 1.24     |
| 2   | B     | 100 | ARG  | CZ-NH1 | -6.80 | 1.23        | 1.32     |
| 1   | A     | 147 | ASN  | CA-CB  | 6.79  | 1.63        | 1.53     |
| 2   | B     | 161 | SER  | N-CA   | -6.78 | 1.36        | 1.45     |
| 2   | B     | 89  | ASN  | CG-ND2 | 6.75  | 1.47        | 1.33     |
| 2   | B     | 338 | THR  | CA-CB  | -6.75 | 1.42        | 1.53     |
| 2   | B     | 220 | GLU  | N-CA   | 6.75  | 1.56        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 379 | ARG  | CZ-NH1 | -6.75 | 1.23        | 1.32     |
| 2   | B     | 350 | GLU  | CA-CB  | 6.73  | 1.63        | 1.53     |
| 2   | B     | 347 | PRO  | N-CA   | 6.73  | 1.54        | 1.46     |
| 1   | A     | 70  | ARG  | N-CA   | 6.71  | 1.54        | 1.46     |
| 1   | A     | 231 | ALA  | CA-C   | -6.70 | 1.44        | 1.52     |
| 2   | B     | 33  | VAL  | CA-CB  | 6.70  | 1.62        | 1.54     |
| 1   | A     | 128 | VAL  | CA-CB  | 6.69  | 1.61        | 1.54     |
| 2   | B     | 97  | LEU  | CB-CG  | -6.69 | 1.40        | 1.53     |
| 2   | B     | 134 | MET  | N-CA   | 6.68  | 1.54        | 1.46     |
| 2   | B     | 55  | ARG  | NE-CZ  | 6.68  | 1.40        | 1.33     |
| 1   | A     | 49  | GLU  | CA-C   | 6.68  | 1.60        | 1.52     |
| 2   | B     | 328 | THR  | CA-C   | 6.67  | 1.62        | 1.53     |
| 2   | B     | 311 | PRO  | C-O    | 6.67  | 1.32        | 1.24     |
| 2   | B     | 262 | ILE  | CA-CB  | -6.67 | 1.46        | 1.54     |
| 2   | B     | 156 | VAL  | C-O    | 6.66  | 1.31        | 1.24     |
| 2   | B     | 195 | HIS  | C-O    | -6.66 | 1.15        | 1.24     |
| 1   | A     | 85  | LEU  | CG-CD1 | 6.66  | 1.74        | 1.52     |
| 2   | B     | 305 | ASP  | CA-C   | 6.65  | 1.61        | 1.52     |
| 1   | A     | 83  | GLU  | CA-CB  | 6.65  | 1.63        | 1.53     |
| 2   | B     | 275 | ARG  | CD-NE  | 6.64  | 1.55        | 1.46     |
| 2   | B     | 183 | THR  | CA-C   | 6.64  | 1.61        | 1.52     |
| 1   | A     | 74  | ALA  | C-O    | -6.63 | 1.15        | 1.24     |
| 1   | A     | 221 | SER  | N-CA   | -6.63 | 1.38        | 1.46     |
| 2   | B     | 90  | GLN  | CA-C   | 6.63  | 1.61        | 1.52     |
| 2   | B     | 218 | ASP  | CA-CB  | 6.63  | 1.63        | 1.53     |
| 2   | B     | 193 | GLY  | CA-C   | 6.61  | 1.61        | 1.51     |
| 1   | A     | 139 | PHE  | CA-C   | 6.61  | 1.61        | 1.52     |
| 2   | B     | 218 | ASP  | CA-C   | -6.59 | 1.44        | 1.52     |
| 2   | B     | 61  | LYS  | CA-C   | -6.59 | 1.44        | 1.52     |
| 1   | A     | 25  | LEU  | N-CA   | 6.59  | 1.54        | 1.46     |
| 2   | B     | 287 | MET  | C-N    | -6.57 | 1.25        | 1.33     |
| 2   | B     | 53  | ALA  | N-CA   | 6.57  | 1.54        | 1.46     |
| 1   | A     | 67  | ALA  | N-CA   | 6.57  | 1.54        | 1.46     |
| 1   | A     | 96  | PRO  | C-O    | 6.56  | 1.30        | 1.23     |
| 2   | B     | 237 | ALA  | CA-CB  | 6.56  | 1.63        | 1.53     |
| 1   | A     | 131 | VAL  | CA-CB  | 6.55  | 1.62        | 1.54     |
| 1   | A     | 259 | VAL  | C-O    | 6.55  | 1.31        | 1.24     |
| 2   | B     | 325 | VAL  | C-O    | 6.53  | 1.32        | 1.23     |
| 2   | B     | 341 | ARG  | CZ-NH1 | 6.53  | 1.41        | 1.32     |
| 2   | B     | 249 | SER  | C-O    | -6.53 | 1.15        | 1.24     |
| 1   | A     | 114 | PHE  | C-O    | 6.52  | 1.31        | 1.24     |
| 2   | B     | 318 | SER  | N-CA   | 6.51  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 296 | GLU  | C-O     | -6.51 | 1.15        | 1.23     |
| 1   | A     | 67  | ALA  | CA-CB   | 6.50  | 1.63        | 1.53     |
| 1   | A     | 220 | VAL  | C-N     | 6.50  | 1.42        | 1.33     |
| 1   | A     | 266 | SER  | N-CA    | 6.48  | 1.54        | 1.46     |
| 2   | B     | 287 | MET  | C-O     | -6.46 | 1.16        | 1.24     |
| 1   | A     | 158 | ALA  | CA-CB   | -6.45 | 1.43        | 1.53     |
| 1   | A     | 236 | ALA  | N-CA    | 6.44  | 1.54        | 1.46     |
| 1   | A     | 115 | TYR  | N-CA    | -6.42 | 1.38        | 1.46     |
| 2   | B     | 212 | THR  | CA-CB   | -6.42 | 1.43        | 1.53     |
| 1   | A     | 36  | ILE  | C-O     | -6.40 | 1.16        | 1.24     |
| 1   | A     | 144 | LEU  | CA-CB   | 6.40  | 1.63        | 1.53     |
| 2   | B     | 326 | SER  | N-CA    | -6.38 | 1.38        | 1.45     |
| 2   | B     | 278 | ILE  | CA-CB   | 6.38  | 1.62        | 1.54     |
| 1   | A     | 240 | ILE  | CG1-CD1 | 6.36  | 1.76        | 1.51     |
| 2   | B     | 185 | HIS  | CE1-NE2 | 6.36  | 1.39        | 1.32     |
| 2   | B     | 382 | LYS  | CA-C    | 6.35  | 1.61        | 1.52     |
| 2   | B     | 327 | ILE  | C-O     | 6.35  | 1.30        | 1.24     |
| 2   | B     | 390 | ILE  | CA-C    | -6.34 | 1.45        | 1.52     |
| 1   | A     | 133 | VAL  | CA-CB   | 6.33  | 1.63        | 1.54     |
| 1   | A     | 47  | ALA  | N-CA    | 6.32  | 1.53        | 1.46     |
| 1   | A     | 257 | SER  | C-O     | 6.32  | 1.31        | 1.24     |
| 2   | B     | 304 | LEU  | CA-C    | 6.32  | 1.61        | 1.52     |
| 2   | B     | 268 | GLY  | C-O     | 6.31  | 1.32        | 1.23     |
| 1   | A     | 29  | GLY  | CA-C    | 6.29  | 1.58        | 1.51     |
| 2   | B     | 217 | LEU  | N-CA    | 6.29  | 1.54        | 1.46     |
| 1   | A     | 15  | ARG  | C-O     | 6.27  | 1.32        | 1.23     |
| 2   | B     | 61  | LYS  | CE-NZ   | 6.27  | 1.68        | 1.49     |
| 2   | B     | 45  | PHE  | N-CA    | 6.26  | 1.53        | 1.46     |
| 2   | B     | 312 | GLN  | N-CA    | 6.26  | 1.54        | 1.46     |
| 1   | A     | 73  | ALA  | N-CA    | 6.26  | 1.54        | 1.46     |
| 2   | B     | 296 | GLU  | N-CA    | 6.25  | 1.53        | 1.45     |
| 1   | A     | 14  | ARG  | C-O     | -6.25 | 1.15        | 1.23     |
| 2   | B     | 167 | LYS  | CA-C    | -6.25 | 1.44        | 1.52     |
| 1   | A     | 70  | ARG  | NE-CZ   | -6.24 | 1.26        | 1.33     |
| 2   | B     | 75  | LEU  | C-O     | -6.24 | 1.16        | 1.24     |
| 2   | B     | 234 | GLY  | C-O     | -6.24 | 1.17        | 1.24     |
| 2   | B     | 46  | ALA  | C-O     | 6.23  | 1.31        | 1.24     |
| 1   | A     | 41  | ILE  | CA-C    | 6.22  | 1.60        | 1.52     |
| 1   | A     | 240 | ILE  | CA-CB   | 6.22  | 1.62        | 1.54     |
| 2   | B     | 208 | ILE  | C-O     | -6.22 | 1.17        | 1.24     |
| 2   | B     | 317 | ASN  | C-O     | 6.22  | 1.31        | 1.24     |
| 2   | B     | 19  | GLN  | CA-CB   | 6.22  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 357 | HIS  | CD2-NE2 | 6.22  | 1.44        | 1.37     |
| 1   | A     | 224 | VAL  | CA-C    | -6.20 | 1.44        | 1.52     |
| 1   | A     | 125 | SER  | CA-C    | 6.19  | 1.60        | 1.52     |
| 2   | B     | 206 | ARG  | NE-CZ   | 6.18  | 1.39        | 1.33     |
| 2   | B     | 122 | ALA  | CA-CB   | -6.18 | 1.43        | 1.53     |
| 2   | B     | 192 | ALA  | CA-CB   | 6.17  | 1.64        | 1.53     |
| 2   | B     | 388 | HIS  | CA-C    | -6.17 | 1.45        | 1.52     |
| 2   | B     | 344 | GLY  | C-O     | 6.16  | 1.33        | 1.24     |
| 2   | B     | 51  | ASN  | CG-ND2  | 6.16  | 1.46        | 1.33     |
| 2   | B     | 253 | ILE  | C-O     | 6.16  | 1.30        | 1.24     |
| 2   | B     | 17  | VAL  | CB-CG2  | 6.14  | 1.72        | 1.52     |
| 2   | B     | 126 | LEU  | CA-C    | 6.13  | 1.61        | 1.52     |
| 1   | A     | 145 | ARG  | NE-CZ   | -6.13 | 1.26        | 1.33     |
| 1   | A     | 9   | ALA  | CA-CB   | -6.13 | 1.43        | 1.53     |
| 2   | B     | 206 | ARG  | CZ-NH2  | 6.13  | 1.41        | 1.33     |
| 1   | A     | 236 | ALA  | CA-CB   | -6.12 | 1.43        | 1.53     |
| 2   | B     | 76  | LYS  | CD-CE   | 6.12  | 1.70        | 1.52     |
| 2   | B     | 136 | ALA  | CA-CB   | 6.12  | 1.63        | 1.53     |
| 2   | B     | 206 | ARG  | CB-CG   | -6.12 | 1.34        | 1.52     |
| 2   | B     | 227 | VAL  | C-N     | 6.12  | 1.41        | 1.33     |
| 1   | A     | 120 | GLN  | N-CA    | 6.11  | 1.53        | 1.46     |
| 2   | B     | 363 | ARG  | N-CA    | 6.11  | 1.54        | 1.46     |
| 2   | B     | 58  | ALA  | CA-CB   | 6.11  | 1.63        | 1.53     |
| 1   | A     | 204 | HIS  | CA-C    | 6.10  | 1.60        | 1.53     |
| 2   | B     | 242 | ALA  | C-O     | 6.09  | 1.31        | 1.24     |
| 2   | B     | 240 | MET  | CA-CB   | 6.09  | 1.63        | 1.53     |
| 1   | A     | 266 | SER  | CA-C    | -6.09 | 1.44        | 1.52     |
| 1   | A     | 175 | TYR  | CA-C    | -6.08 | 1.44        | 1.52     |
| 2   | B     | 125 | LEU  | CG-CD2  | 6.08  | 1.72        | 1.52     |
| 2   | B     | 246 | ASN  | C-O     | 6.08  | 1.32        | 1.24     |
| 1   | A     | 260 | SER  | C-O     | 6.07  | 1.31        | 1.24     |
| 2   | B     | 142 | GLN  | N-CA    | 6.07  | 1.54        | 1.46     |
| 2   | B     | 6   | ASN  | C-N     | -6.06 | 1.28        | 1.33     |
| 2   | B     | 256 | GLU  | CD-OE1  | 6.06  | 1.36        | 1.25     |
| 2   | B     | 327 | ILE  | N-CA    | 6.05  | 1.53        | 1.46     |
| 1   | A     | 121 | VAL  | CB-CG2  | 6.03  | 1.72        | 1.52     |
| 2   | B     | 286 | MET  | CA-CB   | 6.03  | 1.66        | 1.54     |
| 2   | B     | 111 | GLY  | N-CA    | 6.02  | 1.49        | 1.45     |
| 2   | B     | 248 | THR  | N-CA    | 6.02  | 1.54        | 1.46     |
| 1   | A     | 131 | VAL  | C-N     | -6.01 | 1.25        | 1.33     |
| 2   | B     | 11  | GLU  | CG-CD   | 6.01  | 1.67        | 1.52     |
| 2   | B     | 346 | ILE  | C-O     | 6.01  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 238 | ILE  | CB-CG2 | 6.00  | 1.72        | 1.52     |
| 2   | B     | 248 | THR  | C-O    | -6.00 | 1.16        | 1.24     |
| 1   | A     | 40  | LEU  | C-O    | -5.99 | 1.17        | 1.24     |
| 1   | A     | 225 | ARG  | NE-CZ  | 5.99  | 1.39        | 1.33     |
| 1   | A     | 50  | LEU  | N-CA   | -5.98 | 1.38        | 1.46     |
| 2   | B     | 130 | CYS  | C-N    | 5.98  | 1.42        | 1.33     |
| 2   | B     | 143 | SER  | CA-CB  | 5.98  | 1.59        | 1.54     |
| 1   | A     | 68  | ASN  | CA-C   | -5.98 | 1.45        | 1.52     |
| 1   | A     | 107 | PHE  | CA-C   | 5.97  | 1.60        | 1.52     |
| 1   | A     | 22  | PHE  | C-O    | 5.97  | 1.30        | 1.23     |
| 2   | B     | 202 | ARG  | CZ-NH2 | 5.97  | 1.41        | 1.33     |
| 2   | B     | 295 | GLU  | CD-OE2 | 5.97  | 1.36        | 1.25     |
| 1   | A     | 143 | ALA  | N-CA   | 5.96  | 1.53        | 1.46     |
| 2   | B     | 189 | GLY  | CA-C   | 5.95  | 1.57        | 1.51     |
| 2   | B     | 150 | ARG  | C-O    | 5.94  | 1.31        | 1.24     |
| 2   | B     | 164 | ALA  | CA-CB  | 5.93  | 1.62        | 1.53     |
| 2   | B     | 270 | PRO  | CA-CB  | 5.92  | 1.62        | 1.53     |
| 2   | B     | 37  | LYS  | CE-NZ  | 5.91  | 1.67        | 1.49     |
| 2   | B     | 117 | VAL  | CB-CG2 | -5.91 | 1.33        | 1.52     |
| 2   | B     | 243 | ASP  | CA-C   | 5.91  | 1.60        | 1.52     |
| 1   | A     | 62  | PRO  | N-CD   | 5.91  | 1.56        | 1.47     |
| 2   | B     | 241 | PHE  | C-N    | 5.91  | 1.41        | 1.33     |
| 1   | A     | 66  | ASN  | C-O    | 5.89  | 1.31        | 1.24     |
| 2   | B     | 86  | HIS  | CA-CB  | 5.87  | 1.63        | 1.53     |
| 2   | B     | 269 | ALA  | C-O    | 5.86  | 1.31        | 1.24     |
| 1   | A     | 92  | HIS  | CA-C   | 5.86  | 1.59        | 1.52     |
| 1   | A     | 76  | VAL  | CA-CB  | -5.85 | 1.47        | 1.54     |
| 2   | B     | 370 | GLN  | CA-C   | 5.85  | 1.60        | 1.52     |
| 2   | B     | 50  | LYS  | CE-NZ  | 5.85  | 1.66        | 1.49     |
| 1   | A     | 126 | VAL  | CB-CG1 | 5.85  | 1.71        | 1.52     |
| 2   | B     | 233 | GLY  | C-N    | 5.85  | 1.40        | 1.33     |
| 2   | B     | 48  | LEU  | N-CA   | 5.84  | 1.53        | 1.46     |
| 1   | A     | 252 | LEU  | CA-C   | -5.83 | 1.45        | 1.52     |
| 2   | B     | 150 | ARG  | CZ-NH2 | 5.83  | 1.41        | 1.33     |
| 2   | B     | 202 | ARG  | N-CA   | 5.83  | 1.53        | 1.46     |
| 1   | A     | 171 | ARG  | CD-NE  | -5.82 | 1.38        | 1.46     |
| 1   | A     | 70  | ARG  | CZ-NH1 | 5.81  | 1.40        | 1.32     |
| 2   | B     | 15  | MET  | SD-CE  | 5.81  | 1.94        | 1.79     |
| 2   | B     | 150 | ARG  | CZ-NH1 | 5.81  | 1.40        | 1.32     |
| 1   | A     | 251 | MET  | N-CA   | 5.81  | 1.53        | 1.46     |
| 2   | B     | 45  | PHE  | CG-CD1 | 5.81  | 1.51        | 1.38     |
| 1   | A     | 91  | LYS  | C-N    | 5.80  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 107 | PHE  | CD2-CE2 | 5.80  | 1.56        | 1.38     |
| 2   | B     | 363 | ARG  | CA-CB   | -5.79 | 1.43        | 1.53     |
| 2   | B     | 324 | TYR  | CA-C    | -5.79 | 1.45        | 1.52     |
| 1   | A     | 84  | MET  | C-O     | 5.78  | 1.30        | 1.24     |
| 2   | B     | 253 | ILE  | CA-CB   | 5.78  | 1.61        | 1.54     |
| 2   | B     | 324 | TYR  | C-O     | 5.78  | 1.31        | 1.24     |
| 2   | B     | 312 | GLN  | CA-C    | 5.77  | 1.60        | 1.52     |
| 2   | B     | 241 | PHE  | C-O     | -5.77 | 1.16        | 1.24     |
| 1   | A     | 49  | GLU  | N-CA    | 5.76  | 1.53        | 1.46     |
| 2   | B     | 86  | HIS  | C-O     | -5.76 | 1.16        | 1.24     |
| 1   | A     | 231 | ALA  | C-N     | 5.75  | 1.40        | 1.33     |
| 2   | B     | 279 | TYR  | CA-CB   | 5.75  | 1.63        | 1.53     |
| 2   | B     | 297 | SER  | CA-C    | 5.75  | 1.59        | 1.52     |
| 2   | B     | 341 | ARG  | C-O     | -5.75 | 1.16        | 1.24     |
| 2   | B     | 123 | SER  | C-O     | 5.75  | 1.30        | 1.24     |
| 2   | B     | 68  | GLY  | C-O     | 5.75  | 1.32        | 1.24     |
| 1   | A     | 168 | SER  | C-O     | -5.74 | 1.17        | 1.24     |
| 2   | B     | 286 | MET  | N-CA    | 5.74  | 1.53        | 1.45     |
| 2   | B     | 177 | TRP  | NE1-CE2 | 5.74  | 1.43        | 1.37     |
| 1   | A     | 261 | ALA  | CA-C    | -5.74 | 1.44        | 1.52     |
| 2   | B     | 57  | THR  | C-O     | -5.74 | 1.17        | 1.23     |
| 1   | A     | 216 | SER  | C-O     | 5.73  | 1.31        | 1.24     |
| 2   | B     | 216 | ILE  | CA-CB   | -5.73 | 1.47        | 1.54     |
| 2   | B     | 360 | LYS  | CA-CB   | 5.72  | 1.62        | 1.53     |
| 1   | A     | 132 | PRO  | CG-CD   | 5.72  | 1.70        | 1.50     |
| 2   | B     | 203 | GLU  | C-N     | 5.71  | 1.41        | 1.33     |
| 2   | B     | 327 | ILE  | CA-CB   | 5.71  | 1.63        | 1.54     |
| 2   | B     | 143 | SER  | C-O     | -5.71 | 1.18        | 1.24     |
| 2   | B     | 356 | ALA  | N-CA    | 5.70  | 1.53        | 1.46     |
| 1   | A     | 262 | MET  | CA-C    | -5.70 | 1.45        | 1.52     |
| 2   | B     | 291 | ASP  | N-CA    | 5.69  | 1.53        | 1.46     |
| 1   | A     | 55  | SER  | CA-CB   | -5.69 | 1.44        | 1.53     |
| 1   | A     | 35  | LYS  | C-O     | -5.69 | 1.17        | 1.24     |
| 1   | A     | 199 | LYS  | C-O     | 5.69  | 1.30        | 1.24     |
| 2   | B     | 337 | LYS  | CA-CB   | 5.69  | 1.62        | 1.53     |
| 1   | A     | 114 | PHE  | CE2-CZ  | 5.68  | 1.55        | 1.38     |
| 1   | A     | 37  | ILE  | CA-C    | 5.67  | 1.61        | 1.52     |
| 2   | B     | 387 | VAL  | CB-CG2  | 5.67  | 1.71        | 1.52     |
| 2   | B     | 167 | LYS  | CE-NZ   | 5.67  | 1.66        | 1.49     |
| 1   | A     | 158 | ALA  | C-O     | 5.67  | 1.31        | 1.23     |
| 2   | B     | 355 | LEU  | C-O     | 5.66  | 1.30        | 1.24     |
| 2   | B     | 244 | PHE  | CA-C    | 5.66  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 318 | SER  | CA-C    | 5.66  | 1.60        | 1.52     |
| 2   | B     | 374 | VAL  | CA-C    | 5.65  | 1.59        | 1.52     |
| 2   | B     | 166 | LEU  | CG-CD1  | 5.65  | 1.71        | 1.52     |
| 2   | B     | 134 | MET  | CA-C    | 5.65  | 1.59        | 1.52     |
| 2   | B     | 358 | ALA  | CA-CB   | 5.64  | 1.62        | 1.53     |
| 2   | B     | 21  | LEU  | CA-C    | 5.64  | 1.60        | 1.52     |
| 2   | B     | 157 | ILE  | CA-CB   | 5.64  | 1.59        | 1.54     |
| 1   | A     | 83  | GLU  | CG-CD   | 5.63  | 1.66        | 1.52     |
| 2   | B     | 165 | THR  | CA-CB   | 5.63  | 1.62        | 1.53     |
| 2   | B     | 69  | THR  | N-CA    | 5.62  | 1.53        | 1.45     |
| 1   | A     | 75  | GLY  | C-O     | -5.62 | 1.16        | 1.24     |
| 2   | B     | 205 | GLN  | CG-CD   | 5.62  | 1.66        | 1.52     |
| 2   | B     | 150 | ARG  | CB-CG   | 5.62  | 1.69        | 1.52     |
| 2   | B     | 235 | SER  | CB-OG   | 5.62  | 1.53        | 1.42     |
| 1   | A     | 148 | ILE  | CA-C    | 5.62  | 1.59        | 1.52     |
| 2   | B     | 104 | SER  | CB-OG   | 5.62  | 1.53        | 1.42     |
| 2   | B     | 30  | GLU  | CA-C    | 5.61  | 1.60        | 1.52     |
| 1   | A     | 54  | PHE  | C-N     | -5.61 | 1.26        | 1.34     |
| 2   | B     | 136 | ALA  | N-CA    | 5.61  | 1.53        | 1.46     |
| 2   | B     | 140 | GLU  | C-O     | 5.60  | 1.30        | 1.24     |
| 2   | B     | 97  | LEU  | CA-CB   | 5.59  | 1.62        | 1.53     |
| 2   | B     | 11  | GLU  | CA-CB   | 5.59  | 1.63        | 1.53     |
| 1   | A     | 244 | ASN  | CA-C    | -5.58 | 1.45        | 1.53     |
| 2   | B     | 242 | ALA  | CA-C    | -5.58 | 1.45        | 1.52     |
| 2   | B     | 295 | GLU  | CG-CD   | 5.57  | 1.66        | 1.52     |
| 2   | B     | 119 | SER  | CA-CB   | 5.57  | 1.62        | 1.53     |
| 1   | A     | 100 | LEU  | N-CA    | 5.56  | 1.53        | 1.46     |
| 2   | B     | 227 | VAL  | N-CA    | 5.56  | 1.52        | 1.46     |
| 1   | A     | 57  | PRO  | C-N     | 5.55  | 1.42        | 1.33     |
| 2   | B     | 206 | ARG  | CA-C    | 5.54  | 1.60        | 1.52     |
| 1   | A     | 13  | ASP  | CB-CG   | 5.53  | 1.65        | 1.52     |
| 2   | B     | 105 | GLU  | CA-C    | 5.53  | 1.59        | 1.52     |
| 2   | B     | 283 | LYS  | CE-NZ   | 5.53  | 1.66        | 1.49     |
| 2   | B     | 200 | ILE  | CB-CG1  | 5.53  | 1.64        | 1.53     |
| 2   | B     | 21  | LEU  | CG-CD2  | 5.53  | 1.70        | 1.52     |
| 2   | B     | 160 | HIS  | N-CA    | 5.53  | 1.53        | 1.45     |
| 1   | A     | 50  | LEU  | CG-CD2  | 5.52  | 1.70        | 1.52     |
| 1   | A     | 77  | THR  | CB-CG2  | 5.51  | 1.70        | 1.52     |
| 1   | A     | 221 | SER  | CA-CB   | 5.51  | 1.62        | 1.53     |
| 2   | B     | 307 | PRO  | CA-CB   | 5.51  | 1.61        | 1.53     |
| 2   | B     | 10  | GLY  | N-CA    | 5.50  | 1.53        | 1.45     |
| 2   | B     | 346 | ILE  | CG1-CD1 | 5.50  | 1.73        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 6   | ASN  | N-CA    | 5.50  | 1.52        | 1.46     |
| 1   | A     | 79  | ALA  | CA-CB   | -5.50 | 1.44        | 1.53     |
| 2   | B     | 10  | GLY  | C-O     | 5.49  | 1.31        | 1.24     |
| 2   | B     | 71  | THR  | CA-C    | 5.49  | 1.59        | 1.52     |
| 1   | A     | 69  | LEU  | C-O     | 5.48  | 1.30        | 1.24     |
| 2   | B     | 284 | ALA  | CA-C    | 5.48  | 1.61        | 1.53     |
| 2   | B     | 2   | THR  | N-CA    | 5.47  | 1.56        | 1.46     |
| 2   | B     | 172 | GLU  | C-N     | 5.47  | 1.41        | 1.33     |
| 1   | A     | 210 | GLN  | CA-C    | -5.46 | 1.45        | 1.52     |
| 2   | B     | 72  | THR  | N-CA    | 5.46  | 1.52        | 1.46     |
| 2   | B     | 308 | SER  | C-O     | 5.46  | 1.30        | 1.24     |
| 2   | B     | 22  | MET  | C-O     | 5.45  | 1.30        | 1.24     |
| 2   | B     | 64  | ASN  | N-CA    | 5.44  | 1.52        | 1.46     |
| 1   | A     | 225 | ARG  | CZ-NH1  | 5.44  | 1.40        | 1.32     |
| 2   | B     | 288 | GLN  | N-CA    | 5.44  | 1.52        | 1.45     |
| 2   | B     | 360 | LYS  | CD-CE   | -5.43 | 1.36        | 1.52     |
| 2   | B     | 145 | ASN  | C-O     | 5.43  | 1.30        | 1.24     |
| 2   | B     | 272 | LYS  | N-CA    | 5.43  | 1.53        | 1.46     |
| 1   | A     | 39  | THR  | C-N     | 5.43  | 1.41        | 1.33     |
| 2   | B     | 186 | TYR  | C-O     | -5.43 | 1.16        | 1.23     |
| 2   | B     | 338 | THR  | C-O     | -5.43 | 1.17        | 1.24     |
| 1   | A     | 93  | PRO  | CA-C    | 5.42  | 1.60        | 1.52     |
| 2   | B     | 170 | CYS  | N-CA    | 5.42  | 1.53        | 1.46     |
| 2   | B     | 32  | PHE  | N-CA    | 5.41  | 1.52        | 1.46     |
| 1   | A     | 83  | GLU  | CD-OE1  | 5.40  | 1.35        | 1.25     |
| 2   | B     | 167 | LYS  | N-CA    | 5.40  | 1.53        | 1.46     |
| 2   | B     | 100 | ARG  | NE-CZ   | -5.40 | 1.27        | 1.33     |
| 2   | B     | 129 | LYS  | C-O     | 5.40  | 1.30        | 1.24     |
| 2   | B     | 349 | LEU  | CA-C    | 5.40  | 1.60        | 1.52     |
| 2   | B     | 6   | ASN  | C-O     | 5.39  | 1.30        | 1.24     |
| 2   | B     | 316 | LEU  | CA-CB   | 5.39  | 1.62        | 1.53     |
| 2   | B     | 175 | ARG  | CB-CG   | 5.39  | 1.68        | 1.52     |
| 2   | B     | 165 | THR  | C-O     | 5.38  | 1.30        | 1.24     |
| 1   | A     | 76  | VAL  | CA-C    | 5.37  | 1.58        | 1.52     |
| 2   | B     | 315 | TYR  | CD2-CE2 | 5.37  | 1.54        | 1.38     |
| 2   | B     | 181 | TYR  | CZ-OH   | 5.36  | 1.49        | 1.38     |
| 2   | B     | 99  | LYS  | C-O     | 5.36  | 1.30        | 1.24     |
| 1   | A     | 214 | ILE  | C-O     | 5.36  | 1.30        | 1.23     |
| 2   | B     | 24  | ALA  | CA-CB   | -5.36 | 1.45        | 1.53     |
| 2   | B     | 145 | ASN  | CA-C    | 5.36  | 1.59        | 1.52     |
| 2   | B     | 69  | THR  | CB-OG1  | 5.35  | 1.52        | 1.43     |
| 2   | B     | 237 | ALA  | CA-C    | 5.35  | 1.59        | 1.52     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | A     | 37     | ILE  | N-CA    | -5.35 | 1.39        | 1.46     |
| 2   | B     | 148    | ARG  | CZ-NH2  | 5.35  | 1.40        | 1.33     |
| 2   | B     | 81     | LEU  | C-O     | -5.34 | 1.17        | 1.23     |
| 2   | B     | 22     | MET  | CA-CB   | 5.34  | 1.61        | 1.53     |
| 2   | B     | 56     | PRO  | C-O     | 5.34  | 1.33        | 1.23     |
| 2   | B     | 70     | ARG  | CA-C    | 5.34  | 1.60        | 1.52     |
| 2   | B     | 341    | ARG  | CZ-NH2  | 5.33  | 1.40        | 1.33     |
| 2   | B     | 147    | PHE  | C-O     | 5.32  | 1.30        | 1.24     |
| 2   | B     | 97     | LEU  | N-CA    | 5.32  | 1.52        | 1.46     |
| 2   | B     | 117    | VAL  | CA-CB   | 5.32  | 1.60        | 1.54     |
| 2   | B     | 13     | GLY  | C-O     | -5.30 | 1.16        | 1.23     |
| 2   | B     | 112    | ALA  | CA-CB   | 5.30  | 1.62        | 1.53     |
| 2   | B     | 61     | LYS  | CA-CB   | 5.30  | 1.61        | 1.53     |
| 2   | B     | 144    | PRO  | N-CA    | 5.28  | 1.54        | 1.47     |
| 1   | A     | 228    | ALA  | N-CA    | 5.28  | 1.52        | 1.45     |
| 2   | B     | 275    | ARG  | CG-CD   | 5.28  | 1.68        | 1.52     |
| 2   | B     | 337    | LYS  | C-O     | 5.28  | 1.30        | 1.24     |
| 1   | A     | 129    | ALA  | CA-C    | 5.27  | 1.59        | 1.52     |
| 1   | A     | 114    | PHE  | CD1-CE1 | 5.26  | 1.54        | 1.38     |
| 1   | A     | 31     | GLU  | CA-C    | 5.26  | 1.59        | 1.52     |
| 2   | B     | 315    | TYR  | CG-CD1  | 5.26  | 1.50        | 1.39     |
| 1   | A     | 87     | LEU  | CB-CG   | 5.26  | 1.64        | 1.53     |
| 2   | B     | 25     | LEU  | C-N     | 5.26  | 1.41        | 1.33     |
| 2   | B     | 273    | HIS  | CB-CG   | -5.25 | 1.42        | 1.50     |
| 2   | B     | 361    | MET  | CB-CG   | 5.24  | 1.68        | 1.52     |
| 1   | A     | 7      | LEU  | N-CA    | -5.24 | 1.40        | 1.46     |
| 2   | B     | 301[A] | SER  | CA-CB   | 5.21  | 1.60        | 1.53     |
| 2   | B     | 301[B] | SER  | CA-CB   | 5.21  | 1.60        | 1.53     |
| 1   | A     | 125    | SER  | CB-OG   | 5.21  | 1.52        | 1.42     |
| 1   | A     | 263    | LYS  | CA-CB   | 5.21  | 1.61        | 1.53     |
| 2   | B     | 226    | ALA  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | A     | 130    | ASP  | N-CA    | 5.20  | 1.52        | 1.46     |
| 2   | B     | 299    | SER  | C-O     | 5.19  | 1.30        | 1.23     |
| 2   | B     | 314    | ALA  | C-N     | 5.19  | 1.41        | 1.33     |
| 2   | B     | 65     | ILE  | CB-CG2  | 5.18  | 1.69        | 1.52     |
| 2   | B     | 97     | LEU  | CA-C    | 5.18  | 1.59        | 1.52     |
| 2   | B     | 111    | GLY  | CA-C    | 5.18  | 1.55        | 1.51     |
| 2   | B     | 252    | LEU  | CA-C    | -5.17 | 1.46        | 1.52     |
| 2   | B     | 361    | MET  | CA-CB   | 5.17  | 1.61        | 1.53     |
| 1   | A     | 22     | PHE  | CA-CB   | 5.17  | 1.61        | 1.53     |
| 2   | B     | 227    | VAL  | C-O     | 5.16  | 1.29        | 1.24     |
| 2   | B     | 48     | LEU  | CA-C    | 5.16  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 188 | LEU  | CG-CD2 | 5.16  | 1.69        | 1.52     |
| 2   | B     | 235 | SER  | CA-CB  | 5.16  | 1.61        | 1.53     |
| 2   | B     | 354 | ALA  | CA-CB  | 5.16  | 1.61        | 1.53     |
| 1   | A     | 12  | ASN  | CB-CG  | 5.15  | 1.65        | 1.52     |
| 2   | B     | 188 | LEU  | CG-CD1 | 5.15  | 1.69        | 1.52     |
| 1   | A     | 50  | LEU  | C-O    | -5.14 | 1.17        | 1.24     |
| 2   | B     | 96  | LEU  | N-CA   | 5.14  | 1.52        | 1.46     |
| 1   | A     | 31  | GLU  | CA-CB  | 5.14  | 1.61        | 1.53     |
| 2   | B     | 242 | ALA  | CA-CB  | 5.14  | 1.61        | 1.53     |
| 2   | B     | 350 | GLU  | C-O    | -5.14 | 1.18        | 1.24     |
| 2   | B     | 353 | HIS  | CA-CB  | 5.14  | 1.61        | 1.53     |
| 2   | B     | 350 | GLU  | N-CA   | 5.14  | 1.52        | 1.46     |
| 2   | B     | 292 | GLY  | C-N    | 5.13  | 1.40        | 1.33     |
| 2   | B     | 76  | LYS  | C-N    | 5.13  | 1.40        | 1.33     |
| 1   | A     | 138 | PRO  | C-N    | 5.12  | 1.40        | 1.33     |
| 1   | A     | 241 | ILE  | CA-CB  | 5.12  | 1.60        | 1.54     |
| 2   | B     | 276 | VAL  | N-CA   | 5.12  | 1.52        | 1.46     |
| 2   | B     | 293 | GLN  | CA-C   | 5.12  | 1.59        | 1.52     |
| 2   | B     | 24  | ALA  | C-O    | 5.12  | 1.29        | 1.24     |
| 1   | A     | 16  | GLU  | N-CA   | 5.11  | 1.52        | 1.45     |
| 2   | B     | 203 | GLU  | C-O    | 5.11  | 1.30        | 1.24     |
| 2   | B     | 42  | GLN  | C-O    | 5.11  | 1.30        | 1.24     |
| 1   | A     | 82  | PHE  | C-N    | -5.11 | 1.27        | 1.33     |
| 1   | A     | 200 | LEU  | C-O    | 5.10  | 1.30        | 1.24     |
| 1   | A     | 116 | ALA  | CA-CB  | 5.10  | 1.61        | 1.53     |
| 2   | B     | 332 | ALA  | CA-C   | -5.10 | 1.46        | 1.52     |
| 2   | B     | 97  | LEU  | CG-CD2 | 5.09  | 1.69        | 1.52     |
| 2   | B     | 186 | TYR  | CA-C   | -5.09 | 1.46        | 1.52     |
| 1   | A     | 66  | ASN  | CA-C   | 5.08  | 1.59        | 1.52     |
| 2   | B     | 46  | ALA  | CA-C   | -5.08 | 1.46        | 1.52     |
| 1   | A     | 163 | LEU  | N-CA   | 5.08  | 1.52        | 1.46     |
| 2   | B     | 144 | PRO  | CB-CG  | 5.07  | 1.75        | 1.49     |
| 2   | B     | 252 | LEU  | CA-CB  | 5.07  | 1.60        | 1.53     |
| 1   | A     | 208 | ALA  | N-CA   | 5.07  | 1.52        | 1.46     |
| 2   | B     | 300 | ILE  | N-CA   | 5.07  | 1.52        | 1.46     |
| 2   | B     | 133 | TYR  | CA-CB  | 5.07  | 1.60        | 1.53     |
| 2   | B     | 62  | CYS  | N-CA   | 5.06  | 1.53        | 1.46     |
| 1   | A     | 212 | PHE  | CA-CB  | 5.05  | 1.62        | 1.53     |
| 2   | B     | 183 | THR  | C-O    | 5.05  | 1.30        | 1.24     |
| 1   | A     | 35  | LYS  | CA-CB  | 5.04  | 1.61        | 1.53     |
| 2   | B     | 229 | ALA  | CA-C   | -5.04 | 1.46        | 1.52     |
| 1   | A     | 29  | GLY  | N-CA   | 5.03  | 1.51        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 276 | VAL  | CB-CG1 | 5.03  | 1.69        | 1.52     |
| 1   | A     | 54  | PHE  | CG-CD2 | 5.03  | 1.49        | 1.38     |
| 1   | A     | 251 | MET  | C-O    | 5.03  | 1.29        | 1.24     |
| 2   | B     | 353 | HIS  | CA-C   | 5.02  | 1.59        | 1.52     |
| 1   | A     | 171 | ARG  | NE-CZ  | -5.02 | 1.27        | 1.33     |
| 2   | B     | 142 | GLN  | CA-C   | 5.02  | 1.60        | 1.52     |
| 1   | A     | 60  | ASP  | CG-OD1 | 5.01  | 1.34        | 1.25     |
| 2   | B     | 208 | ILE  | C-N    | -5.01 | 1.27        | 1.33     |
| 2   | B     | 305 | ASP  | N-CA   | -5.01 | 1.39        | 1.46     |
| 2   | B     | 86  | HIS  | CA-C   | 5.01  | 1.59        | 1.52     |
| 2   | B     | 391 | LEU  | CA-C   | 5.01  | 1.63        | 1.52     |
| 2   | B     | 309 | VAL  | C-O    | 5.00  | 1.29        | 1.23     |

All (443) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | B     | 152 | MET  | CG-SD-CE  | -12.55 | 73.28       | 100.90   |
| 2   | B     | 303 | GLY  | N-CA-C    | 11.53  | 127.35      | 114.67   |
| 1   | A     | 92  | HIS  | CA-C-N    | 10.85  | 131.21      | 119.28   |
| 1   | A     | 92  | HIS  | C-N-CA    | 10.85  | 131.21      | 119.28   |
| 2   | B     | 206 | ARG  | CD-NE-CZ  | 10.33  | 138.86      | 124.40   |
| 1   | A     | 207 | PRO  | CB-CA-C   | -10.30 | 98.04       | 111.23   |
| 2   | B     | 158 | PRO  | CA-C-N    | -10.28 | 109.67      | 123.14   |
| 2   | B     | 158 | PRO  | C-N-CA    | -10.28 | 109.67      | 123.14   |
| 2   | B     | 206 | ARG  | NE-CZ-NH1 | 10.24  | 131.74      | 121.50   |
| 2   | B     | 321 | ARG  | CA-C-O    | -9.71  | 107.91      | 119.27   |
| 2   | B     | 106 | ILE  | CA-C-O    | 9.65   | 130.59      | 120.36   |
| 2   | B     | 373 | VAL  | CA-CB-CG1 | -9.55  | 94.17       | 110.40   |
| 1   | A     | 143 | ALA  | N-CA-C    | -9.54  | 100.86      | 111.07   |
| 2   | B     | 107 | ILE  | CA-C-O    | -9.38  | 110.11      | 120.71   |
| 2   | B     | 138 | ASP  | CA-C-O    | 9.38   | 130.36      | 120.42   |
| 1   | A     | 84  | MET  | N-CA-CB   | 9.27   | 123.76      | 109.94   |
| 2   | B     | 206 | ARG  | NE-CZ-NH2 | -9.26  | 110.86      | 119.20   |
| 2   | B     | 97  | LEU  | N-CA-C    | -9.19  | 101.34      | 111.36   |
| 1   | A     | 136 | SER  | N-CA-C    | 9.19   | 124.29      | 113.18   |
| 2   | B     | 71  | THR  | CA-CB-CG2 | -9.07  | 95.08       | 110.50   |
| 2   | B     | 319 | ILE  | CA-C-O    | 9.04   | 130.87      | 119.48   |
| 1   | A     | 119 | GLU  | N-CA-C    | -9.04  | 101.51      | 111.36   |
| 1   | A     | 86  | ALA  | CA-C-O    | -9.04  | 110.97      | 120.55   |
| 1   | A     | 61  | GLY  | N-CA-C    | 8.86   | 122.63      | 112.00   |
| 2   | B     | 100 | ARG  | NE-CZ-NH2 | 8.81   | 127.13      | 119.20   |
| 1   | A     | 212 | PHE  | CA-C-N    | -8.81  | 104.17      | 121.53   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 212 | PHE  | C-N-CA     | -8.81 | 104.17      | 121.53   |
| 1   | A     | 154 | CYS  | CA-C-O     | 8.80  | 127.68      | 119.59   |
| 2   | B     | 137 | LYS  | N-CA-C     | -8.78 | 100.89      | 111.69   |
| 1   | A     | 54  | PHE  | N-CA-C     | -8.76 | 95.66       | 109.23   |
| 1   | A     | 7   | LEU  | CD1-CG-CD2 | -8.49 | 92.11       | 110.80   |
| 1   | A     | 109 | ASN  | N-CA-CB    | -8.47 | 97.37       | 110.92   |
| 1   | A     | 93  | PRO  | O-C-N      | 8.27  | 132.89      | 122.22   |
| 2   | B     | 6   | ASN  | N-CA-C     | 8.26  | 120.06      | 109.65   |
| 2   | B     | 92  | LEU  | N-CA-C     | -8.23 | 102.26      | 111.14   |
| 2   | B     | 316 | LEU  | CA-C-O     | -8.22 | 110.51      | 119.97   |
| 1   | A     | 51  | GLY  | CA-C-O     | -8.21 | 113.77      | 120.91   |
| 2   | B     | 218 | ASP  | N-CA-C     | 8.20  | 120.22      | 111.28   |
| 2   | B     | 158 | PRO  | N-CD-CG    | -8.19 | 90.91       | 103.20   |
| 2   | B     | 298 | TYR  | CA-CB-CG   | -8.18 | 99.18       | 113.90   |
| 2   | B     | 65  | ILE  | CA-CB-CG1  | -8.17 | 96.52       | 110.40   |
| 1   | A     | 104 | ASN  | CA-CB-CG   | -8.12 | 104.48      | 112.60   |
| 2   | B     | 349 | LEU  | N-CA-C     | -8.10 | 102.66      | 112.54   |
| 2   | B     | 363 | ARG  | CA-C-O     | -8.07 | 110.69      | 119.97   |
| 1   | A     | 103 | ALA  | N-CA-C     | 8.03  | 120.03      | 111.28   |
| 1   | A     | 220 | VAL  | N-CA-C     | -8.03 | 102.99      | 110.53   |
| 2   | B     | 169 | ALA  | N-CA-CB    | -7.95 | 97.95       | 110.28   |
| 2   | B     | 107 | ILE  | N-CA-C     | 7.95  | 120.03      | 108.58   |
| 1   | A     | 97  | ILE  | CA-C-N     | -7.91 | 114.91      | 122.66   |
| 1   | A     | 97  | ILE  | C-N-CA     | -7.91 | 114.91      | 122.66   |
| 2   | B     | 98  | ALA  | N-CA-C     | -7.91 | 102.74      | 111.36   |
| 2   | B     | 55  | ARG  | CD-NE-CZ   | -7.90 | 113.34      | 124.40   |
| 2   | B     | 62  | CYS  | CA-CB-SG   | -7.88 | 96.26       | 114.40   |
| 2   | B     | 119 | SER  | N-CA-C     | -7.85 | 102.34      | 112.23   |
| 1   | A     | 109 | ASN  | N-CA-C     | -7.77 | 103.11      | 112.59   |
| 2   | B     | 58  | ALA  | O-C-N      | 7.74  | 131.81      | 122.75   |
| 1   | A     | 118 | CYS  | N-CA-CB    | -7.71 | 98.79       | 110.12   |
| 2   | B     | 150 | ARG  | NE-CZ-NH1  | -7.65 | 113.85      | 121.50   |
| 2   | B     | 23  | PRO  | O-C-N      | 7.57  | 131.31      | 122.23   |
| 1   | A     | 114 | PHE  | CA-C-O     | -7.56 | 112.88      | 120.82   |
| 1   | A     | 11  | LEU  | N-CA-C     | -7.56 | 103.04      | 111.28   |
| 1   | A     | 60  | ASP  | N-CA-C     | 7.54  | 122.13      | 109.76   |
| 1   | A     | 16  | GLU  | N-CA-CB    | -7.51 | 97.57       | 111.53   |
| 2   | B     | 348 | ALA  | O-C-N      | 7.45  | 131.97      | 122.81   |
| 2   | B     | 72  | THR  | OG1-CB-CG2 | -7.44 | 94.42       | 109.30   |
| 2   | B     | 44  | GLN  | CA-CB-CG   | -7.38 | 99.34       | 114.10   |
| 2   | B     | 208 | ILE  | O-C-N      | 7.37  | 129.13      | 121.91   |
| 1   | A     | 151 | ILE  | CB-CA-C    | -7.30 | 99.71       | 110.81   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 2   | B     | 119    | SER  | N-CA-CB    | -7.29 | 99.07       | 110.30   |
| 2   | B     | 138    | ASP  | O-C-N      | -7.29 | 113.84      | 122.15   |
| 2   | B     | 48     | LEU  | CA-C-N     | -7.29 | 109.94      | 120.29   |
| 2   | B     | 48     | LEU  | C-N-CA     | -7.29 | 109.94      | 120.29   |
| 2   | B     | 219[A] | LYS  | CA-CB-CG   | -7.29 | 99.53       | 114.10   |
| 2   | B     | 219[B] | LYS  | CA-CB-CG   | -7.29 | 99.53       | 114.10   |
| 1   | A     | 127    | LEU  | N-CA-CB    | -7.27 | 99.13       | 110.55   |
| 2   | B     | 164    | ALA  | N-CA-C     | -7.23 | 102.98      | 112.24   |
| 1   | A     | 152    | PHE  | CA-CB-CG   | -7.22 | 106.58      | 113.80   |
| 2   | B     | 359    | LEU  | N-CA-C     | -7.22 | 103.49      | 111.36   |
| 2   | B     | 31     | ALA  | CA-C-O     | 7.20  | 128.19      | 120.55   |
| 2   | B     | 286    | MET  | N-CA-CB    | -7.19 | 99.04       | 111.55   |
| 1   | A     | 26     | GLY  | N-CA-C     | 7.14  | 124.86      | 115.36   |
| 1   | A     | 229    | ALA  | CA-C-N     | -7.12 | 111.08      | 120.91   |
| 1   | A     | 229    | ALA  | C-N-CA     | -7.12 | 111.08      | 120.91   |
| 2   | B     | 132    | ILE  | CB-CG1-CD1 | -7.12 | 98.85       | 113.80   |
| 2   | B     | 65     | ILE  | N-CA-C     | 7.12  | 117.88      | 110.62   |
| 2   | B     | 251    | GLY  | CA-C-O     | -7.10 | 115.19      | 121.58   |
| 2   | B     | 97     | LEU  | CB-CA-C    | -7.09 | 98.80       | 110.85   |
| 2   | B     | 319    | ILE  | N-CA-C     | 7.08  | 120.95      | 112.80   |
| 2   | B     | 215    | GLN  | CA-CB-CG   | -7.07 | 99.96       | 114.10   |
| 1   | A     | 225    | ARG  | NE-CZ-NH2  | -7.05 | 112.85      | 119.20   |
| 2   | B     | 87     | LYS  | N-CA-C     | -7.05 | 103.78      | 112.38   |
| 2   | B     | 366    | PRO  | CA-C-N     | -7.04 | 111.40      | 122.73   |
| 2   | B     | 366    | PRO  | C-N-CA     | -7.04 | 111.40      | 122.73   |
| 1   | A     | 204    | HIS  | N-CA-CB    | -7.03 | 101.51      | 112.13   |
| 2   | B     | 105    | GLU  | CA-C-O     | -7.02 | 112.90      | 121.11   |
| 2   | B     | 157    | ILE  | N-CA-CB    | -6.98 | 101.95      | 111.86   |
| 2   | B     | 226    | ALA  | CA-C-N     | -6.97 | 113.44      | 123.06   |
| 2   | B     | 226    | ALA  | C-N-CA     | -6.97 | 113.44      | 123.06   |
| 2   | B     | 54     | GLY  | O-C-N      | -6.96 | 114.02      | 122.30   |
| 2   | B     | 83     | GLY  | N-CA-C     | -6.96 | 106.16      | 115.21   |
| 2   | B     | 152    | MET  | CB-CG-SD   | -6.94 | 91.88       | 112.70   |
| 2   | B     | 341    | ARG  | N-CA-CB    | -6.92 | 99.64       | 110.44   |
| 2   | B     | 25     | LEU  | CD1-CG-CD2 | -6.92 | 95.57       | 110.80   |
| 1   | A     | 260    | SER  | CA-CB-OG   | -6.92 | 97.26       | 111.10   |
| 2   | B     | 321    | ARG  | O-C-N      | 6.90  | 131.91      | 122.46   |
| 2   | B     | 214    | ALA  | N-CA-C     | -6.88 | 103.84      | 111.82   |
| 2   | B     | 38     | ASP  | CA-C-N     | -6.82 | 112.67      | 119.56   |
| 2   | B     | 38     | ASP  | C-N-CA     | -6.82 | 112.67      | 119.56   |
| 2   | B     | 355    | LEU  | CA-C-O     | -6.81 | 113.20      | 120.42   |
| 2   | B     | 295    | GLU  | CB-CA-C    | -6.79 | 97.50       | 111.22   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 166 | VAL  | CA-C-N     | -6.79 | 110.65      | 120.29   |
| 1   | A     | 166 | VAL  | C-N-CA     | -6.79 | 110.65      | 120.29   |
| 2   | B     | 169 | ALA  | N-CA-C     | 6.77  | 119.68      | 111.82   |
| 2   | B     | 22  | MET  | CA-C-O     | 6.76  | 124.90      | 118.34   |
| 1   | A     | 57  | PRO  | CB-CA-C    | 6.76  | 122.28      | 113.09   |
| 2   | B     | 297 | SER  | O-C-N      | 6.74  | 131.08      | 123.19   |
| 2   | B     | 57  | THR  | CA-C-N     | -6.74 | 109.48      | 120.87   |
| 2   | B     | 57  | THR  | C-N-CA     | -6.74 | 109.48      | 120.87   |
| 2   | B     | 143 | SER  | N-CA-C     | 6.72  | 122.64      | 113.77   |
| 2   | B     | 278 | ILE  | O-C-N      | -6.71 | 116.20      | 123.18   |
| 1   | A     | 79  | ALA  | O-C-N      | -6.71 | 115.11      | 122.09   |
| 2   | B     | 367 | GLU  | N-CA-CB    | -6.70 | 100.71      | 110.70   |
| 1   | A     | 82  | PHE  | CA-CB-CG   | -6.70 | 107.10      | 113.80   |
| 2   | B     | 265 | GLY  | CA-C-O     | -6.69 | 112.33      | 118.95   |
| 2   | B     | 278 | ILE  | CA-C-O     | 6.68  | 127.02      | 120.27   |
| 2   | B     | 248 | THR  | CA-C-O     | -6.66 | 110.40      | 119.05   |
| 2   | B     | 320 | GLY  | CA-C-N     | -6.65 | 109.96      | 121.66   |
| 2   | B     | 320 | GLY  | C-N-CA     | -6.65 | 109.96      | 121.66   |
| 1   | A     | 56  | ASP  | CA-CB-CG   | -6.64 | 105.96      | 112.60   |
| 2   | B     | 286 | MET  | CA-CB-CG   | 6.64  | 127.37      | 114.10   |
| 1   | A     | 157 | ASN  | N-CA-CB    | -6.62 | 100.32      | 110.92   |
| 2   | B     | 367 | GLU  | CB-CA-C    | 6.61  | 121.85      | 110.94   |
| 2   | B     | 150 | ARG  | NH1-CZ-NH2 | 6.61  | 127.89      | 119.30   |
| 2   | B     | 159 | VAL  | CA-CB-CG2  | -6.60 | 99.18       | 110.40   |
| 1   | A     | 155 | PRO  | CB-CA-C    | 6.59  | 118.96      | 110.92   |
| 1   | A     | 194 | HIS  | N-CA-C     | -6.59 | 104.13      | 111.71   |
| 2   | B     | 139 | VAL  | CB-CA-C    | -6.59 | 103.25      | 112.14   |
| 1   | A     | 242 | GLU  | N-CA-C     | -6.58 | 104.03      | 111.07   |
| 1   | A     | 102 | TYR  | CA-CB-CG   | -6.58 | 102.06      | 113.90   |
| 2   | B     | 254 | GLY  | CA-C-N     | -6.57 | 114.36      | 123.10   |
| 2   | B     | 254 | GLY  | C-N-CA     | -6.57 | 114.36      | 123.10   |
| 2   | B     | 118 | ALA  | CA-C-O     | 6.54  | 128.24      | 120.92   |
| 2   | B     | 355 | LEU  | O-C-N      | 6.53  | 129.59      | 122.15   |
| 1   | A     | 260 | SER  | N-CA-C     | 6.52  | 119.22      | 111.33   |
| 2   | B     | 294 | ILE  | CA-C-O     | 6.51  | 129.29      | 121.02   |
| 2   | B     | 34  | SER  | N-CA-C     | 6.48  | 118.35      | 111.28   |
| 2   | B     | 340 | CYS  | CA-C-N     | -6.48 | 110.26      | 121.66   |
| 2   | B     | 340 | CYS  | C-N-CA     | -6.48 | 110.26      | 121.66   |
| 2   | B     | 317 | ASN  | N-CA-CB    | -6.47 | 100.69      | 110.07   |
| 1   | A     | 49  | GLU  | N-CA-C     | -6.44 | 97.78       | 108.34   |
| 2   | B     | 226 | ALA  | O-C-N      | 6.43  | 130.68      | 123.48   |
| 2   | B     | 376 | LEU  | CA-C-O     | 6.42  | 128.77      | 121.58   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 106 | ILE  | O-C-N      | -6.41 | 116.27      | 123.20   |
| 2   | B     | 130 | CYS  | CA-C-N     | -6.41 | 112.75      | 122.81   |
| 2   | B     | 130 | CYS  | C-N-CA     | -6.41 | 112.75      | 122.81   |
| 2   | B     | 44  | GLN  | O-C-N      | 6.41  | 128.67      | 122.07   |
| 1   | A     | 216 | SER  | N-CA-CB    | -6.39 | 104.39      | 111.10   |
| 2   | B     | 241 | PHE  | CA-C-N     | -6.37 | 111.74      | 120.28   |
| 2   | B     | 241 | PHE  | C-N-CA     | -6.37 | 111.74      | 120.28   |
| 2   | B     | 285 | PRO  | CB-CA-C    | -6.37 | 103.55      | 111.64   |
| 1   | A     | 198 | GLU  | CB-CG-CD   | 6.37  | 123.42      | 112.60   |
| 1   | A     | 161 | ASP  | N-CA-C     | -6.36 | 104.43      | 111.36   |
| 1   | A     | 211 | GLY  | O-C-N      | -6.34 | 117.78      | 123.29   |
| 1   | A     | 55  | SER  | CA-C-O     | -6.33 | 112.95      | 120.10   |
| 2   | B     | 303 | GLY  | CA-C-O     | 6.33  | 127.23      | 119.01   |
| 1   | A     | 150 | PRO  | CA-C-N     | -6.31 | 114.96      | 123.10   |
| 1   | A     | 150 | PRO  | C-N-CA     | -6.31 | 114.96      | 123.10   |
| 2   | B     | 363 | ARG  | NE-CZ-NH1  | -6.31 | 115.19      | 121.50   |
| 2   | B     | 280 | PHE  | CA-C-N     | -6.30 | 112.18      | 122.20   |
| 2   | B     | 280 | PHE  | C-N-CA     | -6.30 | 112.18      | 122.20   |
| 2   | B     | 58  | ALA  | CA-C-O     | -6.30 | 114.94      | 121.87   |
| 2   | B     | 284 | ALA  | N-CA-C     | -6.30 | 102.46      | 108.13   |
| 2   | B     | 244 | PHE  | N-CA-C     | -6.29 | 104.87      | 113.30   |
| 1   | A     | 104 | ASN  | N-CA-C     | 6.28  | 119.79      | 111.75   |
| 1   | A     | 138 | PRO  | N-CD-CG    | -6.28 | 93.78       | 103.20   |
| 2   | B     | 158 | PRO  | CA-C-O     | -6.27 | 113.79      | 121.31   |
| 2   | B     | 141 | ARG  | N-CA-C     | 6.25  | 120.91      | 113.16   |
| 1   | A     | 92  | HIS  | O-C-N      | -6.24 | 116.28      | 121.27   |
| 1   | A     | 64  | ILE  | N-CA-C     | 6.22  | 116.97      | 110.62   |
| 1   | A     | 49  | GLU  | CA-CB-CG   | -6.21 | 101.68      | 114.10   |
| 1   | A     | 210 | GLN  | CA-C-N     | -6.21 | 116.94      | 122.47   |
| 1   | A     | 210 | GLN  | C-N-CA     | -6.21 | 116.94      | 122.47   |
| 1   | A     | 231 | ALA  | O-C-N      | -6.20 | 116.07      | 123.27   |
| 2   | B     | 7   | PRO  | CA-C-O     | -6.20 | 111.41      | 118.98   |
| 2   | B     | 128 | LEU  | CA-C-O     | 6.20  | 128.16      | 121.16   |
| 2   | B     | 58  | ALA  | N-CA-C     | 6.20  | 118.55      | 110.43   |
| 2   | B     | 379 | ARG  | NE-CZ-NH2  | 6.20  | 124.78      | 119.20   |
| 2   | B     | 7   | PRO  | O-C-N      | 6.18  | 132.50      | 122.36   |
| 2   | B     | 372 | LEU  | CD1-CG-CD2 | 6.18  | 124.40      | 110.80   |
| 2   | B     | 376 | LEU  | CB-CG-CD2  | -6.13 | 92.30       | 110.70   |
| 2   | B     | 325 | VAL  | CG1-CB-CG2 | -6.13 | 97.32       | 110.80   |
| 2   | B     | 208 | ILE  | CA-C-N     | -6.12 | 113.27      | 120.00   |
| 2   | B     | 208 | ILE  | C-N-CA     | -6.12 | 113.27      | 120.00   |
| 1   | A     | 124 | ASP  | CA-CB-CG   | -6.11 | 106.49      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 45  | PHE  | CD1-CE1-CZ | -6.09 | 109.03      | 120.00   |
| 2   | B     | 362 | MET  | O-C-N      | 6.09  | 128.67      | 122.09   |
| 2   | B     | 106 | ILE  | N-CA-C     | -6.08 | 99.36       | 108.12   |
| 1   | A     | 54  | PHE  | CE1-CZ-CE2 | 6.08  | 130.94      | 120.00   |
| 2   | B     | 72  | THR  | N-CA-CB    | -6.06 | 101.06      | 110.57   |
| 2   | B     | 216 | ILE  | CA-CB-CG2  | 6.05  | 120.79      | 110.50   |
| 1   | A     | 216 | SER  | CA-C-O     | 6.04  | 126.00      | 120.26   |
| 2   | B     | 228 | ILE  | CA-CB-CG1  | -6.04 | 100.14      | 110.40   |
| 2   | B     | 106 | ILE  | CA-C-N     | 6.03  | 130.15      | 122.37   |
| 2   | B     | 106 | ILE  | C-N-CA     | 6.03  | 130.15      | 122.37   |
| 1   | A     | 38  | ASP  | N-CA-C     | -6.02 | 104.83      | 111.82   |
| 2   | B     | 135 | GLY  | CA-C-O     | 6.02  | 126.71      | 121.41   |
| 2   | B     | 309 | VAL  | O-C-N      | 6.02  | 128.21      | 122.97   |
| 2   | B     | 368 | LYS  | N-CA-C     | -6.02 | 100.19      | 109.76   |
| 1   | A     | 31  | GLU  | N-CA-C     | -6.01 | 104.64      | 111.14   |
| 1   | A     | 116 | ALA  | N-CA-C     | 6.01  | 118.63      | 111.71   |
| 2   | B     | 96  | LEU  | N-CA-C     | -6.01 | 104.80      | 111.36   |
| 1   | A     | 10  | GLN  | N-CA-CB    | 6.01  | 118.78      | 110.07   |
| 2   | B     | 98  | ALA  | O-C-N      | 6.00  | 128.99      | 122.15   |
| 1   | A     | 64  | ILE  | CB-CA-C    | 5.99  | 120.23      | 112.14   |
| 1   | A     | 232 | ILE  | N-CA-C     | 5.99  | 116.56      | 108.17   |
| 1   | A     | 256 | ARG  | NE-CZ-NH1  | -5.98 | 115.52      | 121.50   |
| 1   | A     | 106 | VAL  | CA-C-O     | 5.97  | 126.19      | 119.92   |
| 2   | B     | 129 | LYS  | N-CA-CB    | -5.97 | 100.14      | 110.17   |
| 1   | A     | 48  | LEU  | CA-C-O     | 5.96  | 128.09      | 121.11   |
| 2   | B     | 137 | LYS  | CA-C-N     | -5.96 | 111.82      | 120.29   |
| 2   | B     | 137 | LYS  | C-N-CA     | -5.96 | 111.82      | 120.29   |
| 2   | B     | 146 | VAL  | CA-C-N     | -5.96 | 111.25      | 120.31   |
| 2   | B     | 146 | VAL  | C-N-CA     | -5.96 | 111.25      | 120.31   |
| 1   | A     | 52  | VAL  | N-CA-CB    | -5.96 | 102.87      | 111.21   |
| 2   | B     | 292 | GLY  | O-C-N      | -5.95 | 115.48      | 122.38   |
| 2   | B     | 322 | ALA  | N-CA-CB    | -5.95 | 101.56      | 111.20   |
| 2   | B     | 22  | MET  | CA-C-N     | -5.94 | 112.45      | 119.05   |
| 2   | B     | 22  | MET  | C-N-CA     | -5.94 | 112.45      | 119.05   |
| 1   | A     | 7   | LEU  | N-CA-C     | 5.94  | 118.24      | 111.11   |
| 2   | B     | 40  | GLU  | N-CA-C     | -5.93 | 104.90      | 111.36   |
| 1   | A     | 140 | ARG  | CG-CD-NE   | -5.91 | 98.99       | 112.00   |
| 1   | A     | 15  | ARG  | CA-C-N     | -5.91 | 112.54      | 122.29   |
| 1   | A     | 15  | ARG  | C-N-CA     | -5.91 | 112.54      | 122.29   |
| 1   | A     | 122 | GLY  | CA-C-O     | 5.90  | 125.24      | 118.98   |
| 2   | B     | 44  | GLN  | N-CA-C     | -5.90 | 104.75      | 111.07   |
| 1   | A     | 87  | LEU  | CA-CB-CG   | 5.89  | 136.92      | 116.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 304 | LEU  | CA-C-O     | -5.87 | 112.57      | 120.15   |
| 1   | A     | 163 | LEU  | N-CA-C     | 5.86  | 118.43      | 111.33   |
| 2   | B     | 244 | PHE  | CA-C-N     | -5.86 | 112.44      | 120.46   |
| 2   | B     | 244 | PHE  | C-N-CA     | -5.86 | 112.44      | 120.46   |
| 2   | B     | 56  | PRO  | N-CA-CB    | -5.84 | 96.17       | 102.60   |
| 2   | B     | 61  | LYS  | CA-CB-CG   | -5.84 | 102.41      | 114.10   |
| 1   | A     | 166 | VAL  | N-CA-C     | -5.83 | 104.68      | 110.62   |
| 2   | B     | 227 | VAL  | N-CA-C     | -5.83 | 100.09      | 108.48   |
| 2   | B     | 386 | THR  | O-C-N      | -5.82 | 115.51      | 122.15   |
| 2   | B     | 390 | ILE  | CB-CA-C    | -5.82 | 104.40      | 112.02   |
| 2   | B     | 367 | GLU  | N-CA-C     | 5.81  | 119.35      | 112.72   |
| 2   | B     | 309 | VAL  | CA-C-N     | -5.81 | 112.75      | 121.87   |
| 2   | B     | 309 | VAL  | C-N-CA     | -5.81 | 112.75      | 121.87   |
| 1   | A     | 35  | LYS  | CG-CD-CE   | 5.81  | 124.66      | 111.30   |
| 2   | B     | 152 | MET  | CA-CB-CG   | -5.80 | 102.49      | 114.10   |
| 2   | B     | 158 | PRO  | CA-CB-CG   | -5.80 | 93.48       | 104.50   |
| 1   | A     | 32  | GLN  | N-CA-CB    | 5.78  | 118.61      | 110.12   |
| 2   | B     | 364 | GLU  | CA-C-O     | -5.76 | 113.34      | 119.97   |
| 1   | A     | 3   | ARG  | N-CA-C     | -5.75 | 105.15      | 111.82   |
| 2   | B     | 326 | SER  | N-CA-C     | 5.75  | 118.93      | 109.85   |
| 1   | A     | 156 | PRO  | CB-CA-C    | -5.74 | 103.26      | 112.21   |
| 2   | B     | 58  | ALA  | CA-C-N     | -5.74 | 114.69      | 123.07   |
| 2   | B     | 58  | ALA  | C-N-CA     | -5.74 | 114.69      | 123.07   |
| 2   | B     | 69  | THR  | O-C-N      | -5.74 | 115.08      | 122.94   |
| 2   | B     | 238 | ILE  | N-CA-C     | -5.73 | 103.92      | 111.09   |
| 1   | A     | 127 | LEU  | CA-C-N     | -5.73 | 115.57      | 122.90   |
| 1   | A     | 127 | LEU  | C-N-CA     | -5.73 | 115.57      | 122.90   |
| 1   | A     | 72  | PHE  | N-CA-C     | -5.72 | 105.13      | 111.36   |
| 1   | A     | 206 | ALA  | CA-C-N     | -5.70 | 113.91      | 119.78   |
| 1   | A     | 206 | ALA  | C-N-CA     | -5.70 | 113.91      | 119.78   |
| 2   | B     | 148 | ARG  | CG-CD-NE   | 5.69  | 124.53      | 112.00   |
| 2   | B     | 82  | HIS  | CA-C-O     | -5.68 | 115.54      | 120.88   |
| 2   | B     | 202 | ARG  | CD-NE-CZ   | -5.67 | 116.46      | 124.40   |
| 1   | A     | 63  | THR  | OG1-CB-CG2 | -5.67 | 97.96       | 109.30   |
| 2   | B     | 388 | HIS  | CA-C-N     | 5.67  | 128.92      | 120.31   |
| 2   | B     | 388 | HIS  | C-N-CA     | 5.67  | 128.92      | 120.31   |
| 2   | B     | 53  | ALA  | N-CA-C     | 5.65  | 120.24      | 113.23   |
| 2   | B     | 132 | ILE  | O-C-N      | -5.64 | 117.17      | 123.26   |
| 2   | B     | 387 | VAL  | N-CA-C     | -5.63 | 104.16      | 112.04   |
| 2   | B     | 92  | LEU  | O-C-N      | -5.63 | 116.01      | 122.09   |
| 2   | B     | 373 | VAL  | N-CA-CB    | -5.62 | 103.66      | 111.41   |
| 1   | A     | 10  | GLN  | CA-C-O     | -5.61 | 114.92      | 120.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 321 | ARG  | CB-CA-C    | -5.61 | 98.17       | 109.55   |
| 1   | A     | 222 | ALA  | CA-C-N     | -5.61 | 112.77      | 120.28   |
| 1   | A     | 222 | ALA  | C-N-CA     | -5.61 | 112.77      | 120.28   |
| 1   | A     | 12  | ASN  | N-CA-C     | -5.60 | 105.17      | 112.23   |
| 2   | B     | 283 | LYS  | N-CA-C     | -5.60 | 99.39       | 108.52   |
| 1   | A     | 229 | ALA  | N-CA-C     | -5.59 | 106.45      | 113.28   |
| 2   | B     | 293 | GLN  | CA-C-O     | -5.59 | 114.65      | 121.36   |
| 2   | B     | 385 | PHE  | CB-CA-C    | -5.59 | 98.43       | 109.67   |
| 2   | B     | 388 | HIS  | N-CA-CB    | 5.59  | 118.17      | 110.07   |
| 2   | B     | 251 | GLY  | O-C-N      | 5.59  | 128.59      | 122.84   |
| 2   | B     | 168 | ASP  | CA-CB-CG   | -5.58 | 107.02      | 112.60   |
| 2   | B     | 176 | ASP  | N-CA-CB    | -5.58 | 101.91      | 110.16   |
| 2   | B     | 54  | GLY  | CA-C-N     | 5.57  | 129.15      | 120.68   |
| 2   | B     | 54  | GLY  | C-N-CA     | 5.57  | 129.15      | 120.68   |
| 1   | A     | 135 | GLU  | CB-CA-C    | -5.57 | 101.31      | 110.72   |
| 2   | B     | 87  | LYS  | O-C-N      | 5.56  | 129.61      | 122.39   |
| 1   | A     | 199 | LYS  | N-CA-C     | 5.54  | 117.00      | 111.07   |
| 2   | B     | 188 | LEU  | CA-C-N     | -5.54 | 113.88      | 122.30   |
| 2   | B     | 188 | LEU  | C-N-CA     | -5.54 | 113.88      | 122.30   |
| 2   | B     | 304 | LEU  | O-C-N      | 5.54  | 129.34      | 122.19   |
| 2   | B     | 74  | TYR  | N-CA-CB    | -5.54 | 102.32      | 110.85   |
| 2   | B     | 306 | PHE  | O-C-N      | -5.54 | 116.03      | 121.18   |
| 1   | A     | 87  | LEU  | CA-C-O     | -5.52 | 114.56      | 120.42   |
| 1   | A     | 155 | PRO  | CA-C-N     | 5.52  | 125.35      | 119.28   |
| 1   | A     | 155 | PRO  | C-N-CA     | 5.52  | 125.35      | 119.28   |
| 1   | A     | 259 | VAL  | N-CA-C     | 5.52  | 116.25      | 110.62   |
| 2   | B     | 166 | LEU  | CD1-CG-CD2 | -5.51 | 98.67       | 110.80   |
| 2   | B     | 231 | VAL  | CB-CA-C    | 5.51  | 117.21      | 111.09   |
| 1   | A     | 177 | LEU  | N-CA-C     | 5.50  | 126.41      | 111.00   |
| 2   | B     | 122 | ALA  | N-CA-C     | -5.50 | 105.36      | 111.36   |
| 2   | B     | 390 | ILE  | N-CA-C     | -5.50 | 105.36      | 110.53   |
| 1   | A     | 199 | LYS  | N-CA-CB    | 5.49  | 117.97      | 110.01   |
| 2   | B     | 63  | GLN  | N-CA-C     | 5.49  | 118.18      | 111.82   |
| 2   | B     | 33  | VAL  | O-C-N      | 5.48  | 127.19      | 121.87   |
| 2   | B     | 153 | GLY  | CA-C-N     | -5.47 | 112.31      | 121.39   |
| 2   | B     | 153 | GLY  | C-N-CA     | -5.47 | 112.31      | 121.39   |
| 2   | B     | 105 | GLU  | O-C-N      | 5.45  | 129.94      | 123.24   |
| 1   | A     | 148 | ILE  | CB-CA-C    | -5.44 | 102.55      | 110.81   |
| 2   | B     | 297 | SER  | N-CA-C     | -5.43 | 100.85      | 109.76   |
| 1   | A     | 55  | SER  | N-CA-C     | -5.41 | 105.48      | 111.71   |
| 2   | B     | 170 | CYS  | N-CA-C     | -5.41 | 105.49      | 111.71   |
| 2   | B     | 341 | ARG  | CG-CD-NE   | 5.41  | 123.91      | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 345 | ILE  | CA-C-N     | -5.41 | 116.69      | 122.85   |
| 2   | B     | 345 | ILE  | C-N-CA     | -5.41 | 116.69      | 122.85   |
| 1   | A     | 55  | SER  | CA-C-N     | -5.40 | 116.62      | 123.15   |
| 1   | A     | 55  | SER  | C-N-CA     | -5.40 | 116.62      | 123.15   |
| 1   | A     | 130 | ASP  | CA-CB-CG   | 5.40  | 118.00      | 112.60   |
| 2   | B     | 48  | LEU  | O-C-N      | 5.39  | 128.30      | 122.15   |
| 2   | B     | 198 | PRO  | CA-N-CD    | 5.39  | 119.55      | 112.00   |
| 1   | A     | 47  | ALA  | N-CA-C     | -5.39 | 100.73      | 108.60   |
| 1   | A     | 214 | ILE  | N-CA-CB    | -5.39 | 106.08      | 111.90   |
| 2   | B     | 61  | LYS  | CG-CD-CE   | 5.38  | 123.68      | 111.30   |
| 1   | A     | 255 | LEU  | CB-CG-CD2  | -5.36 | 94.63       | 110.70   |
| 2   | B     | 266 | GLU  | N-CA-CB    | -5.34 | 101.66      | 110.53   |
| 1   | A     | 197 | ILE  | O-C-N      | -5.34 | 116.33      | 121.83   |
| 1   | A     | 238 | VAL  | CA-CB-CG2  | -5.34 | 101.32      | 110.40   |
| 2   | B     | 176 | ASP  | CB-CG-OD2  | 5.34  | 130.68      | 118.40   |
| 1   | A     | 232 | ILE  | O-C-N      | -5.33 | 117.58      | 123.18   |
| 1   | A     | 255 | LEU  | CA-C-O     | -5.33 | 114.90      | 120.55   |
| 2   | B     | 158 | PRO  | CB-CA-C    | -5.33 | 104.12      | 111.21   |
| 1   | A     | 8   | PHE  | N-CA-C     | -5.33 | 105.52      | 112.23   |
| 1   | A     | 93  | PRO  | N-CD-CG    | -5.32 | 95.22       | 103.20   |
| 2   | B     | 365 | GLN  | CA-C-O     | 5.32  | 127.13      | 121.28   |
| 2   | B     | 334 | GLU  | N-CA-C     | 5.31  | 117.07      | 111.28   |
| 1   | A     | 106 | VAL  | O-C-N      | -5.31 | 114.07      | 122.04   |
| 1   | A     | 218 | GLU  | CA-C-O     | 5.30  | 125.90      | 119.38   |
| 1   | A     | 103 | ALA  | CA-C-N     | -5.30 | 112.65      | 120.38   |
| 1   | A     | 103 | ALA  | C-N-CA     | -5.30 | 112.65      | 120.38   |
| 2   | B     | 361 | MET  | CA-CB-CG   | -5.30 | 103.51      | 114.10   |
| 2   | B     | 89  | ASN  | CB-CA-C    | -5.29 | 102.01      | 110.79   |
| 2   | B     | 215 | GLN  | N-CA-C     | -5.28 | 105.19      | 111.69   |
| 2   | B     | 317 | ASN  | OD1-CG-ND2 | 5.28  | 127.88      | 122.60   |
| 2   | B     | 51  | ASN  | CA-C-O     | -5.28 | 112.90      | 119.18   |
| 1   | A     | 214 | ILE  | CB-CA-C    | -5.28 | 106.21      | 111.80   |
| 2   | B     | 17  | VAL  | CA-C-N     | -5.28 | 114.35      | 119.78   |
| 2   | B     | 17  | VAL  | C-N-CA     | -5.28 | 114.35      | 119.78   |
| 2   | B     | 87  | LYS  | CB-CG-CD   | -5.27 | 99.17       | 111.30   |
| 2   | B     | 40  | GLU  | N-CA-CB    | 5.27  | 117.96      | 110.16   |
| 2   | B     | 132 | ILE  | N-CA-C     | 5.27  | 115.48      | 108.11   |
| 2   | B     | 348 | ALA  | CA-C-O     | -5.27 | 115.97      | 121.55   |
| 2   | B     | 258 | GLY  | CA-C-N     | 5.26  | 129.14      | 120.25   |
| 2   | B     | 258 | GLY  | C-N-CA     | 5.26  | 129.14      | 120.25   |
| 1   | A     | 215 | SER  | N-CA-C     | 5.24  | 119.43      | 112.30   |
| 1   | A     | 228 | ALA  | O-C-N      | -5.24 | 116.81      | 122.79   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 124 | ASP  | N-CA-CB    | -5.23 | 103.40      | 110.67   |
| 2   | B     | 351 | SER  | O-C-N      | 5.23  | 127.66      | 122.12   |
| 1   | A     | 109 | ASN  | CA-C-O     | -5.22 | 113.78      | 119.95   |
| 2   | B     | 242 | ALA  | N-CA-CB    | -5.22 | 102.44      | 110.12   |
| 1   | A     | 100 | LEU  | CD1-CG-CD2 | -5.22 | 99.31       | 110.80   |
| 2   | B     | 48  | LEU  | N-CA-C     | -5.21 | 105.68      | 111.36   |
| 2   | B     | 101 | MET  | N-CA-C     | -5.21 | 106.77      | 113.02   |
| 1   | A     | 66  | ASN  | CA-C-N     | -5.20 | 113.31      | 120.28   |
| 1   | A     | 66  | ASN  | C-N-CA     | -5.20 | 113.31      | 120.28   |
| 1   | A     | 218 | GLU  | CA-C-N     | -5.20 | 112.51      | 121.66   |
| 1   | A     | 218 | GLU  | C-N-CA     | -5.20 | 112.51      | 121.66   |
| 2   | B     | 158 | PRO  | N-CA-C     | 5.20  | 119.35      | 111.19   |
| 1   | A     | 59  | ALA  | CB-CA-C    | -5.20 | 101.70      | 110.64   |
| 2   | B     | 134 | MET  | CB-CG-SD   | -5.19 | 97.12       | 112.70   |
| 1   | A     | 242 | GLU  | CB-CA-C    | -5.19 | 102.73      | 110.88   |
| 2   | B     | 337 | LYS  | CB-CA-C    | -5.19 | 102.03      | 110.85   |
| 2   | B     | 14  | GLY  | O-C-N      | 5.18  | 128.74      | 122.98   |
| 2   | B     | 81  | LEU  | O-C-N      | 5.18  | 128.98      | 122.86   |
| 2   | B     | 149 | MET  | CA-C-N     | -5.18 | 112.93      | 120.29   |
| 2   | B     | 149 | MET  | C-N-CA     | -5.18 | 112.93      | 120.29   |
| 2   | B     | 183 | THR  | CB-CA-C    | -5.18 | 100.97      | 109.99   |
| 1   | A     | 82  | PHE  | CZ-CE2-CD2 | -5.18 | 110.68      | 120.00   |
| 2   | B     | 343 | GLU  | CB-CG-CD   | 5.17  | 121.40      | 112.60   |
| 1   | A     | 93  | PRO  | N-CA-C     | 5.16  | 120.62      | 113.65   |
| 2   | B     | 77  | ARG  | N-CA-C     | 5.16  | 117.15      | 110.65   |
| 2   | B     | 204 | PHE  | CD1-CE1-CZ | -5.16 | 110.72      | 120.00   |
| 1   | A     | 247 | SER  | CA-C-O     | 5.15  | 126.21      | 120.34   |
| 1   | A     | 9   | ALA  | N-CA-C     | -5.15 | 105.75      | 111.36   |
| 2   | B     | 170 | CYS  | CB-CA-C    | -5.15 | 101.11      | 110.63   |
| 2   | B     | 71  | THR  | N-CA-C     | -5.14 | 100.93      | 109.46   |
| 2   | B     | 293 | GLN  | CA-C-N     | -5.13 | 114.30      | 122.50   |
| 2   | B     | 293 | GLN  | C-N-CA     | -5.13 | 114.30      | 122.50   |
| 2   | B     | 57  | THR  | O-C-N      | 5.13  | 129.00      | 123.10   |
| 2   | B     | 190 | THR  | CA-C-O     | -5.12 | 115.86      | 121.14   |
| 2   | B     | 5   | LEU  | CA-C-O     | 5.12  | 127.43      | 121.44   |
| 2   | B     | 255 | VAL  | N-CA-CB    | -5.12 | 104.98      | 111.64   |
| 2   | B     | 298 | TYR  | CE1-CZ-CE2 | 5.12  | 130.54      | 120.30   |
| 2   | B     | 70  | ARG  | CA-CB-CG   | -5.12 | 103.87      | 114.10   |
| 2   | B     | 138 | ASP  | CA-C-N     | -5.11 | 113.46      | 120.46   |
| 2   | B     | 138 | ASP  | C-N-CA     | -5.11 | 113.46      | 120.46   |
| 2   | B     | 76  | LYS  | CA-C-N     | -5.11 | 114.79      | 122.24   |
| 2   | B     | 76  | LYS  | C-N-CA     | -5.11 | 114.79      | 122.24   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | A     | 220    | VAL  | CA-C-O     | 5.10  | 126.71      | 121.05   |
| 2   | B     | 34     | SER  | CA-C-O     | 5.10  | 125.95      | 120.55   |
| 2   | B     | 285    | PRO  | CA-C-O     | -5.10 | 115.77      | 121.32   |
| 2   | B     | 317    | ASN  | CA-CB-CG   | -5.10 | 107.50      | 112.60   |
| 2   | B     | 168    | ASP  | CA-C-N     | -5.09 | 112.57      | 120.31   |
| 2   | B     | 168    | ASP  | C-N-CA     | -5.09 | 112.57      | 120.31   |
| 2   | B     | 388    | HIS  | N-CA-C     | 5.09  | 116.64      | 111.14   |
| 2   | B     | 222    | ARG  | NE-CZ-NH1  | -5.09 | 116.41      | 121.50   |
| 2   | B     | 263    | GLU  | CG-CD-OE2  | -5.08 | 106.71      | 118.40   |
| 1   | A     | 162    | LEU  | CA-C-N     | -5.08 | 113.42      | 120.38   |
| 1   | A     | 162    | LEU  | C-N-CA     | -5.08 | 113.42      | 120.38   |
| 2   | B     | 19     | GLN  | CA-C-N     | -5.08 | 113.21      | 121.54   |
| 2   | B     | 19     | GLN  | C-N-CA     | -5.08 | 113.21      | 121.54   |
| 1   | A     | 216    | SER  | CB-CA-C    | -5.08 | 103.52      | 110.22   |
| 2   | B     | 199    | THR  | N-CA-C     | 5.08  | 116.62      | 111.14   |
| 1   | A     | 75     | GLY  | N-CA-C     | -5.07 | 108.24      | 115.64   |
| 2   | B     | 198    | PRO  | N-CD-CG    | -5.06 | 95.61       | 103.20   |
| 2   | B     | 281    | GLY  | CA-C-N     | -5.06 | 113.57      | 121.87   |
| 2   | B     | 281    | GLY  | C-N-CA     | -5.06 | 113.57      | 121.87   |
| 2   | B     | 242    | ALA  | CA-C-O     | -5.06 | 115.19      | 120.55   |
| 1   | A     | 243    | LYS  | N-CA-C     | 5.06  | 118.55      | 112.38   |
| 1   | A     | 197    | ILE  | CG1-CB-CG2 | -5.05 | 95.53       | 110.70   |
| 2   | B     | 70     | ARG  | O-C-N      | 5.05  | 128.71      | 122.19   |
| 2   | B     | 46     | ALA  | CA-C-N     | -5.04 | 113.13      | 120.29   |
| 2   | B     | 46     | ALA  | C-N-CA     | -5.04 | 113.13      | 120.29   |
| 2   | B     | 229    | ALA  | O-C-N      | -5.04 | 117.23      | 123.33   |
| 2   | B     | 65     | ILE  | N-CA-CB    | -5.04 | 103.69      | 110.54   |
| 2   | B     | 368    | LYS  | CA-CB-CG   | -5.03 | 104.03      | 114.10   |
| 1   | A     | 99     | LEU  | CD1-CG-CD2 | 5.03  | 121.86      | 110.80   |
| 2   | B     | 132    | ILE  | N-CA-CB    | -5.02 | 104.48      | 111.41   |
| 1   | A     | 175    | TYR  | CA-C-N     | -5.02 | 116.09      | 122.77   |
| 1   | A     | 175    | TYR  | C-N-CA     | -5.02 | 116.09      | 122.77   |
| 2   | B     | 16     | TYR  | CA-C-N     | -5.02 | 114.86      | 122.24   |
| 2   | B     | 16     | TYR  | C-N-CA     | -5.02 | 114.86      | 122.24   |
| 2   | B     | 301[A] | SER  | O-C-N      | -5.02 | 117.36      | 123.13   |
| 2   | B     | 301[B] | SER  | O-C-N      | -5.02 | 117.36      | 123.13   |
| 2   | B     | 81     | LEU  | CA-C-N     | -5.00 | 113.31      | 121.97   |
| 2   | B     | 81     | LEU  | C-N-CA     | -5.00 | 113.31      | 121.97   |
| 2   | B     | 322    | ALA  | CA-C-O     | -5.00 | 115.61      | 121.46   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 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     | 1917  | 0        | 1927     | 46      | 0            |
| 2   | B     | 2959  | 0        | 2933     | 69      | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 15    | 0        | 7        | 1       | 0            |
| 5   | A     | 139   | 0        | 0        | 2       | 0            |
| 5   | B     | 295   | 0        | 0        | 2       | 0            |
| All | All   | 5326  | 0        | 4867     | 113     | 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 12.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:240:ILE:CD1 | 1:A:240:ILE:CG1  | 1.76                     | 1.64              |
| 1:A:111:ILE:CA  | 1:A:111:ILE:CB   | 1.75                     | 1.62              |
| 2:B:217:LEU:CD2 | 2:B:217:LEU:CG   | 1.79                     | 1.61              |
| 1:A:85:LEU:CG   | 1:A:85:LEU:CD1   | 1.74                     | 1.59              |
| 1:A:140:ARG:CD  | 1:A:140:ARG:CG   | 1.78                     | 1.58              |
| 1:A:117:ARG:CG  | 1:A:117:ARG:CD   | 1.75                     | 1.58              |
| 2:B:376:LEU:CD2 | 2:B:376:LEU:CG   | 1.76                     | 1.57              |
| 2:B:139:VAL:CB  | 2:B:139:VAL:CG2  | 1.76                     | 1.57              |
| 2:B:97:LEU:CD1  | 2:B:97:LEU:CG    | 1.77                     | 1.56              |
| 2:B:63:GLN:CD   | 2:B:63:GLN:CG    | 1.74                     | 1.55              |
| 2:B:390:ILE:CG2 | 2:B:390:ILE:CB   | 1.86                     | 1.52              |
| 2:B:61:LYS:CE   | 2:B:61:LYS:NZ    | 1.68                     | 1.51              |
| 2:B:144:PRO:CG  | 2:B:144:PRO:CB   | 1.75                     | 1.50              |
| 1:A:262:MET:CG  | 1:A:262:MET:SD   | 2.02                     | 1.47              |
| 2:B:376:LEU:CD2 | 2:B:376:LEU:CB   | 2.37                     | 1.02              |
| 1:A:193:LEU:HG  | 1:A:197:ILE:HD12 | 1.54                     | 0.86              |
| 2:B:97:LEU:CD1  | 2:B:97:LEU:CB    | 2.53                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:337:LYS:HE3  | 2:B:391:LEU:HD21 | 1.58                     | 0.84              |
| 2:B:61:LYS:NZ    | 2:B:61:LYS:CD    | 2.44                     | 0.80              |
| 1:A:211:GLY:O    | 1:A:212:PHE:CB   | 2.29                     | 0.80              |
| 1:A:262:MET:SD   | 1:A:262:MET:CB   | 2.71                     | 0.79              |
| 2:B:182:GLU:HG3  | 5:B:738:HOH:O    | 1.80                     | 0.79              |
| 1:A:85:LEU:CD1   | 1:A:85:LEU:CD2   | 2.63                     | 0.77              |
| 1:A:140:ARG:CG   | 1:A:140:ARG:NE   | 2.49                     | 0.76              |
| 2:B:337:LYS:CE   | 2:B:391:LEU:HD21 | 2.15                     | 0.75              |
| 2:B:376:LEU:CD2  | 2:B:376:LEU:CD1  | 2.65                     | 0.74              |
| 2:B:63:GLN:CD    | 2:B:63:GLN:CB    | 2.62                     | 0.73              |
| 1:A:85:LEU:CD1   | 1:A:85:LEU:CB    | 2.66                     | 0.71              |
| 1:A:111:ILE:CB   | 1:A:111:ILE:C    | 2.61                     | 0.70              |
| 2:B:139:VAL:CG2  | 2:B:139:VAL:CG1  | 2.69                     | 0.68              |
| 2:B:337:LYS:NZ   | 2:B:391:LEU:CD2  | 2.58                     | 0.67              |
| 2:B:217:LEU:CD2  | 2:B:217:LEU:CD1  | 2.69                     | 0.66              |
| 1:A:111:ILE:CB   | 1:A:111:ILE:N    | 2.57                     | 0.66              |
| 1:A:117:ARG:CD   | 1:A:117:ARG:CB   | 2.71                     | 0.65              |
| 1:A:240:ILE:CD1  | 1:A:240:ILE:CB   | 2.72                     | 0.65              |
| 2:B:54:GLY:O     | 5:B:777:HOH:O    | 2.14                     | 0.64              |
| 2:B:337:LYS:NZ   | 2:B:391:LEU:HD21 | 2.14                     | 0.63              |
| 1:A:203:TYR:O    | 1:A:204:HIS:HB2  | 1.99                     | 0.62              |
| 2:B:337:LYS:HE3  | 2:B:391:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:117:ARG:NH1  | 1:A:120:GLN:OE1  | 2.31                     | 0.61              |
| 2:B:337:LYS:CE   | 2:B:391:LEU:HD11 | 2.31                     | 0.61              |
| 2:B:139:VAL:CG2  | 2:B:139:VAL:CA   | 2.77                     | 0.60              |
| 1:A:111:ILE:CA   | 1:A:111:ILE:CG1  | 2.77                     | 0.60              |
| 2:B:390:ILE:CG2  | 2:B:390:ILE:C    | 2.74                     | 0.60              |
| 1:A:112:ASP:OD1  | 1:A:146:HIS:HE1  | 1.85                     | 0.59              |
| 1:A:239:LYS:O    | 1:A:243:LYS:HG3  | 2.02                     | 0.58              |
| 2:B:177:TRP:N    | 2:B:178:PRO:CD   | 2.65                     | 0.58              |
| 2:B:206:ARG:HD3  | 2:B:210:GLU:OE2  | 2.03                     | 0.57              |
| 2:B:337:LYS:NZ   | 2:B:391:LEU:HD22 | 2.19                     | 0.57              |
| 2:B:337:LYS:HZ1  | 2:B:391:LEU:HD22 | 1.70                     | 0.57              |
| 2:B:300:ILE:HD11 | 2:B:390:ILE:CD1  | 2.36                     | 0.55              |
| 1:A:20:VAL:HB    | 1:A:232:ILE:HG12 | 1.87                     | 0.55              |
| 2:B:20:ILE:HD13  | 2:B:178:PRO:HB3  | 1.88                     | 0.55              |
| 1:A:15:ARG:O     | 1:A:268:ALA:HB2  | 2.08                     | 0.54              |
| 1:A:58:LEU:C     | 1:A:58:LEU:HD12  | 2.32                     | 0.54              |
| 2:B:38:ASP:OD1   | 2:B:38:ASP:C     | 2.51                     | 0.54              |
| 2:B:390:ILE:CG2  | 2:B:390:ILE:CA   | 2.83                     | 0.53              |
| 2:B:62:CYS:SG    | 2:B:75:LEU:HG    | 2.48                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:61:LYS:NZ    | 2:B:61:LYS:HD2     | 2.22                     | 0.53              |
| 2:B:11:GLU:O     | 2:B:11:GLU:HG2     | 2.10                     | 0.52              |
| 2:B:376:LEU:CD2  | 2:B:376:LEU:HB3    | 2.37                     | 0.52              |
| 1:A:140:ARG:CD   | 1:A:140:ARG:CB     | 2.76                     | 0.51              |
| 1:A:157:ASN:OD1  | 1:A:157:ASN:C      | 2.51                     | 0.51              |
| 1:A:215:SER:N    | 1:A:219:GLN:OE1    | 2.26                     | 0.51              |
| 1:A:213:GLY:N    | 5:A:281:HOH:O      | 2.43                     | 0.51              |
| 2:B:206:ARG:CD   | 2:B:210:GLU:OE2    | 2.59                     | 0.51              |
| 1:A:111:ILE:CA   | 1:A:111:ILE:CG2    | 2.82                     | 0.50              |
| 2:B:115:HIS:CE1  | 2:B:189:GLY:HA2    | 2.47                     | 0.49              |
| 2:B:337:LYS:CE   | 2:B:391:LEU:CD2    | 2.89                     | 0.49              |
| 1:A:31:GLU:HA    | 1:A:31:GLU:OE1     | 2.12                     | 0.49              |
| 2:B:390:ILE:O    | 2:B:391:LEU:C      | 2.55                     | 0.49              |
| 2:B:217:LEU:CD2  | 2:B:217:LEU:CB     | 2.82                     | 0.48              |
| 2:B:143:SER:HB2  | 2:B:144:PRO:HD3    | 1.94                     | 0.48              |
| 1:A:1:MET:HG2    | 1:A:149:ALA:HB2    | 1.95                     | 0.47              |
| 1:A:34:LEU:HD11  | 1:A:87:LEU:HD12    | 1.97                     | 0.47              |
| 2:B:87:LYS:NZ    | 4:B:400:PLP:O3     | 2.47                     | 0.47              |
| 1:A:262:MET:CG   | 1:A:262:MET:CE     | 2.92                     | 0.46              |
| 1:A:127:LEU:C    | 1:A:127:LEU:HD23   | 2.41                     | 0.45              |
| 1:A:117:ARG:CG   | 1:A:117:ARG:NE     | 2.66                     | 0.45              |
| 2:B:61:LYS:HE3   | 2:B:63:GLN:CG      | 2.46                     | 0.45              |
| 1:A:82:PHE:CE1   | 1:A:117:ARG:HG3    | 2.52                     | 0.45              |
| 2:B:63:GLN:CG    | 2:B:63:GLN:NE2     | 2.64                     | 0.45              |
| 2:B:384:ILE:HG13 | 2:B:385:PHE:N      | 2.30                     | 0.45              |
| 2:B:300:ILE:HD11 | 2:B:390:ILE:HD13   | 1.98                     | 0.45              |
| 1:A:69:LEU:HD22  | 1:A:69:LEU:HA      | 1.68                     | 0.45              |
| 2:B:387:VAL:O    | 2:B:387:VAL:HG12   | 2.16                     | 0.45              |
| 1:A:104:ASN:HB2  | 2:B:278:ILE:O      | 2.17                     | 0.45              |
| 2:B:97:LEU:HA    | 2:B:97:LEU:HD23    | 1.60                     | 0.45              |
| 2:B:379:ARG:HH11 | 2:B:379:ARG:HD3    | 1.56                     | 0.44              |
| 2:B:390:ILE:CG2  | 2:B:390:ILE:CG1    | 2.81                     | 0.44              |
| 2:B:337:LYS:HZ2  | 2:B:391:LEU:CD2    | 2.31                     | 0.44              |
| 2:B:22:MET:HB3   | 2:B:22:MET:HE3     | 1.76                     | 0.44              |
| 1:A:258:PHE:O    | 1:A:262:MET:HG2    | 2.18                     | 0.44              |
| 2:B:106:ILE:HG21 | 2:B:187[A]:MET:HE2 | 1.98                     | 0.44              |
| 2:B:87:LYS:HD2   | 2:B:114:GLN:HG3    | 1.98                     | 0.44              |
| 2:B:61:LYS:HE3   | 2:B:63:GLN:HG3     | 1.99                     | 0.43              |
| 1:A:157:ASN:O    | 1:A:158:ALA:C      | 2.60                     | 0.43              |
| 2:B:138:ASP:O    | 2:B:139:VAL:C      | 2.58                     | 0.43              |
| 1:A:64:ILE:HD11  | 1:A:234:GLY:O      | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:132:ILE:HD13 | 2:B:132:ILE:HG21 | 1.77                     | 0.43              |
| 1:A:132:PRO:HD3  | 2:B:17:VAL:O     | 2.19                     | 0.42              |
| 2:B:261:GLY:O    | 2:B:262:ILE:C    | 2.61                     | 0.42              |
| 2:B:86:HIS:CE1   | 2:B:236:ASN:HB3  | 2.54                     | 0.42              |
| 2:B:227:VAL:C    | 2:B:228:ILE:HG13 | 2.44                     | 0.42              |
| 1:A:11:LEU:HA    | 1:A:11:LEU:HD23  | 1.70                     | 0.42              |
| 1:A:82:PHE:CD1   | 1:A:117:ARG:HG3  | 2.54                     | 0.42              |
| 1:A:212:PHE:CA   | 5:A:281:HOH:O    | 2.67                     | 0.42              |
| 2:B:238:ILE:HD12 | 2:B:238:ILE:HA   | 1.91                     | 0.41              |
| 2:B:90:GLN:HA    | 2:B:204:PHE:HB3  | 2.02                     | 0.41              |
| 1:A:115:TYR:CD1  | 1:A:143:ALA:HA   | 2.56                     | 0.41              |
| 2:B:197:TYR:N    | 2:B:198:PRO:CD   | 2.84                     | 0.41              |
| 2:B:79:ASP:HB2   | 2:B:379:ARG:HB3  | 2.03                     | 0.40              |
| 2:B:55:ARG:HA    | 2:B:56:PRO:C     | 2.46                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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     | 250/268 (93%) | 244 (98%) | 3 (1%)  | 3 (1%)   | 10          | 2   |
| 2   | B     | 391/396 (99%) | 380 (97%) | 11 (3%) | 0        | 100         | 100 |
| All | All   | 641/664 (96%) | 624 (97%) | 14 (2%) | 3 (0%)   | 24          | 12  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | ASN  |
| 1   | A     | 212 | PHE  |
| 1   | A     | 2   | GLU  |

### 5.3.2 Protein sidechains ⓘ

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     | 198/208 (95%)  | 189 (96%) | 9 (4%)   | 24          | 9  |
| 2   | B     | 309/310 (100%) | 303 (98%) | 6 (2%)   | 50          | 34 |
| All | All   | 507/518 (98%)  | 492 (97%) | 15 (3%)  | 36          | 19 |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | PRO  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 132 | PRO  |
| 1   | A     | 196 | LEU  |
| 1   | A     | 197 | ILE  |
| 1   | A     | 237 | ILE  |
| 1   | A     | 247 | SER  |
| 1   | A     | 248 | PRO  |
| 1   | A     | 249 | LYS  |
| 2   | B     | 65  | ILE  |
| 2   | B     | 107 | ILE  |
| 2   | B     | 143 | SER  |
| 2   | B     | 196 | PRO  |
| 2   | B     | 297 | SER  |
| 2   | B     | 390 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | GLN  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 195 | HIS  |
| 2   | B     | 27  | GLN  |
| 2   | B     | 44  | GLN  |
| 2   | B     | 51  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 236 | ASN  |
| 2   | B     | 375 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 4   | PLP  | B     | 400 | 2    | 15,15,16     | 2.37 | 6 (40%)     | 21,22,23    | 2.73 | 8 (38%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 4   | PLP  | B     | 400 | 2    | -       | 0/6/6/8  | 0/1/1/1 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | B     | 400 | PLP  | C2A-C2  | 5.59  | 1.59        | 1.50     |
| 4   | B     | 400 | PLP  | C5A-C5  | 4.01  | 1.61        | 1.50     |
| 4   | B     | 400 | PLP  | C4A-C4  | -3.31 | 1.45        | 1.51     |
| 4   | B     | 400 | PLP  | C6-C5   | -2.69 | 1.32        | 1.37     |
| 4   | B     | 400 | PLP  | O4P-C5A | 2.12  | 1.52        | 1.44     |
| 4   | B     | 400 | PLP  | P-O1P   | -2.02 | 1.44        | 1.50     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | B     | 400 | PLP  | C5A-C5-C6  | 6.45  | 129.88      | 119.36   |
| 4   | B     | 400 | PLP  | O4P-C5A-C5 | 6.32  | 121.20      | 109.36   |
| 4   | B     | 400 | PLP  | C6-C5-C4   | -4.26 | 114.60      | 118.10   |
| 4   | B     | 400 | PLP  | C5A-C5-C4  | -3.61 | 115.51      | 122.64   |
| 4   | B     | 400 | PLP  | C5-C6-N1   | 3.35  | 129.29      | 123.83   |
| 4   | B     | 400 | PLP  | C2A-C2-C3  | 2.71  | 123.97      | 120.80   |
| 4   | B     | 400 | PLP  | C4A-C4-C5  | -2.49 | 118.37      | 120.94   |
| 4   | B     | 400 | PLP  | O4P-P-O1P  | -2.14 | 100.67      | 106.44   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 400 | PLP  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9  |
|-----|-------|---------------|--------|---------------|-----------------------|--------|
| 1   | A     | 254/268 (94%) | 0.50   | 14 (5%) 30 34 | 13, 23, 44, 72        | 0      |
| 2   | B     | 390/396 (98%) | -0.06  | 9 (2%) 61 65  | 10, 16, 28, 49        | 3 (0%) |
| All | All   | 644/664 (96%) | 0.16   | 23 (3%) 46 50 | 10, 19, 38, 72        | 3 (0%) |

All (23) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 192 | PRO  | 5.7  |
| 1   | A     | 212 | PHE  | 5.5  |
| 1   | A     | 194 | HIS  | 4.5  |
| 1   | A     | 268 | ALA  | 4.1  |
| 2   | B     | 391 | LEU  | 3.8  |
| 2   | B     | 385 | PHE  | 3.6  |
| 1   | A     | 213 | GLY  | 3.6  |
| 1   | A     | 247 | SER  | 3.5  |
| 2   | B     | 147 | PHE  | 3.1  |
| 1   | A     | 1   | MET  | 3.0  |
| 2   | B     | 390 | ILE  | 3.0  |
| 2   | B     | 388 | HIS  | 3.0  |
| 2   | B     | 62  | CYS  | 2.9  |
| 1   | A     | 193 | LEU  | 2.9  |
| 1   | A     | 246 | ALA  | 2.8  |
| 1   | A     | 250 | GLN  | 2.6  |
| 1   | A     | 87  | LEU  | 2.5  |
| 1   | A     | 69  | LEU  | 2.4  |
| 2   | B     | 263 | GLU  | 2.3  |
| 1   | A     | 243 | LYS  | 2.3  |
| 2   | B     | 184 | ALA  | 2.2  |
| 2   | B     | 2   | THR  | 2.2  |
| 1   | A     | 257 | SER  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | NA   | B     | 500 | 1/1   | 0.99 | 0.04 | 14,14,14,14                 | 0     |
| 4   | PLP  | B     | 400 | 15/16 | 0.99 | 0.05 | 9,14,27,31                  | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.