



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 1CHG / pdb\_00001chg  
Title : CHYMOTRYPSINOGEN,2.5 ANGSTROMS CRYSTAL STRUCTURE,  
COMPARISON WITH ALPHA-CHYMOTRYPSIN,AND IMPLICATIONS  
FOR ZYMOGEN ACTIVATION  
Authors : Freer, S.T.; Kraut, J.; Robertus, J.D.; Wright, H.T.; Xuong, N.H.  
Deposited on : 1975-03-01  
Resolution : 2.50 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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

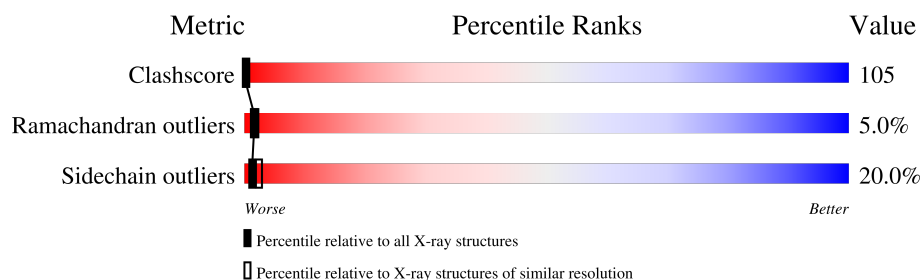
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |

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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 245    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1643 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 CHYMOTRYPSINOGEN A.

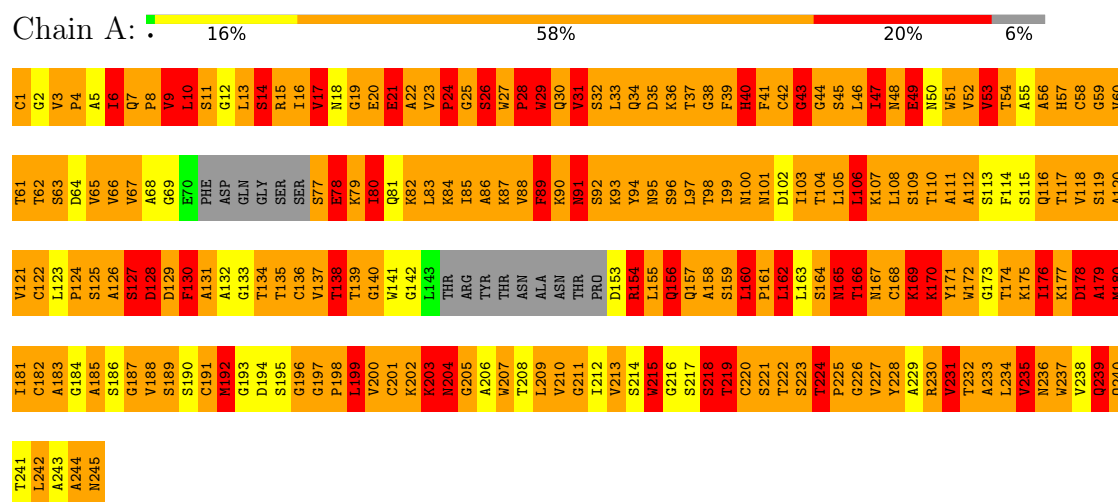
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 1   | A     | 230      | 1643  | 1034 | 279 | 318 | 12 | 0       | 0       | 5     |

### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

#### • Molecule 1: CHYMOTRYPSINOGEN A



## 4 Data and refinement statistics

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

| Property                                                 | Value                                        | Source    |
|----------------------------------------------------------|----------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 52.00Å 63.90Å 77.10Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 2.50                       | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-2.50)       | Depositor |
| $R_{merge}$                                              | (Not available)                              | Depositor |
| $R_{sym}$                                                | (Not available)                              | Depositor |
| Refinement program                                       | unknown                                      | Depositor |
| R, $R_{free}$                                            | 0.430 , (Not available)                      | Depositor |
| Estimated twinning fraction                              | No twinning to report.                       | Xtriage   |
| Total number of atoms                                    | 1643                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 0.0                                          | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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     | 5.25         | 464/1673 (27.7%) | 4.71        | 596/2277 (26.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 9                   |

All (464) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 15  | ARG  | N-CA    | -31.48 | 1.05        | 1.46     |
| 1   | A     | 9   | VAL  | CA-CB   | -22.52 | 1.23        | 1.54     |
| 1   | A     | 125 | SER  | CA-C    | 21.94  | 1.81        | 1.52     |
| 1   | A     | 114 | PHE  | C-O     | -20.82 | 0.98        | 1.23     |
| 1   | A     | 126 | ALA  | N-CA    | -20.73 | 1.18        | 1.46     |
| 1   | A     | 53  | VAL  | N-CA    | -19.63 | 1.22        | 1.46     |
| 1   | A     | 241 | THR  | C-O     | -19.28 | 1.01        | 1.24     |
| 1   | A     | 54  | THR  | C-N     | -19.19 | 1.05        | 1.33     |
| 1   | A     | 9   | VAL  | N-CA    | 18.53  | 1.69        | 1.46     |
| 1   | A     | 53  | VAL  | C-O     | -18.42 | 1.03        | 1.24     |
| 1   | A     | 207 | TRP  | C-O     | -18.09 | 1.02        | 1.23     |
| 1   | A     | 43  | GLY  | CA-C    | 17.27  | 1.76        | 1.51     |
| 1   | A     | 209 | LEU  | C-N     | -16.71 | 1.17        | 1.33     |
| 1   | A     | 117 | THR  | C-O     | -16.36 | 1.02        | 1.24     |
| 1   | A     | 91  | ASN  | N-CA    | -16.27 | 1.25        | 1.45     |
| 1   | A     | 51  | TRP  | NE1-CE2 | -16.15 | 1.19        | 1.37     |
| 1   | A     | 60  | VAL  | C-O     | -16.12 | 1.04        | 1.24     |
| 1   | A     | 207 | TRP  | NE1-CE2 | -15.73 | 1.20        | 1.37     |
| 1   | A     | 27  | TRP  | CA-CB   | 15.67  | 1.70        | 1.53     |
| 1   | A     | 155 | LEU  | C-O     | -15.42 | 1.05        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 209 | LEU  | CA-C   | 14.97  | 1.71        | 1.52     |
| 1   | A     | 220 | CYS  | C-N    | 14.74  | 1.53        | 1.33     |
| 1   | A     | 19  | GLY  | CA-C   | 14.70  | 1.71        | 1.52     |
| 1   | A     | 204 | ASN  | C-O    | -14.60 | 1.04        | 1.23     |
| 1   | A     | 123 | LEU  | C-O    | -13.92 | 1.05        | 1.24     |
| 1   | A     | 5   | ALA  | C-O    | -13.85 | 1.07        | 1.24     |
| 1   | A     | 3   | VAL  | C-O    | -13.79 | 1.07        | 1.24     |
| 1   | A     | 211 | GLY  | CA-C   | 13.79  | 1.63        | 1.51     |
| 1   | A     | 239 | GLN  | C-O    | -13.49 | 1.08        | 1.24     |
| 1   | A     | 236 | ASN  | C-O    | -13.32 | 1.07        | 1.24     |
| 1   | A     | 22  | ALA  | C-N    | -13.28 | 1.22        | 1.33     |
| 1   | A     | 131 | ALA  | C-N    | -13.11 | 1.16        | 1.33     |
| 1   | A     | 185 | ALA  | C-O    | -13.09 | 1.07        | 1.24     |
| 1   | A     | 59  | GLY  | C-N    | -13.07 | 1.15        | 1.33     |
| 1   | A     | 142 | GLY  | C-N    | -13.03 | 1.15        | 1.33     |
| 1   | A     | 112 | ALA  | C-N    | -13.01 | 1.14        | 1.33     |
| 1   | A     | 32  | SER  | C-N    | -13.00 | 1.17        | 1.33     |
| 1   | A     | 124 | PRO  | CA-CB  | 12.96  | 1.72        | 1.53     |
| 1   | A     | 242 | LEU  | C-N    | -12.79 | 1.15        | 1.33     |
| 1   | A     | 159 | SER  | CA-C   | 12.78  | 1.68        | 1.52     |
| 1   | A     | 168 | CYS  | C-O    | -12.74 | 1.09        | 1.24     |
| 1   | A     | 38  | GLY  | C-N    | -12.63 | 1.16        | 1.33     |
| 1   | A     | 127 | SER  | C-O    | -12.60 | 1.06        | 1.23     |
| 1   | A     | 117 | THR  | CA-C   | 12.48  | 1.69        | 1.52     |
| 1   | A     | 213 | VAL  | C-O    | -12.47 | 1.11        | 1.24     |
| 1   | A     | 114 | PHE  | CA-C   | 12.45  | 1.69        | 1.52     |
| 1   | A     | 204 | ASN  | CA-CB  | 12.39  | 1.73        | 1.53     |
| 1   | A     | 61  | THR  | C-O    | -12.39 | 1.08        | 1.24     |
| 1   | A     | 106 | LEU  | CA-CB  | 12.32  | 1.77        | 1.53     |
| 1   | A     | 93  | LYS  | CA-C   | 12.27  | 1.71        | 1.52     |
| 1   | A     | 137 | VAL  | N-CA   | 12.27  | 1.60        | 1.46     |
| 1   | A     | 130 | PHE  | N-CA   | 12.24  | 1.61        | 1.46     |
| 1   | A     | 236 | ASN  | N-CA   | -12.06 | 1.31        | 1.46     |
| 1   | A     | 194 | ASP  | C-N    | -11.95 | 1.17        | 1.33     |
| 1   | A     | 127 | SER  | CB-OG  | -11.88 | 1.18        | 1.42     |
| 1   | A     | 139 | THR  | C-O    | -11.80 | 1.09        | 1.23     |
| 1   | A     | 178 | ASP  | CG-OD2 | 11.71  | 1.47        | 1.25     |
| 1   | A     | 51  | TRP  | CA-C   | 11.66  | 1.67        | 1.52     |
| 1   | A     | 204 | ASN  | CG-OD1 | -11.59 | 1.01        | 1.23     |
| 1   | A     | 134 | THR  | N-CA   | -11.50 | 1.31        | 1.46     |
| 1   | A     | 223 | SER  | N-CA   | 11.49  | 1.60        | 1.46     |
| 1   | A     | 191 | CYS  | C-N    | -11.48 | 1.18        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 106 | LEU  | C-O     | -11.45 | 1.10        | 1.24     |
| 1   | A     | 64  | ASP  | CA-CB   | -11.44 | 1.33        | 1.53     |
| 1   | A     | 94  | TYR  | C-N     | -11.44 | 1.17        | 1.33     |
| 1   | A     | 141 | TRP  | NE1-CE2 | -11.40 | 1.25        | 1.37     |
| 1   | A     | 91  | ASN  | CA-C    | 11.39  | 1.66        | 1.52     |
| 1   | A     | 205 | GLY  | C-N     | -11.39 | 1.17        | 1.33     |
| 1   | A     | 237 | TRP  | N-CA    | -11.38 | 1.32        | 1.46     |
| 1   | A     | 112 | ALA  | CA-C    | 11.37  | 1.66        | 1.52     |
| 1   | A     | 83  | LEU  | CA-C    | 11.37  | 1.66        | 1.52     |
| 1   | A     | 239 | GLN  | C-N     | -11.35 | 1.18        | 1.33     |
| 1   | A     | 92  | SER  | C-O     | -11.35 | 1.09        | 1.24     |
| 1   | A     | 128 | ASP  | CG-OD2  | -11.29 | 1.03        | 1.25     |
| 1   | A     | 175 | LYS  | C-N     | -11.25 | 1.18        | 1.33     |
| 1   | A     | 165 | ASN  | C-N     | -11.18 | 1.18        | 1.33     |
| 1   | A     | 164 | SER  | C-O     | 11.18  | 1.37        | 1.23     |
| 1   | A     | 58  | CYS  | C-O     | 11.12  | 1.38        | 1.24     |
| 1   | A     | 30  | GLN  | C-O     | -11.11 | 1.10        | 1.23     |
| 1   | A     | 12  | GLY  | C-O     | 11.02  | 1.37        | 1.23     |
| 1   | A     | 221 | SER  | N-CA    | -10.96 | 1.31        | 1.46     |
| 1   | A     | 160 | LEU  | C-N     | -10.90 | 1.19        | 1.33     |
| 1   | A     | 67  | VAL  | N-CA    | -10.89 | 1.32        | 1.46     |
| 1   | A     | 209 | LEU  | C-O     | -10.88 | 1.10        | 1.24     |
| 1   | A     | 125 | SER  | C-O     | -10.74 | 1.10        | 1.23     |
| 1   | A     | 67  | VAL  | C-N     | -10.73 | 1.19        | 1.33     |
| 1   | A     | 37  | THR  | CA-CB   | -10.71 | 1.38        | 1.53     |
| 1   | A     | 156 | GLN  | C-O     | -10.70 | 1.09        | 1.23     |
| 1   | A     | 224 | THR  | C-O     | 10.69  | 1.37        | 1.24     |
| 1   | A     | 203 | LYS  | C-O     | -10.69 | 1.10        | 1.24     |
| 1   | A     | 85  | ILE  | CA-C    | -10.68 | 1.40        | 1.52     |
| 1   | A     | 68  | ALA  | C-O     | -10.66 | 1.11        | 1.24     |
| 1   | A     | 85  | ILE  | CA-CB   | 10.61  | 1.67        | 1.54     |
| 1   | A     | 9   | VAL  | C-N     | -10.54 | 1.16        | 1.33     |
| 1   | A     | 59  | GLY  | C-O     | -10.54 | 1.09        | 1.23     |
| 1   | A     | 94  | TYR  | CA-C    | 10.48  | 1.66        | 1.52     |
| 1   | A     | 202 | LYS  | C-N     | -10.46 | 1.19        | 1.33     |
| 1   | A     | 128 | ASP  | CB-CG   | 10.45  | 1.78        | 1.52     |
| 1   | A     | 241 | THR  | CA-C    | 10.34  | 1.66        | 1.52     |
| 1   | A     | 242 | LEU  | N-CA    | -10.34 | 1.26        | 1.46     |
| 1   | A     | 86  | ALA  | CA-C    | 10.33  | 1.64        | 1.52     |
| 1   | A     | 20  | GLU  | C-O     | -10.32 | 1.11        | 1.23     |
| 1   | A     | 104 | THR  | C-N     | -10.31 | 1.18        | 1.33     |
| 1   | A     | 138 | THR  | C-O     | -10.31 | 1.11        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 46  | LEU  | C-O     | -10.30 | 1.11        | 1.23     |
| 1   | A     | 22  | ALA  | CA-CB   | 10.30  | 1.69        | 1.53     |
| 1   | A     | 194 | ASP  | CG-OD1  | -10.29 | 1.05        | 1.25     |
| 1   | A     | 21  | GLU  | C-O     | -10.27 | 1.11        | 1.24     |
| 1   | A     | 59  | GLY  | CA-C    | 10.26  | 1.66        | 1.51     |
| 1   | A     | 201 | CYS  | C-O     | -10.24 | 1.11        | 1.24     |
| 1   | A     | 43  | GLY  | C-N     | -10.18 | 1.21        | 1.33     |
| 1   | A     | 157 | GLN  | C-O     | -10.11 | 1.12        | 1.24     |
| 1   | A     | 109 | SER  | N-CA    | -10.06 | 1.33        | 1.46     |
| 1   | A     | 86  | ALA  | C-O     | -10.03 | 1.10        | 1.23     |
| 1   | A     | 141 | TRP  | CD2-CE2 | 10.02  | 1.58        | 1.41     |
| 1   | A     | 237 | TRP  | C-N     | -9.94  | 1.22        | 1.33     |
| 1   | A     | 218 | SER  | C-O     | 9.87   | 1.36        | 1.24     |
| 1   | A     | 155 | LEU  | C-N     | 9.82   | 1.46        | 1.33     |
| 1   | A     | 104 | THR  | C-O     | 9.81   | 1.35        | 1.23     |
| 1   | A     | 207 | TRP  | CD2-CE2 | -9.80  | 1.24        | 1.41     |
| 1   | A     | 92  | SER  | C-N     | -9.80  | 1.21        | 1.33     |
| 1   | A     | 24  | PRO  | C-O     | -9.78  | 1.11        | 1.24     |
| 1   | A     | 52  | VAL  | C-O     | 9.78   | 1.33        | 1.24     |
| 1   | A     | 102 | ASP  | CA-CB   | 9.73   | 1.67        | 1.52     |
| 1   | A     | 236 | ASN  | CA-CB   | 9.72   | 1.69        | 1.53     |
| 1   | A     | 78  | GLU  | C-O     | -9.71  | 1.12        | 1.23     |
| 1   | A     | 54  | THR  | C-O     | -9.71  | 1.14        | 1.24     |
| 1   | A     | 180 | MET  | C-O     | -9.69  | 1.12        | 1.23     |
| 1   | A     | 20  | GLU  | N-CA    | -9.68  | 1.33        | 1.46     |
| 1   | A     | 189 | SER  | N-CA    | -9.63  | 1.34        | 1.46     |
| 1   | A     | 67  | VAL  | CA-C    | 9.62   | 1.63        | 1.52     |
| 1   | A     | 37  | THR  | C-O     | -9.60  | 1.11        | 1.23     |
| 1   | A     | 32  | SER  | N-CA    | -9.59  | 1.34        | 1.45     |
| 1   | A     | 160 | LEU  | N-CA    | 9.55   | 1.68        | 1.45     |
| 1   | A     | 80  | ILE  | C-N     | -9.48  | 1.20        | 1.33     |
| 1   | A     | 222 | THR  | CB-OG1  | -9.47  | 1.28        | 1.43     |
| 1   | A     | 113 | SER  | C-N     | -9.41  | 1.20        | 1.33     |
| 1   | A     | 85  | ILE  | N-CA    | 9.39   | 1.57        | 1.46     |
| 1   | A     | 191 | CYS  | C-O     | -9.39  | 1.11        | 1.24     |
| 1   | A     | 29  | TRP  | CD1-NE1 | 9.39   | 1.57        | 1.37     |
| 1   | A     | 141 | TRP  | CZ2-CH2 | 9.35   | 1.55        | 1.37     |
| 1   | A     | 93  | LYS  | C-O     | -9.33  | 1.12        | 1.24     |
| 1   | A     | 170 | LYS  | CA-C    | 9.31   | 1.65        | 1.52     |
| 1   | A     | 82  | LYS  | C-O     | -9.27  | 1.13        | 1.24     |
| 1   | A     | 92  | SER  | N-CA    | -9.26  | 1.34        | 1.46     |
| 1   | A     | 26  | SER  | C-N     | -9.20  | 1.22        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 222 | THR  | N-CA    | -9.20 | 1.33        | 1.46     |
| 1   | A     | 18  | ASN  | C-O     | -9.18 | 1.11        | 1.23     |
| 1   | A     | 67  | VAL  | C-O     | -9.18 | 1.13        | 1.24     |
| 1   | A     | 78  | GLU  | CD-OE1  | -9.15 | 1.07        | 1.25     |
| 1   | A     | 107 | LYS  | CA-CB   | -9.11 | 1.41        | 1.53     |
| 1   | A     | 41  | PHE  | C-N     | -9.03 | 1.22        | 1.33     |
| 1   | A     | 83  | LEU  | C-O     | -9.01 | 1.13        | 1.24     |
| 1   | A     | 154 | ARG  | CD-NE   | 9.00  | 1.58        | 1.46     |
| 1   | A     | 183 | ALA  | CA-C    | 8.93  | 1.63        | 1.52     |
| 1   | A     | 114 | PHE  | CG-CD1  | -8.91 | 1.20        | 1.38     |
| 1   | A     | 34  | GLN  | CD-NE2  | -8.90 | 1.14        | 1.33     |
| 1   | A     | 30  | GLN  | CD-OE1  | -8.89 | 1.06        | 1.23     |
| 1   | A     | 44  | GLY  | C-O     | -8.85 | 1.11        | 1.24     |
| 1   | A     | 198 | PRO  | N-CA    | -8.83 | 1.36        | 1.47     |
| 1   | A     | 122 | CYS  | CA-C    | 8.83  | 1.65        | 1.53     |
| 1   | A     | 101 | ASN  | C-O     | -8.80 | 1.12        | 1.23     |
| 1   | A     | 123 | LEU  | CA-CB   | -8.78 | 1.41        | 1.53     |
| 1   | A     | 40  | HIS  | C-O     | -8.77 | 1.13        | 1.24     |
| 1   | A     | 81  | GLN  | N-CA    | 8.77  | 1.56        | 1.46     |
| 1   | A     | 215 | TRP  | C-O     | -8.76 | 1.15        | 1.23     |
| 1   | A     | 47  | ILE  | N-CA    | 8.73  | 1.54        | 1.46     |
| 1   | A     | 203 | LYS  | C-N     | -8.71 | 1.21        | 1.33     |
| 1   | A     | 231 | VAL  | C-O     | -8.68 | 1.13        | 1.24     |
| 1   | A     | 40  | HIS  | CD2-NE2 | -8.58 | 1.28        | 1.37     |
| 1   | A     | 77  | SER  | C-O     | -8.56 | 1.06        | 1.23     |
| 1   | A     | 124 | PRO  | N-CA    | -8.53 | 1.36        | 1.47     |
| 1   | A     | 5   | ALA  | N-CA    | 8.50  | 1.57        | 1.46     |
| 1   | A     | 187 | GLY  | C-N     | -8.50 | 1.21        | 1.33     |
| 1   | A     | 44  | GLY  | N-CA    | 8.48  | 1.54        | 1.45     |
| 1   | A     | 238 | VAL  | C-O     | -8.47 | 1.14        | 1.24     |
| 1   | A     | 82  | LYS  | C-N     | -8.46 | 1.22        | 1.33     |
| 1   | A     | 226 | GLY  | C-O     | -8.43 | 1.12        | 1.23     |
| 1   | A     | 134 | THR  | CA-C    | 8.41  | 1.63        | 1.52     |
| 1   | A     | 215 | TRP  | CG-CD2  | -8.40 | 1.28        | 1.43     |
| 1   | A     | 224 | THR  | CB-OG1  | -8.39 | 1.30        | 1.43     |
| 1   | A     | 20  | GLU  | CD-OE2  | -8.33 | 1.09        | 1.25     |
| 1   | A     | 198 | PRO  | N-CD    | 8.30  | 1.59        | 1.47     |
| 1   | A     | 86  | ALA  | C-N     | -8.26 | 1.23        | 1.33     |
| 1   | A     | 52  | VAL  | CA-C    | -8.23 | 1.42        | 1.52     |
| 1   | A     | 105 | LEU  | C-O     | -8.22 | 1.14        | 1.23     |
| 1   | A     | 7   | GLN  | CA-C    | -8.21 | 1.41        | 1.52     |
| 1   | A     | 65  | VAL  | CA-CB   | -8.21 | 1.44        | 1.54     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 57  | HIS  | C-O    | 8.20  | 1.34        | 1.24     |
| 1   | A     | 95  | ASN  | CA-CB  | 8.18  | 1.64        | 1.53     |
| 1   | A     | 16  | ILE  | C-N    | -8.18 | 1.22        | 1.33     |
| 1   | A     | 17  | VAL  | CA-CB  | 8.14  | 1.65        | 1.54     |
| 1   | A     | 89  | PHE  | C-N    | -8.13 | 1.22        | 1.33     |
| 1   | A     | 84  | LYS  | CA-C   | 8.11  | 1.63        | 1.52     |
| 1   | A     | 7   | GLN  | CD-NE2 | 8.09  | 1.50        | 1.33     |
| 1   | A     | 41  | PHE  | C-O    | -8.07 | 1.15        | 1.24     |
| 1   | A     | 107 | LYS  | CA-C   | 8.07  | 1.62        | 1.52     |
| 1   | A     | 33  | LEU  | C-O    | -8.05 | 1.14        | 1.23     |
| 1   | A     | 97  | LEU  | C-N    | -8.05 | 1.22        | 1.33     |
| 1   | A     | 210 | VAL  | N-CA   | 8.05  | 1.56        | 1.46     |
| 1   | A     | 84  | LYS  | C-O    | -8.04 | 1.14        | 1.23     |
| 1   | A     | 37  | THR  | CA-C   | 8.04  | 1.63        | 1.53     |
| 1   | A     | 173 | GLY  | N-CA   | -8.04 | 1.33        | 1.45     |
| 1   | A     | 135 | THR  | CA-CB  | -8.04 | 1.41        | 1.52     |
| 1   | A     | 24  | PRO  | N-CA   | -8.03 | 1.37        | 1.47     |
| 1   | A     | 101 | ASN  | N-CA   | -8.02 | 1.34        | 1.46     |
| 1   | A     | 113 | SER  | CA-CB  | -7.98 | 1.41        | 1.52     |
| 1   | A     | 77  | SER  | C-N    | 7.90  | 1.43        | 1.33     |
| 1   | A     | 155 | LEU  | N-CA   | 7.89  | 1.56        | 1.46     |
| 1   | A     | 26  | SER  | C-O    | -7.86 | 1.15        | 1.24     |
| 1   | A     | 24  | PRO  | CA-C   | 7.84  | 1.63        | 1.52     |
| 1   | A     | 225 | PRO  | C-O    | -7.80 | 1.15        | 1.23     |
| 1   | A     | 154 | ARG  | CA-C   | -7.79 | 1.42        | 1.53     |
| 1   | A     | 117 | THR  | N-CA   | -7.78 | 1.35        | 1.46     |
| 1   | A     | 113 | SER  | N-CA   | 7.76  | 1.57        | 1.46     |
| 1   | A     | 205 | GLY  | CA-C   | 7.75  | 1.62        | 1.51     |
| 1   | A     | 132 | ALA  | C-O    | 7.74  | 1.33        | 1.23     |
| 1   | A     | 64  | ASP  | CA-C   | 7.73  | 1.61        | 1.52     |
| 1   | A     | 131 | ALA  | N-CA   | -7.72 | 1.36        | 1.46     |
| 1   | A     | 46  | LEU  | N-CA   | 7.71  | 1.55        | 1.46     |
| 1   | A     | 49  | GLU  | C-O    | -7.70 | 1.14        | 1.24     |
| 1   | A     | 194 | ASP  | CA-CB  | -7.70 | 1.40        | 1.53     |
| 1   | A     | 218 | SER  | CA-C   | -7.68 | 1.42        | 1.52     |
| 1   | A     | 124 | PRO  | CA-C   | 7.68  | 1.63        | 1.52     |
| 1   | A     | 6   | ILE  | CB-CG1 | -7.66 | 1.38        | 1.53     |
| 1   | A     | 209 | LEU  | CA-CB  | -7.64 | 1.43        | 1.53     |
| 1   | A     | 19  | GLY  | N-CA   | -7.62 | 1.33        | 1.45     |
| 1   | A     | 64  | ASP  | N-CA   | -7.61 | 1.36        | 1.45     |
| 1   | A     | 194 | ASP  | CB-CG  | 7.59  | 1.71        | 1.52     |
| 1   | A     | 27  | TRP  | C-O    | -7.59 | 1.15        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 200 | VAL  | C-N     | 7.57  | 1.44        | 1.33     |
| 1   | A     | 167 | ASN  | C-N     | -7.56 | 1.24        | 1.33     |
| 1   | A     | 170 | LYS  | C-N     | -7.55 | 1.22        | 1.33     |
| 1   | A     | 88  | VAL  | C-O     | -7.52 | 1.16        | 1.24     |
| 1   | A     | 182 | CYS  | CA-C    | -7.49 | 1.44        | 1.52     |
| 1   | A     | 178 | ASP  | C-O     | 7.42  | 1.33        | 1.24     |
| 1   | A     | 38  | GLY  | N-CA    | 7.41  | 1.56        | 1.45     |
| 1   | A     | 169 | LYS  | CA-C    | 7.40  | 1.62        | 1.52     |
| 1   | A     | 127 | SER  | N-CA    | -7.40 | 1.36        | 1.46     |
| 1   | A     | 65  | VAL  | C-N     | -7.39 | 1.23        | 1.33     |
| 1   | A     | 57  | HIS  | C-N     | -7.38 | 1.24        | 1.33     |
| 1   | A     | 142 | GLY  | C-O     | 7.38  | 1.38        | 1.23     |
| 1   | A     | 27  | TRP  | CD2-CE2 | -7.36 | 1.28        | 1.41     |
| 1   | A     | 235 | VAL  | CB-CG2  | -7.32 | 1.28        | 1.52     |
| 1   | A     | 41  | PHE  | N-CA    | -7.31 | 1.37        | 1.46     |
| 1   | A     | 128 | ASP  | CA-C    | -7.31 | 1.43        | 1.52     |
| 1   | A     | 218 | SER  | CB-OG   | -7.31 | 1.27        | 1.42     |
| 1   | A     | 188 | VAL  | N-CA    | 7.30  | 1.54        | 1.46     |
| 1   | A     | 82  | LYS  | CA-C    | 7.27  | 1.61        | 1.52     |
| 1   | A     | 239 | GLN  | CD-OE1  | -7.25 | 1.09        | 1.23     |
| 1   | A     | 136 | CYS  | C-N     | -7.25 | 1.23        | 1.33     |
| 1   | A     | 189 | SER  | C-O     | -7.20 | 1.15        | 1.24     |
| 1   | A     | 239 | GLN  | N-CA    | -7.19 | 1.38        | 1.46     |
| 1   | A     | 21  | GLU  | CD-OE1  | 7.18  | 1.39        | 1.25     |
| 1   | A     | 99  | ILE  | N-CA    | -7.17 | 1.37        | 1.46     |
| 1   | A     | 239 | GLN  | CA-C    | 7.17  | 1.62        | 1.52     |
| 1   | A     | 49  | GLU  | N-CA    | -7.15 | 1.37        | 1.46     |
| 1   | A     | 111 | ALA  | N-CA    | -7.15 | 1.36        | 1.46     |
| 1   | A     | 57  | HIS  | CG-CD2  | -7.14 | 1.27        | 1.35     |
| 1   | A     | 203 | LYS  | CA-C    | 7.13  | 1.62        | 1.52     |
| 1   | A     | 55  | ALA  | N-CA    | 7.12  | 1.54        | 1.45     |
| 1   | A     | 182 | CYS  | C-O     | -7.10 | 1.15        | 1.23     |
| 1   | A     | 165 | ASN  | CG-ND2  | -7.08 | 1.18        | 1.33     |
| 1   | A     | 240 | GLN  | C-O     | -7.08 | 1.15        | 1.24     |
| 1   | A     | 88  | VAL  | C-N     | -7.07 | 1.21        | 1.33     |
| 1   | A     | 78  | GLU  | N-CA    | -7.07 | 1.38        | 1.46     |
| 1   | A     | 97  | LEU  | N-CA    | -7.06 | 1.37        | 1.46     |
| 1   | A     | 183 | ALA  | N-CA    | -7.03 | 1.38        | 1.46     |
| 1   | A     | 124 | PRO  | C-O     | -7.03 | 1.14        | 1.24     |
| 1   | A     | 242 | LEU  | C-O     | 7.00  | 1.37        | 1.23     |
| 1   | A     | 31  | VAL  | C-O     | -6.99 | 1.16        | 1.23     |
| 1   | A     | 172 | TRP  | C-O     | -6.98 | 1.16        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 232 | THR  | CA-C    | -6.97 | 1.43        | 1.52     |
| 1   | A     | 36  | LYS  | CA-C    | -6.97 | 1.43        | 1.52     |
| 1   | A     | 176 | ILE  | CA-CB   | -6.94 | 1.45        | 1.54     |
| 1   | A     | 136 | CYS  | N-CA    | 6.94  | 1.54        | 1.45     |
| 1   | A     | 40  | HIS  | CG-ND1  | -6.93 | 1.30        | 1.38     |
| 1   | A     | 30  | GLN  | C-N     | -6.92 | 1.24        | 1.33     |
| 1   | A     | 160 | LEU  | C-O     | 6.92  | 1.35        | 1.25     |
| 1   | A     | 40  | HIS  | CE1-NE2 | 6.91  | 1.39        | 1.32     |
| 1   | A     | 89  | PHE  | CB-CG   | 6.90  | 1.66        | 1.50     |
| 1   | A     | 234 | LEU  | CB-CG   | 6.88  | 1.67        | 1.53     |
| 1   | A     | 219 | THR  | C-O     | -6.88 | 1.15        | 1.24     |
| 1   | A     | 34  | GLN  | C-N     | -6.88 | 1.22        | 1.33     |
| 1   | A     | 35  | ASP  | C-O     | -6.87 | 1.15        | 1.23     |
| 1   | A     | 6   | ILE  | C-O     | -6.86 | 1.16        | 1.24     |
| 1   | A     | 94  | TYR  | CA-CB   | -6.83 | 1.42        | 1.53     |
| 1   | A     | 29  | TRP  | CD2-CE3 | -6.81 | 1.29        | 1.40     |
| 1   | A     | 27  | TRP  | CA-C    | -6.80 | 1.45        | 1.53     |
| 1   | A     | 100 | ASN  | C-O     | -6.78 | 1.15        | 1.23     |
| 1   | A     | 215 | TRP  | C-N     | 6.78  | 1.43        | 1.33     |
| 1   | A     | 48  | ASN  | C-N     | -6.76 | 1.24        | 1.34     |
| 1   | A     | 228 | TYR  | CA-C    | -6.74 | 1.44        | 1.52     |
| 1   | A     | 161 | PRO  | N-CA    | 6.73  | 1.55        | 1.47     |
| 1   | A     | 108 | LEU  | CA-CB   | 6.70  | 1.63        | 1.53     |
| 1   | A     | 237 | TRP  | C-O     | -6.70 | 1.16        | 1.24     |
| 1   | A     | 87  | LYS  | CA-C    | -6.69 | 1.44        | 1.52     |
| 1   | A     | 198 | PRO  | C-O     | 6.68  | 1.30        | 1.23     |
| 1   | A     | 57  | HIS  | CE1-NE2 | 6.62  | 1.39        | 1.32     |
| 1   | A     | 134 | THR  | CB-OG1  | -6.62 | 1.33        | 1.43     |
| 1   | A     | 116 | GLN  | CA-CB   | 6.59  | 1.63        | 1.53     |
| 1   | A     | 199 | LEU  | C-O     | 6.59  | 1.31        | 1.24     |
| 1   | A     | 64  | ASP  | CG-OD2  | -6.58 | 1.12        | 1.25     |
| 1   | A     | 51  | TRP  | CD2-CE3 | 6.57  | 1.50        | 1.40     |
| 1   | A     | 17  | VAL  | C-N     | -6.57 | 1.24        | 1.33     |
| 1   | A     | 163 | LEU  | N-CA    | 6.56  | 1.55        | 1.46     |
| 1   | A     | 46  | LEU  | CA-CB   | -6.56 | 1.43        | 1.53     |
| 1   | A     | 130 | PHE  | C-O     | -6.55 | 1.15        | 1.24     |
| 1   | A     | 208 | THR  | C-N     | -6.54 | 1.24        | 1.33     |
| 1   | A     | 57  | HIS  | CB-CG   | 6.54  | 1.59        | 1.50     |
| 1   | A     | 48  | ASN  | CA-CB   | 6.53  | 1.63        | 1.53     |
| 1   | A     | 222 | THR  | CA-C    | -6.51 | 1.43        | 1.52     |
| 1   | A     | 214 | SER  | N-CA    | -6.50 | 1.38        | 1.46     |
| 1   | A     | 4   | PRO  | C-N     | -6.47 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 155 | LEU  | CA-C   | 6.46  | 1.60        | 1.52     |
| 1   | A     | 18  | ASN  | CG-OD1 | -6.46 | 1.11        | 1.23     |
| 1   | A     | 103 | ILE  | C-N    | -6.43 | 1.25        | 1.33     |
| 1   | A     | 88  | VAL  | N-CA   | -6.42 | 1.38        | 1.46     |
| 1   | A     | 134 | THR  | C-O    | -6.39 | 1.16        | 1.24     |
| 1   | A     | 68  | ALA  | CA-C   | 6.38  | 1.60        | 1.52     |
| 1   | A     | 161 | PRO  | C-N    | 6.37  | 1.42        | 1.33     |
| 1   | A     | 63  | SER  | C-O    | -6.36 | 1.14        | 1.23     |
| 1   | A     | 237 | TRP  | CA-C   | 6.36  | 1.61        | 1.52     |
| 1   | A     | 28  | PRO  | CA-C   | 6.35  | 1.61        | 1.52     |
| 1   | A     | 199 | LEU  | N-CA   | 6.34  | 1.53        | 1.46     |
| 1   | A     | 202 | LYS  | C-O    | 6.33  | 1.31        | 1.23     |
| 1   | A     | 105 | LEU  | N-CA   | 6.33  | 1.53        | 1.45     |
| 1   | A     | 66  | VAL  | CA-C   | -6.33 | 1.45        | 1.52     |
| 1   | A     | 94  | TYR  | CZ-OH  | 6.26  | 1.51        | 1.38     |
| 1   | A     | 33  | LEU  | CA-CB  | -6.25 | 1.43        | 1.53     |
| 1   | A     | 169 | LYS  | C-N    | -6.25 | 1.25        | 1.33     |
| 1   | A     | 237 | TRP  | CA-CB  | 6.24  | 1.63        | 1.53     |
| 1   | A     | 179 | ALA  | CA-C   | 6.23  | 1.61        | 1.52     |
| 1   | A     | 108 | LEU  | N-CA   | -6.15 | 1.37        | 1.46     |
| 1   | A     | 62  | THR  | N-CA   | 6.13  | 1.54        | 1.46     |
| 1   | A     | 224 | THR  | N-CA   | 6.10  | 1.55        | 1.45     |
| 1   | A     | 23  | VAL  | CA-C   | -6.10 | 1.48        | 1.53     |
| 1   | A     | 126 | ALA  | CA-CB  | 6.10  | 1.63        | 1.53     |
| 1   | A     | 245 | ASN  | CA-C   | 6.10  | 1.65        | 1.52     |
| 1   | A     | 177 | LYS  | N-CA   | 6.08  | 1.52        | 1.45     |
| 1   | A     | 195 | SER  | N-CA   | 6.07  | 1.53        | 1.45     |
| 1   | A     | 240 | GLN  | CA-C   | -6.06 | 1.45        | 1.52     |
| 1   | A     | 202 | LYS  | CB-CG  | 6.05  | 1.70        | 1.52     |
| 1   | A     | 6   | ILE  | CA-C   | -6.05 | 1.45        | 1.52     |
| 1   | A     | 96  | SER  | C-O    | -6.05 | 1.16        | 1.24     |
| 1   | A     | 176 | ILE  | C-O    | -6.04 | 1.16        | 1.24     |
| 1   | A     | 245 | ASN  | C-O    | -6.04 | 1.11        | 1.23     |
| 1   | A     | 33  | LEU  | N-CA   | 5.99  | 1.53        | 1.46     |
| 1   | A     | 130 | PHE  | CG-CD1 | -5.99 | 1.26        | 1.38     |
| 1   | A     | 14  | SER  | CA-CB  | -5.99 | 1.43        | 1.53     |
| 1   | A     | 245 | ASN  | CB-CG  | 5.99  | 1.67        | 1.52     |
| 1   | A     | 234 | LEU  | C-O    | -5.97 | 1.16        | 1.24     |
| 1   | A     | 167 | ASN  | CG-OD1 | -5.96 | 1.12        | 1.23     |
| 1   | A     | 176 | ILE  | C-N    | -5.96 | 1.25        | 1.33     |
| 1   | A     | 37  | THR  | N-CA   | 5.96  | 1.53        | 1.46     |
| 1   | A     | 104 | THR  | N-CA   | -5.94 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 13  | LEU  | CB-CG  | -5.93 | 1.41        | 1.53     |
| 1   | A     | 6   | ILE  | CA-CB  | -5.92 | 1.47        | 1.54     |
| 1   | A     | 120 | ALA  | C-O    | -5.92 | 1.16        | 1.24     |
| 1   | A     | 162 | LEU  | N-CA   | -5.92 | 1.38        | 1.45     |
| 1   | A     | 68  | ALA  | C-N    | -5.91 | 1.25        | 1.33     |
| 1   | A     | 135 | THR  | CB-OG1 | -5.91 | 1.34        | 1.43     |
| 1   | A     | 203 | LYS  | CE-NZ  | 5.91  | 1.67        | 1.49     |
| 1   | A     | 42  | CYS  | CA-C   | -5.90 | 1.45        | 1.52     |
| 1   | A     | 188 | VAL  | CA-C   | 5.90  | 1.60        | 1.52     |
| 1   | A     | 87  | LYS  | N-CA   | 5.90  | 1.53        | 1.45     |
| 1   | A     | 115 | SER  | C-N    | -5.88 | 1.25        | 1.33     |
| 1   | A     | 159 | SER  | C-O    | -5.88 | 1.16        | 1.24     |
| 1   | A     | 221 | SER  | CA-C   | -5.88 | 1.45        | 1.52     |
| 1   | A     | 82  | LYS  | CD-CE  | 5.87  | 1.70        | 1.52     |
| 1   | A     | 214 | SER  | CA-C   | -5.85 | 1.47        | 1.53     |
| 1   | A     | 68  | ALA  | N-CA   | 5.84  | 1.53        | 1.46     |
| 1   | A     | 110 | THR  | CA-CB  | 5.84  | 1.62        | 1.53     |
| 1   | A     | 46  | LEU  | C-N    | -5.83 | 1.27        | 1.33     |
| 1   | A     | 90  | LYS  | C-O    | -5.83 | 1.16        | 1.23     |
| 1   | A     | 162 | LEU  | CA-CB  | 5.83  | 1.63        | 1.53     |
| 1   | A     | 162 | LEU  | C-N    | -5.80 | 1.25        | 1.33     |
| 1   | A     | 228 | TYR  | C-N    | -5.80 | 1.25        | 1.33     |
| 1   | A     | 37  | THR  | C-N    | -5.79 | 1.27        | 1.33     |
| 1   | A     | 171 | TYR  | CZ-OH  | 5.78  | 1.50        | 1.38     |
| 1   | A     | 99  | ILE  | CA-C   | -5.78 | 1.45        | 1.52     |
| 1   | A     | 33  | LEU  | C-N    | -5.76 | 1.25        | 1.33     |
| 1   | A     | 194 | ASP  | CG-OD2 | -5.76 | 1.14        | 1.25     |
| 1   | A     | 63  | SER  | C-N    | -5.76 | 1.25        | 1.33     |
| 1   | A     | 153 | ASP  | C-O    | -5.75 | 1.12        | 1.23     |
| 1   | A     | 122 | CYS  | C-O    | -5.74 | 1.16        | 1.23     |
| 1   | A     | 4   | PRO  | N-CA   | 5.73  | 1.54        | 1.47     |
| 1   | A     | 78  | GLU  | CA-CB  | 5.73  | 1.64        | 1.53     |
| 1   | A     | 219 | THR  | CB-OG1 | -5.71 | 1.34        | 1.43     |
| 1   | A     | 168 | CYS  | CA-C   | 5.69  | 1.60        | 1.52     |
| 1   | A     | 199 | LEU  | C-N    | -5.69 | 1.25        | 1.33     |
| 1   | A     | 27  | TRP  | N-CA   | 5.68  | 1.52        | 1.46     |
| 1   | A     | 157 | GLN  | C-N    | 5.67  | 1.42        | 1.33     |
| 1   | A     | 16  | ILE  | C-O    | 5.67  | 1.31        | 1.23     |
| 1   | A     | 93  | LYS  | N-CA   | -5.67 | 1.39        | 1.46     |
| 1   | A     | 69  | GLY  | N-CA   | -5.66 | 1.36        | 1.45     |
| 1   | A     | 43  | GLY  | N-CA   | -5.66 | 1.37        | 1.45     |
| 1   | A     | 221 | SER  | CB-OG  | -5.66 | 1.30        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 133 | GLY  | CA-C    | 5.63  | 1.59        | 1.51     |
| 1   | A     | 62  | THR  | C-O     | 5.62  | 1.32        | 1.24     |
| 1   | A     | 197 | GLY  | N-CA    | -5.61 | 1.37        | 1.44     |
| 1   | A     | 130 | PHE  | CE1-CZ  | 5.61  | 1.55        | 1.38     |
| 1   | A     | 49  | GLU  | CD-OE1  | -5.60 | 1.14        | 1.25     |
| 1   | A     | 89  | PHE  | CG-CD2  | -5.60 | 1.27        | 1.38     |
| 1   | A     | 53  | VAL  | C-N     | 5.59  | 1.40        | 1.33     |
| 1   | A     | 192 | MET  | CA-C    | -5.59 | 1.44        | 1.52     |
| 1   | A     | 141 | TRP  | C-O     | -5.59 | 1.16        | 1.24     |
| 1   | A     | 223 | SER  | C-O     | -5.58 | 1.16        | 1.24     |
| 1   | A     | 194 | ASP  | CA-C    | 5.57  | 1.60        | 1.52     |
| 1   | A     | 55  | ALA  | C-N     | 5.55  | 1.42        | 1.33     |
| 1   | A     | 15  | ARG  | C-N     | -5.54 | 1.24        | 1.33     |
| 1   | A     | 118 | VAL  | C-N     | -5.54 | 1.26        | 1.33     |
| 1   | A     | 245 | ASN  | C-OXT   | -5.53 | 1.12        | 1.23     |
| 1   | A     | 121 | VAL  | N-CA    | -5.53 | 1.38        | 1.46     |
| 1   | A     | 30  | GLN  | CA-C    | -5.53 | 1.45        | 1.52     |
| 1   | A     | 172 | TRP  | CD1-NE1 | -5.50 | 1.26        | 1.37     |
| 1   | A     | 125 | SER  | N-CA    | 5.50  | 1.52        | 1.45     |
| 1   | A     | 57  | HIS  | CG-ND1  | -5.46 | 1.32        | 1.38     |
| 1   | A     | 129 | ASP  | CG-OD2  | -5.46 | 1.15        | 1.25     |
| 1   | A     | 24  | PRO  | N-CD    | 5.46  | 1.55        | 1.47     |
| 1   | A     | 1   | CYS  | C-N     | -5.45 | 1.26        | 1.33     |
| 1   | A     | 66  | VAL  | C-O     | -5.42 | 1.18        | 1.24     |
| 1   | A     | 81  | GLN  | CD-OE1  | 5.41  | 1.33        | 1.23     |
| 1   | A     | 68  | ALA  | CA-CB   | 5.41  | 1.63        | 1.53     |
| 1   | A     | 112 | ALA  | C-O     | -5.40 | 1.17        | 1.24     |
| 1   | A     | 175 | LYS  | C-O     | 5.39  | 1.31        | 1.24     |
| 1   | A     | 99  | ILE  | CA-CB   | 5.38  | 1.61        | 1.54     |
| 1   | A     | 155 | LEU  | CA-CB   | 5.38  | 1.61        | 1.53     |
| 1   | A     | 15  | ARG  | CA-C    | -5.37 | 1.45        | 1.52     |
| 1   | A     | 129 | ASP  | C-O     | 5.31  | 1.30        | 1.23     |
| 1   | A     | 230 | ARG  | CD-NE   | -5.31 | 1.38        | 1.46     |
| 1   | A     | 31  | VAL  | N-CA    | -5.30 | 1.40        | 1.46     |
| 1   | A     | 105 | LEU  | CA-C    | 5.30  | 1.59        | 1.52     |
| 1   | A     | 137 | VAL  | C-N     | 5.30  | 1.40        | 1.33     |
| 1   | A     | 191 | CYS  | CA-C    | 5.29  | 1.59        | 1.52     |
| 1   | A     | 25  | GLY  | CA-C    | -5.29 | 1.43        | 1.51     |
| 1   | A     | 167 | ASN  | CA-C    | -5.29 | 1.46        | 1.52     |
| 1   | A     | 235 | VAL  | CB-CG1  | 5.28  | 1.70        | 1.52     |
| 1   | A     | 195 | SER  | C-N     | -5.26 | 1.25        | 1.33     |
| 1   | A     | 61  | THR  | CB-OG1  | -5.26 | 1.35        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 110 | THR  | C-N     | -5.25 | 1.26        | 1.33     |
| 1   | A     | 98  | THR  | C-N     | -5.24 | 1.26        | 1.33     |
| 1   | A     | 229 | ALA  | C-O     | -5.23 | 1.17        | 1.24     |
| 1   | A     | 89  | PHE  | CE2-CZ  | 5.22  | 1.54        | 1.38     |
| 1   | A     | 244 | ALA  | C-N     | -5.21 | 1.26        | 1.33     |
| 1   | A     | 141 | TRP  | CD2-CE3 | -5.21 | 1.31        | 1.40     |
| 1   | A     | 30  | GLN  | N-CA    | -5.20 | 1.39        | 1.46     |
| 1   | A     | 115 | SER  | C-O     | -5.19 | 1.19        | 1.24     |
| 1   | A     | 29  | TRP  | C-O     | 5.17  | 1.30        | 1.24     |
| 1   | A     | 226 | GLY  | N-CA    | -5.15 | 1.38        | 1.45     |
| 1   | A     | 93  | LYS  | CA-CB   | -5.14 | 1.45        | 1.53     |
| 1   | A     | 44  | GLY  | CA-C    | 5.14  | 1.57        | 1.51     |
| 1   | A     | 49  | GLU  | CA-CB   | 5.13  | 1.61        | 1.53     |
| 1   | A     | 156 | GLN  | C-N     | -5.13 | 1.26        | 1.33     |
| 1   | A     | 160 | LEU  | CA-C    | -5.12 | 1.47        | 1.53     |
| 1   | A     | 27  | TRP  | CZ2-CH2 | 5.10  | 1.47        | 1.37     |
| 1   | A     | 236 | ASN  | CB-CG   | 5.10  | 1.64        | 1.52     |
| 1   | A     | 230 | ARG  | CZ-NH2  | -5.07 | 1.26        | 1.33     |
| 1   | A     | 202 | LYS  | CE-NZ   | 5.06  | 1.64        | 1.49     |
| 1   | A     | 207 | TRP  | CZ2-CH2 | -5.05 | 1.27        | 1.37     |
| 1   | A     | 80  | ILE  | N-CA    | -5.04 | 1.40        | 1.46     |
| 1   | A     | 14  | SER  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | A     | 116 | GLN  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | A     | 28  | PRO  | C-O     | -5.02 | 1.17        | 1.24     |

All (596) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 9   | VAL  | CB-CA-C   | 23.92  | 150.53      | 111.29   |
| 1   | A     | 18  | ASN  | CA-CB-CG  | -18.54 | 94.06       | 112.60   |
| 1   | A     | 9   | VAL  | CA-CB-CG1 | -17.65 | 80.39       | 110.40   |
| 1   | A     | 22  | ALA  | N-CA-C    | 17.22  | 132.74      | 110.53   |
| 1   | A     | 138 | THR  | CB-CA-C   | 17.00  | 139.99      | 109.38   |
| 1   | A     | 34  | GLN  | O-C-N     | 16.52  | 142.10      | 123.10   |
| 1   | A     | 114 | PHE  | O-C-N     | 16.36  | 143.06      | 122.93   |
| 1   | A     | 49  | GLU  | CA-C-O    | 15.93  | 138.29      | 119.97   |
| 1   | A     | 89  | PHE  | CA-CB-CG  | -15.54 | 98.26       | 113.80   |
| 1   | A     | 59  | GLY  | O-C-N     | 15.14  | 142.38      | 122.70   |
| 1   | A     | 194 | ASP  | CA-CB-CG  | 15.01  | 127.61      | 112.60   |
| 1   | A     | 125 | SER  | O-C-N     | 14.77  | 139.72      | 123.03   |
| 1   | A     | 17  | VAL  | CA-C-N    | 14.62  | 146.66      | 122.54   |
| 1   | A     | 17  | VAL  | C-N-CA    | 14.62  | 146.66      | 122.54   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 93  | LYS  | N-CA-C    | -14.60 | 96.08       | 112.72   |
| 1   | A     | 174 | THR  | CB-CA-C   | 14.55  | 134.00      | 109.55   |
| 1   | A     | 23  | VAL  | CA-C-O    | 14.18  | 130.03      | 119.25   |
| 1   | A     | 195 | SER  | N-CA-CB   | -14.13 | 89.83       | 110.17   |
| 1   | A     | 55  | ALA  | CB-CA-C   | 14.05  | 134.42      | 109.83   |
| 1   | A     | 86  | ALA  | O-C-N     | 14.05  | 140.60      | 122.19   |
| 1   | A     | 34  | GLN  | CB-CG-CD  | -14.04 | 88.73       | 112.60   |
| 1   | A     | 97  | LEU  | N-CA-C    | -13.93 | 96.10       | 111.28   |
| 1   | A     | 52  | VAL  | CA-C-O    | 13.66  | 135.78      | 120.76   |
| 1   | A     | 29  | TRP  | CA-C-O    | -13.37 | 104.34      | 119.05   |
| 1   | A     | 94  | TYR  | N-CA-CB   | 13.34  | 133.04      | 110.49   |
| 1   | A     | 230 | ARG  | CA-C-O    | 13.29  | 139.51      | 120.51   |
| 1   | A     | 9   | VAL  | CA-C-O    | -13.18 | 104.30      | 120.78   |
| 1   | A     | 230 | ARG  | N-CA-C    | 13.18  | 138.88      | 110.80   |
| 1   | A     | 224 | THR  | CA-C-N    | 12.89  | 133.91      | 119.99   |
| 1   | A     | 224 | THR  | C-N-CA    | 12.89  | 133.91      | 119.99   |
| 1   | A     | 215 | TRP  | CB-CG-CD1 | -12.74 | 107.80      | 126.90   |
| 1   | A     | 8   | PRO  | CA-C-N    | 12.70  | 144.82      | 121.97   |
| 1   | A     | 8   | PRO  | C-N-CA    | 12.70  | 144.82      | 121.97   |
| 1   | A     | 57  | HIS  | CA-CB-CG  | -12.63 | 101.17      | 113.80   |
| 1   | A     | 204 | ASN  | CB-CA-C   | 12.53  | 130.09      | 111.80   |
| 1   | A     | 209 | LEU  | O-C-N     | 12.47  | 137.47      | 123.13   |
| 1   | A     | 88  | VAL  | CB-CA-C   | 12.47  | 127.25      | 110.42   |
| 1   | A     | 107 | LYS  | N-CA-CB   | 12.43  | 131.05      | 110.17   |
| 1   | A     | 237 | TRP  | CA-C-O    | -12.36 | 107.45      | 120.55   |
| 1   | A     | 130 | PHE  | N-CA-CB   | 12.28  | 130.58      | 110.32   |
| 1   | A     | 88  | VAL  | N-CA-CB   | -12.27 | 95.13       | 111.82   |
| 1   | A     | 89  | PHE  | N-CA-CB   | 12.26  | 130.62      | 110.39   |
| 1   | A     | 32  | SER  | CA-C-N    | -12.26 | 104.25      | 122.39   |
| 1   | A     | 32  | SER  | C-N-CA    | -12.26 | 104.25      | 122.39   |
| 1   | A     | 207 | TRP  | CA-C-O    | 12.21  | 134.35      | 120.80   |
| 1   | A     | 160 | LEU  | CA-C-N    | 12.18  | 132.15      | 119.85   |
| 1   | A     | 160 | LEU  | C-N-CA    | 12.18  | 132.15      | 119.85   |
| 1   | A     | 231 | VAL  | CB-CA-C   | 12.11  | 131.16      | 111.29   |
| 1   | A     | 159 | SER  | O-C-N     | 12.10  | 138.57      | 123.21   |
| 1   | A     | 52  | VAL  | N-CA-C    | -12.03 | 90.64       | 108.45   |
| 1   | A     | 125 | SER  | CA-C-O    | -11.71 | 107.37      | 121.66   |
| 1   | A     | 229 | ALA  | N-CA-C    | 11.50  | 127.25      | 108.96   |
| 1   | A     | 35  | ASP  | CA-CB-CG  | 11.45  | 124.05      | 112.60   |
| 1   | A     | 200 | VAL  | CA-CB-CG1 | 11.42  | 129.81      | 110.40   |
| 1   | A     | 112 | ALA  | O-C-N     | 11.38  | 136.19      | 123.22   |
| 1   | A     | 202 | LYS  | O-C-N     | -11.33 | 110.37      | 123.06   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 85  | ILE  | N-CA-CB    | -11.31 | 94.76       | 110.26   |
| 1   | A     | 160 | LEU  | CB-CA-C    | -11.31 | 95.11       | 110.16   |
| 1   | A     | 93  | LYS  | N-CA-CB    | 11.29  | 127.52      | 110.70   |
| 1   | A     | 54  | THR  | N-CA-CB    | 11.23  | 128.48      | 110.97   |
| 1   | A     | 55  | ALA  | N-CA-CB    | -11.22 | 92.51       | 110.46   |
| 1   | A     | 132 | ALA  | CB-CA-C    | 11.17  | 130.10      | 109.54   |
| 1   | A     | 54  | THR  | CA-C-O     | -11.10 | 109.39      | 121.05   |
| 1   | A     | 241 | THR  | O-C-N      | 11.09  | 134.79      | 122.15   |
| 1   | A     | 200 | VAL  | N-CA-CB    | -11.02 | 91.54       | 111.93   |
| 1   | A     | 197 | GLY  | CA-C-N     | 11.02  | 132.58      | 120.13   |
| 1   | A     | 197 | GLY  | C-N-CA     | 11.02  | 132.58      | 120.13   |
| 1   | A     | 129 | ASP  | N-CA-CB    | -11.00 | 93.94       | 111.43   |
| 1   | A     | 32  | SER  | N-CA-CB    | 10.97  | 127.74      | 110.85   |
| 1   | A     | 27  | TRP  | CB-CA-C    | 10.95  | 125.52      | 110.96   |
| 1   | A     | 180 | MET  | CB-CA-C    | 10.95  | 128.00      | 109.50   |
| 1   | A     | 10  | LEU  | CB-CA-C    | -10.89 | 93.36       | 110.78   |
| 1   | A     | 67  | VAL  | CA-C-N     | -10.71 | 107.89      | 122.99   |
| 1   | A     | 67  | VAL  | C-N-CA     | -10.71 | 107.89      | 122.99   |
| 1   | A     | 220 | CYS  | CB-CA-C    | -10.68 | 96.51       | 112.11   |
| 1   | A     | 169 | LYS  | CB-CA-C    | 10.63  | 131.58      | 110.42   |
| 1   | A     | 96  | SER  | CB-CA-C    | -10.62 | 88.71       | 110.38   |
| 1   | A     | 136 | CYS  | CA-C-N     | -10.57 | 106.93      | 122.58   |
| 1   | A     | 136 | CYS  | C-N-CA     | -10.57 | 106.93      | 122.58   |
| 1   | A     | 53  | VAL  | O-C-N      | -10.53 | 112.40      | 123.14   |
| 1   | A     | 158 | ALA  | CA-C-O     | -10.49 | 108.84      | 121.11   |
| 1   | A     | 237 | TRP  | O-C-N      | 10.44  | 133.19      | 122.12   |
| 1   | A     | 160 | LEU  | O-C-N      | -10.39 | 109.53      | 121.79   |
| 1   | A     | 107 | LYS  | CA-C-O     | -10.37 | 108.81      | 120.43   |
| 1   | A     | 124 | PRO  | CB-CA-C    | -10.36 | 94.47       | 111.56   |
| 1   | A     | 116 | GLN  | OE1-CD-NE2 | -10.29 | 112.31      | 122.60   |
| 1   | A     | 161 | PRO  | O-C-N      | -10.28 | 110.41      | 123.06   |
| 1   | A     | 7   | GLN  | CA-C-O     | 10.27  | 131.11      | 119.61   |
| 1   | A     | 107 | LYS  | CB-CA-C    | -10.23 | 93.14       | 110.22   |
| 1   | A     | 222 | THR  | CA-C-O     | 10.20  | 132.48      | 119.12   |
| 1   | A     | 89  | PHE  | CZ-CE2-CD2 | -10.12 | 101.79      | 120.00   |
| 1   | A     | 212 | ILE  | N-CA-C     | -10.09 | 93.90       | 108.53   |
| 1   | A     | 213 | VAL  | CB-CA-C    | -10.07 | 97.84       | 111.33   |
| 1   | A     | 64  | ASP  | CA-C-O     | -10.06 | 109.79      | 121.16   |
| 1   | A     | 218 | SER  | O-C-N      | -10.06 | 109.21      | 122.59   |
| 1   | A     | 135 | THR  | CA-CB-OG1  | 9.92   | 124.48      | 109.60   |
| 1   | A     | 192 | MET  | N-CA-C     | -9.90  | 100.46      | 112.54   |
| 1   | A     | 189 | SER  | CA-C-O     | 9.89   | 131.20      | 120.71   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 93  | LYS  | CB-CA-C    | 9.88  | 127.24      | 110.94   |
| 1   | A     | 192 | MET  | CA-C-O     | 9.87  | 131.52      | 119.38   |
| 1   | A     | 159 | SER  | CA-C-N     | -9.82 | 102.95      | 122.40   |
| 1   | A     | 159 | SER  | C-N-CA     | -9.82 | 102.95      | 122.40   |
| 1   | A     | 123 | LEU  | CB-CA-C    | 9.78  | 123.60      | 108.84   |
| 1   | A     | 155 | LEU  | CA-C-N     | -9.75 | 105.59      | 123.05   |
| 1   | A     | 155 | LEU  | C-N-CA     | -9.75 | 105.59      | 123.05   |
| 1   | A     | 129 | ASP  | CA-C-N     | -9.69 | 105.89      | 121.58   |
| 1   | A     | 129 | ASP  | C-N-CA     | -9.69 | 105.89      | 121.58   |
| 1   | A     | 67  | VAL  | O-C-N      | 9.65  | 136.14      | 122.62   |
| 1   | A     | 206 | ALA  | N-CA-C     | -9.59 | 95.56       | 110.42   |
| 1   | A     | 204 | ASN  | N-CA-C     | -9.58 | 98.51       | 111.54   |
| 1   | A     | 164 | SER  | CB-CA-C    | -9.57 | 94.96       | 109.90   |
| 1   | A     | 97  | LEU  | CB-CA-C    | 9.56  | 126.66      | 110.79   |
| 1   | A     | 229 | ALA  | O-C-N      | 9.56  | 134.12      | 123.13   |
| 1   | A     | 47  | ILE  | N-CA-C     | -9.56 | 104.16      | 113.53   |
| 1   | A     | 20  | GLU  | CB-CG-CD   | -9.54 | 96.37       | 112.60   |
| 1   | A     | 185 | ALA  | CB-CA-C    | -9.54 | 91.43       | 110.42   |
| 1   | A     | 23  | VAL  | N-CA-CB    | -9.51 | 100.09      | 111.31   |
| 1   | A     | 162 | LEU  | O-C-N      | 9.44  | 133.61      | 122.85   |
| 1   | A     | 88  | VAL  | O-C-N      | 9.40  | 132.96      | 123.18   |
| 1   | A     | 32  | SER  | CB-CA-C    | -9.38 | 92.82       | 109.71   |
| 1   | A     | 130 | PHE  | CA-C-O     | 9.37  | 131.41      | 119.98   |
| 1   | A     | 225 | PRO  | CA-C-N     | 9.21  | 131.29      | 122.36   |
| 1   | A     | 225 | PRO  | C-N-CA     | 9.21  | 131.29      | 122.36   |
| 1   | A     | 191 | CYS  | CA-C-O     | -9.19 | 107.10      | 119.05   |
| 1   | A     | 64  | ASP  | CA-C-N     | -9.18 | 110.39      | 123.06   |
| 1   | A     | 64  | ASP  | C-N-CA     | -9.18 | 110.39      | 123.06   |
| 1   | A     | 100 | ASN  | CA-CB-CG   | -9.14 | 103.46      | 112.60   |
| 1   | A     | 50  | ASN  | N-CA-CB    | -9.13 | 97.23       | 110.65   |
| 1   | A     | 236 | ASN  | OD1-CG-ND2 | 9.08  | 131.68      | 122.60   |
| 1   | A     | 171 | TYR  | N-CA-CB    | 9.04  | 124.28      | 110.80   |
| 1   | A     | 171 | TYR  | CB-CA-C    | -9.03 | 94.27       | 109.99   |
| 1   | A     | 20  | GLU  | N-CA-CB    | -9.03 | 96.13       | 111.21   |
| 1   | A     | 177 | LYS  | N-CA-CB    | -9.03 | 96.95       | 110.85   |
| 1   | A     | 167 | ASN  | N-CA-C     | -9.02 | 101.02      | 111.03   |
| 1   | A     | 218 | SER  | CA-C-N     | 9.01  | 135.14      | 120.63   |
| 1   | A     | 218 | SER  | C-N-CA     | 9.01  | 135.14      | 120.63   |
| 1   | A     | 54  | THR  | O-C-N      | 9.00  | 133.07      | 122.72   |
| 1   | A     | 183 | ALA  | N-CA-C     | 8.91  | 122.93      | 108.32   |
| 1   | A     | 240 | GLN  | CB-CA-C    | -8.87 | 95.77       | 110.85   |
| 1   | A     | 136 | CYS  | N-CA-C     | 8.81  | 123.78      | 109.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 242 | LEU  | CB-CA-C     | -8.79 | 93.39       | 110.10   |
| 1   | A     | 64  | ASP  | O-C-N       | 8.79  | 134.23      | 123.16   |
| 1   | A     | 141 | TRP  | CA-C-O      | 8.79  | 128.92      | 119.34   |
| 1   | A     | 134 | THR  | N-CA-CB     | 8.79  | 123.57      | 109.95   |
| 1   | A     | 27  | TRP  | CB-CG-CD2   | 8.72  | 139.01      | 126.80   |
| 1   | A     | 23  | VAL  | N-CA-C      | -8.70 | 98.94       | 107.55   |
| 1   | A     | 228 | TYR  | N-CA-CB     | -8.70 | 97.11       | 111.20   |
| 1   | A     | 82  | LYS  | CA-C-O      | -8.68 | 110.77      | 120.32   |
| 1   | A     | 186 | SER  | O-C-N       | 8.68  | 131.24      | 122.30   |
| 1   | A     | 61  | THR  | N-CA-CB     | 8.67  | 125.80      | 111.31   |
| 1   | A     | 13  | LEU  | N-CA-C      | -8.67 | 100.84      | 111.33   |
| 1   | A     | 30  | GLN  | N-CA-CB     | 8.67  | 122.96      | 109.69   |
| 1   | A     | 101 | ASN  | CA-CB-CG    | -8.64 | 103.96      | 112.60   |
| 1   | A     | 161 | PRO  | CA-C-O      | 8.62  | 132.19      | 121.67   |
| 1   | A     | 202 | LYS  | N-CA-C      | 8.62  | 124.02      | 110.32   |
| 1   | A     | 179 | ALA  | CA-C-O      | -8.61 | 108.20      | 120.51   |
| 1   | A     | 200 | VAL  | CB-CA-C     | 8.60  | 124.46      | 110.69   |
| 1   | A     | 209 | LEU  | CA-C-O      | -8.60 | 110.80      | 120.43   |
| 1   | A     | 245 | ASN  | CA-CB-CG    | -8.59 | 104.01      | 112.60   |
| 1   | A     | 23  | VAL  | CA-C-N      | 8.58  | 130.57      | 119.84   |
| 1   | A     | 23  | VAL  | C-N-CA      | 8.58  | 130.57      | 119.84   |
| 1   | A     | 181 | ILE  | CB-CA-C     | -8.57 | 97.82       | 110.33   |
| 1   | A     | 174 | THR  | N-CA-CB     | -8.56 | 98.06       | 110.65   |
| 1   | A     | 127 | SER  | CA-C-O      | 8.56  | 130.14      | 119.78   |
| 1   | A     | 175 | LYS  | N-CA-CB     | -8.56 | 98.75       | 110.56   |
| 1   | A     | 32  | SER  | CA-C-O      | -8.54 | 111.22      | 121.56   |
| 1   | A     | 29  | TRP  | CE3-CZ3-CH2 | -8.53 | 110.02      | 121.10   |
| 1   | A     | 176 | ILE  | N-CA-CB     | -8.52 | 97.18       | 111.23   |
| 1   | A     | 219 | THR  | N-CA-C      | -8.52 | 101.27      | 112.34   |
| 1   | A     | 116 | GLN  | CB-CA-C     | -8.47 | 96.46       | 110.85   |
| 1   | A     | 91  | ASN  | N-CA-CB     | -8.44 | 96.00       | 111.37   |
| 1   | A     | 200 | VAL  | CA-C-O      | 8.44  | 131.06      | 121.28   |
| 1   | A     | 240 | GLN  | N-CA-CB     | 8.43  | 122.64      | 110.16   |
| 1   | A     | 168 | CYS  | CA-CB-SG    | -8.42 | 95.04       | 114.40   |
| 1   | A     | 90  | LYS  | O-C-N       | -8.38 | 112.29      | 123.10   |
| 1   | A     | 203 | LYS  | CA-C-N      | 8.38  | 134.05      | 122.07   |
| 1   | A     | 203 | LYS  | C-N-CA      | 8.38  | 134.05      | 122.07   |
| 1   | A     | 58  | CYS  | N-CA-CB     | 8.35  | 124.51      | 110.32   |
| 1   | A     | 37  | THR  | N-CA-C      | 8.34  | 123.27      | 112.26   |
| 1   | A     | 103 | ILE  | N-CA-C      | 8.31  | 120.75      | 108.45   |
| 1   | A     | 29  | TRP  | O-C-N       | 8.31  | 132.57      | 122.35   |
| 1   | A     | 138 | THR  | N-CA-C      | -8.29 | 96.24       | 109.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 23  | VAL  | CB-CA-C     | -8.28 | 101.27      | 111.04   |
| 1   | A     | 20  | GLU  | CA-C-O      | 8.26  | 130.12      | 121.36   |
| 1   | A     | 183 | ALA  | CB-CA-C     | -8.26 | 95.94       | 109.89   |
| 1   | A     | 68  | ALA  | N-CA-CB     | -8.24 | 96.84       | 110.68   |
| 1   | A     | 167 | ASN  | CB-CG-ND2   | -8.21 | 104.08      | 116.40   |
| 1   | A     | 122 | CYS  | CA-C-O      | -8.21 | 111.46      | 121.89   |
| 1   | A     | 80  | ILE  | O-C-N       | 8.20  | 132.86      | 122.61   |
| 1   | A     | 80  | ILE  | N-CA-CB     | -8.19 | 95.71       | 110.95   |
| 1   | A     | 25  | GLY  | CA-C-O      | 8.19  | 127.72      | 119.04   |
| 1   | A     | 162 | LEU  | N-CA-CB     | 8.18  | 122.88      | 110.45   |
| 1   | A     | 128 | ASP  | O-C-N       | -8.17 | 111.72      | 122.59   |
| 1   | A     | 50  | ASN  | CB-CA-C     | 8.15  | 123.24      | 109.55   |
| 1   | A     | 189 | SER  | N-CA-C      | 8.13  | 122.69      | 109.59   |
| 1   | A     | 6   | ILE  | O-C-N       | -8.11 | 114.51      | 123.26   |
| 1   | A     | 223 | SER  | CA-C-O      | 8.05  | 129.09      | 119.59   |
| 1   | A     | 119 | SER  | N-CA-CB     | 8.04  | 123.52      | 110.97   |
| 1   | A     | 141 | TRP  | CG-CD2-CE3  | 8.02  | 141.92      | 133.90   |
| 1   | A     | 68  | ALA  | CB-CA-C     | 8.00  | 124.34      | 109.71   |
| 1   | A     | 42  | CYS  | CA-C-N      | -7.98 | 105.76      | 121.41   |
| 1   | A     | 42  | CYS  | C-N-CA      | -7.98 | 105.76      | 121.41   |
| 1   | A     | 49  | GLU  | CB-CG-CD    | -7.97 | 99.05       | 112.60   |
| 1   | A     | 131 | ALA  | O-C-N       | -7.92 | 112.22      | 123.07   |
| 1   | A     | 98  | THR  | N-CA-C      | 7.91  | 124.09      | 113.97   |
| 1   | A     | 22  | ALA  | O-C-N       | 7.90  | 132.37      | 122.65   |
| 1   | A     | 80  | ILE  | CB-CA-C     | 7.90  | 123.45      | 111.68   |
| 1   | A     | 127 | SER  | N-CA-C      | -7.89 | 103.26      | 113.12   |
| 1   | A     | 90  | LYS  | CA-C-N      | -7.88 | 110.33      | 122.62   |
| 1   | A     | 90  | LYS  | C-N-CA      | -7.88 | 110.33      | 122.62   |
| 1   | A     | 218 | SER  | CA-C-O      | 7.87  | 131.77      | 120.51   |
| 1   | A     | 85  | ILE  | CA-CB-CG2   | -7.85 | 97.15       | 110.50   |
| 1   | A     | 85  | ILE  | N-CA-C      | 7.85  | 119.89      | 109.21   |
| 1   | A     | 123 | LEU  | CA-C-O      | 7.82  | 129.71      | 120.41   |
| 1   | A     | 237 | TRP  | CZ3-CH2-CZ2 | 7.80  | 131.65      | 121.50   |
| 1   | A     | 60  | VAL  | N-CA-CB     | -7.79 | 98.38       | 111.23   |
| 1   | A     | 26  | SER  | O-C-N       | 7.78  | 130.41      | 122.08   |
| 1   | A     | 224 | THR  | OG1-CB-CG2  | 7.78  | 124.85      | 109.30   |
| 1   | A     | 189 | SER  | CA-C-N      | 7.77  | 130.55      | 120.44   |
| 1   | A     | 189 | SER  | C-N-CA      | 7.77  | 130.55      | 120.44   |
| 1   | A     | 163 | LEU  | CA-C-O      | 7.76  | 130.49      | 121.49   |
| 1   | A     | 227 | VAL  | CA-CB-CG2   | -7.75 | 97.22       | 110.40   |
| 1   | A     | 53  | VAL  | N-CA-C      | -7.72 | 97.34       | 108.53   |
| 1   | A     | 16  | ILE  | N-CA-CB     | -7.70 | 97.30       | 112.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 232 | THR  | CB-CA-C     | 7.70  | 125.74      | 110.42   |
| 1   | A     | 13  | LEU  | O-C-N       | -7.69 | 113.97      | 122.12   |
| 1   | A     | 124 | PRO  | N-CA-CB     | -7.68 | 95.19       | 103.25   |
| 1   | A     | 118 | VAL  | N-CA-CB     | -7.67 | 100.63      | 111.99   |
| 1   | A     | 203 | LYS  | O-C-N       | 7.67  | 132.79      | 122.59   |
| 1   | A     | 44  | GLY  | O-C-N       | 7.66  | 131.47      | 123.81   |
| 1   | A     | 40  | HIS  | ND1-CG-CD2  | 7.63  | 113.73      | 106.10   |
| 1   | A     | 29  | TRP  | CD2-CE2-CZ2 | -7.63 | 114.77      | 122.40   |
| 1   | A     | 207 | TRP  | CG-CD2-CE3  | -7.58 | 126.32      | 133.90   |
| 1   | A     | 111 | ALA  | N-CA-CB     | -7.58 | 97.68       | 110.49   |
| 1   | A     | 18  | ASN  | N-CA-C      | -7.55 | 103.66      | 113.17   |
| 1   | A     | 208 | THR  | CA-CB-OG1   | 7.54  | 120.91      | 109.60   |
| 1   | A     | 13  | LEU  | CB-CA-C     | 7.54  | 123.49      | 110.68   |
| 1   | A     | 86  | ALA  | CA-C-O      | -7.54 | 109.58      | 120.13   |
| 1   | A     | 77  | SER  | O-C-N       | 7.53  | 135.04      | 123.00   |
| 1   | A     | 34  | GLN  | CA-CB-CG    | 7.51  | 129.13      | 114.10   |
| 1   | A     | 29  | TRP  | N-CA-C      | -7.51 | 103.96      | 113.72   |
| 1   | A     | 90  | LYS  | N-CA-C      | -7.49 | 98.53       | 110.14   |
| 1   | A     | 137 | VAL  | CB-CA-C     | -7.49 | 97.31       | 110.71   |
| 1   | A     | 191 | CYS  | O-C-N       | 7.47  | 132.76      | 122.46   |
| 1   | A     | 20  | GLU  | CA-CB-CG    | 7.46  | 129.02      | 114.10   |
| 1   | A     | 245 | ASN  | N-CA-CB     | -7.46 | 97.82       | 110.50   |
| 1   | A     | 194 | ASP  | O-C-N       | -7.43 | 112.70      | 122.59   |
| 1   | A     | 180 | MET  | CA-C-O      | -7.43 | 112.52      | 121.28   |
| 1   | A     | 215 | TRP  | CG-CD2-CE3  | 7.42  | 141.32      | 133.90   |
| 1   | A     | 53  | VAL  | CG1-CB-CG2  | -7.42 | 94.49       | 110.80   |
| 1   | A     | 169 | LYS  | N-CA-C      | -7.42 | 95.01       | 110.80   |
| 1   | A     | 51  | TRP  | CA-C-O      | -7.40 | 112.78      | 121.44   |
| 1   | A     | 213 | VAL  | N-CA-C      | 7.38  | 118.59      | 108.84   |
| 1   | A     | 162 | LEU  | CB-CA-C     | -7.38 | 95.07       | 109.76   |
| 1   | A     | 237 | TRP  | CE3-CZ3-CH2 | -7.38 | 111.51      | 121.10   |
| 1   | A     | 166 | THR  | CA-C-N      | 7.37  | 130.65      | 120.63   |
| 1   | A     | 166 | THR  | C-N-CA      | 7.37  | 130.65      | 120.63   |
| 1   | A     | 82  | LYS  | N-CA-C      | -7.36 | 96.52       | 108.52   |
| 1   | A     | 13  | LEU  | CA-C-N      | 7.33  | 135.55      | 121.54   |
| 1   | A     | 13  | LEU  | C-N-CA      | 7.33  | 135.55      | 121.54   |
| 1   | A     | 197 | GLY  | O-C-N       | 7.33  | 129.10      | 121.77   |
| 1   | A     | 88  | VAL  | CA-CB-CG2   | 7.32  | 122.84      | 110.40   |
| 1   | A     | 67  | VAL  | CA-C-O      | -7.31 | 111.14      | 120.86   |
| 1   | A     | 207 | TRP  | CG-CD1-NE1  | -7.30 | 100.71      | 110.20   |
| 1   | A     | 97  | LEU  | N-CA-CB     | -7.29 | 99.40       | 110.12   |
| 1   | A     | 202 | LYS  | CA-C-N      | 7.29  | 135.46      | 121.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 202 | LYS  | C-N-CA      | 7.29  | 135.46      | 121.54   |
| 1   | A     | 157 | GLN  | CA-C-O      | 7.28  | 128.40      | 120.32   |
| 1   | A     | 52  | VAL  | CA-C-N      | 7.27  | 132.48      | 123.10   |
| 1   | A     | 52  | VAL  | C-N-CA      | 7.27  | 132.48      | 123.10   |
| 1   | A     | 61  | THR  | CA-C-N      | -7.27 | 107.76      | 122.31   |
| 1   | A     | 61  | THR  | C-N-CA      | -7.27 | 107.76      | 122.31   |
| 1   | A     | 93  | LYS  | CA-C-O      | 7.27  | 128.43      | 119.78   |
| 1   | A     | 47  | ILE  | N-CA-CB     | -7.26 | 102.31      | 112.12   |
| 1   | A     | 132 | ALA  | N-CA-CB     | -7.26 | 99.72       | 110.17   |
| 1   | A     | 185 | ALA  | N-CA-CB     | 7.25  | 122.74      | 110.49   |
| 1   | A     | 33  | LEU  | CB-CA-C     | 7.24  | 121.29      | 110.14   |
| 1   | A     | 57  | HIS  | CB-CG-CD2   | -7.24 | 121.79      | 131.20   |
| 1   | A     | 110 | THR  | CA-CB-OG1   | -7.24 | 98.75       | 109.60   |
| 1   | A     | 27  | TRP  | CA-C-N      | 7.22  | 128.86      | 119.84   |
| 1   | A     | 27  | TRP  | C-N-CA      | 7.22  | 128.86      | 119.84   |
| 1   | A     | 7   | GLN  | CA-C-N      | 7.22  | 127.65      | 119.93   |
| 1   | A     | 7   | GLN  | C-N-CA      | 7.22  | 127.65      | 119.93   |
| 1   | A     | 195 | SER  | CB-CA-C     | 7.22  | 122.82      | 109.54   |
| 1   | A     | 154 | ARG  | N-CA-CB     | 7.20  | 121.36      | 110.42   |
| 1   | A     | 87  | LYS  | CA-CB-CG    | -7.16 | 99.77       | 114.10   |
| 1   | A     | 54  | THR  | CA-CB-OG1   | 7.16  | 120.34      | 109.60   |
| 1   | A     | 120 | ALA  | N-CA-C      | 7.14  | 121.09      | 109.59   |
| 1   | A     | 30  | GLN  | CA-C-O      | 7.13  | 129.04      | 120.92   |
| 1   | A     | 100 | ASN  | CB-CG-ND2   | -7.12 | 105.72      | 116.40   |
| 1   | A     | 83  | LEU  | CB-CG-CD2   | -7.12 | 89.35       | 110.70   |
| 1   | A     | 17  | VAL  | O-C-N       | -7.11 | 113.69      | 122.57   |
| 1   | A     | 39  | PHE  | CA-C-O      | 7.10  | 128.12      | 120.38   |
| 1   | A     | 108 | LEU  | N-CA-CB     | -7.08 | 98.76       | 110.23   |
| 1   | A     | 125 | SER  | N-CA-C      | -7.04 | 99.51       | 110.42   |
| 1   | A     | 135 | THR  | N-CA-CB     | -7.04 | 100.47      | 110.46   |
| 1   | A     | 237 | TRP  | CB-CA-C     | 7.03  | 122.46      | 110.79   |
| 1   | A     | 205 | GLY  | O-C-N       | 7.03  | 131.03      | 122.32   |
| 1   | A     | 132 | ALA  | N-CA-C      | -7.03 | 100.59      | 110.50   |
| 1   | A     | 9   | VAL  | N-CA-C      | -7.02 | 94.74       | 109.34   |
| 1   | A     | 174 | THR  | CA-C-O      | 7.02  | 126.77      | 119.05   |
| 1   | A     | 225 | PRO  | N-CA-CB     | 7.01  | 109.85      | 103.19   |
| 1   | A     | 99  | ILE  | O-C-N       | -7.01 | 113.81      | 122.57   |
| 1   | A     | 154 | ARG  | CD-NE-CZ    | -7.00 | 114.60      | 124.40   |
| 1   | A     | 166 | THR  | CA-CB-CG2   | 7.00  | 122.40      | 110.50   |
| 1   | A     | 11  | SER  | CA-C-N      | 6.99  | 127.74      | 119.98   |
| 1   | A     | 11  | SER  | C-N-CA      | 6.99  | 127.74      | 119.98   |
| 1   | A     | 141 | TRP  | CD2-CE3-CZ3 | 6.98  | 127.68      | 118.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 24  | PRO  | CB-CA-C    | 6.98  | 123.08      | 111.56   |
| 1   | A     | 31  | VAL  | CA-C-N     | 6.97  | 135.19      | 122.92   |
| 1   | A     | 31  | VAL  | C-N-CA     | 6.97  | 135.19      | 122.92   |
| 1   | A     | 44  | GLY  | CA-C-N     | -6.96 | 111.89      | 122.81   |
| 1   | A     | 44  | GLY  | C-N-CA     | -6.96 | 111.89      | 122.81   |
| 1   | A     | 195 | SER  | CA-C-N     | 6.96  | 134.64      | 122.05   |
| 1   | A     | 195 | SER  | C-N-CA     | 6.96  | 134.64      | 122.05   |
| 1   | A     | 223 | SER  | N-CA-CB    | -6.96 | 99.95       | 110.73   |
| 1   | A     | 27  | TRP  | CB-CG-CD1  | -6.95 | 116.47      | 126.90   |
| 1   | A     | 141 | TRP  | CG-CD1-NE1 | -6.94 | 101.17      | 110.20   |
| 1   | A     | 195 | SER  | O-C-N      | -6.92 | 114.69      | 122.86   |
| 1   | A     | 108 | LEU  | CB-CA-C    | 6.91  | 120.93      | 109.53   |
| 1   | A     | 98  | THR  | CA-CB-OG1  | 6.90  | 119.95      | 109.60   |
| 1   | A     | 200 | VAL  | O-C-N      | -6.89 | 115.63      | 123.00   |
| 1   | A     | 57  | HIS  | O-C-N      | -6.89 | 114.35      | 122.20   |
| 1   | A     | 123 | LEU  | O-C-N      | -6.86 | 114.91      | 121.57   |
| 1   | A     | 7   | GLN  | N-CA-C     | 6.83  | 119.53      | 109.62   |
| 1   | A     | 231 | VAL  | CA-C-O     | 6.83  | 129.32      | 120.78   |
| 1   | A     | 81  | GLN  | CA-C-N     | -6.83 | 113.50      | 123.05   |
| 1   | A     | 81  | GLN  | C-N-CA     | -6.83 | 113.50      | 123.05   |
| 1   | A     | 178 | ASP  | N-CA-CB    | 6.83  | 122.03      | 110.49   |
| 1   | A     | 43  | GLY  | N-CA-C     | -6.82 | 97.01       | 113.18   |
| 1   | A     | 138 | THR  | CA-CB-CG2  | 6.82  | 122.09      | 110.50   |
| 1   | A     | 68  | ALA  | O-C-N      | 6.81  | 131.41      | 123.30   |
| 1   | A     | 106 | LEU  | CB-CA-C    | -6.80 | 97.39       | 109.70   |
| 1   | A     | 80  | ILE  | N-CA-C     | 6.80  | 119.86      | 109.12   |
| 1   | A     | 131 | ALA  | CA-C-N     | 6.79  | 131.60      | 120.94   |
| 1   | A     | 131 | ALA  | C-N-CA     | 6.79  | 131.60      | 120.94   |
| 1   | A     | 187 | GLY  | N-CA-C     | -6.79 | 106.61      | 114.69   |
| 1   | A     | 159 | SER  | N-CA-CB    | -6.77 | 99.79       | 110.69   |
| 1   | A     | 27  | TRP  | CA-C-O     | 6.77  | 129.26      | 120.87   |
| 1   | A     | 182 | CYS  | CA-C-O     | 6.75  | 128.79      | 121.16   |
| 1   | A     | 180 | MET  | N-CA-C     | -6.75 | 99.30       | 110.17   |
| 1   | A     | 130 | PHE  | O-C-N      | 6.74  | 131.62      | 123.26   |
| 1   | A     | 204 | ASN  | CA-C-O     | 6.74  | 129.36      | 121.54   |
| 1   | A     | 61  | THR  | O-C-N      | 6.73  | 131.73      | 122.78   |
| 1   | A     | 134 | THR  | CA-C-N     | 6.73  | 134.16      | 122.32   |
| 1   | A     | 134 | THR  | C-N-CA     | 6.73  | 134.16      | 122.32   |
| 1   | A     | 214 | SER  | N-CA-CB    | 6.71  | 122.29      | 110.27   |
| 1   | A     | 41  | PHE  | CA-C-O     | 6.69  | 126.09      | 118.47   |
| 1   | A     | 129 | ASP  | O-C-N      | 6.68  | 132.09      | 122.94   |
| 1   | A     | 47  | ILE  | CA-C-O     | 6.68  | 125.86      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 212 | ILE  | CA-CB-CG1   | 6.68  | 121.75      | 110.40   |
| 1   | A     | 206 | ALA  | CB-CA-C     | 6.67  | 120.80      | 109.80   |
| 1   | A     | 51  | TRP  | O-C-N       | 6.65  | 131.79      | 123.15   |
| 1   | A     | 103 | ILE  | CA-C-N      | 6.63  | 133.44      | 121.89   |
| 1   | A     | 103 | ILE  | C-N-CA      | 6.63  | 133.44      | 121.89   |
| 1   | A     | 26  | SER  | CA-C-N      | -6.63 | 115.32      | 123.21   |
| 1   | A     | 26  | SER  | C-N-CA      | -6.63 | 115.32      | 123.21   |
| 1   | A     | 129 | ASP  | CA-CB-CG    | 6.63  | 119.23      | 112.60   |
| 1   | A     | 203 | LYS  | CA-CB-CG    | -6.62 | 100.86      | 114.10   |
| 1   | A     | 166 | THR  | CA-CB-OG1   | 6.61  | 119.52      | 109.60   |
| 1   | A     | 239 | GLN  | O-C-N       | 6.61  | 129.15      | 122.08   |
| 1   | A     | 134 | THR  | CA-CB-OG1   | 6.60  | 119.49      | 109.60   |
| 1   | A     | 141 | TRP  | CD1-NE1-CE2 | 6.59  | 120.77      | 108.90   |
| 1   | A     | 225 | PRO  | CA-C-O      | 6.59  | 129.39      | 121.48   |
| 1   | A     | 104 | THR  | O-C-N       | 6.59  | 131.54      | 123.44   |
| 1   | A     | 124 | PRO  | CA-N-CD     | 6.57  | 121.20      | 112.00   |
| 1   | A     | 51  | TRP  | N-CA-C      | 6.54  | 119.65      | 109.52   |
| 1   | A     | 203 | LYS  | CA-C-O      | 6.53  | 129.85      | 120.51   |
| 1   | A     | 208 | THR  | N-CA-CB     | -6.53 | 99.49       | 111.37   |
| 1   | A     | 215 | TRP  | CD1-CG-CD2  | 6.52  | 116.73      | 106.30   |
| 1   | A     | 139 | THR  | N-CA-C      | -6.51 | 99.60       | 109.95   |
| 1   | A     | 194 | ASP  | OD1-CG-OD2  | 6.50  | 138.51      | 122.90   |
| 1   | A     | 121 | VAL  | N-CA-C      | -6.49 | 102.98      | 110.05   |
| 1   | A     | 192 | MET  | N-CA-CB     | 6.49  | 121.16      | 110.39   |
| 1   | A     | 3   | VAL  | N-CA-CB     | -6.48 | 102.14      | 111.21   |
| 1   | A     | 65  | VAL  | N-CA-CB     | -6.47 | 100.13      | 111.39   |
| 1   | A     | 116 | GLN  | CG-CD-NE2   | 6.47  | 126.11      | 116.40   |
| 1   | A     | 175 | LYS  | N-CA-C      | 6.46  | 120.17      | 112.93   |
| 1   | A     | 204 | ASN  | CA-CB-CG    | -6.46 | 106.14      | 112.60   |
| 1   | A     | 14  | SER  | N-CA-CB     | 6.43  | 121.35      | 110.49   |
| 1   | A     | 29  | TRP  | CB-CA-C     | 6.42  | 120.34      | 109.55   |
| 1   | A     | 52  | VAL  | CB-CA-C     | 6.41  | 121.80      | 110.71   |
| 1   | A     | 81  | GLN  | CA-C-O      | 6.41  | 127.37      | 120.32   |
| 1   | A     | 7   | GLN  | N-CA-CB     | -6.38 | 100.08      | 109.90   |
| 1   | A     | 175 | LYS  | CA-C-N      | 6.36  | 133.41      | 121.97   |
| 1   | A     | 175 | LYS  | C-N-CA      | 6.36  | 133.41      | 121.97   |
| 1   | A     | 244 | ALA  | CB-CA-C     | -6.35 | 100.97      | 110.50   |
| 1   | A     | 9   | VAL  | CG1-CB-CG2  | 6.35  | 124.76      | 110.80   |
| 1   | A     | 226 | GLY  | CA-C-N      | -6.32 | 114.86      | 123.14   |
| 1   | A     | 226 | GLY  | C-N-CA      | -6.32 | 114.86      | 123.14   |
| 1   | A     | 220 | CYS  | CA-C-O      | 6.31  | 129.92      | 122.03   |
| 1   | A     | 112 | ALA  | CA-C-O      | -6.31 | 113.41      | 120.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 204 | ASN  | O-C-N       | 6.31  | 130.66      | 122.40   |
| 1   | A     | 22  | ALA  | CA-C-N      | 6.29  | 130.02      | 122.85   |
| 1   | A     | 22  | ALA  | C-N-CA      | 6.29  | 130.02      | 122.85   |
| 1   | A     | 16  | ILE  | N-CA-C      | 6.29  | 118.85      | 109.17   |
| 1   | A     | 42  | CYS  | O-C-N       | -6.29 | 116.23      | 123.33   |
| 1   | A     | 85  | ILE  | CA-C-O      | 6.28  | 128.59      | 121.11   |
| 1   | A     | 114 | PHE  | CA-C-O      | -6.28 | 113.59      | 120.81   |
| 1   | A     | 242 | LEU  | N-CA-CB     | 6.26  | 121.14      | 110.50   |
| 1   | A     | 125 | SER  | N-CA-CB     | 6.26  | 120.32      | 110.56   |
| 1   | A     | 155 | LEU  | CB-CG-CD2   | -6.25 | 91.95       | 110.70   |
| 1   | A     | 112 | ALA  | N-CA-CB     | 6.25  | 120.47      | 110.16   |
| 1   | A     | 188 | VAL  | N-CA-C      | -6.24 | 99.26       | 108.99   |
| 1   | A     | 211 | GLY  | N-CA-C      | -6.24 | 100.55      | 111.46   |
| 1   | A     | 142 | GLY  | CA-C-O      | -6.23 | 107.71      | 120.80   |
| 1   | A     | 84  | LYS  | CA-C-N      | -6.21 | 112.39      | 121.71   |
| 1   | A     | 84  | LYS  | C-N-CA      | -6.21 | 112.39      | 121.71   |
| 1   | A     | 119 | SER  | CA-C-O      | 6.21  | 127.57      | 121.05   |
| 1   | A     | 30  | GLN  | CA-C-N      | 6.21  | 132.48      | 122.68   |
| 1   | A     | 30  | GLN  | C-N-CA      | 6.21  | 132.48      | 122.68   |
| 1   | A     | 155 | LEU  | CB-CA-C     | -6.21 | 99.62       | 109.80   |
| 1   | A     | 186 | SER  | CB-CA-C     | 6.20  | 125.78      | 110.46   |
| 1   | A     | 180 | MET  | CA-C-N      | 6.19  | 131.59      | 122.99   |
| 1   | A     | 180 | MET  | C-N-CA      | 6.19  | 131.59      | 122.99   |
| 1   | A     | 29  | TRP  | CD2-CE3-CZ3 | 6.18  | 126.64      | 118.60   |
| 1   | A     | 167 | ASN  | CA-CB-CG    | -6.18 | 106.42      | 112.60   |
| 1   | A     | 190 | SER  | CA-C-N      | 6.17  | 133.40      | 121.18   |
| 1   | A     | 190 | SER  | C-N-CA      | 6.17  | 133.40      | 121.18   |
| 1   | A     | 8   | PRO  | N-CA-C      | -6.16 | 101.23      | 111.26   |
| 1   | A     | 227 | VAL  | CG1-CB-CG2  | 6.14  | 124.32      | 110.80   |
| 1   | A     | 106 | LEU  | CA-C-N      | -6.12 | 114.04      | 122.30   |
| 1   | A     | 106 | LEU  | C-N-CA      | -6.12 | 114.04      | 122.30   |
| 1   | A     | 110 | THR  | CA-CB-CG2   | -6.12 | 100.10      | 110.50   |
| 1   | A     | 209 | LEU  | N-CA-C      | -6.10 | 99.26       | 108.96   |
| 1   | A     | 198 | PRO  | N-CA-CB     | 6.09  | 108.42      | 103.36   |
| 1   | A     | 199 | LEU  | CB-CA-C     | 6.08  | 119.81      | 110.62   |
| 1   | A     | 128 | ASP  | CA-CB-CG    | 6.08  | 118.68      | 112.60   |
| 1   | A     | 107 | LYS  | CA-CB-CG    | 6.08  | 126.25      | 114.10   |
| 1   | A     | 170 | LYS  | N-CA-CB     | -6.05 | 100.26      | 110.49   |
| 1   | A     | 204 | ASN  | N-CA-CB     | -6.03 | 102.85      | 111.84   |
| 1   | A     | 207 | TRP  | N-CA-C      | -6.01 | 99.91       | 109.76   |
| 1   | A     | 220 | CYS  | O-C-N       | -6.00 | 115.77      | 122.91   |
| 1   | A     | 103 | ILE  | O-C-N       | -5.99 | 116.40      | 123.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 123 | LEU  | CB-CG-CD2   | 5.98  | 128.63      | 110.70   |
| 1   | A     | 237 | TRP  | CE2-CD2-CG  | 5.96  | 114.36      | 107.20   |
| 1   | A     | 94  | TYR  | CB-CG-CD1   | -5.95 | 111.87      | 120.80   |
| 1   | A     | 230 | ARG  | N-CA-CB     | -5.95 | 100.44      | 110.49   |
| 1   | A     | 245 | ASN  | CB-CA-C     | 5.95  | 121.40      | 110.10   |
| 1   | A     | 162 | LEU  | CA-C-O      | -5.92 | 114.83      | 121.81   |
| 1   | A     | 129 | ASP  | N-CA-C      | -5.91 | 100.42      | 109.41   |
| 1   | A     | 38  | GLY  | N-CA-C      | -5.90 | 102.36      | 114.16   |
| 1   | A     | 109 | SER  | N-CA-C      | 5.89  | 118.45      | 111.33   |
| 1   | A     | 127 | SER  | CA-C-N      | -5.89 | 110.29      | 121.54   |
| 1   | A     | 127 | SER  | C-N-CA      | -5.89 | 110.29      | 121.54   |
| 1   | A     | 238 | VAL  | CA-C-N      | 5.88  | 128.97      | 120.79   |
| 1   | A     | 238 | VAL  | C-N-CA      | 5.88  | 128.97      | 120.79   |
| 1   | A     | 102 | ASP  | CA-CB-CG    | 5.88  | 118.47      | 112.60   |
| 1   | A     | 18  | ASN  | O-C-N       | 5.86  | 129.66      | 122.34   |
| 1   | A     | 174 | THR  | OG1-CB-CG2  | 5.84  | 120.98      | 109.30   |
| 1   | A     | 91  | ASN  | CB-CA-C     | -5.84 | 97.18       | 109.38   |
| 1   | A     | 166 | THR  | CA-C-O      | 5.82  | 125.82      | 119.24   |
| 1   | A     | 215 | TRP  | CB-CG-CD2   | 5.81  | 134.93      | 126.80   |
| 1   | A     | 158 | ALA  | CB-CA-C     | -5.79 | 97.27       | 109.38   |
| 1   | A     | 234 | LEU  | CB-CA-C     | 5.79  | 118.16      | 109.13   |
| 1   | A     | 27  | TRP  | CG-CD2-CE3  | -5.78 | 128.12      | 133.90   |
| 1   | A     | 124 | PRO  | O-C-N       | 5.77  | 130.43      | 122.64   |
| 1   | A     | 237 | TRP  | CD2-CE2-CZ2 | 5.77  | 128.17      | 122.40   |
| 1   | A     | 8   | PRO  | CA-N-CD     | 5.77  | 120.07      | 112.00   |
| 1   | A     | 244 | ALA  | O-C-N       | 5.77  | 132.23      | 123.00   |
| 1   | A     | 114 | PHE  | CA-C-N      | -5.73 | 112.24      | 122.32   |
| 1   | A     | 114 | PHE  | C-N-CA      | -5.73 | 112.24      | 122.32   |
| 1   | A     | 192 | MET  | CA-CB-CG    | 5.72  | 125.53      | 114.10   |
| 1   | A     | 179 | ALA  | O-C-N       | -5.71 | 114.99      | 122.59   |
| 1   | A     | 33  | LEU  | N-CA-C      | -5.71 | 98.79       | 108.26   |
| 1   | A     | 113 | SER  | N-CA-CB     | 5.70  | 120.00      | 110.53   |
| 1   | A     | 171 | TYR  | O-C-N       | 5.70  | 128.92      | 122.20   |
| 1   | A     | 122 | CYS  | N-CA-C      | -5.69 | 102.04      | 110.46   |
| 1   | A     | 161 | PRO  | N-CA-C      | -5.66 | 102.38      | 111.38   |
| 1   | A     | 138 | THR  | CA-C-O      | 5.66  | 126.70      | 120.71   |
| 1   | A     | 215 | TRP  | CA-C-O      | 5.65  | 127.59      | 121.26   |
| 1   | A     | 57  | HIS  | CA-C-O      | 5.64  | 126.52      | 120.20   |
| 1   | A     | 117 | THR  | N-CA-CB     | 5.64  | 119.32      | 110.46   |
| 1   | A     | 221 | SER  | N-CA-CB     | -5.64 | 101.55      | 110.06   |
| 1   | A     | 35  | ASP  | N-CA-CB     | 5.63  | 119.34      | 110.39   |
| 1   | A     | 53  | VAL  | CA-C-O      | -5.62 | 114.31      | 120.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 49  | GLU  | N-CA-CB     | -5.61 | 101.58      | 110.28   |
| 1   | A     | 183 | ALA  | CA-C-O      | 5.61  | 126.98      | 120.14   |
| 1   | A     | 202 | LYS  | CG-CD-CE    | -5.61 | 98.40       | 111.30   |
| 1   | A     | 56  | ALA  | N-CA-C      | -5.61 | 105.56      | 112.90   |
| 1   | A     | 50  | ASN  | CA-CB-CG    | 5.59  | 118.19      | 112.60   |
| 1   | A     | 231 | VAL  | N-CA-CB     | -5.59 | 102.01      | 111.23   |
| 1   | A     | 91  | ASN  | CA-C-N      | 5.58  | 132.21      | 121.54   |
| 1   | A     | 91  | ASN  | C-N-CA      | 5.58  | 132.21      | 121.54   |
| 1   | A     | 103 | ILE  | CB-CA-C     | 5.58  | 120.35      | 110.71   |
| 1   | A     | 110 | THR  | N-CA-CB     | -5.57 | 102.21      | 110.90   |
| 1   | A     | 176 | ILE  | CB-CA-C     | 5.57  | 120.42      | 111.29   |
| 1   | A     | 232 | THR  | N-CA-CB     | -5.56 | 101.09      | 110.49   |
| 1   | A     | 140 | GLY  | CA-C-N      | -5.56 | 113.24      | 122.08   |
| 1   | A     | 140 | GLY  | C-N-CA      | -5.56 | 113.24      | 122.08   |
| 1   | A     | 157 | GLN  | CA-CB-CG    | -5.56 | 102.97      | 114.10   |
| 1   | A     | 222 | THR  | O-C-N       | 5.56  | 130.62      | 122.39   |
| 1   | A     | 212 | ILE  | CA-CB-CG2   | -5.55 | 101.06      | 110.50   |
| 1   | A     | 27  | TRP  | CD2-CE2-CZ2 | -5.54 | 116.86      | 122.40   |
| 1   | A     | 41  | PHE  | CA-C-N      | 5.54  | 131.66      | 121.85   |
| 1   | A     | 41  | PHE  | C-N-CA      | 5.54  | 131.66      | 121.85   |
| 1   | A     | 103 | ILE  | N-CA-CB     | -5.53 | 102.38      | 111.45   |
| 1   | A     | 87  | LYS  | CB-CA-C     | 5.53  | 122.33      | 110.45   |
| 1   | A     | 88  | VAL  | N-CA-C      | -5.53 | 99.59       | 107.77   |
| 1   | A     | 104 | THR  | OG1-CB-CG2  | 5.53  | 120.35      | 109.30   |
| 1   | A     | 140 | GLY  | CA-C-O      | 5.53  | 127.18      | 121.38   |
| 1   | A     | 4   | PRO  | CB-CA-C     | -5.51 | 104.17      | 111.23   |
| 1   | A     | 238 | VAL  | CA-CB-CG2   | -5.51 | 101.03      | 110.40   |
| 1   | A     | 238 | VAL  | N-CA-C      | -5.51 | 104.50      | 110.23   |
| 1   | A     | 140 | GLY  | N-CA-C      | 5.51  | 118.57      | 110.80   |
| 1   | A     | 116 | GLN  | N-CA-C      | 5.48  | 117.34      | 111.36   |
| 1   | A     | 57  | HIS  | ND1-CG-CD2  | 5.48  | 111.58      | 106.10   |
| 1   | A     | 62  | THR  | CB-CA-C     | -5.48 | 100.23      | 110.36   |
| 1   | A     | 233 | ALA  | O-C-N       | 5.47  | 130.41      | 122.43   |
| 1   | A     | 101 | ASN  | N-CA-C      | -5.46 | 104.11      | 111.54   |
| 1   | A     | 177 | LYS  | CA-C-O      | 5.46  | 128.17      | 121.56   |
| 1   | A     | 29  | TRP  | CZ3-CH2-CZ2 | 5.45  | 128.59      | 121.50   |
| 1   | A     | 227 | VAL  | N-CA-CB     | -5.45 | 103.89      | 111.41   |
| 1   | A     | 43  | GLY  | CA-C-O      | -5.45 | 111.09      | 120.57   |
| 1   | A     | 17  | VAL  | CA-CB-CG2   | -5.45 | 101.14      | 110.40   |
| 1   | A     | 196 | GLY  | N-CA-C      | -5.45 | 107.80      | 115.32   |
| 1   | A     | 9   | VAL  | CA-C-N      | 5.45  | 129.92      | 122.84   |
| 1   | A     | 9   | VAL  | C-N-CA      | 5.45  | 129.92      | 122.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 229 | ALA  | N-CA-CB     | -5.44 | 101.02      | 110.17   |
| 1   | A     | 3   | VAL  | O-C-N       | 5.44  | 127.30      | 121.10   |
| 1   | A     | 68  | ALA  | N-CA-C      | 5.43  | 117.75      | 108.90   |
| 1   | A     | 66  | VAL  | CB-CA-C     | 5.42  | 117.52      | 110.96   |
| 1   | A     | 180 | MET  | N-CA-CB     | 5.42  | 119.46      | 110.63   |
| 1   | A     | 141 | TRP  | CE2-CD2-CE3 | -5.41 | 113.39      | 118.80   |
| 1   | A     | 122 | CYS  | O-C-N       | 5.40  | 129.11      | 122.84   |
| 1   | A     | 110 | THR  | OG1-CB-CG2  | -5.39 | 98.52       | 109.30   |
| 1   | A     | 79  | LYS  | N-CA-C      | -5.38 | 106.56      | 113.02   |
| 1   | A     | 89  | PHE  | CE1-CZ-CE2  | 5.38  | 129.69      | 120.00   |
| 1   | A     | 241 | THR  | CA-C-O      | -5.38 | 114.72      | 120.42   |
| 1   | A     | 117 | THR  | CA-CB-CG2   | -5.37 | 101.36      | 110.50   |
| 1   | A     | 4   | PRO  | N-CA-CB     | 5.37  | 108.02      | 103.35   |
| 1   | A     | 12  | GLY  | CA-C-O      | -5.36 | 115.22      | 120.75   |
| 1   | A     | 95  | ASN  | CA-C-O      | 5.36  | 126.22      | 120.32   |
| 1   | A     | 30  | GLN  | CB-CG-CD    | 5.36  | 121.71      | 112.60   |
| 1   | A     | 228 | TYR  | CA-C-N      | 5.36  | 129.53      | 122.30   |
| 1   | A     | 228 | TYR  | C-N-CA      | 5.36  | 129.53      | 122.30   |
| 1   | A     | 230 | ARG  | O-C-N       | 5.36  | 129.71      | 122.59   |
| 1   | A     | 235 | VAL  | CA-CB-CG1   | -5.36 | 101.29      | 110.40   |
| 1   | A     | 27  | TRP  | CE2-CD2-CE3 | 5.34  | 124.14      | 118.80   |
| 1   | A     | 111 | ALA  | N-CA-C      | 5.34  | 122.17      | 110.80   |
| 1   | A     | 35  | ASP  | CA-C-O      | -5.31 | 114.86      | 121.50   |
| 1   | A     | 178 | ASP  | CB-CA-C     | -5.29 | 99.89       | 110.42   |
| 1   | A     | 45  | SER  | N-CA-C      | 5.28  | 118.17      | 109.72   |
| 1   | A     | 58  | CYS  | CB-CA-C     | -5.27 | 99.20       | 110.32   |
| 1   | A     | 233 | ALA  | N-CA-CB     | 5.27  | 119.26      | 110.41   |
| 1   | A     | 235 | VAL  | CA-C-N      | -5.26 | 111.58      | 120.58   |
| 1   | A     | 235 | VAL  | C-N-CA      | -5.26 | 111.58      | 120.58   |
| 1   | A     | 34  | GLN  | CA-C-N      | -5.26 | 112.86      | 122.12   |
| 1   | A     | 34  | GLN  | C-N-CA      | -5.26 | 112.86      | 122.12   |
| 1   | A     | 80  | ILE  | CB-CG1-CD1  | -5.26 | 102.76      | 113.80   |
| 1   | A     | 109 | SER  | CA-CB-OG    | 5.25  | 121.61      | 111.10   |
| 1   | A     | 21  | GLU  | N-CA-CB     | -5.25 | 101.87      | 110.43   |
| 1   | A     | 205 | GLY  | N-CA-C      | 5.25  | 123.16      | 115.08   |
| 1   | A     | 36  | LYS  | CA-C-O      | -5.25 | 114.17      | 120.10   |
| 1   | A     | 23  | VAL  | CA-CB-CG2   | 5.24  | 119.31      | 110.40   |
| 1   | A     | 232 | THR  | CA-CB-OG1   | 5.24  | 117.46      | 109.60   |
| 1   | A     | 25  | GLY  | CA-C-N      | 5.23  | 128.06      | 120.79   |
| 1   | A     | 25  | GLY  | C-N-CA      | 5.23  | 128.06      | 120.79   |
| 1   | A     | 29  | TRP  | N-CA-CB     | -5.22 | 102.97      | 110.65   |
| 1   | A     | 89  | PHE  | CG-CD1-CE1  | -5.22 | 111.82      | 120.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 236 | ASN  | CA-CB-CG   | -5.22 | 107.38      | 112.60   |
| 1   | A     | 91  | ASN  | CA-CB-CG   | 5.21  | 117.81      | 112.60   |
| 1   | A     | 28  | PRO  | CB-CA-C    | -5.20 | 102.98      | 111.56   |
| 1   | A     | 131 | ALA  | CB-CA-C    | -5.19 | 102.84      | 110.06   |
| 1   | A     | 119 | SER  | CA-C-N     | -5.18 | 115.42      | 122.93   |
| 1   | A     | 119 | SER  | C-N-CA     | -5.18 | 115.42      | 122.93   |
| 1   | A     | 168 | CYS  | O-C-N      | 5.17  | 127.47      | 122.09   |
| 1   | A     | 17  | VAL  | CA-CB-CG1  | -5.16 | 101.64      | 110.40   |
| 1   | A     | 86  | ALA  | CA-C-N     | -5.16 | 112.83      | 121.75   |
| 1   | A     | 86  | ALA  | C-N-CA     | -5.16 | 112.83      | 121.75   |
| 1   | A     | 213 | VAL  | N-CA-CB    | 5.14  | 116.53      | 110.82   |
| 1   | A     | 30  | GLN  | CB-CA-C    | 5.14  | 117.92      | 109.90   |
| 1   | A     | 47  | ILE  | CB-CG1-CD1 | -5.14 | 103.01      | 113.80   |
| 1   | A     | 21  | GLU  | N-CA-C     | 5.11  | 117.57      | 109.24   |
| 1   | A     | 182 | CYS  | CA-C-N     | 5.11  | 130.32      | 121.64   |
| 1   | A     | 182 | CYS  | C-N-CA     | 5.11  | 130.32      | 121.64   |
| 1   | A     | 88  | VAL  | CA-CB-CG1  | -5.11 | 101.72      | 110.40   |
| 1   | A     | 131 | ALA  | N-CA-C     | 5.11  | 117.96      | 110.30   |
| 1   | A     | 194 | ASP  | CB-CA-C    | 5.10  | 120.57      | 110.42   |
| 1   | A     | 91  | ASN  | CB-CG-ND2  | -5.10 | 108.76      | 116.40   |
| 1   | A     | 244 | ALA  | N-CA-C     | 5.07  | 125.21      | 111.00   |
| 1   | A     | 139 | THR  | CA-CB-OG1  | 5.07  | 117.20      | 109.60   |
| 1   | A     | 16  | ILE  | CA-C-N     | 5.06  | 131.08      | 121.97   |
| 1   | A     | 16  | ILE  | C-N-CA     | 5.06  | 131.08      | 121.97   |
| 1   | A     | 242 | LEU  | CD1-CG-CD2 | -5.05 | 99.68       | 110.80   |
| 1   | A     | 162 | LEU  | N-CA-C     | -5.05 | 103.73      | 110.55   |
| 1   | A     | 175 | LYS  | O-C-N      | 5.05  | 128.83      | 122.37   |
| 1   | A     | 220 | CYS  | CA-CB-SG   | -5.05 | 102.79      | 114.40   |
| 1   | A     | 165 | ASN  | CB-CG-ND2  | 5.04  | 123.96      | 116.40   |
| 1   | A     | 139 | THR  | CA-CB-CG2  | -5.04 | 101.94      | 110.50   |
| 1   | A     | 81  | GLN  | CB-CA-C    | 5.04  | 118.45      | 110.19   |
| 1   | A     | 94  | TYR  | CA-C-O     | -5.02 | 113.33      | 120.51   |
| 1   | A     | 171 | TYR  | CB-CG-CD1  | -5.02 | 113.27      | 120.80   |
| 1   | A     | 50  | ASN  | N-CA-C     | 5.02  | 120.24      | 113.72   |
| 1   | A     | 123 | LEU  | N-CA-C     | -5.01 | 102.43      | 110.10   |
| 1   | A     | 231 | VAL  | CA-CB-CG2  | 5.01  | 118.92      | 110.40   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 154 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 160 | LEU  | Mainchain |
| 1   | A     | 179 | ALA  | Mainchain |
| 1   | A     | 242 | LEU  | Mainchain |
| 1   | A     | 29  | TRP  | Mainchain |
| 1   | A     | 32  | SER  | Mainchain |
| 1   | A     | 43  | GLY  | Mainchain |
| 1   | A     | 53  | VAL  | Mainchain |
| 1   | A     | 9   | VAL  | Mainchain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1643  | 0        | 1610     | 340     | 52           |
| All | All   | 1643  | 0        | 1610     | 340     | 52           |

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 105.

All (340) 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:106:LEU:CB   | 1:A:106:LEU:CA   | 1.77                     | 1.59              |
| 1:A:128:ASP:CG   | 1:A:128:ASP:CB   | 1.78                     | 1.55              |
| 1:A:160:LEU:N    | 1:A:160:LEU:CA   | 1.68                     | 1.53              |
| 1:A:9:VAL:N      | 1:A:9:VAL:CA     | 1.69                     | 1.52              |
| 1:A:125:SER:C    | 1:A:125:SER:CA   | 1.81                     | 1.52              |
| 1:A:43:GLY:C     | 1:A:43:GLY:CA    | 1.76                     | 1.50              |
| 1:A:174:THR:O    | 1:A:177:LYS:NZ   | 1.58                     | 1.32              |
| 1:A:54:THR:OG1   | 1:A:196:GLY:HA3  | 1.28                     | 1.28              |
| 1:A:25:GLY:O     | 1:A:28:PRO:HD3   | 1.32                     | 1.26              |
| 1:A:23:VAL:O     | 1:A:26:SER:CB    | 1.86                     | 1.23              |
| 1:A:189:SER:O    | 1:A:192:MET:HE1  | 1.40                     | 1.20              |
| 1:A:162:LEU:HD13 | 1:A:181:ILE:HD11 | 1.24                     | 1.13              |
| 1:A:20:GLU:C     | 1:A:156:GLN:HG3  | 1.74                     | 1.11              |
| 1:A:35:ASP:OD1   | 1:A:39:PHE:HB3   | 1.50                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:34:GLN:OE1   | 1:A:38:GLY:HA2   | 1.52                     | 1.08              |
| 1:A:136:CYS:HB3  | 1:A:200:VAL:O    | 1.50                     | 1.08              |
| 1:A:20:GLU:O     | 1:A:156:GLN:HG3  | 1.53                     | 1.08              |
| 1:A:23:VAL:O     | 1:A:26:SER:HB2   | 0.93                     | 1.08              |
| 1:A:165:ASN:O    | 1:A:169:LYS:HE3  | 1.53                     | 1.08              |
| 1:A:224:THR:CG2  | 1:A:225:PRO:HD2  | 1.86                     | 1.05              |
| 1:A:239:GLN:HA   | 1:A:239:GLN:OE1  | 1.49                     | 1.05              |
| 1:A:2:GLY:O      | 1:A:4:PRO:HD3    | 1.56                     | 1.05              |
| 1:A:159:SER:C    | 1:A:160:LEU:CA   | 2.33                     | 1.00              |
| 1:A:224:THR:HG22 | 1:A:225:PRO:HD2  | 1.39                     | 1.00              |
| 1:A:243:ALA:CA   | 1:A:244:ALA:N    | 2.25                     | 1.00              |
| 1:A:165:ASN:O    | 1:A:169:LYS:HB2  | 1.63                     | 0.99              |
| 1:A:11:SER:OG    | 1:A:20:GLU:OE1   | 1.80                     | 0.99              |
| 1:A:95:ASN:O     | 1:A:99:ILE:N     | 1.96                     | 0.97              |
| 1:A:87:LYS:HG2   | 1:A:88:VAL:H     | 1.28                     | 0.97              |
| 1:A:131:ALA:HB3  | 1:A:134:THR:OG1  | 1.64                     | 0.97              |
| 1:A:46:LEU:HD23  | 1:A:52:VAL:CG2   | 1.95                     | 0.96              |
| 1:A:54:THR:OG1   | 1:A:196:GLY:CA   | 2.13                     | 0.95              |
| 1:A:23:VAL:C     | 1:A:26:SER:HB2   | 1.92                     | 0.95              |
| 1:A:20:GLU:C     | 1:A:156:GLN:CG   | 2.40                     | 0.95              |
| 1:A:34:GLN:HA    | 1:A:39:PHE:O     | 1.66                     | 0.94              |
| 1:A:20:GLU:O     | 1:A:156:GLN:CG   | 2.16                     | 0.94              |
| 1:A:172:TRP:HB2  | 1:A:176:ILE:CD1  | 1.98                     | 0.93              |
| 1:A:16:ILE:HG22  | 1:A:17:VAL:HG23  | 1.51                     | 0.92              |
| 1:A:27:TRP:CG    | 1:A:139:THR:HG21 | 2.03                     | 0.92              |
| 1:A:171:TYR:CD2  | 1:A:225:PRO:HG3  | 2.05                     | 0.91              |
| 1:A:34:GLN:HE22  | 1:A:82:LYS:HE3   | 1.35                     | 0.91              |
| 1:A:46:LEU:HD23  | 1:A:52:VAL:HG22  | 1.53                     | 0.91              |
| 1:A:16:ILE:CG2   | 1:A:17:VAL:HG23  | 2.00                     | 0.91              |
| 1:A:87:LYS:HG2   | 1:A:88:VAL:N     | 1.83                     | 0.90              |
| 1:A:15:ARG:O     | 1:A:188:VAL:HB   | 1.71                     | 0.89              |
| 1:A:177:LYS:O    | 1:A:178:ASP:C    | 2.13                     | 0.89              |
| 1:A:34:GLN:NE2   | 1:A:82:LYS:HE3   | 1.90                     | 0.86              |
| 1:A:9:VAL:N      | 1:A:9:VAL:CB     | 2.38                     | 0.86              |
| 1:A:189:SER:O    | 1:A:192:MET:CE   | 2.23                     | 0.85              |
| 1:A:22:ALA:HB2   | 1:A:157:GLN:OE1  | 1.76                     | 0.84              |
| 1:A:27:TRP:CB    | 1:A:139:THR:HG21 | 2.06                     | 0.84              |
| 1:A:65:VAL:HG11  | 1:A:82:LYS:HG2   | 1.57                     | 0.84              |
| 1:A:25:GLY:O     | 1:A:28:PRO:CD    | 2.22                     | 0.83              |
| 1:A:2:GLY:C      | 1:A:4:PRO:HD3    | 2.02                     | 0.83              |
| 1:A:43:GLY:C     | 1:A:43:GLY:N     | 2.35                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:106:LEU:CB   | 1:A:106:LEU:C    | 2.52                     | 0.82              |
| 1:A:35:ASP:CG    | 1:A:39:PHE:HB3   | 2.03                     | 0.82              |
| 1:A:65:VAL:CG1   | 1:A:82:LYS:HG2   | 2.10                     | 0.82              |
| 1:A:108:LEU:N    | 1:A:108:LEU:HD12 | 1.95                     | 0.81              |
| 1:A:26:SER:O     | 1:A:28:PRO:HD2   | 1.80                     | 0.81              |
| 1:A:134:THR:O    | 1:A:161:PRO:HA   | 1.81                     | 0.81              |
| 1:A:172:TRP:HB2  | 1:A:176:ILE:HD13 | 1.62                     | 0.81              |
| 1:A:54:THR:HG1   | 1:A:196:GLY:HA3  | 1.46                     | 0.81              |
| 1:A:100:ASN:ND2  | 1:A:177:LYS:HB2  | 1.96                     | 0.80              |
| 1:A:203:LYS:HG3  | 1:A:204:ASN:OD1  | 1.80                     | 0.80              |
| 1:A:44:GLY:HA2   | 1:A:196:GLY:O    | 1.81                     | 0.79              |
| 1:A:164:SER:HB3  | 1:A:167:ASN:HB2  | 1.65                     | 0.79              |
| 1:A:10:LEU:N     | 1:A:10:LEU:HD23  | 1.97                     | 0.79              |
| 1:A:47:ILE:C     | 1:A:120:ALA:HB1  | 2.07                     | 0.79              |
| 1:A:11:SER:O     | 1:A:14:SER:HB2   | 1.82                     | 0.79              |
| 1:A:159:SER:C    | 1:A:160:LEU:HA   | 2.05                     | 0.79              |
| 1:A:9:VAL:N      | 1:A:9:VAL:C      | 2.41                     | 0.78              |
| 1:A:47:ILE:CA    | 1:A:120:ALA:HB1  | 2.15                     | 0.77              |
| 1:A:172:TRP:HB2  | 1:A:176:ILE:HD11 | 1.67                     | 0.76              |
| 1:A:235:VAL:O    | 1:A:239:GLN:HG2  | 1.85                     | 0.76              |
| 1:A:176:ILE:C    | 1:A:177:LYS:HD3  | 2.09                     | 0.76              |
| 1:A:224:THR:HG23 | 1:A:225:PRO:HD2  | 1.67                     | 0.76              |
| 1:A:61:THR:OG1   | 1:A:62:THR:N     | 2.18                     | 0.76              |
| 1:A:127:SER:O    | 1:A:128:ASP:C    | 2.23                     | 0.76              |
| 1:A:26:SER:C     | 1:A:28:PRO:CD    | 2.60                     | 0.75              |
| 1:A:200:VAL:HG13 | 1:A:207:TRP:HB3  | 1.66                     | 0.75              |
| 1:A:175:LYS:O    | 1:A:180:MET:SD   | 2.44                     | 0.75              |
| 1:A:6:ILE:HD11   | 1:A:116:GLN:HB3  | 1.69                     | 0.75              |
| 1:A:174:THR:O    | 1:A:177:LYS:CE   | 2.36                     | 0.74              |
| 1:A:218:SER:C    | 1:A:220:CYS:H    | 1.93                     | 0.74              |
| 1:A:224:THR:CG2  | 1:A:225:PRO:CD   | 2.65                     | 0.74              |
| 1:A:160:LEU:N    | 1:A:160:LEU:HA   | 1.98                     | 0.74              |
| 1:A:185:ALA:HB2  | 1:A:225:PRO:N    | 2.03                     | 0.73              |
| 1:A:224:THR:HG22 | 1:A:225:PRO:CD   | 2.17                     | 0.73              |
| 1:A:49:GLU:HA    | 1:A:112:ALA:HB3  | 1.70                     | 0.73              |
| 1:A:91:ASN:HB2   | 1:A:237:TRP:CZ2  | 2.24                     | 0.73              |
| 1:A:172:TRP:CB   | 1:A:176:ILE:CD1  | 2.66                     | 0.73              |
| 1:A:162:LEU:HD13 | 1:A:181:ILE:CD1  | 2.13                     | 0.72              |
| 1:A:92:SER:C     | 1:A:94:TYR:H     | 1.97                     | 0.72              |
| 1:A:2:GLY:O      | 1:A:4:PRO:CD     | 2.37                     | 0.72              |
| 1:A:164:SER:HB3  | 1:A:167:ASN:H    | 1.53                     | 0.72              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:160:LEU:HB3  | 1:A:184:GLY:HA2 | 1.71                     | 0.71              |
| 1:A:202:LYS:O    | 1:A:203:LYS:HB2 | 1.89                     | 0.71              |
| 1:A:35:ASP:OD1   | 1:A:39:PHE:CB   | 2.36                     | 0.71              |
| 1:A:7:GLN:O      | 1:A:9:VAL:HG23  | 1.91                     | 0.70              |
| 1:A:87:LYS:CG    | 1:A:88:VAL:H    | 2.02                     | 0.70              |
| 1:A:85:ILE:HG21  | 1:A:88:VAL:CG2  | 2.21                     | 0.70              |
| 1:A:24:PRO:C     | 1:A:26:SER:H    | 1.99                     | 0.70              |
| 1:A:30:GLN:NE2   | 1:A:198:PRO:CD  | 2.55                     | 0.70              |
| 1:A:52:VAL:O     | 1:A:106:LEU:N   | 2.25                     | 0.69              |
| 1:A:46:LEU:CD2   | 1:A:52:VAL:CG2  | 2.70                     | 0.68              |
| 1:A:136:CYS:CB   | 1:A:200:VAL:O   | 2.36                     | 0.68              |
| 1:A:164:SER:HB3  | 1:A:167:ASN:CB  | 2.23                     | 0.68              |
| 1:A:164:SER:CB   | 1:A:167:ASN:HB2 | 2.24                     | 0.68              |
| 1:A:199:LEU:HD23 | 1:A:211:GLY:HA3 | 1.74                     | 0.68              |
| 1:A:178:ASP:OD2  | 1:A:179:ALA:HB2 | 1.94                     | 0.67              |
| 1:A:51:TRP:HZ2   | 1:A:245:ASN:O   | 1.76                     | 0.67              |
| 1:A:181:ILE:HG23 | 1:A:181:ILE:O   | 1.93                     | 0.67              |
| 1:A:47:ILE:C     | 1:A:120:ALA:CB  | 2.68                     | 0.67              |
| 1:A:203:LYS:C    | 1:A:205:GLY:N   | 2.46                     | 0.67              |
| 1:A:26:SER:C     | 1:A:28:PRO:HD2  | 2.19                     | 0.67              |
| 1:A:53:VAL:HG13  | 1:A:53:VAL:O    | 1.94                     | 0.67              |
| 1:A:165:ASN:O    | 1:A:169:LYS:CE  | 2.38                     | 0.67              |
| 1:A:233:ALA:C    | 1:A:234:LEU:HG  | 2.20                     | 0.66              |
| 1:A:228:TYR:CD1  | 1:A:228:TYR:N   | 2.62                     | 0.66              |
| 1:A:98:THR:O     | 1:A:99:ILE:HB   | 1.94                     | 0.66              |
| 1:A:8:PRO:HA     | 1:A:26:SER:OG   | 1.96                     | 0.66              |
| 1:A:178:ASP:CG   | 1:A:179:ALA:N   | 2.50                     | 0.66              |
| 1:A:6:ILE:N      | 1:A:6:ILE:HD12  | 2.11                     | 0.66              |
| 1:A:16:ILE:HG23  | 1:A:17:VAL:HG23 | 1.77                     | 0.66              |
| 1:A:239:GLN:OE1  | 1:A:239:GLN:CA  | 2.35                     | 0.66              |
| 1:A:10:LEU:N     | 1:A:10:LEU:CD2  | 2.59                     | 0.65              |
| 1:A:91:ASN:OD1   | 1:A:91:ASN:C    | 2.39                     | 0.65              |
| 1:A:171:TYR:CD1  | 1:A:225:PRO:HD3 | 2.31                     | 0.65              |
| 1:A:45:SER:O     | 1:A:53:VAL:HG12 | 1.95                     | 0.65              |
| 1:A:27:TRP:CG    | 1:A:139:THR:CG2 | 2.80                     | 0.65              |
| 1:A:89:PHE:N     | 1:A:89:PHE:CD2  | 2.60                     | 0.65              |
| 1:A:8:PRO:HB2    | 1:A:10:LEU:HD21 | 1.79                     | 0.65              |
| 1:A:125:SER:CA   | 1:A:126:ALA:N   | 2.57                     | 0.65              |
| 1:A:9:VAL:HB     | 1:A:23:VAL:HG21 | 1.79                     | 0.64              |
| 1:A:136:CYS:HB3  | 1:A:200:VAL:C   | 2.21                     | 0.64              |
| 1:A:46:LEU:HD23  | 1:A:52:VAL:HG23 | 1.77                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:172:TRP:CB  | 1:A:176:ILE:HD11 | 2.24                     | 0.64              |
| 1:A:172:TRP:CZ3 | 1:A:215:TRP:NE1  | 2.65                     | 0.64              |
| 1:A:218:SER:C   | 1:A:220:CYS:N    | 2.51                     | 0.64              |
| 1:A:162:LEU:CD1 | 1:A:181:ILE:HD11 | 2.15                     | 0.64              |
| 1:A:25:GLY:C    | 1:A:28:PRO:HD3   | 2.20                     | 0.64              |
| 1:A:125:SER:C   | 1:A:125:SER:N    | 2.55                     | 0.64              |
| 1:A:201:CYS:SG  | 1:A:210:VAL:HG21 | 2.38                     | 0.64              |
| 1:A:244:ALA:HB1 | 1:A:245:ASN:OD1  | 1.97                     | 0.63              |
| 1:A:21:GLU:N    | 1:A:156:GLN:HG3  | 2.12                     | 0.63              |
| 1:A:77:SER:C    | 1:A:78:GLU:CG    | 2.71                     | 0.63              |
| 1:A:66:VAL:HG21 | 1:A:108:LEU:HD21 | 1.80                     | 0.63              |
| 1:A:67:VAL:HG22 | 1:A:82:LYS:HG3   | 1.80                     | 0.63              |
| 1:A:191:CYS:C   | 1:A:193:GLY:H    | 1.98                     | 0.63              |
| 1:A:125:SER:CA  | 1:A:125:SER:O    | 2.38                     | 0.63              |
| 1:A:33:LEU:N    | 1:A:42:CYS:O     | 2.31                     | 0.62              |
| 1:A:53:VAL:O    | 1:A:53:VAL:CG1   | 2.44                     | 0.62              |
| 1:A:108:LEU:N   | 1:A:108:LEU:CD1  | 2.60                     | 0.62              |
| 1:A:52:VAL:HB   | 1:A:106:LEU:HG   | 1.82                     | 0.62              |
| 1:A:27:TRP:CD1  | 1:A:139:THR:CG2  | 2.82                     | 0.62              |
| 1:A:16:ILE:O    | 1:A:19:GLY:HA2   | 1.98                     | 0.62              |
| 1:A:106:LEU:CB  | 1:A:106:LEU:N    | 2.58                     | 0.62              |
| 1:A:191:CYS:C   | 1:A:193:GLY:N    | 2.48                     | 0.62              |
| 1:A:47:ILE:HA   | 1:A:120:ALA:HB1  | 1.79                     | 0.62              |
| 1:A:107:LYS:C   | 1:A:108:LEU:HD12 | 2.24                     | 0.62              |
| 1:A:185:ALA:HB2 | 1:A:224:THR:C    | 2.24                     | 0.61              |
| 1:A:127:SER:O   | 1:A:128:ASP:O    | 2.18                     | 0.61              |
| 1:A:159:SER:O   | 1:A:160:LEU:HA   | 2.01                     | 0.61              |
| 1:A:171:TYR:CG  | 1:A:225:PRO:HG3  | 2.35                     | 0.61              |
| 1:A:79:LYS:HD3  | 1:A:117:THR:HG21 | 1.83                     | 0.61              |
| 1:A:236:ASN:HA  | 1:A:239:GLN:HB2  | 1.82                     | 0.61              |
| 1:A:168:CYS:O   | 1:A:169:LYS:C    | 2.44                     | 0.61              |
| 1:A:33:LEU:O    | 1:A:41:PHE:CD2   | 2.54                     | 0.60              |
| 1:A:217:SER:O   | 1:A:220:CYS:HA   | 2.01                     | 0.60              |
| 1:A:86:ALA:HB2  | 1:A:109:SER:HA   | 1.84                     | 0.60              |
| 1:A:244:ALA:HB3 | 1:A:245:ASN:ND2  | 2.16                     | 0.60              |
| 1:A:52:VAL:O    | 1:A:105:LEU:HA   | 2.02                     | 0.59              |
| 1:A:140:GLY:CA  | 1:A:155:LEU:HD12 | 2.32                     | 0.59              |
| 1:A:79:LYS:O    | 1:A:79:LYS:HG2   | 2.00                     | 0.59              |
| 1:A:221:SER:C   | 1:A:223:SER:N    | 2.55                     | 0.59              |
| 1:A:177:LYS:N   | 1:A:177:LYS:CD   | 2.65                     | 0.59              |
| 1:A:230:ARG:NH1 | 1:A:230:ARG:HG3  | 2.18                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:SER:C    | 1:A:128:ASP:O    | 2.45                     | 0.59              |
| 1:A:20:GLU:C     | 1:A:156:GLN:HG2  | 2.28                     | 0.59              |
| 1:A:178:ASP:OD2  | 1:A:179:ALA:N    | 2.35                     | 0.59              |
| 1:A:244:ALA:HB3  | 1:A:245:ASN:CG   | 2.28                     | 0.59              |
| 1:A:34:GLN:CD    | 1:A:38:GLY:HA2   | 2.26                     | 0.58              |
| 1:A:77:SER:C     | 1:A:78:GLU:HG2   | 2.28                     | 0.58              |
| 1:A:203:LYS:CG   | 1:A:204:ASN:OD1  | 2.50                     | 0.58              |
| 1:A:166:THR:HA   | 1:A:169:LYS:HB2  | 1.86                     | 0.58              |
| 1:A:39:PHE:HE2   | 1:A:41:PHE:HB3   | 1.68                     | 0.58              |
| 1:A:26:SER:C     | 1:A:28:PRO:HD3   | 2.29                     | 0.57              |
| 1:A:125:SER:C    | 1:A:125:SER:CB   | 2.71                     | 0.57              |
| 1:A:218:SER:O    | 1:A:220:CYS:N    | 2.38                     | 0.57              |
| 1:A:27:TRP:HB2   | 1:A:139:THR:HG21 | 1.85                     | 0.57              |
| 1:A:87:LYS:HD3   | 1:A:89:PHE:CE1   | 2.39                     | 0.57              |
| 1:A:201:CYS:O    | 1:A:207:TRP:HA   | 2.03                     | 0.57              |
| 1:A:100:ASN:HD22 | 1:A:177:LYS:HB2  | 1.67                     | 0.57              |
| 1:A:158:ALA:HB2  | 1:A:192:MET:HE2  | 1.86                     | 0.57              |
| 1:A:9:VAL:HG12   | 1:A:9:VAL:O      | 2.05                     | 0.56              |
| 1:A:27:TRP:CD1   | 1:A:139:THR:HG21 | 2.40                     | 0.56              |
| 1:A:41:PHE:HE1   | 1:A:58:CYS:O     | 1.88                     | 0.56              |
| 1:A:95:ASN:O     | 1:A:99:ILE:CA    | 2.54                     | 0.56              |
| 1:A:230:ARG:HH11 | 1:A:230:ARG:CG   | 2.19                     | 0.56              |
| 1:A:34:GLN:HE22  | 1:A:82:LYS:CE    | 2.14                     | 0.56              |
| 1:A:66:VAL:HB    | 1:A:83:LEU:HB2   | 1.88                     | 0.56              |
| 1:A:137:VAL:HG12 | 1:A:138:THR:N    | 2.21                     | 0.56              |
| 1:A:235:VAL:HG13 | 1:A:236:ASN:N    | 2.20                     | 0.55              |
| 1:A:199:LEU:HD22 | 1:A:228:TYR:CD2  | 2.41                     | 0.55              |
| 1:A:30:GLN:NE2   | 1:A:198:PRO:HD2  | 2.21                     | 0.55              |
| 1:A:177:LYS:HD3  | 1:A:177:LYS:N    | 2.21                     | 0.55              |
| 1:A:172:TRP:CE3  | 1:A:215:TRP:CZ2  | 2.95                     | 0.55              |
| 1:A:87:LYS:CG    | 1:A:88:VAL:N     | 2.60                     | 0.54              |
| 1:A:47:ILE:O     | 1:A:120:ALA:CB   | 2.56                     | 0.54              |
| 1:A:35:ASP:N     | 1:A:39:PHE:O     | 2.40                     | 0.54              |
| 1:A:26:SER:O     | 1:A:28:PRO:CD    | 2.53                     | 0.54              |
| 1:A:27:TRP:CD1   | 1:A:139:THR:HG22 | 2.43                     | 0.54              |
| 1:A:83:LEU:CD2   | 1:A:110:THR:O    | 2.56                     | 0.54              |
| 1:A:39:PHE:C     | 1:A:39:PHE:CD2   | 2.86                     | 0.53              |
| 1:A:171:TYR:CG   | 1:A:225:PRO:CG   | 2.92                     | 0.53              |
| 1:A:235:VAL:CG1  | 1:A:236:ASN:N    | 2.71                     | 0.53              |
| 1:A:140:GLY:C    | 1:A:155:LEU:HD12 | 2.33                     | 0.53              |
| 1:A:95:ASN:OD1   | 1:A:98:THR:OG1   | 2.25                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:LYS:O     | 1:A:101:ASN:HB2  | 2.09                     | 0.53              |
| 1:A:131:ALA:HB3  | 1:A:134:THR:HG1  | 1.73                     | 0.53              |
| 1:A:24:PRO:C     | 1:A:26:SER:N     | 2.65                     | 0.53              |
| 1:A:199:LEU:C    | 1:A:200:VAL:HG23 | 2.34                     | 0.53              |
| 1:A:8:PRO:HB3    | 1:A:27:TRP:CZ2   | 2.44                     | 0.53              |
| 1:A:9:VAL:N      | 1:A:9:VAL:CG2    | 2.73                     | 0.52              |
| 1:A:49:GLU:O     | 1:A:112:ALA:N    | 2.39                     | 0.52              |
| 1:A:30:GLN:OE1   | 1:A:155:LEU:HD11 | 2.09                     | 0.52              |
| 1:A:90:LYS:HA    | 1:A:104:THR:OG1  | 2.10                     | 0.52              |
| 1:A:83:LEU:HB3   | 1:A:108:LEU:HD23 | 1.90                     | 0.51              |
| 1:A:221:SER:C    | 1:A:223:SER:H    | 1.91                     | 0.51              |
| 1:A:30:GLN:HE22  | 1:A:198:PRO:HD2  | 1.76                     | 0.51              |
| 1:A:65:VAL:HG12  | 1:A:82:LYS:HG2   | 1.89                     | 0.51              |
| 1:A:33:LEU:HD21  | 1:A:106:LEU:HD11 | 1.91                     | 0.51              |
| 1:A:124:PRO:O    | 1:A:235:VAL:HG21 | 2.11                     | 0.51              |
| 1:A:244:ALA:CB   | 1:A:245:ASN:CG   | 2.84                     | 0.51              |
| 1:A:175:LYS:O    | 1:A:180:MET:CE   | 2.59                     | 0.51              |
| 1:A:85:ILE:HG21  | 1:A:88:VAL:HG23  | 1.92                     | 0.50              |
| 1:A:3:VAL:HG12   | 1:A:3:VAL:O      | 2.11                     | 0.50              |
| 1:A:181:ILE:O    | 1:A:181:ILE:CG2  | 2.59                     | 0.50              |
| 1:A:230:ARG:HG3  | 1:A:230:ARG:HH11 | 1.76                     | 0.50              |
| 1:A:125:SER:N    | 1:A:125:SER:O    | 2.44                     | 0.50              |
| 1:A:182:CYS:SG   | 1:A:227:VAL:HG22 | 2.52                     | 0.50              |
| 1:A:9:VAL:HB     | 1:A:23:VAL:CG2   | 2.41                     | 0.49              |
| 1:A:39:PHE:CE2   | 1:A:41:PHE:HB3   | 2.47                     | 0.49              |
| 1:A:60:VAL:O     | 1:A:60:VAL:HG13  | 2.12                     | 0.49              |
| 1:A:66:VAL:HG21  | 1:A:108:LEU:CD2  | 2.41                     | 0.49              |
| 1:A:200:VAL:HG22 | 1:A:209:LEU:HA   | 1.93                     | 0.49              |
| 1:A:230:ARG:O    | 1:A:231:VAL:C    | 2.56                     | 0.49              |
| 1:A:6:ILE:HD12   | 1:A:6:ILE:H      | 1.78                     | 0.48              |
| 1:A:66:VAL:O     | 1:A:83:LEU:N     | 2.40                     | 0.48              |
| 1:A:171:TYR:CD1  | 1:A:225:PRO:CD   | 2.96                     | 0.48              |
| 1:A:90:LYS:HG2   | 1:A:91:ASN:N     | 2.29                     | 0.48              |
| 1:A:230:ARG:NH1  | 1:A:230:ARG:CG   | 2.75                     | 0.48              |
| 1:A:197:GLY:O    | 1:A:213:VAL:HG23 | 2.14                     | 0.47              |
| 1:A:244:ALA:CB   | 1:A:245:ASN:OD1  | 2.61                     | 0.47              |
| 1:A:23:VAL:O     | 1:A:24:PRO:C     | 2.58                     | 0.47              |
| 1:A:83:LEU:HD21  | 1:A:110:THR:O    | 2.15                     | 0.47              |
| 1:A:129:ASP:C    | 1:A:130:PHE:CD1  | 2.92                     | 0.47              |
| 1:A:199:LEU:HD22 | 1:A:228:TYR:CG   | 2.50                     | 0.47              |
| 1:A:51:TRP:CE3   | 1:A:105:LEU:HD22 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:SER:HB3   | 1:A:159:SER:HB2  | 1.97                     | 0.46              |
| 1:A:27:TRP:N     | 1:A:28:PRO:CD    | 2.69                     | 0.46              |
| 1:A:203:LYS:C    | 1:A:205:GLY:H    | 2.14                     | 0.46              |
| 1:A:9:VAL:CA     | 1:A:9:VAL:H      | 2.07                     | 0.46              |
| 1:A:124:PRO:CG   | 1:A:231:VAL:HG12 | 2.46                     | 0.46              |
| 1:A:22:ALA:HB1   | 1:A:26:SER:HB3   | 1.97                     | 0.45              |
| 1:A:85:ILE:CG2   | 1:A:88:VAL:HG23  | 2.47                     | 0.45              |
| 1:A:91:ASN:HB2   | 1:A:237:TRP:CE2  | 2.50                     | 0.45              |
| 1:A:188:VAL:HG22 | 1:A:189:SER:N    | 2.32                     | 0.45              |
| 1:A:95:ASN:CG    | 1:A:98:THR:HG1   | 2.25                     | 0.45              |
| 1:A:7:GLN:HA     | 1:A:8:PRO:HD3    | 1.42                     | 0.45              |
| 1:A:100:ASN:HD21 | 1:A:177:LYS:HB2  | 1.77                     | 0.45              |
| 1:A:22:ALA:HB1   | 1:A:26:SER:CB    | 2.47                     | 0.45              |
| 1:A:29:TRP:HB3   | 1:A:119:SER:O    | 2.17                     | 0.45              |
| 1:A:103:ILE:HG21 | 1:A:234:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:31:VAL:HG23  | 1:A:33:LEU:CD1   | 2.47                     | 0.45              |
| 1:A:129:ASP:O    | 1:A:130:PHE:CG   | 2.70                     | 0.45              |
| 1:A:79:LYS:O     | 1:A:79:LYS:CG    | 2.65                     | 0.44              |
| 1:A:56:ALA:O     | 1:A:59:GLY:N     | 2.43                     | 0.44              |
| 1:A:139:THR:OG1  | 1:A:198:PRO:HG2  | 2.16                     | 0.44              |
| 1:A:189:SER:C    | 1:A:192:MET:HE1  | 2.27                     | 0.44              |
| 1:A:138:THR:O    | 1:A:157:GLN:HA   | 2.18                     | 0.44              |
| 1:A:200:VAL:CG1  | 1:A:207:TRP:HB3  | 2.40                     | 0.44              |
| 1:A:165:ASN:HA   | 1:A:168:CYS:HB3  | 1.99                     | 0.44              |
| 1:A:9:VAL:CB     | 1:A:23:VAL:HG21  | 2.45                     | 0.44              |
| 1:A:99:ILE:HG22  | 1:A:99:ILE:O     | 2.18                     | 0.44              |
| 1:A:125:SER:HB3  | 1:A:128:ASP:CG   | 2.43                     | 0.44              |
| 1:A:98:THR:O     | 1:A:99:ILE:CB    | 2.56                     | 0.44              |
| 1:A:47:ILE:HG13  | 1:A:48:ASN:HD22  | 1.82                     | 0.44              |
| 1:A:51:TRP:CZ3   | 1:A:89:PHE:CE2   | 3.06                     | 0.43              |
| 1:A:172:TRP:HB3  | 1:A:176:ILE:CD1  | 2.48                     | 0.43              |
| 1:A:1:CYS:C      | 1:A:3:VAL:H      | 2.25                     | 0.43              |
| 1:A:20:GLU:O     | 1:A:157:GLN:N    | 2.37                     | 0.43              |
| 1:A:23:VAL:HA    | 1:A:24:PRO:HD2   | 1.58                     | 0.43              |
| 1:A:61:THR:HG23  | 1:A:63:SER:H     | 1.84                     | 0.43              |
| 1:A:57:HIS:O     | 1:A:58:CYS:C     | 2.61                     | 0.43              |
| 1:A:91:ASN:O     | 1:A:94:TYR:N     | 2.51                     | 0.43              |
| 1:A:160:LEU:HD22 | 1:A:184:GLY:HA3  | 2.00                     | 0.43              |
| 1:A:171:TYR:CE1  | 1:A:225:PRO:HD3  | 2.54                     | 0.43              |
| 1:A:224:THR:HA   | 1:A:225:PRO:HD3  | 1.89                     | 0.43              |
| 1:A:21:GLU:HB2   | 1:A:156:GLN:NE2  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:GLY:CA    | 1:A:43:GLY:O     | 2.51                     | 0.42              |
| 1:A:20:GLU:O     | 1:A:156:GLN:HG2  | 2.09                     | 0.42              |
| 1:A:121:VAL:HG22 | 1:A:122:CYS:H    | 1.84                     | 0.42              |
| 1:A:9:VAL:N      | 1:A:9:VAL:HG23   | 2.34                     | 0.42              |
| 1:A:51:TRP:CZ2   | 1:A:245:ASN:O    | 2.66                     | 0.42              |
| 1:A:187:GLY:O    | 1:A:222:THR:HB   | 2.18                     | 0.42              |
| 1:A:188:VAL:HG22 | 1:A:189:SER:H    | 1.84                     | 0.42              |
| 1:A:29:TRP:CD2   | 1:A:121:VAL:HB   | 2.54                     | 0.42              |
| 1:A:65:VAL:HG11  | 1:A:82:LYS:CG    | 2.39                     | 0.42              |
| 1:A:21:GLU:HA    | 1:A:156:GLN:HA   | 2.01                     | 0.42              |
| 1:A:166:THR:HA   | 1:A:169:LYS:CB   | 2.50                     | 0.42              |
| 1:A:183:ALA:HB3  | 1:A:228:TYR:CE1  | 2.55                     | 0.42              |
| 1:A:227:VAL:C    | 1:A:228:TYR:CD1  | 2.98                     | 0.42              |
| 1:A:230:ARG:O    | 1:A:233:ALA:N    | 2.35                     | 0.42              |
| 1:A:28:PRO:O     | 1:A:118:VAL:HA   | 2.19                     | 0.42              |
| 1:A:48:ASN:HD21  | 1:A:51:TRP:CD1   | 2.38                     | 0.42              |
| 1:A:13:LEU:HD23  | 1:A:13:LEU:HA    | 2.01                     | 0.42              |
| 1:A:47:ILE:O     | 1:A:120:ALA:HB1  | 2.13                     | 0.42              |
| 1:A:167:ASN:O    | 1:A:170:LYS:HB3  | 2.20                     | 0.42              |
| 1:A:235:VAL:HG22 | 1:A:239:GLN:HG2  | 2.01                     | 0.41              |
| 1:A:175:LYS:H    | 1:A:175:LYS:HG3  | 1.52                     | 0.41              |
| 1:A:30:GLN:HE21  | 1:A:198:PRO:HD3  | 1.86                     | 0.41              |
| 1:A:106:LEU:HB2  | 1:A:108:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:215:TRP:CD1  | 1:A:216:GLY:N    | 2.88                     | 0.41              |
| 1:A:31:VAL:CG1   | 1:A:46:LEU:HG    | 2.51                     | 0.41              |
| 1:A:172:TRP:CE3  | 1:A:215:TRP:HZ2  | 2.37                     | 0.41              |
| 1:A:215:TRP:CD1  | 1:A:215:TRP:C    | 2.99                     | 0.41              |
| 1:A:9:VAL:C      | 1:A:10:LEU:HD23  | 2.43                     | 0.41              |
| 1:A:85:ILE:HD11  | 1:A:106:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:226:GLY:C    | 1:A:227:VAL:HG23 | 2.40                     | 0.41              |
| 1:A:21:GLU:CA    | 1:A:156:GLN:HG3  | 2.50                     | 0.40              |
| 1:A:13:LEU:O     | 1:A:16:ILE:N     | 2.49                     | 0.40              |
| 1:A:39:PHE:CE2   | 1:A:40:HIS:O     | 2.75                     | 0.40              |
| 1:A:221:SER:HB3  | 1:A:224:THR:OG1  | 2.21                     | 0.40              |
| 1:A:16:ILE:HG22  | 1:A:17:VAL:CG2   | 2.37                     | 0.40              |
| 1:A:169:LYS:O    | 1:A:171:TYR:N    | 2.54                     | 0.40              |
| 1:A:6:ILE:CD1    | 1:A:116:GLN:O    | 2.69                     | 0.40              |
| 1:A:176:ILE:C    | 1:A:177:LYS:CD   | 2.87                     | 0.40              |
| 1:A:218:SER:O    | 1:A:219:THR:C    | 2.65                     | 0.40              |

All (52) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:36:LYS:C   | 1:A:174:THR:OG1[3_655] | 0.73                     | 1.47              |
| 1:A:78:GLU:OE2 | 1:A:99:ILE:CA[3_655]   | 0.89                     | 1.31              |
| 1:A:36:LYS:O   | 1:A:174:THR:CA[3_655]  | 1.02                     | 1.18              |
| 1:A:78:GLU:N   | 1:A:94:TYR:CE2[3_655]  | 1.05                     | 1.15              |
| 1:A:65:VAL:CG1 | 1:A:175:LYS:NZ[3_655]  | 1.23                     | 0.97              |
| 1:A:36:LYS:CA  | 1:A:174:THR:CB[3_655]  | 1.25                     | 0.95              |
| 1:A:37:THR:N   | 1:A:174:THR:OG1[3_655] | 1.26                     | 0.94              |
| 1:A:78:GLU:CD  | 1:A:99:ILE:CA[3_655]   | 1.29                     | 0.91              |
| 1:A:80:ILE:CD1 | 1:A:97:LEU:CD2[3_655]  | 1.30                     | 0.90              |
| 1:A:80:ILE:CD1 | 1:A:97:LEU:CG[3_655]   | 1.33                     | 0.87              |
| 1:A:36:LYS:C   | 1:A:174:THR:CB[3_655]  | 1.34                     | 0.86              |
| 1:A:36:LYS:O   | 1:A:174:THR:CB[3_655]  | 1.35                     | 0.85              |
| 1:A:78:GLU:OE1 | 1:A:99:ILE:C[3_655]    | 1.36                     | 0.84              |
| 1:A:78:GLU:OE2 | 1:A:99:ILE:N[3_655]    | 1.41                     | 0.79              |
| 1:A:77:SER:C   | 1:A:94:TYR:CD2[3_655]  | 1.45                     | 0.75              |
| 1:A:36:LYS:CA  | 1:A:174:THR:OG1[3_655] | 1.47                     | 0.73              |
| 1:A:65:VAL:CG2 | 1:A:175:LYS:CE[3_655]  | 1.48                     | 0.72              |
| 1:A:79:LYS:N   | 1:A:96:SER:OG[3_655]   | 1.55                     | 0.65              |
| 1:A:78:GLU:OE1 | 1:A:99:ILE:CA[3_655]   | 1.62                     | 0.58              |
| 1:A:36:LYS:O   | 1:A:174:THR:OG1[3_655] | 1.70                     | 0.50              |
| 1:A:80:ILE:CG2 | 1:A:96:SER:O[3_655]    | 1.73                     | 0.47              |
| 1:A:77:SER:C   | 1:A:94:TYR:CG[3_655]   | 1.74                     | 0.46              |
| 1:A:65:VAL:CB  | 1:A:175:LYS:NZ[3_655]  | 1.80                     | 0.40              |
| 1:A:78:GLU:N   | 1:A:94:TYR:CZ[3_655]   | 1.84                     | 0.36              |
| 1:A:78:GLU:OE2 | 1:A:99:ILE:CB[3_655]   | 1.84                     | 0.36              |
| 1:A:80:ILE:CG2 | 1:A:96:SER:C[3_655]    | 1.84                     | 0.36              |
| 1:A:78:GLU:CG  | 1:A:94:TYR:CE1[3_655]  | 1.85                     | 0.35              |
| 1:A:65:VAL:CG2 | 1:A:175:LYS:NZ[3_655]  | 1.87                     | 0.33              |
| 1:A:78:GLU:N   | 1:A:94:TYR:CD2[3_655]  | 1.87                     | 0.33              |
| 1:A:77:SER:C   | 1:A:94:TYR:CE2[3_655]  | 1.88                     | 0.32              |
| 1:A:77:SER:O   | 1:A:94:TYR:O[3_655]    | 1.89                     | 0.31              |
| 1:A:78:GLU:C   | 1:A:96:SER:OG[3_655]   | 1.90                     | 0.30              |
| 1:A:36:LYS:O   | 1:A:174:THR:C[3_655]   | 1.92                     | 0.28              |
| 1:A:78:GLU:OE1 | 1:A:100:ASN:N[3_655]   | 1.92                     | 0.28              |
| 1:A:78:GLU:CB  | 1:A:96:SER:CA[3_655]   | 1.92                     | 0.28              |
| 1:A:80:ILE:CG2 | 1:A:97:LEU:N[3_655]    | 1.92                     | 0.28              |
| 1:A:78:GLU:CA  | 1:A:96:SER:OG[3_655]   | 1.95                     | 0.25              |
| 1:A:84:LYS:NZ  | 1:A:172:TRP:CZ3[3_655] | 1.95                     | 0.25              |
| 1:A:78:GLU:CD  | 1:A:99:ILE:C[3_655]    | 1.96                     | 0.24              |
| 1:A:36:LYS:N   | 1:A:174:THR:OG1[3_655] | 1.97                     | 0.23              |
| 1:A:13:LEU:CD2 | 1:A:240:GLN:CB[2_564]  | 1.98                     | 0.22              |
| 1:A:80:ILE:CG2 | 1:A:97:LEU:CA[3_655]   | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:78:GLU:CD   | 1:A:99:ILE:N[3_655]    | 2.06                     | 0.14              |
| 1:A:80:ILE:CB   | 1:A:96:SER:CB[3_655]   | 2.06                     | 0.14              |
| 1:A:78:GLU:CD   | 1:A:95:ASN:O[3_655]    | 2.07                     | 0.13              |
| 1:A:110:THR:OG1 | 1:A:218:SER:OG[3_655]  | 2.09                     | 0.11              |
| 1:A:35:ASP:O    | 1:A:174:THR:OG1[3_655] | 2.10                     | 0.10              |
| 1:A:84:LYS:NZ   | 1:A:172:TRP:CE3[3_655] | 2.10                     | 0.10              |
| 1:A:36:LYS:C    | 1:A:174:THR:CA[3_655]  | 2.15                     | 0.05              |
| 1:A:78:GLU:CG   | 1:A:94:TYR:CZ[3_655]   | 2.16                     | 0.04              |
| 1:A:36:LYS:CA   | 1:A:174:THR:CG2[3_655] | 2.17                     | 0.03              |
| 1:A:17:VAL:CG2  | 1:A:243:ALA:CA[2_564]  | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles                         |
|-----|-------|---------------|-----------|----------|----------|-------------------------------------|
| 1   | A     | 222/245 (91%) | 181 (82%) | 30 (14%) | 11 (5%)  | <a href="#">1</a> <a href="#">2</a> |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 111 | ALA  |
| 1   | A     | 128 | ASP  |
| 1   | A     | 178 | ASP  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 28  | PRO  |
| 1   | A     | 170 | LYS  |
| 1   | A     | 218 | SER  |
| 1   | A     | 231 | VAL  |
| 1   | A     | 219 | THR  |
| 1   | A     | 24  | PRO  |
| 1   | A     | 235 | VAL  |

### 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     | 180/200 (90%) | 144 (80%) | 36 (20%) | <b>1</b> <b>2</b> |

All (36) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ILE  |
| 1   | A     | 10  | LEU  |
| 1   | A     | 14  | SER  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 21  | GLU  |
| 1   | A     | 26  | SER  |
| 1   | A     | 31  | VAL  |
| 1   | A     | 40  | HIS  |
| 1   | A     | 47  | ILE  |
| 1   | A     | 49  | GLU  |
| 1   | A     | 78  | GLU  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 89  | PHE  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 127 | SER  |
| 1   | A     | 130 | PHE  |
| 1   | A     | 135 | THR  |
| 1   | A     | 138 | THR  |
| 1   | A     | 154 | ARG  |
| 1   | A     | 156 | GLN  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 166 | THR  |
| 1   | A     | 169 | LYS  |
| 1   | A     | 176 | ILE  |
| 1   | A     | 180 | MET  |
| 1   | A     | 192 | MET  |
| 1   | A     | 199 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 203 | LYS  |
| 1   | A     | 204 | ASN  |
| 1   | A     | 215 | TRP  |
| 1   | A     | 224 | THR  |
| 1   | A     | 232 | THR  |
| 1   | A     | 239 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 156 | GLN  |
| 1   | A     | 165 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 22               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 80:ILE    | C      | 81:GLN    | N      | 1.20         |
| 1     | A     | 67:VAL    | C      | 68:ALA    | N      | 1.19         |
| 1     | A     | 160:LEU   | C      | 161:PRO   | N      | 1.19         |
| 1     | A     | 202:LYS   | C      | 203:LYS   | N      | 1.19         |
| 1     | A     | 104:THR   | C      | 105:LEU   | N      | 1.18         |
| 1     | A     | 165:ASN   | C      | 166:THR   | N      | 1.18         |
| 1     | A     | 175:LYS   | C      | 176:ILE   | N      | 1.18         |
| 1     | A     | 191:CYS   | C      | 192:MET   | N      | 1.18         |
| 1     | A     | 239:GLN   | C      | 240:GLN   | N      | 1.18         |
| 1     | A     | 32:SER    | C      | 33:LEU    | N      | 1.17         |
| 1     | A     | 94:TYR    | C      | 95:ASN    | N      | 1.17         |
| 1     | A     | 194:ASP   | C      | 195:SER   | N      | 1.17         |
| 1     | A     | 205:GLY   | C      | 206:ALA   | N      | 1.17         |
| 1     | A     | 209:LEU   | C      | 210:VAL   | N      | 1.17         |
| 1     | A     | 9:VAL     | C      | 10:LEU    | N      | 1.16         |
| 1     | A     | 38:GLY    | C      | 39:PHE    | N      | 1.16         |
| 1     | A     | 131:ALA   | C      | 132:ALA   | N      | 1.16         |
| 1     | A     | 59:GLY    | C      | 60:VAL    | N      | 1.15         |
| 1     | A     | 142:GLY   | C      | 143:LEU   | N      | 1.15         |
| 1     | A     | 242:LEU   | C      | 243:ALA   | N      | 1.15         |
| 1     | A     | 112:ALA   | C      | 113:SER   | N      | 1.13         |
| 1     | A     | 54:THR    | C      | 55:ALA    | N      | 1.05         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.