



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:39 AM UTC

PDB ID : 1SBT / pdb\_00001sbt  
Title : ATOMIC COORDINATES FOR SUBTILISIN BPN (OR NOVO)  
Authors : Alden, R.A.; Birktoft, J.J.; Kraut, J.; Robertus, J.D.; Wright, C.S.  
Deposited on : 1972-08-11  
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

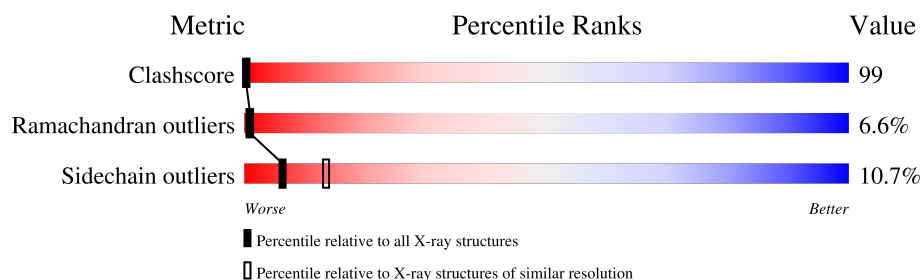
# 1 Overall quality at a glance

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     | 275    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1955 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 SUBTILISIN BPN'.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1938  | 1204 | 335 | 394 | 5 |         |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 56      | PRO      | ASN    | conflict | UNP P00782 |
| A     | 57      | ASN      | PRO    | conflict | UNP P00782 |
| A     | 61      | ASP      | ASN    | conflict | UNP P00782 |
| A     | 88      | SER      | ALA    | conflict | UNP P00782 |
| A     | 89      | ALA      | SER    | conflict | UNP P00782 |
| A     | 98      | ASP      | ALA    | conflict | UNP P00782 |
| A     | 99      | ALA      | ASP    | conflict | UNP P00782 |
| A     | 158     | SER      | THR    | conflict | UNP P00782 |
| A     | 159     | THR      | SER    | conflict | UNP P00782 |
| A     | 251     | GLN      | GLU    | conflict | UNP P00782 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |

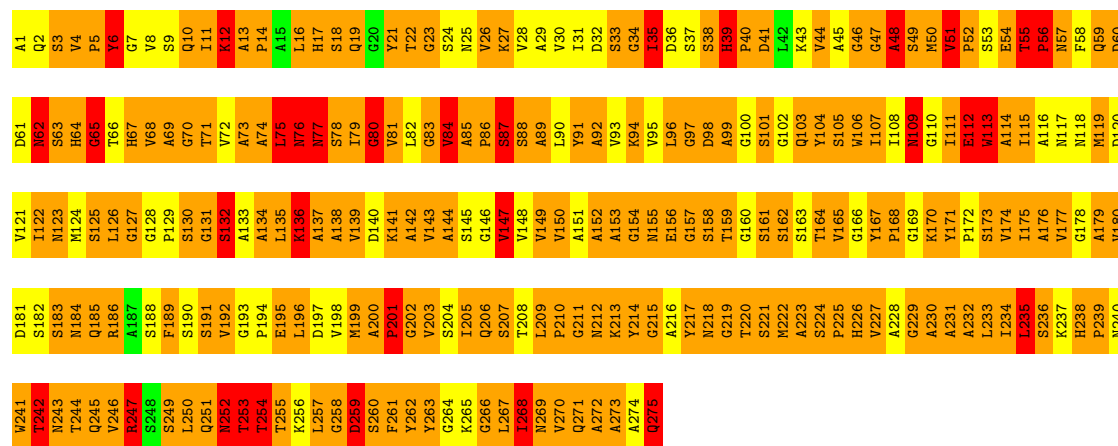
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: SUBTILISIN BPN'

Chain A:  24% 62% 12%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                        | Source    |
|----------------------------------------------------------|----------------------------------------------|-----------|
| Space group                                              | C 1 2 1                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 66.70Å 54.40Å 62.90Å<br>90.00° 91.90° 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, $R_{free}$                                            | (Not available) , (Not available)            | Depositor |
| Estimated twinning fraction                              | No twinning to report.                       | Xtriage   |
| Total number of atoms                                    | 1955                                         | 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     | 15.59        | 581/1976 (29.4%) | 4.02        | 482/2697 (17.9%) |

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                   | 19                  |

All (581) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 76  | ASN  | CG-OD1  | 650.42 | 13.59       | 1.23     |
| 1   | A     | 76  | ASN  | CB-CG   | 41.26  | 2.55        | 1.52     |
| 1   | A     | 111 | ILE  | CA-CB   | 28.04  | 1.84        | 1.54     |
| 1   | A     | 226 | HIS  | CE1-NE2 | 21.20  | 1.53        | 1.32     |
| 1   | A     | 96  | LEU  | CA-C    | 20.32  | 1.77        | 1.52     |
| 1   | A     | 79  | ILE  | C-N     | 19.74  | 1.62        | 1.33     |
| 1   | A     | 163 | SER  | C-O     | -19.16 | 0.99        | 1.24     |
| 1   | A     | 26  | VAL  | C-N     | 18.94  | 1.58        | 1.33     |
| 1   | A     | 76  | ASN  | CG-ND2  | 18.41  | 1.72        | 1.33     |
| 1   | A     | 84  | VAL  | CA-CB   | 17.19  | 1.76        | 1.54     |
| 1   | A     | 224 | SER  | CA-C    | 16.98  | 1.74        | 1.52     |
| 1   | A     | 155 | ASN  | C-N     | 16.84  | 1.50        | 1.33     |
| 1   | A     | 139 | VAL  | C-N     | 16.71  | 1.54        | 1.33     |
| 1   | A     | 201 | PRO  | N-CA    | -16.54 | 1.26        | 1.47     |
| 1   | A     | 168 | PRO  | N-CD    | 16.35  | 1.70        | 1.47     |
| 1   | A     | 219 | GLY  | C-N     | -16.28 | 1.12        | 1.33     |
| 1   | A     | 201 | PRO  | CA-C    | 16.18  | 1.75        | 1.52     |
| 1   | A     | 190 | SER  | CA-C    | 15.90  | 1.72        | 1.52     |
| 1   | A     | 207 | SER  | CA-C    | 15.87  | 1.74        | 1.53     |
| 1   | A     | 197 | ASP  | N-CA    | 15.84  | 1.65        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 91  | TYR  | C-O     | 15.47  | 1.42        | 1.23     |
| 1   | A     | 196 | LEU  | C-N     | -15.22 | 1.14        | 1.33     |
| 1   | A     | 151 | ALA  | C-O     | -15.10 | 1.04        | 1.23     |
| 1   | A     | 122 | ILE  | CA-C    | 15.06  | 1.71        | 1.52     |
| 1   | A     | 213 | LYS  | CA-C    | 14.95  | 1.71        | 1.52     |
| 1   | A     | 140 | ASP  | N-CA    | -14.91 | 1.28        | 1.46     |
| 1   | A     | 263 | TYR  | C-N     | -14.91 | 1.14        | 1.33     |
| 1   | A     | 71  | THR  | C-O     | 14.89  | 1.42        | 1.24     |
| 1   | A     | 147 | VAL  | C-O     | 14.89  | 1.44        | 1.24     |
| 1   | A     | 49  | SER  | C-O     | 14.55  | 1.41        | 1.24     |
| 1   | A     | 134 | ALA  | N-CA    | 14.55  | 1.63        | 1.46     |
| 1   | A     | 227 | VAL  | CA-CB   | 14.46  | 1.70        | 1.54     |
| 1   | A     | 60  | ASP  | CA-CB   | 14.43  | 1.75        | 1.53     |
| 1   | A     | 105 | SER  | CA-C    | 14.26  | 1.72        | 1.52     |
| 1   | A     | 118 | ASN  | C-N     | -14.24 | 1.14        | 1.33     |
| 1   | A     | 36  | ASP  | N-CA    | 13.99  | 1.63        | 1.46     |
| 1   | A     | 7   | GLY  | CA-C    | 13.93  | 1.71        | 1.51     |
| 1   | A     | 259 | ASP  | N-CA    | -13.70 | 1.28        | 1.46     |
| 1   | A     | 57  | ASN  | CG-ND2  | 13.69  | 1.62        | 1.33     |
| 1   | A     | 224 | SER  | C-O     | -13.65 | 1.06        | 1.24     |
| 1   | A     | 87  | SER  | C-O     | 13.61  | 1.42        | 1.24     |
| 1   | A     | 186 | ARG  | CZ-NH1  | 13.59  | 1.51        | 1.32     |
| 1   | A     | 38  | SER  | CA-C    | 13.54  | 1.72        | 1.52     |
| 1   | A     | 39  | HIS  | ND1-CE1 | 13.50  | 1.46        | 1.32     |
| 1   | A     | 177 | VAL  | C-N     | -13.46 | 1.18        | 1.33     |
| 1   | A     | 34  | GLY  | CA-C    | -13.45 | 1.36        | 1.52     |
| 1   | A     | 76  | ASN  | C-O     | -13.30 | 1.07        | 1.24     |
| 1   | A     | 55  | THR  | C-O     | -13.29 | 1.07        | 1.24     |
| 1   | A     | 178 | GLY  | CA-C    | 13.28  | 1.69        | 1.52     |
| 1   | A     | 126 | LEU  | CA-CB   | -13.17 | 1.31        | 1.53     |
| 1   | A     | 4   | VAL  | C-N     | -13.04 | 1.18        | 1.33     |
| 1   | A     | 179 | ALA  | N-CA    | 12.93  | 1.62        | 1.46     |
| 1   | A     | 212 | ASN  | CA-C    | 12.90  | 1.70        | 1.53     |
| 1   | A     | 182 | SER  | C-N     | -12.88 | 1.17        | 1.33     |
| 1   | A     | 53  | SER  | N-CA    | 12.82  | 1.62        | 1.46     |
| 1   | A     | 67  | HIS  | CE1-NE2 | 12.81  | 1.45        | 1.32     |
| 1   | A     | 180 | VAL  | C-N     | 12.76  | 1.53        | 1.33     |
| 1   | A     | 60  | ASP  | N-CA    | -12.69 | 1.31        | 1.46     |
| 1   | A     | 31  | ILE  | CA-C    | 12.66  | 1.64        | 1.53     |
| 1   | A     | 209 | LEU  | CA-C    | 12.66  | 1.67        | 1.52     |
| 1   | A     | 72  | VAL  | N-CA    | -12.62 | 1.32        | 1.46     |
| 1   | A     | 56  | PRO  | C-N     | 12.57  | 1.52        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 260 | SER  | CA-C    | 12.53  | 1.69        | 1.52     |
| 1   | A     | 173 | SER  | C-O     | -12.49 | 1.07        | 1.24     |
| 1   | A     | 158 | SER  | C-N     | -12.49 | 1.16        | 1.33     |
| 1   | A     | 98  | ASP  | C-N     | 12.45  | 1.51        | 1.33     |
| 1   | A     | 218 | ASN  | N-CA    | 12.44  | 1.61        | 1.46     |
| 1   | A     | 82  | LEU  | N-CA    | -12.30 | 1.31        | 1.46     |
| 1   | A     | 220 | THR  | C-N     | 12.21  | 1.49        | 1.33     |
| 1   | A     | 155 | ASN  | N-CA    | -12.20 | 1.30        | 1.46     |
| 1   | A     | 124 | MET  | C-N     | -12.20 | 1.18        | 1.33     |
| 1   | A     | 154 | GLY  | N-CA    | -12.17 | 1.27        | 1.45     |
| 1   | A     | 119 | MET  | N-CA    | 12.08  | 1.61        | 1.45     |
| 1   | A     | 92  | ALA  | C-N     | 12.06  | 1.49        | 1.33     |
| 1   | A     | 35  | ILE  | N-CA    | 12.03  | 1.61        | 1.46     |
| 1   | A     | 76  | ASN  | N-CA    | 12.02  | 1.61        | 1.46     |
| 1   | A     | 87  | SER  | CA-CB   | 11.91  | 1.72        | 1.53     |
| 1   | A     | 191 | SER  | C-N     | 11.82  | 1.49        | 1.33     |
| 1   | A     | 112 | GLU  | CG-CD   | -11.81 | 1.22        | 1.52     |
| 1   | A     | 71  | THR  | CB-OG1  | -11.75 | 1.25        | 1.43     |
| 1   | A     | 154 | GLY  | C-N     | 11.73  | 1.50        | 1.33     |
| 1   | A     | 101 | SER  | CB-OG   | -11.69 | 1.18        | 1.42     |
| 1   | A     | 55  | THR  | CA-CB   | -11.67 | 1.34        | 1.53     |
| 1   | A     | 155 | ASN  | CA-C    | 11.65  | 1.68        | 1.52     |
| 1   | A     | 113 | TRP  | N-CA    | -11.61 | 1.31        | 1.46     |
| 1   | A     | 172 | PRO  | CA-CB   | 11.54  | 1.70        | 1.53     |
| 1   | A     | 106 | TRP  | CD1-NE1 | 11.50  | 1.62        | 1.37     |
| 1   | A     | 150 | VAL  | CA-C    | 11.47  | 1.66        | 1.52     |
| 1   | A     | 67  | HIS  | ND1-CE1 | 11.43  | 1.44        | 1.32     |
| 1   | A     | 182 | SER  | C-O     | 11.39  | 1.40        | 1.24     |
| 1   | A     | 176 | ALA  | CA-CB   | 11.32  | 1.69        | 1.53     |
| 1   | A     | 111 | ILE  | CA-C    | -11.32 | 1.39        | 1.52     |
| 1   | A     | 72  | VAL  | CA-C    | 11.31  | 1.66        | 1.52     |
| 1   | A     | 58  | PHE  | CA-CB   | 11.27  | 1.68        | 1.53     |
| 1   | A     | 78  | SER  | C-N     | -11.24 | 1.18        | 1.33     |
| 1   | A     | 174 | VAL  | N-CA    | -11.19 | 1.31        | 1.46     |
| 1   | A     | 218 | ASN  | CA-CB   | -11.18 | 1.38        | 1.53     |
| 1   | A     | 129 | PRO  | CA-CB   | 11.12  | 1.69        | 1.53     |
| 1   | A     | 93  | VAL  | C-O     | 11.10  | 1.36        | 1.24     |
| 1   | A     | 147 | VAL  | C-N     | -11.10 | 1.18        | 1.33     |
| 1   | A     | 201 | PRO  | N-CD    | 11.06  | 1.63        | 1.47     |
| 1   | A     | 131 | GLY  | C-O     | 11.03  | 1.36        | 1.24     |
| 1   | A     | 64  | HIS  | CG-ND1  | -11.00 | 1.26        | 1.38     |
| 1   | A     | 219 | GLY  | N-CA    | 10.83  | 1.61        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 67  | HIS  | CG-ND1 | 10.79  | 1.50        | 1.38     |
| 1   | A     | 51  | VAL  | N-CA   | -10.78 | 1.38        | 1.46     |
| 1   | A     | 199 | MET  | CA-C   | -10.74 | 1.40        | 1.52     |
| 1   | A     | 189 | PHE  | CG-CD1 | 10.73  | 1.61        | 1.38     |
| 1   | A     | 158 | SER  | CA-C   | 10.71  | 1.68        | 1.53     |
| 1   | A     | 218 | ASN  | C-N    | -10.67 | 1.18        | 1.33     |
| 1   | A     | 17  | HIS  | C-O    | 10.65  | 1.36        | 1.24     |
| 1   | A     | 195 | GLU  | CA-CB  | 10.59  | 1.72        | 1.53     |
| 1   | A     | 272 | ALA  | CA-C   | 10.57  | 1.66        | 1.52     |
| 1   | A     | 78  | SER  | N-CA   | 10.57  | 1.59        | 1.46     |
| 1   | A     | 183 | SER  | CA-C   | 10.56  | 1.67        | 1.52     |
| 1   | A     | 82  | LEU  | CA-CB  | 10.56  | 1.71        | 1.52     |
| 1   | A     | 215 | GLY  | CA-C   | 10.53  | 1.62        | 1.51     |
| 1   | A     | 258 | GLY  | N-CA   | 10.50  | 1.56        | 1.45     |
| 1   | A     | 129 | PRO  | CA-C   | 10.41  | 1.67        | 1.52     |
| 1   | A     | 265 | LYS  | C-N    | -10.40 | 1.20        | 1.32     |
| 1   | A     | 201 | PRO  | C-O    | -10.39 | 1.10        | 1.24     |
| 1   | A     | 102 | GLY  | C-O    | 10.38  | 1.38        | 1.23     |
| 1   | A     | 146 | GLY  | C-O    | 10.38  | 1.38        | 1.23     |
| 1   | A     | 57  | ASN  | N-CA   | -10.37 | 1.32        | 1.46     |
| 1   | A     | 127 | GLY  | C-O    | 10.36  | 1.38        | 1.23     |
| 1   | A     | 257 | LEU  | CA-C   | -10.35 | 1.39        | 1.52     |
| 1   | A     | 193 | GLY  | C-O    | -10.35 | 1.09        | 1.24     |
| 1   | A     | 129 | PRO  | C-N    | -10.28 | 1.19        | 1.33     |
| 1   | A     | 167 | TYR  | CA-C   | 10.22  | 1.66        | 1.52     |
| 1   | A     | 86  | PRO  | N-CD   | 10.18  | 1.62        | 1.47     |
| 1   | A     | 194 | PRO  | N-CD   | 10.18  | 1.62        | 1.47     |
| 1   | A     | 79  | ILE  | CA-C   | 10.18  | 1.65        | 1.52     |
| 1   | A     | 164 | THR  | N-CA   | 10.15  | 1.57        | 1.46     |
| 1   | A     | 49  | SER  | C-N    | -10.15 | 1.20        | 1.33     |
| 1   | A     | 26  | VAL  | C-O    | 10.12  | 1.37        | 1.24     |
| 1   | A     | 156 | GLU  | C-N    | -10.09 | 1.18        | 1.33     |
| 1   | A     | 214 | TYR  | C-O    | -10.06 | 1.11        | 1.23     |
| 1   | A     | 77  | ASN  | CA-CB  | 10.05  | 1.70        | 1.53     |
| 1   | A     | 97  | GLY  | CA-C   | -10.03 | 1.39        | 1.52     |
| 1   | A     | 9   | SER  | CA-C   | 9.98   | 1.65        | 1.52     |
| 1   | A     | 136 | LYS  | CD-CE  | 9.98   | 1.82        | 1.52     |
| 1   | A     | 226 | HIS  | C-N    | -9.96  | 1.21        | 1.33     |
| 1   | A     | 35  | ILE  | CA-C   | 9.94   | 1.65        | 1.52     |
| 1   | A     | 12  | LYS  | C-O    | 9.91   | 1.36        | 1.24     |
| 1   | A     | 177 | VAL  | C-O    | 9.90   | 1.34        | 1.24     |
| 1   | A     | 3   | SER  | C-O    | -9.89  | 1.12        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 197 | ASP  | CB-CG   | -9.89 | 1.27        | 1.52     |
| 1   | A     | 215 | GLY  | C-N     | -9.85 | 1.19        | 1.33     |
| 1   | A     | 50  | MET  | C-N     | 9.84  | 1.43        | 1.33     |
| 1   | A     | 254 | THR  | C-N     | -9.83 | 1.19        | 1.33     |
| 1   | A     | 198 | VAL  | C-O     | 9.81  | 1.35        | 1.23     |
| 1   | A     | 200 | ALA  | C-O     | 9.76  | 1.36        | 1.24     |
| 1   | A     | 19  | GLN  | C-O     | 9.71  | 1.36        | 1.24     |
| 1   | A     | 2   | GLN  | CA-C    | 9.70  | 1.64        | 1.52     |
| 1   | A     | 163 | SER  | CA-C    | 9.70  | 1.64        | 1.52     |
| 1   | A     | 267 | LEU  | C-N     | 9.70  | 1.45        | 1.33     |
| 1   | A     | 221 | SER  | CA-C    | 9.65  | 1.65        | 1.52     |
| 1   | A     | 218 | ASN  | CG-OD1  | 9.64  | 1.41        | 1.23     |
| 1   | A     | 154 | GLY  | C-O     | -9.64 | 1.10        | 1.23     |
| 1   | A     | 225 | PRO  | N-CA    | -9.64 | 1.34        | 1.47     |
| 1   | A     | 4   | VAL  | CA-CB   | 9.62  | 1.66        | 1.54     |
| 1   | A     | 52  | PRO  | C-O     | 9.62  | 1.36        | 1.24     |
| 1   | A     | 156 | GLU  | CD-OE1  | 9.62  | 1.43        | 1.25     |
| 1   | A     | 196 | LEU  | C-O     | -9.62 | 1.12        | 1.24     |
| 1   | A     | 85  | ALA  | C-N     | -9.61 | 1.11        | 1.33     |
| 1   | A     | 174 | VAL  | CA-CB   | 9.60  | 1.69        | 1.54     |
| 1   | A     | 107 | ILE  | N-CA    | -9.57 | 1.35        | 1.46     |
| 1   | A     | 67  | HIS  | CD2-NE2 | -9.56 | 1.27        | 1.37     |
| 1   | A     | 238 | HIS  | CD2-NE2 | -9.56 | 1.27        | 1.37     |
| 1   | A     | 103 | GLN  | N-CA    | -9.54 | 1.34        | 1.46     |
| 1   | A     | 66  | THR  | N-CA    | 9.47  | 1.57        | 1.46     |
| 1   | A     | 36  | ASP  | C-N     | 9.45  | 1.48        | 1.33     |
| 1   | A     | 116 | ALA  | CA-C    | 9.45  | 1.66        | 1.52     |
| 1   | A     | 185 | GLN  | N-CA    | 9.44  | 1.58        | 1.46     |
| 1   | A     | 211 | GLY  | C-N     | -9.43 | 1.21        | 1.33     |
| 1   | A     | 181 | ASP  | CA-C    | 9.39  | 1.66        | 1.53     |
| 1   | A     | 137 | ALA  | C-N     | -9.35 | 1.21        | 1.33     |
| 1   | A     | 214 | TYR  | CA-C    | 9.31  | 1.64        | 1.52     |
| 1   | A     | 165 | VAL  | C-N     | -9.24 | 1.21        | 1.33     |
| 1   | A     | 158 | SER  | N-CA    | 9.24  | 1.56        | 1.45     |
| 1   | A     | 24  | SER  | N-CA    | 9.19  | 1.56        | 1.46     |
| 1   | A     | 104 | TYR  | N-CA    | -9.19 | 1.34        | 1.46     |
| 1   | A     | 226 | HIS  | N-CA    | 9.19  | 1.56        | 1.46     |
| 1   | A     | 172 | PRO  | CA-C    | 9.14  | 1.65        | 1.52     |
| 1   | A     | 85  | ALA  | C-O     | 9.11  | 1.34        | 1.24     |
| 1   | A     | 105 | SER  | C-N     | -9.10 | 1.20        | 1.33     |
| 1   | A     | 65  | GLY  | N-CA    | 9.10  | 1.58        | 1.45     |
| 1   | A     | 109 | ASN  | CG-OD1  | 9.08  | 1.40        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 117 | ASN  | N-CA    | 9.05  | 1.56        | 1.46     |
| 1   | A     | 28  | VAL  | C-N     | -9.02 | 1.20        | 1.33     |
| 1   | A     | 148 | VAL  | CA-C    | 9.01  | 1.64        | 1.52     |
| 1   | A     | 65  | GLY  | CA-C    | 8.92  | 1.64        | 1.51     |
| 1   | A     | 170 | LYS  | CA-C    | -8.91 | 1.40        | 1.52     |
| 1   | A     | 185 | GLN  | CA-CB   | -8.89 | 1.39        | 1.53     |
| 1   | A     | 179 | ALA  | C-N     | -8.88 | 1.23        | 1.33     |
| 1   | A     | 123 | ASN  | CB-CG   | 8.87  | 1.74        | 1.52     |
| 1   | A     | 129 | PRO  | N-CD    | -8.85 | 1.35        | 1.47     |
| 1   | A     | 169 | GLY  | CA-C    | 8.85  | 1.62        | 1.52     |
| 1   | A     | 113 | TRP  | CD2-CE3 | 8.84  | 1.54        | 1.40     |
| 1   | A     | 112 | GLU  | CB-CG   | 8.78  | 1.78        | 1.52     |
| 1   | A     | 261 | PHE  | CA-C    | 8.70  | 1.64        | 1.52     |
| 1   | A     | 151 | ALA  | CA-CB   | 8.70  | 1.69        | 1.53     |
| 1   | A     | 88  | SER  | CA-C    | -8.66 | 1.41        | 1.52     |
| 1   | A     | 222 | MET  | CA-CB   | -8.66 | 1.40        | 1.53     |
| 1   | A     | 139 | VAL  | N-CA    | -8.65 | 1.36        | 1.46     |
| 1   | A     | 124 | MET  | CA-C    | 8.64  | 1.65        | 1.53     |
| 1   | A     | 106 | TRP  | CA-CB   | -8.62 | 1.39        | 1.53     |
| 1   | A     | 189 | PHE  | CA-CB   | 8.62  | 1.68        | 1.53     |
| 1   | A     | 72  | VAL  | C-O     | -8.61 | 1.14        | 1.24     |
| 1   | A     | 52  | PRO  | C-N     | -8.60 | 1.21        | 1.33     |
| 1   | A     | 232 | ALA  | CA-C    | -8.60 | 1.41        | 1.52     |
| 1   | A     | 109 | ASN  | CA-C    | 8.59  | 1.64        | 1.52     |
| 1   | A     | 218 | ASN  | C-O     | 8.57  | 1.34        | 1.24     |
| 1   | A     | 127 | GLY  | N-CA    | 8.57  | 1.53        | 1.45     |
| 1   | A     | 177 | VAL  | CA-CB   | 8.55  | 1.64        | 1.54     |
| 1   | A     | 121 | VAL  | CA-C    | 8.54  | 1.63        | 1.52     |
| 1   | A     | 273 | ALA  | N-CA    | 8.52  | 1.56        | 1.46     |
| 1   | A     | 96  | LEU  | C-N     | 8.50  | 1.43        | 1.33     |
| 1   | A     | 186 | ARG  | C-O     | 8.50  | 1.34        | 1.24     |
| 1   | A     | 226 | HIS  | CD2-NE2 | -8.49 | 1.28        | 1.37     |
| 1   | A     | 84  | VAL  | C-O     | 8.49  | 1.34        | 1.24     |
| 1   | A     | 11  | ILE  | CA-C    | 8.48  | 1.61        | 1.52     |
| 1   | A     | 212 | ASN  | C-N     | -8.47 | 1.22        | 1.33     |
| 1   | A     | 226 | HIS  | C-O     | 8.47  | 1.33        | 1.24     |
| 1   | A     | 119 | MET  | C-O     | 8.44  | 1.34        | 1.23     |
| 1   | A     | 175 | ILE  | N-CA    | 8.44  | 1.57        | 1.46     |
| 1   | A     | 224 | SER  | N-CA    | -8.44 | 1.34        | 1.46     |
| 1   | A     | 231 | ALA  | C-N     | 8.41  | 1.44        | 1.33     |
| 1   | A     | 238 | HIS  | ND1-CE1 | -8.41 | 1.24        | 1.32     |
| 1   | A     | 39  | HIS  | C-O     | 8.40  | 1.34        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 107 | ILE  | CA-CB  | -8.40 | 1.45        | 1.54     |
| 1   | A     | 96  | LEU  | C-O    | -8.37 | 1.14        | 1.23     |
| 1   | A     | 65  | GLY  | C-O    | -8.37 | 1.12        | 1.23     |
| 1   | A     | 120 | ASP  | C-N    | -8.35 | 1.22        | 1.33     |
| 1   | A     | 67  | HIS  | CG-CD2 | 8.34  | 1.45        | 1.35     |
| 1   | A     | 66  | THR  | CB-OG1 | -8.31 | 1.30        | 1.43     |
| 1   | A     | 133 | ALA  | CA-C   | -8.30 | 1.41        | 1.52     |
| 1   | A     | 161 | SER  | C-O    | 8.29  | 1.34        | 1.24     |
| 1   | A     | 210 | PRO  | CA-CB  | -8.29 | 1.43        | 1.53     |
| 1   | A     | 58  | PHE  | N-CA   | -8.27 | 1.36        | 1.46     |
| 1   | A     | 93  | VAL  | N-CA   | -8.27 | 1.36        | 1.46     |
| 1   | A     | 181 | ASP  | CA-CB  | -8.27 | 1.39        | 1.53     |
| 1   | A     | 202 | GLY  | CA-C   | 8.27  | 1.63        | 1.51     |
| 1   | A     | 257 | LEU  | C-N    | -8.18 | 1.23        | 1.32     |
| 1   | A     | 232 | ALA  | CA-CB  | 8.17  | 1.66        | 1.53     |
| 1   | A     | 113 | TRP  | C-N    | 8.15  | 1.45        | 1.33     |
| 1   | A     | 75  | LEU  | C-O    | 8.14  | 1.34        | 1.24     |
| 1   | A     | 244 | THR  | C-N    | -8.13 | 1.23        | 1.33     |
| 1   | A     | 77  | ASN  | CG-ND2 | -8.12 | 1.16        | 1.33     |
| 1   | A     | 267 | LEU  | CA-C   | -8.11 | 1.43        | 1.52     |
| 1   | A     | 149 | VAL  | CA-C   | 8.10  | 1.62        | 1.52     |
| 1   | A     | 91  | TYR  | CG-CD1 | 8.09  | 1.56        | 1.39     |
| 1   | A     | 30  | VAL  | N-CA   | -8.09 | 1.36        | 1.46     |
| 1   | A     | 35  | ILE  | C-O    | -8.07 | 1.14        | 1.24     |
| 1   | A     | 137 | ALA  | CA-C   | 8.04  | 1.63        | 1.52     |
| 1   | A     | 82  | LEU  | C-O    | -8.03 | 1.14        | 1.23     |
| 1   | A     | 55  | THR  | CA-C   | 8.02  | 1.62        | 1.52     |
| 1   | A     | 161 | SER  | N-CA   | 7.99  | 1.57        | 1.45     |
| 1   | A     | 91  | TYR  | CZ-OH  | -7.99 | 1.21        | 1.38     |
| 1   | A     | 112 | GLU  | CD-OE1 | 7.95  | 1.40        | 1.25     |
| 1   | A     | 45  | ALA  | CA-C   | -7.94 | 1.42        | 1.52     |
| 1   | A     | 44  | VAL  | C-N    | -7.94 | 1.23        | 1.33     |
| 1   | A     | 6   | TYR  | CG-CD2 | 7.93  | 1.56        | 1.39     |
| 1   | A     | 80  | GLY  | N-CA   | -7.93 | 1.33        | 1.45     |
| 1   | A     | 57  | ASN  | CA-C   | 7.90  | 1.63        | 1.52     |
| 1   | A     | 221 | SER  | C-N    | -7.89 | 1.23        | 1.33     |
| 1   | A     | 112 | GLU  | CA-C   | -7.87 | 1.42        | 1.52     |
| 1   | A     | 30  | VAL  | C-N    | 7.87  | 1.41        | 1.33     |
| 1   | A     | 112 | GLU  | N-CA   | 7.86  | 1.56        | 1.46     |
| 1   | A     | 74  | ALA  | N-CA   | 7.84  | 1.55        | 1.46     |
| 1   | A     | 119 | MET  | C-N    | -7.81 | 1.23        | 1.33     |
| 1   | A     | 269 | ASN  | C-N    | -7.79 | 1.24        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 8   | VAL  | C-O    | -7.76 | 1.15        | 1.24     |
| 1   | A     | 84  | VAL  | C-N    | -7.76 | 1.24        | 1.33     |
| 1   | A     | 159 | THR  | CA-CB  | 7.76  | 1.66        | 1.53     |
| 1   | A     | 33  | SER  | CA-CB  | -7.75 | 1.42        | 1.53     |
| 1   | A     | 208 | THR  | CA-CB  | -7.74 | 1.40        | 1.53     |
| 1   | A     | 79  | ILE  | CA-CB  | -7.71 | 1.44        | 1.54     |
| 1   | A     | 264 | GLY  | N-CA   | 7.70  | 1.57        | 1.45     |
| 1   | A     | 195 | GLU  | CA-C   | 7.68  | 1.63        | 1.52     |
| 1   | A     | 55  | THR  | C-N    | 7.65  | 1.42        | 1.33     |
| 1   | A     | 219 | GLY  | C-O    | 7.64  | 1.34        | 1.23     |
| 1   | A     | 177 | VAL  | CA-C   | -7.64 | 1.43        | 1.52     |
| 1   | A     | 60  | ASP  | CA-C   | 7.64  | 1.62        | 1.52     |
| 1   | A     | 216 | ALA  | CA-CB  | 7.61  | 1.71        | 1.53     |
| 1   | A     | 64  | HIS  | C-O    | 7.60  | 1.33        | 1.24     |
| 1   | A     | 34  | GLY  | C-N    | 7.60  | 1.44        | 1.33     |
| 1   | A     | 246 | VAL  | CA-CB  | -7.57 | 1.43        | 1.54     |
| 1   | A     | 130 | SER  | CB-OG  | 7.57  | 1.57        | 1.42     |
| 1   | A     | 140 | ASP  | CG-OD1 | 7.57  | 1.39        | 1.25     |
| 1   | A     | 40  | PRO  | N-CA   | 7.54  | 1.56        | 1.47     |
| 1   | A     | 29  | ALA  | CA-C   | 7.54  | 1.62        | 1.52     |
| 1   | A     | 201 | PRO  | CA-CB  | 7.53  | 1.64        | 1.53     |
| 1   | A     | 62  | ASN  | CG-ND2 | -7.50 | 1.17        | 1.33     |
| 1   | A     | 67  | HIS  | CB-CG  | -7.44 | 1.39        | 1.50     |
| 1   | A     | 206 | GLN  | C-O    | -7.44 | 1.15        | 1.24     |
| 1   | A     | 210 | PRO  | N-CA   | -7.42 | 1.38        | 1.47     |
| 1   | A     | 83  | GLY  | C-O    | 7.42  | 1.33        | 1.23     |
| 1   | A     | 17  | HIS  | CG-CD2 | 7.39  | 1.44        | 1.35     |
| 1   | A     | 64  | HIS  | CG-CD2 | -7.38 | 1.27        | 1.35     |
| 1   | A     | 151 | ALA  | CA-C   | 7.37  | 1.62        | 1.52     |
| 1   | A     | 254 | THR  | CA-C   | -7.34 | 1.43        | 1.52     |
| 1   | A     | 86  | PRO  | C-O    | 7.33  | 1.33        | 1.24     |
| 1   | A     | 11  | ILE  | C-O    | 7.33  | 1.31        | 1.23     |
| 1   | A     | 258 | GLY  | C-O    | 7.32  | 1.33        | 1.23     |
| 1   | A     | 257 | LEU  | CB-CG  | 7.32  | 1.68        | 1.53     |
| 1   | A     | 195 | GLU  | C-N    | 7.30  | 1.43        | 1.33     |
| 1   | A     | 39  | HIS  | CA-C   | 7.28  | 1.62        | 1.52     |
| 1   | A     | 210 | PRO  | N-CD   | 7.27  | 1.57        | 1.47     |
| 1   | A     | 152 | ALA  | CA-CB  | 7.27  | 1.64        | 1.53     |
| 1   | A     | 196 | LEU  | CA-C   | 7.27  | 1.62        | 1.52     |
| 1   | A     | 182 | SER  | CA-CB  | 7.26  | 1.65        | 1.53     |
| 1   | A     | 115 | ILE  | C-N    | -7.26 | 1.24        | 1.33     |
| 1   | A     | 60  | ASP  | C-N    | 7.25  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 221 | SER  | C-O    | -7.23 | 1.14        | 1.24     |
| 1   | A     | 99  | ALA  | CA-CB  | 7.22  | 1.65        | 1.53     |
| 1   | A     | 216 | ALA  | N-CA   | 7.21  | 1.54        | 1.45     |
| 1   | A     | 155 | ASN  | C-O    | -7.20 | 1.15        | 1.24     |
| 1   | A     | 275 | GLN  | C-OXT  | 7.19  | 1.38        | 1.23     |
| 1   | A     | 130 | SER  | N-CA   | 7.18  | 1.54        | 1.45     |
| 1   | A     | 154 | GLY  | CA-C   | 7.18  | 1.62        | 1.51     |
| 1   | A     | 157 | GLY  | CA-C   | 7.18  | 1.62        | 1.51     |
| 1   | A     | 160 | GLY  | C-N    | -7.17 | 1.22        | 1.33     |
| 1   | A     | 190 | SER  | N-CA   | -7.17 | 1.36        | 1.46     |
| 1   | A     | 167 | TYR  | CG-CD1 | 7.17  | 1.54        | 1.39     |
| 1   | A     | 64  | HIS  | CA-C   | -7.16 | 1.43        | 1.52     |
| 1   | A     | 249 | SER  | C-O    | -7.15 | 1.15        | 1.24     |
| 1   | A     | 62  | ASN  | C-O    | -7.14 | 1.15        | 1.24     |
| 1   | A     | 122 | ILE  | CA-CB  | -7.13 | 1.45        | 1.54     |
| 1   | A     | 246 | VAL  | C-N    | -7.13 | 1.24        | 1.33     |
| 1   | A     | 264 | GLY  | C-N    | -7.10 | 1.24        | 1.33     |
| 1   | A     | 173 | SER  | CA-C   | 7.09  | 1.63        | 1.52     |
| 1   | A     | 184 | ASN  | C-O    | -7.09 | 1.12        | 1.24     |
| 1   | A     | 33  | SER  | C-N    | 7.06  | 1.43        | 1.32     |
| 1   | A     | 111 | ILE  | C-O    | 7.03  | 1.31        | 1.24     |
| 1   | A     | 56  | PRO  | C-O    | -7.02 | 1.14        | 1.23     |
| 1   | A     | 261 | PHE  | CG-CD2 | -7.00 | 1.24        | 1.38     |
| 1   | A     | 98  | ASP  | C-O    | 7.00  | 1.32        | 1.23     |
| 1   | A     | 5   | PRO  | C-O    | 6.99  | 1.32        | 1.23     |
| 1   | A     | 105 | SER  | N-CA   | -6.99 | 1.36        | 1.46     |
| 1   | A     | 31  | ILE  | CA-CB  | -6.99 | 1.44        | 1.53     |
| 1   | A     | 198 | VAL  | C-N    | -6.99 | 1.23        | 1.33     |
| 1   | A     | 85  | ALA  | N-CA   | -6.98 | 1.39        | 1.46     |
| 1   | A     | 226 | HIS  | CA-C   | -6.97 | 1.44        | 1.52     |
| 1   | A     | 27  | LYS  | C-O    | 6.96  | 1.32        | 1.24     |
| 1   | A     | 18  | SER  | C-O    | 6.95  | 1.34        | 1.24     |
| 1   | A     | 199 | MET  | C-O    | 6.94  | 1.32        | 1.23     |
| 1   | A     | 101 | SER  | C-N    | 6.94  | 1.43        | 1.33     |
| 1   | A     | 41  | ASP  | N-CA   | -6.92 | 1.36        | 1.46     |
| 1   | A     | 125 | SER  | C-O    | 6.90  | 1.34        | 1.23     |
| 1   | A     | 156 | GLU  | N-CA   | -6.90 | 1.34        | 1.45     |
| 1   | A     | 123 | ASN  | CG-OD1 | -6.89 | 1.10        | 1.23     |
| 1   | A     | 32  | ASP  | CG-OD2 | -6.89 | 1.12        | 1.25     |
| 1   | A     | 61  | ASP  | CG-OD2 | -6.89 | 1.12        | 1.25     |
| 1   | A     | 78  | SER  | CA-C   | 6.89  | 1.62        | 1.52     |
| 1   | A     | 174 | VAL  | CA-C   | -6.89 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 231 | ALA  | CA-CB   | 6.89  | 1.64        | 1.53     |
| 1   | A     | 106 | TRP  | C-N     | 6.86  | 1.42        | 1.33     |
| 1   | A     | 75  | LEU  | CA-C    | -6.82 | 1.43        | 1.52     |
| 1   | A     | 131 | GLY  | C-N     | -6.82 | 1.24        | 1.33     |
| 1   | A     | 136 | LYS  | C-N     | -6.82 | 1.24        | 1.33     |
| 1   | A     | 256 | LYS  | N-CA    | 6.81  | 1.54        | 1.46     |
| 1   | A     | 2   | GLN  | CD-OE1  | 6.80  | 1.36        | 1.23     |
| 1   | A     | 9   | SER  | C-N     | 6.79  | 1.43        | 1.33     |
| 1   | A     | 27  | LYS  | CB-CG   | 6.78  | 1.72        | 1.52     |
| 1   | A     | 267 | LEU  | N-CA    | -6.75 | 1.38        | 1.46     |
| 1   | A     | 186 | ARG  | CD-NE   | -6.73 | 1.36        | 1.46     |
| 1   | A     | 261 | PHE  | N-CA    | -6.72 | 1.37        | 1.46     |
| 1   | A     | 241 | TRP  | NE1-CE2 | -6.71 | 1.30        | 1.37     |
| 1   | A     | 217 | TYR  | CG-CD2  | 6.70  | 1.53        | 1.39     |
| 1   | A     | 119 | MET  | CB-CG   | -6.70 | 1.32        | 1.52     |
| 1   | A     | 145 | SER  | C-N     | -6.69 | 1.23        | 1.33     |
| 1   | A     | 108 | ILE  | CA-C    | 6.68  | 1.60        | 1.52     |
| 1   | A     | 266 | GLY  | C-N     | 6.68  | 1.42        | 1.33     |
| 1   | A     | 178 | GLY  | C-N     | -6.67 | 1.24        | 1.33     |
| 1   | A     | 126 | LEU  | CA-C    | 6.66  | 1.61        | 1.52     |
| 1   | A     | 69  | ALA  | C-O     | 6.65  | 1.32        | 1.24     |
| 1   | A     | 132 | SER  | C-O     | 6.65  | 1.32        | 1.24     |
| 1   | A     | 68  | VAL  | C-O     | 6.65  | 1.31        | 1.24     |
| 1   | A     | 9   | SER  | C-O     | -6.64 | 1.16        | 1.24     |
| 1   | A     | 186 | ARG  | NE-CZ   | -6.64 | 1.25        | 1.33     |
| 1   | A     | 182 | SER  | CB-OG   | -6.62 | 1.28        | 1.42     |
| 1   | A     | 112 | GLU  | CD-OE2  | 6.62  | 1.38        | 1.25     |
| 1   | A     | 6   | TYR  | CA-CB   | -6.62 | 1.43        | 1.53     |
| 1   | A     | 77  | ASN  | N-CA    | 6.61  | 1.54        | 1.46     |
| 1   | A     | 191 | SER  | C-O     | 6.61  | 1.33        | 1.23     |
| 1   | A     | 61  | ASP  | CA-CB   | -6.60 | 1.43        | 1.53     |
| 1   | A     | 76  | ASN  | C-N     | 6.60  | 1.43        | 1.33     |
| 1   | A     | 19  | GLN  | C-N     | 6.58  | 1.44        | 1.33     |
| 1   | A     | 97  | GLY  | C-O     | 6.58  | 1.30        | 1.23     |
| 1   | A     | 205 | ILE  | C-N     | -6.58 | 1.24        | 1.33     |
| 1   | A     | 167 | TYR  | CB-CG   | -6.57 | 1.37        | 1.51     |
| 1   | A     | 107 | ILE  | C-N     | 6.57  | 1.41        | 1.33     |
| 1   | A     | 113 | TRP  | CA-C    | -6.56 | 1.44        | 1.52     |
| 1   | A     | 53  | SER  | C-O     | -6.55 | 1.15        | 1.23     |
| 1   | A     | 117 | ASN  | CA-CB   | 6.54  | 1.62        | 1.53     |
| 1   | A     | 141 | LYS  | C-O     | 6.54  | 1.31        | 1.24     |
| 1   | A     | 106 | TRP  | CZ3-CH2 | -6.52 | 1.24        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 89  | ALA  | C-O     | 6.51  | 1.31        | 1.24     |
| 1   | A     | 222 | MET  | N-CA    | 6.50  | 1.54        | 1.46     |
| 1   | A     | 142 | ALA  | CA-C    | -6.49 | 1.43        | 1.52     |
| 1   | A     | 156 | GLU  | CA-C    | 6.47  | 1.61        | 1.53     |
| 1   | A     | 268 | ILE  | CA-C    | -6.46 | 1.45        | 1.52     |
| 1   | A     | 22  | THR  | C-O     | 6.45  | 1.32        | 1.24     |
| 1   | A     | 95  | VAL  | N-CA    | -6.45 | 1.38        | 1.46     |
| 1   | A     | 264 | GLY  | C-O     | 6.44  | 1.31        | 1.24     |
| 1   | A     | 22  | THR  | CA-C    | 6.44  | 1.61        | 1.52     |
| 1   | A     | 62  | ASN  | C-N     | 6.43  | 1.42        | 1.33     |
| 1   | A     | 25  | ASN  | CA-C    | 6.42  | 1.63        | 1.52     |
| 1   | A     | 181 | ASP  | CB-CG   | 6.41  | 1.68        | 1.52     |
| 1   | A     | 39  | HIS  | CE1-NE2 | -6.40 | 1.26        | 1.32     |
| 1   | A     | 222 | MET  | C-O     | 6.40  | 1.32        | 1.24     |
| 1   | A     | 142 | ALA  | N-CA    | 6.38  | 1.54        | 1.46     |
| 1   | A     | 43  | LYS  | CA-CB   | 6.38  | 1.62        | 1.53     |
| 1   | A     | 21  | TYR  | CB-CG   | 6.38  | 1.65        | 1.51     |
| 1   | A     | 12  | LYS  | N-CA    | 6.36  | 1.54        | 1.46     |
| 1   | A     | 209 | LEU  | CA-CB   | -6.35 | 1.43        | 1.53     |
| 1   | A     | 115 | ILE  | CA-CB   | 6.35  | 1.61        | 1.54     |
| 1   | A     | 194 | PRO  | C-N     | -6.33 | 1.24        | 1.33     |
| 1   | A     | 176 | ALA  | N-CA    | -6.32 | 1.38        | 1.46     |
| 1   | A     | 57  | ASN  | C-O     | 6.29  | 1.32        | 1.24     |
| 1   | A     | 240 | ASN  | CA-C    | 6.29  | 1.61        | 1.52     |
| 1   | A     | 120 | ASP  | C-O     | 6.28  | 1.32        | 1.23     |
| 1   | A     | 16  | LEU  | C-O     | 6.27  | 1.31        | 1.24     |
| 1   | A     | 103 | GLN  | C-N     | 6.25  | 1.42        | 1.34     |
| 1   | A     | 113 | TRP  | CB-CG   | 6.23  | 1.69        | 1.50     |
| 1   | A     | 146 | GLY  | N-CA    | 6.23  | 1.54        | 1.45     |
| 1   | A     | 48  | ALA  | C-N     | -6.22 | 1.25        | 1.33     |
| 1   | A     | 163 | SER  | C-N     | 6.20  | 1.41        | 1.33     |
| 1   | A     | 213 | LYS  | CB-CG   | 6.20  | 1.71        | 1.52     |
| 1   | A     | 24  | SER  | C-O     | 6.19  | 1.31        | 1.24     |
| 1   | A     | 83  | GLY  | CA-C    | -6.18 | 1.42        | 1.52     |
| 1   | A     | 181 | ASP  | C-N     | -6.18 | 1.24        | 1.33     |
| 1   | A     | 73  | ALA  | C-O     | -6.17 | 1.16        | 1.24     |
| 1   | A     | 200 | ALA  | CA-CB   | 6.16  | 1.63        | 1.54     |
| 1   | A     | 53  | SER  | CB-OG   | 6.12  | 1.54        | 1.42     |
| 1   | A     | 64  | HIS  | N-CA    | -6.12 | 1.38        | 1.46     |
| 1   | A     | 255 | THR  | CA-CB   | -6.11 | 1.45        | 1.53     |
| 1   | A     | 159 | THR  | N-CA    | 6.11  | 1.54        | 1.46     |
| 1   | A     | 174 | VAL  | C-N     | -6.11 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 50  | MET  | C-O     | -6.10 | 1.16        | 1.24     |
| 1   | A     | 210 | PRO  | C-O     | 6.09  | 1.31        | 1.23     |
| 1   | A     | 61  | ASP  | CG-OD1  | 6.04  | 1.36        | 1.25     |
| 1   | A     | 134 | ALA  | CA-CB   | -6.03 | 1.44        | 1.53     |
| 1   | A     | 180 | VAL  | N-CA    | 6.03  | 1.53        | 1.46     |
| 1   | A     | 14  | PRO  | C-N     | 6.01  | 1.41        | 1.33     |
| 1   | A     | 17  | HIS  | CB-CG   | 6.01  | 1.58        | 1.50     |
| 1   | A     | 94  | LYS  | CG-CD   | 6.00  | 1.70        | 1.52     |
| 1   | A     | 206 | GLN  | CA-C    | -5.98 | 1.45        | 1.52     |
| 1   | A     | 262 | TYR  | CB-CG   | 5.96  | 1.64        | 1.51     |
| 1   | A     | 267 | LEU  | C-O     | 5.95  | 1.31        | 1.24     |
| 1   | A     | 213 | LYS  | C-N     | -5.95 | 1.26        | 1.33     |
| 1   | A     | 167 | TYR  | N-CA    | -5.93 | 1.36        | 1.46     |
| 1   | A     | 117 | ASN  | C-N     | 5.93  | 1.40        | 1.33     |
| 1   | A     | 185 | GLN  | CG-CD   | 5.93  | 1.66        | 1.52     |
| 1   | A     | 186 | ARG  | CZ-NH2  | 5.93  | 1.41        | 1.33     |
| 1   | A     | 1   | ALA  | N-CA    | -5.93 | 1.34        | 1.46     |
| 1   | A     | 52  | PRO  | N-CA    | -5.93 | 1.39        | 1.47     |
| 1   | A     | 51  | VAL  | C-O     | 5.92  | 1.31        | 1.24     |
| 1   | A     | 245 | GLN  | CA-C    | -5.92 | 1.45        | 1.52     |
| 1   | A     | 172 | PRO  | N-CD    | 5.90  | 1.56        | 1.47     |
| 1   | A     | 155 | ASN  | CG-ND2  | -5.90 | 1.20        | 1.33     |
| 1   | A     | 37  | SER  | CA-C    | 5.89  | 1.60        | 1.52     |
| 1   | A     | 100 | GLY  | N-CA    | -5.89 | 1.36        | 1.45     |
| 1   | A     | 113 | TRP  | CZ2-CH2 | 5.89  | 1.48        | 1.37     |
| 1   | A     | 157 | GLY  | N-CA    | -5.89 | 1.36        | 1.45     |
| 1   | A     | 245 | GLN  | N-CA    | 5.88  | 1.53        | 1.46     |
| 1   | A     | 97  | GLY  | N-CA    | -5.88 | 1.35        | 1.45     |
| 1   | A     | 90  | LEU  | CA-C    | -5.88 | 1.45        | 1.52     |
| 1   | A     | 168 | PRO  | C-O     | 5.87  | 1.34        | 1.23     |
| 1   | A     | 106 | TRP  | C-O     | 5.87  | 1.31        | 1.24     |
| 1   | A     | 207 | SER  | C-N     | -5.84 | 1.25        | 1.33     |
| 1   | A     | 132 | SER  | CB-OG   | 5.80  | 1.53        | 1.42     |
| 1   | A     | 268 | ILE  | N-CA    | 5.79  | 1.53        | 1.46     |
| 1   | A     | 189 | PHE  | CE2-CZ  | 5.79  | 1.56        | 1.38     |
| 1   | A     | 53  | SER  | CA-C    | 5.79  | 1.60        | 1.52     |
| 1   | A     | 162 | SER  | CA-CB   | 5.78  | 1.63        | 1.53     |
| 1   | A     | 14  | PRO  | CA-C    | 5.76  | 1.62        | 1.52     |
| 1   | A     | 108 | ILE  | N-CA    | 5.74  | 1.53        | 1.46     |
| 1   | A     | 145 | SER  | C-O     | 5.74  | 1.30        | 1.24     |
| 1   | A     | 118 | ASN  | C-O     | 5.73  | 1.31        | 1.23     |
| 1   | A     | 123 | ASN  | N-CA    | 5.73  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 229 | GLY  | C-O    | -5.71 | 1.16        | 1.23     |
| 1   | A     | 63  | SER  | C-N    | 5.71  | 1.42        | 1.33     |
| 1   | A     | 25  | ASN  | CA-CB  | 5.67  | 1.62        | 1.53     |
| 1   | A     | 242 | THR  | CA-CB  | 5.67  | 1.62        | 1.53     |
| 1   | A     | 196 | LEU  | N-CA   | -5.66 | 1.39        | 1.46     |
| 1   | A     | 234 | ILE  | C-O    | -5.66 | 1.18        | 1.24     |
| 1   | A     | 28  | VAL  | C-O    | 5.65  | 1.30        | 1.24     |
| 1   | A     | 71  | THR  | N-CA   | 5.65  | 1.53        | 1.46     |
| 1   | A     | 21  | TYR  | N-CA   | 5.62  | 1.53        | 1.46     |
| 1   | A     | 32  | ASP  | CA-CB  | -5.62 | 1.44        | 1.53     |
| 1   | A     | 44  | VAL  | CA-CB  | 5.61  | 1.61        | 1.54     |
| 1   | A     | 113 | TRP  | CG-CD1 | -5.61 | 1.23        | 1.36     |
| 1   | A     | 109 | ASN  | C-O    | 5.61  | 1.31        | 1.24     |
| 1   | A     | 47  | GLY  | CA-C   | -5.61 | 1.44        | 1.51     |
| 1   | A     | 126 | LEU  | N-CA   | 5.61  | 1.53        | 1.46     |
| 1   | A     | 240 | ASN  | CG-ND2 | 5.60  | 1.45        | 1.33     |
| 1   | A     | 121 | VAL  | CA-CB  | -5.60 | 1.47        | 1.54     |
| 1   | A     | 150 | VAL  | CB-CG1 | 5.60  | 1.71        | 1.52     |
| 1   | A     | 89  | ALA  | C-N    | -5.60 | 1.26        | 1.33     |
| 1   | A     | 226 | HIS  | CA-CB  | 5.59  | 1.62        | 1.53     |
| 1   | A     | 139 | VAL  | CA-CB  | -5.59 | 1.47        | 1.54     |
| 1   | A     | 208 | THR  | C-O    | -5.58 | 1.17        | 1.23     |
| 1   | A     | 94  | LYS  | N-CA   | -5.53 | 1.39        | 1.46     |
| 1   | A     | 23  | GLY  | CA-C   | 5.53  | 1.58        | 1.51     |
| 1   | A     | 132 | SER  | CA-C   | -5.53 | 1.45        | 1.52     |
| 1   | A     | 158 | SER  | CA-CB  | 5.53  | 1.61        | 1.53     |
| 1   | A     | 133 | ALA  | N-CA   | -5.52 | 1.39        | 1.46     |
| 1   | A     | 80  | GLY  | C-N    | -5.51 | 1.26        | 1.33     |
| 1   | A     | 181 | ASP  | CG-OD2 | -5.50 | 1.15        | 1.25     |
| 1   | A     | 1   | ALA  | CA-C   | 5.48  | 1.64        | 1.52     |
| 1   | A     | 153 | ALA  | CA-CB  | -5.47 | 1.45        | 1.53     |
| 1   | A     | 135 | LEU  | CA-CB  | 5.47  | 1.62        | 1.53     |
| 1   | A     | 149 | VAL  | CA-CB  | -5.47 | 1.47        | 1.54     |
| 1   | A     | 145 | SER  | CB-OG  | -5.47 | 1.31        | 1.42     |
| 1   | A     | 44  | VAL  | C-O    | 5.45  | 1.31        | 1.24     |
| 1   | A     | 228 | ALA  | C-O    | 5.44  | 1.30        | 1.24     |
| 1   | A     | 192 | VAL  | CA-C   | 5.44  | 1.59        | 1.52     |
| 1   | A     | 214 | TYR  | C-N    | 5.43  | 1.40        | 1.33     |
| 1   | A     | 224 | SER  | CA-CB  | 5.43  | 1.62        | 1.53     |
| 1   | A     | 246 | VAL  | C-O    | 5.41  | 1.30        | 1.24     |
| 1   | A     | 66  | THR  | CA-C   | 5.41  | 1.59        | 1.52     |
| 1   | A     | 47  | GLY  | C-O    | 5.41  | 1.31        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 128 | GLY  | N-CA    | 5.40  | 1.52        | 1.44     |
| 1   | A     | 91  | TYR  | C-N     | -5.40 | 1.25        | 1.33     |
| 1   | A     | 4   | VAL  | C-O     | 5.39  | 1.31        | 1.24     |
| 1   | A     | 79  | ILE  | N-CA    | 5.39  | 1.53        | 1.46     |
| 1   | A     | 68  | VAL  | C-N     | -5.39 | 1.26        | 1.33     |
| 1   | A     | 257 | LEU  | C-O     | 5.38  | 1.31        | 1.23     |
| 1   | A     | 56  | PRO  | CA-C    | -5.38 | 1.46        | 1.52     |
| 1   | A     | 197 | ASP  | CA-CB   | 5.37  | 1.62        | 1.53     |
| 1   | A     | 125 | SER  | N-CA    | 5.36  | 1.53        | 1.46     |
| 1   | A     | 113 | TRP  | CD1-NE1 | 5.36  | 1.49        | 1.37     |
| 1   | A     | 262 | TYR  | CE2-CZ  | 5.36  | 1.51        | 1.38     |
| 1   | A     | 48  | ALA  | N-CA    | 5.35  | 1.53        | 1.46     |
| 1   | A     | 114 | ALA  | C-N     | -5.35 | 1.27        | 1.33     |
| 1   | A     | 10  | GLN  | C-N     | -5.34 | 1.27        | 1.33     |
| 1   | A     | 50  | MET  | CB-CG   | -5.33 | 1.36        | 1.52     |
| 1   | A     | 59  | GLN  | N-CA    | 5.33  | 1.53        | 1.46     |
| 1   | A     | 102 | GLY  | N-CA    | 5.33  | 1.53        | 1.45     |
| 1   | A     | 95  | VAL  | CA-CB   | 5.32  | 1.61        | 1.54     |
| 1   | A     | 164 | THR  | CA-CB   | 5.31  | 1.60        | 1.53     |
| 1   | A     | 271 | GLN  | CA-C    | 5.30  | 1.59        | 1.52     |
| 1   | A     | 101 | SER  | CA-C    | -5.30 | 1.45        | 1.52     |
| 1   | A     | 262 | TYR  | CG-CD1  | 5.29  | 1.50        | 1.39     |
| 1   | A     | 106 | TRP  | CG-CD2  | -5.28 | 1.34        | 1.43     |
| 1   | A     | 196 | LEU  | CA-CB   | -5.28 | 1.46        | 1.53     |
| 1   | A     | 235 | LEU  | C-O     | -5.27 | 1.17        | 1.24     |
| 1   | A     | 197 | ASP  | CG-OD2  | 5.27  | 1.35        | 1.25     |
| 1   | A     | 262 | TYR  | CA-C    | -5.26 | 1.45        | 1.52     |
| 1   | A     | 113 | TRP  | CZ3-CH2 | -5.25 | 1.27        | 1.40     |
| 1   | A     | 164 | THR  | CB-OG1  | -5.25 | 1.35        | 1.43     |
| 1   | A     | 59  | GLN  | CD-OE1  | 5.23  | 1.33        | 1.23     |
| 1   | A     | 241 | TRP  | CA-CB   | -5.23 | 1.45        | 1.53     |
| 1   | A     | 148 | VAL  | N-CA    | -5.22 | 1.40        | 1.46     |
| 1   | A     | 231 | ALA  | N-CA    | -5.22 | 1.40        | 1.46     |
| 1   | A     | 242 | THR  | CB-OG1  | 5.22  | 1.52        | 1.43     |
| 1   | A     | 106 | TRP  | N-CA    | -5.21 | 1.39        | 1.46     |
| 1   | A     | 141 | LYS  | CB-CG   | 5.21  | 1.68        | 1.52     |
| 1   | A     | 14  | PRO  | CA-CB   | -5.20 | 1.45        | 1.53     |
| 1   | A     | 127 | GLY  | CA-C    | 5.18  | 1.56        | 1.51     |
| 1   | A     | 21  | TYR  | C-O     | 5.16  | 1.30        | 1.24     |
| 1   | A     | 153 | ALA  | CA-C    | 5.16  | 1.59        | 1.52     |
| 1   | A     | 34  | GLY  | C-O     | -5.16 | 1.16        | 1.23     |
| 1   | A     | 134 | ALA  | C-N     | -5.13 | 1.27        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 153 | ALA  | C-O    | 5.13  | 1.30        | 1.24     |
| 1   | A     | 185 | GLN  | CD-NE2 | -5.11 | 1.22        | 1.33     |
| 1   | A     | 124 | MET  | C-O    | -5.10 | 1.18        | 1.23     |
| 1   | A     | 137 | ALA  | N-CA   | 5.10  | 1.52        | 1.46     |
| 1   | A     | 70  | GLY  | C-N    | 5.09  | 1.41        | 1.33     |
| 1   | A     | 86  | PRO  | N-CA   | -5.09 | 1.40        | 1.47     |
| 1   | A     | 6   | TYR  | CE1-CZ | 5.08  | 1.50        | 1.38     |
| 1   | A     | 44  | VAL  | CA-C   | -5.07 | 1.46        | 1.52     |
| 1   | A     | 96  | LEU  | CG-CD2 | 5.07  | 1.69        | 1.52     |
| 1   | A     | 122 | ILE  | CB-CG1 | 5.05  | 1.63        | 1.53     |
| 1   | A     | 261 | PHE  | CG-CD1 | 5.05  | 1.49        | 1.38     |
| 1   | A     | 166 | GLY  | N-CA   | -5.04 | 1.39        | 1.45     |
| 1   | A     | 22  | THR  | CA-CB  | 5.02  | 1.62        | 1.54     |
| 1   | A     | 3   | SER  | CA-C   | 5.01  | 1.58        | 1.52     |
| 1   | A     | 99  | ALA  | N-CA   | -5.00 | 1.39        | 1.46     |

All (482) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 76  | ASN  | OD1-CG-ND2 | -38.34 | 84.26       | 122.60   |
| 1   | A     | 232 | ALA  | O-C-N      | 24.67  | 152.05      | 122.20   |
| 1   | A     | 79  | ILE  | N-CA-CB    | 17.23  | 139.66      | 111.23   |
| 1   | A     | 26  | VAL  | CA-C-N     | -16.80 | 99.30       | 122.99   |
| 1   | A     | 26  | VAL  | C-N-CA     | -16.80 | 99.30       | 122.99   |
| 1   | A     | 246 | VAL  | N-CA-C     | 15.66  | 130.62      | 111.05   |
| 1   | A     | 234 | ILE  | N-CA-C     | -15.62 | 95.74       | 110.42   |
| 1   | A     | 224 | SER  | CA-C-O     | 14.65  | 140.24      | 120.16   |
| 1   | A     | 247 | ARG  | N-CA-C     | -14.39 | 92.67       | 111.24   |
| 1   | A     | 62  | ASN  | OD1-CG-ND2 | 14.24  | 136.84      | 122.60   |
| 1   | A     | 139 | VAL  | O-C-N      | -14.20 | 107.98      | 121.89   |
| 1   | A     | 177 | VAL  | CA-C-N     | 14.18  | 136.73      | 120.71   |
| 1   | A     | 177 | VAL  | C-N-CA     | 14.18  | 136.73      | 120.71   |
| 1   | A     | 63  | SER  | N-CA-CB    | -13.99 | 98.22       | 114.17   |
| 1   | A     | 182 | SER  | CA-C-O     | -13.24 | 97.72       | 118.91   |
| 1   | A     | 167 | TYR  | CA-C-O     | -13.12 | 107.98      | 120.19   |
| 1   | A     | 213 | LYS  | CB-CA-C    | -13.08 | 80.81       | 111.95   |
| 1   | A     | 158 | SER  | N-CA-CB    | -13.02 | 89.55       | 110.51   |
| 1   | A     | 96  | LEU  | O-C-N      | 12.99  | 138.39      | 123.19   |
| 1   | A     | 38  | SER  | N-CA-C     | -12.84 | 97.13       | 112.92   |
| 1   | A     | 181 | ASP  | O-C-N      | 12.65  | 136.12      | 122.20   |
| 1   | A     | 203 | VAL  | CA-C-O     | 12.62  | 135.11      | 120.72   |
| 1   | A     | 63  | SER  | CB-CA-C    | 12.52  | 128.09      | 110.06   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 130 | SER  | CA-C-O     | 12.35  | 135.11      | 121.16   |
| 1   | A     | 188 | SER  | CB-CA-C    | -12.34 | 86.52       | 110.46   |
| 1   | A     | 210 | PRO  | CA-C-N     | 12.05  | 145.03      | 121.41   |
| 1   | A     | 210 | PRO  | C-N-CA     | 12.05  | 145.03      | 121.41   |
| 1   | A     | 19  | GLN  | N-CA-C     | -11.91 | 98.86       | 113.50   |
| 1   | A     | 186 | ARG  | NE-CZ-NH2  | 11.84  | 129.86      | 119.20   |
| 1   | A     | 199 | MET  | O-C-N      | -11.84 | 108.24      | 123.16   |
| 1   | A     | 62  | ASN  | N-CA-C     | 11.84  | 126.83      | 112.38   |
| 1   | A     | 71  | THR  | N-CA-C     | -11.83 | 97.14       | 111.69   |
| 1   | A     | 10  | GLN  | CA-C-N     | -11.70 | 111.32      | 122.66   |
| 1   | A     | 10  | GLN  | C-N-CA     | -11.70 | 111.32      | 122.66   |
| 1   | A     | 36  | ASP  | CA-CB-CG   | -11.61 | 100.99      | 112.60   |
| 1   | A     | 215 | GLY  | O-C-N      | 11.59  | 136.88      | 123.66   |
| 1   | A     | 215 | GLY  | CA-C-O     | -11.59 | 109.16      | 121.56   |
| 1   | A     | 76  | ASN  | CB-CG-OD1  | 11.49  | 143.78      | 120.80   |
| 1   | A     | 141 | LYS  | O-C-N      | -11.47 | 108.32      | 122.20   |
| 1   | A     | 89  | ALA  | CB-CA-C    | 11.40  | 128.66      | 110.19   |
| 1   | A     | 139 | VAL  | CA-C-O     | 11.25  | 132.75      | 121.05   |
| 1   | A     | 92  | ALA  | CA-C-O     | 11.23  | 133.93      | 121.02   |
| 1   | A     | 224 | SER  | O-C-N      | -11.18 | 108.46      | 121.32   |
| 1   | A     | 197 | ASP  | CB-CA-C    | 11.14  | 129.24      | 110.86   |
| 1   | A     | 7   | GLY  | O-C-N      | 10.96  | 136.51      | 122.71   |
| 1   | A     | 210 | PRO  | N-CA-CB    | 10.94  | 112.51      | 103.32   |
| 1   | A     | 200 | ALA  | N-CA-C     | 10.87  | 118.00      | 108.22   |
| 1   | A     | 182 | SER  | N-CA-C     | -10.80 | 100.34      | 113.19   |
| 1   | A     | 57  | ASN  | OD1-CG-ND2 | -10.80 | 111.80      | 122.60   |
| 1   | A     | 74  | ALA  | N-CA-CB    | -10.75 | 93.59       | 109.83   |
| 1   | A     | 84  | VAL  | CA-C-O     | -10.74 | 107.81      | 119.20   |
| 1   | A     | 208 | THR  | N-CA-CB    | 10.74  | 125.76      | 109.97   |
| 1   | A     | 183 | SER  | N-CA-CB    | 10.68  | 128.01      | 110.92   |
| 1   | A     | 75  | LEU  | CB-CA-C    | -10.67 | 89.18       | 110.42   |
| 1   | A     | 64  | HIS  | CB-CG-CD2  | -10.66 | 117.34      | 131.20   |
| 1   | A     | 161 | SER  | N-CA-CB    | -10.65 | 96.92       | 110.98   |
| 1   | A     | 32  | ASP  | CA-CB-CG   | 10.45  | 123.05      | 112.60   |
| 1   | A     | 4   | VAL  | CA-C-N     | 10.36  | 131.02      | 119.83   |
| 1   | A     | 4   | VAL  | C-N-CA     | 10.36  | 131.02      | 119.83   |
| 1   | A     | 174 | VAL  | N-CA-C     | 10.28  | 125.13      | 109.20   |
| 1   | A     | 164 | THR  | N-CA-CB    | -10.23 | 94.54       | 110.92   |
| 1   | A     | 133 | ALA  | CA-C-O     | 10.10  | 131.71      | 120.90   |
| 1   | A     | 78  | SER  | CA-C-O     | -10.09 | 106.08      | 120.51   |
| 1   | A     | 194 | PRO  | O-C-N      | 10.07  | 135.21      | 122.22   |
| 1   | A     | 84  | VAL  | CB-CA-C    | -10.05 | 92.75       | 110.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 133 | ALA  | O-C-N       | -9.99 | 111.70      | 122.09   |
| 1   | A     | 94  | LYS  | O-C-N       | -9.98 | 111.66      | 123.13   |
| 1   | A     | 181 | ASP  | CA-C-O      | -9.94 | 109.86      | 120.89   |
| 1   | A     | 64  | HIS  | CA-CB-CG    | 9.86  | 123.66      | 113.80   |
| 1   | A     | 88  | SER  | CA-C-O      | 9.79  | 134.51      | 120.51   |
| 1   | A     | 11  | ILE  | N-CA-C      | -9.61 | 104.11      | 111.90   |
| 1   | A     | 111 | ILE  | CA-CB-CG2   | -9.61 | 94.16       | 110.50   |
| 1   | A     | 7   | GLY  | CA-C-O      | -9.60 | 108.12      | 119.45   |
| 1   | A     | 82  | LEU  | CB-CA-C     | -9.60 | 98.66       | 110.94   |
| 1   | A     | 34  | GLY  | CA-C-O      | 9.56  | 132.46      | 121.47   |
| 1   | A     | 200 | ALA  | CA-C-N      | 9.45  | 131.65      | 119.84   |
| 1   | A     | 200 | ALA  | C-N-CA      | 9.45  | 131.65      | 119.84   |
| 1   | A     | 226 | HIS  | CA-C-N      | 9.43  | 132.76      | 120.60   |
| 1   | A     | 226 | HIS  | C-N-CA      | 9.43  | 132.76      | 120.60   |
| 1   | A     | 243 | ASN  | N-CA-C      | -9.42 | 100.89      | 111.82   |
| 1   | A     | 116 | ALA  | CA-C-N      | -9.36 | 107.53      | 122.79   |
| 1   | A     | 116 | ALA  | C-N-CA      | -9.36 | 107.53      | 122.79   |
| 1   | A     | 163 | SER  | N-CA-CB     | -9.36 | 94.54       | 110.83   |
| 1   | A     | 156 | GLU  | CA-C-O      | -9.35 | 110.94      | 119.91   |
| 1   | A     | 92  | ALA  | O-C-N       | -9.34 | 109.77      | 122.48   |
| 1   | A     | 50  | MET  | N-CA-C      | 9.29  | 123.31      | 112.72   |
| 1   | A     | 28  | VAL  | CB-CA-C     | 9.27  | 123.45      | 110.84   |
| 1   | A     | 81  | VAL  | N-CA-C      | 9.18  | 128.44      | 109.34   |
| 1   | A     | 151 | ALA  | O-C-N       | 9.12  | 134.45      | 122.96   |
| 1   | A     | 122 | ILE  | N-CA-CB     | 9.08  | 123.95      | 111.41   |
| 1   | A     | 102 | GLY  | CA-C-O      | -9.05 | 104.81      | 120.57   |
| 1   | A     | 137 | ALA  | O-C-N       | 8.99  | 134.55      | 122.59   |
| 1   | A     | 89  | ALA  | N-CA-C      | -8.95 | 94.14       | 108.73   |
| 1   | A     | 139 | VAL  | CB-CA-C     | -8.85 | 100.45      | 112.04   |
| 1   | A     | 164 | THR  | CA-C-O      | -8.84 | 109.51      | 119.95   |
| 1   | A     | 259 | ASP  | CA-C-N      | 8.84  | 138.43      | 121.54   |
| 1   | A     | 259 | ASP  | C-N-CA      | 8.84  | 138.43      | 121.54   |
| 1   | A     | 113 | TRP  | CE3-CZ3-CH2 | 8.73  | 132.45      | 121.10   |
| 1   | A     | 163 | SER  | CA-C-N      | -8.68 | 108.86      | 122.67   |
| 1   | A     | 163 | SER  | C-N-CA      | -8.68 | 108.86      | 122.67   |
| 1   | A     | 90  | LEU  | N-CA-CB     | -8.65 | 97.16       | 110.65   |
| 1   | A     | 163 | SER  | O-C-N       | 8.61  | 134.43      | 123.23   |
| 1   | A     | 10  | GLN  | N-CA-C      | 8.59  | 123.18      | 112.87   |
| 1   | A     | 254 | THR  | CA-C-N      | 8.58  | 133.88      | 122.30   |
| 1   | A     | 254 | THR  | C-N-CA      | 8.58  | 133.88      | 122.30   |
| 1   | A     | 65  | GLY  | N-CA-C      | -8.57 | 92.87       | 113.18   |
| 1   | A     | 157 | GLY  | CA-C-N      | -8.54 | 107.53      | 122.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 157 | GLY  | C-N-CA      | -8.54 | 107.53      | 122.64   |
| 1   | A     | 216 | ALA  | N-CA-C      | 8.53  | 123.37      | 109.72   |
| 1   | A     | 109 | ASN  | CB-CG-ND2   | 8.51  | 129.16      | 116.40   |
| 1   | A     | 125 | SER  | N-CA-CB     | 8.45  | 122.93      | 110.25   |
| 1   | A     | 10  | GLN  | O-C-N       | 8.44  | 133.66      | 122.43   |
| 1   | A     | 123 | ASN  | CB-CG-ND2   | -8.40 | 103.80      | 116.40   |
| 1   | A     | 98  | ASP  | CA-C-O      | 8.37  | 130.48      | 121.44   |
| 1   | A     | 135 | LEU  | O-C-N       | 8.32  | 132.27      | 122.20   |
| 1   | A     | 96  | LEU  | CA-C-N      | -8.28 | 111.36      | 120.71   |
| 1   | A     | 96  | LEU  | C-N-CA      | -8.28 | 111.36      | 120.71   |
| 1   | A     | 60  | ASP  | CA-C-O      | 8.28  | 129.09      | 120.40   |
| 1   | A     | 106 | TRP  | CD2-CE2-CZ2 | 8.24  | 130.64      | 122.40   |
| 1   | A     | 141 | LYS  | CB-CG-CD    | -8.12 | 92.63       | 111.30   |
| 1   | A     | 222 | MET  | N-CA-C      | -8.11 | 103.52      | 113.41   |
| 1   | A     | 232 | ALA  | N-CA-C      | 8.05  | 124.58      | 111.37   |
| 1   | A     | 193 | GLY  | CA-C-O      | 8.03  | 133.01      | 121.52   |
| 1   | A     | 3   | SER  | N-CA-C      | 8.00  | 122.28      | 108.76   |
| 1   | A     | 252 | ASN  | N-CA-C      | 7.96  | 127.76      | 110.80   |
| 1   | A     | 85  | ALA  | CB-CA-C     | 7.95  | 121.54      | 110.96   |
| 1   | A     | 70  | GLY  | CA-C-N      | -7.93 | 107.02      | 120.58   |
| 1   | A     | 70  | GLY  | C-N-CA      | -7.93 | 107.02      | 120.58   |
| 1   | A     | 88  | SER  | O-C-N       | -7.91 | 112.07      | 122.59   |
| 1   | A     | 221 | SER  | CA-C-O      | -7.90 | 110.27      | 119.59   |
| 1   | A     | 159 | THR  | N-CA-C      | -7.88 | 94.01       | 110.80   |
| 1   | A     | 216 | ALA  | N-CA-CB     | -7.87 | 97.62       | 111.08   |
| 1   | A     | 252 | ASN  | OD1-CG-ND2  | -7.87 | 114.73      | 122.60   |
| 1   | A     | 153 | ALA  | N-CA-C      | -7.83 | 102.65      | 112.90   |
| 1   | A     | 177 | VAL  | CB-CA-C     | 7.79  | 122.34      | 110.96   |
| 1   | A     | 180 | VAL  | CA-C-O      | 7.78  | 129.92      | 121.67   |
| 1   | A     | 115 | ILE  | N-CA-C      | -7.76 | 102.77      | 110.30   |
| 1   | A     | 35  | ILE  | O-C-N       | 7.76  | 132.27      | 122.57   |
| 1   | A     | 90  | LEU  | CB-CA-C     | 7.76  | 123.04      | 110.16   |
| 1   | A     | 13  | ALA  | CA-C-O      | 7.75  | 125.49      | 117.98   |
| 1   | A     | 218 | ASN  | CB-CA-C     | 7.74  | 122.88      | 110.19   |
| 1   | A     | 105 | SER  | N-CA-C      | -7.73 | 103.31      | 112.89   |
| 1   | A     | 118 | ASN  | OD1-CG-ND2  | 7.70  | 130.30      | 122.60   |
| 1   | A     | 124 | MET  | CA-C-O      | -7.67 | 108.04      | 120.85   |
| 1   | A     | 215 | GLY  | CA-C-N      | -7.66 | 110.78      | 122.81   |
| 1   | A     | 215 | GLY  | C-N-CA      | -7.66 | 110.78      | 122.81   |
| 1   | A     | 120 | ASP  | CA-CB-CG    | -7.64 | 104.96      | 112.60   |
| 1   | A     | 183 | SER  | N-CA-C      | -7.62 | 103.29      | 112.59   |
| 1   | A     | 67  | HIS  | CG-CD2-NE2  | 7.62  | 114.82      | 107.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 77  | ASN  | O-C-N       | 7.62  | 132.72      | 122.59   |
| 1   | A     | 170 | LYS  | N-CA-CB     | -7.62 | 97.37       | 110.32   |
| 1   | A     | 232 | ALA  | CA-C-O      | -7.61 | 112.11      | 121.02   |
| 1   | A     | 111 | ILE  | N-CA-C      | -7.60 | 102.33      | 110.23   |
| 1   | A     | 106 | TRP  | NE1-CE2-CZ2 | -7.57 | 118.74      | 130.10   |
| 1   | A     | 273 | ALA  | N-CA-C      | 7.52  | 120.36      | 111.71   |
| 1   | A     | 190 | SER  | CA-C-O      | 7.51  | 129.03      | 120.54   |
| 1   | A     | 196 | LEU  | CA-C-O      | -7.51 | 112.11      | 120.60   |
| 1   | A     | 50  | MET  | N-CA-CB     | -7.47 | 99.57       | 110.70   |
| 1   | A     | 117 | ASN  | CB-CA-C     | 7.47  | 123.09      | 111.28   |
| 1   | A     | 58  | PHE  | CB-CA-C     | -7.47 | 98.53       | 111.23   |
| 1   | A     | 144 | ALA  | CA-C-O      | 7.45  | 128.64      | 120.82   |
| 1   | A     | 70  | GLY  | O-C-N       | 7.39  | 132.31      | 122.70   |
| 1   | A     | 109 | ASN  | CA-CB-CG    | -7.37 | 105.23      | 112.60   |
| 1   | A     | 261 | PHE  | CB-CG-CD1   | -7.34 | 108.22      | 120.70   |
| 1   | A     | 147 | VAL  | CA-CB-CG1   | -7.32 | 97.95       | 110.40   |
| 1   | A     | 48  | ALA  | CA-C-N      | -7.28 | 112.37      | 122.93   |
| 1   | A     | 48  | ALA  | C-N-CA      | -7.28 | 112.37      | 122.93   |
| 1   | A     | 226 | HIS  | CA-C-O      | -7.28 | 113.06      | 121.07   |
| 1   | A     | 11  | ILE  | CA-CB-CG2   | -7.28 | 98.13       | 110.50   |
| 1   | A     | 155 | ASN  | OD1-CG-ND2  | -7.24 | 115.36      | 122.60   |
| 1   | A     | 181 | ASP  | CA-C-N      | -7.23 | 104.61      | 121.52   |
| 1   | A     | 181 | ASP  | C-N-CA      | -7.23 | 104.61      | 121.52   |
| 1   | A     | 132 | SER  | CA-C-O      | 7.22  | 130.84      | 120.51   |
| 1   | A     | 156 | GLU  | CB-CG-CD    | 7.19  | 124.82      | 112.60   |
| 1   | A     | 57  | ASN  | N-CA-CB     | -7.18 | 99.46       | 110.44   |
| 1   | A     | 73  | ALA  | N-CA-C      | 7.18  | 126.09      | 110.80   |
| 1   | A     | 194 | PRO  | CA-C-N      | 7.17  | 135.35      | 122.38   |
| 1   | A     | 194 | PRO  | C-N-CA      | 7.17  | 135.35      | 122.38   |
| 1   | A     | 162 | SER  | N-CA-C      | -7.16 | 95.55       | 110.80   |
| 1   | A     | 179 | ALA  | O-C-N       | 7.16  | 131.36      | 123.27   |
| 1   | A     | 75  | LEU  | CA-C-N      | 7.14  | 135.17      | 121.54   |
| 1   | A     | 75  | LEU  | C-N-CA      | 7.14  | 135.17      | 121.54   |
| 1   | A     | 201 | PRO  | N-CA-CB     | 7.13  | 110.74      | 103.25   |
| 1   | A     | 145 | SER  | N-CA-C      | -7.12 | 103.52      | 111.28   |
| 1   | A     | 218 | ASN  | CB-CG-ND2   | 7.09  | 127.04      | 116.40   |
| 1   | A     | 64  | HIS  | ND1-CG-CD2  | 7.09  | 113.19      | 106.10   |
| 1   | A     | 261 | PHE  | N-CA-C      | 7.09  | 121.68      | 112.89   |
| 1   | A     | 172 | PRO  | CB-CA-C     | -7.08 | 99.88       | 111.56   |
| 1   | A     | 196 | LEU  | O-C-N       | 7.08  | 132.02      | 122.82   |
| 1   | A     | 148 | VAL  | N-CA-CB     | -7.07 | 102.58      | 111.41   |
| 1   | A     | 82  | LEU  | O-C-N       | 7.06  | 131.83      | 123.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 246 | VAL  | CB-CA-C     | -7.04 | 101.25      | 112.16   |
| 1   | A     | 185 | GLN  | CB-CA-C     | 7.02  | 121.40      | 109.53   |
| 1   | A     | 203 | VAL  | O-C-N       | -7.01 | 115.99      | 123.14   |
| 1   | A     | 84  | VAL  | CA-CB-CG1   | -6.98 | 98.54       | 110.40   |
| 1   | A     | 71  | THR  | CA-C-N      | 6.97  | 129.90      | 120.77   |
| 1   | A     | 71  | THR  | C-N-CA      | 6.97  | 129.90      | 120.77   |
| 1   | A     | 186 | ARG  | CD-NE-CZ    | 6.96  | 134.14      | 124.40   |
| 1   | A     | 195 | GLU  | CB-CG-CD    | -6.96 | 100.78      | 112.60   |
| 1   | A     | 189 | PHE  | O-C-N       | -6.95 | 113.43      | 122.39   |
| 1   | A     | 205 | ILE  | N-CA-C      | -6.93 | 97.18       | 107.51   |
| 1   | A     | 200 | ALA  | N-CA-CB     | -6.92 | 103.83      | 111.10   |
| 1   | A     | 9   | SER  | O-C-N       | 6.88  | 129.99      | 122.15   |
| 1   | A     | 46  | GLY  | O-C-N       | -6.87 | 118.10      | 123.80   |
| 1   | A     | 106 | TRP  | CA-C-N      | 6.84  | 129.25      | 120.70   |
| 1   | A     | 106 | TRP  | C-N-CA      | 6.84  | 129.25      | 120.70   |
| 1   | A     | 232 | ALA  | N-CA-CB     | -6.84 | 98.10       | 109.72   |
| 1   | A     | 231 | ALA  | N-CA-C      | 6.83  | 119.31      | 111.11   |
| 1   | A     | 89  | ALA  | O-C-N       | -6.83 | 115.43      | 123.22   |
| 1   | A     | 165 | VAL  | N-CA-CB     | -6.83 | 100.91      | 110.26   |
| 1   | A     | 106 | TRP  | CB-CG-CD1   | -6.82 | 116.67      | 126.90   |
| 1   | A     | 213 | LYS  | CA-CB-CG    | -6.81 | 100.47      | 114.10   |
| 1   | A     | 23  | GLY  | CA-C-O      | 6.80  | 127.84      | 119.88   |
| 1   | A     | 35  | ILE  | CA-C-N      | -6.78 | 111.81      | 121.50   |
| 1   | A     | 35  | ILE  | C-N-CA      | -6.78 | 111.81      | 121.50   |
| 1   | A     | 221 | SER  | O-C-N       | 6.78  | 130.32      | 122.25   |
| 1   | A     | 164 | THR  | CB-CA-C     | 6.77  | 121.92      | 111.02   |
| 1   | A     | 222 | MET  | O-C-N       | 6.77  | 131.97      | 122.36   |
| 1   | A     | 177 | VAL  | N-CA-CB     | -6.76 | 102.94      | 111.46   |
| 1   | A     | 245 | GLN  | OE1-CD-NE2  | -6.75 | 115.85      | 122.60   |
| 1   | A     | 10  | GLN  | CG-CD-NE2   | -6.74 | 106.29      | 116.40   |
| 1   | A     | 10  | GLN  | OE1-CD-NE2  | 6.74  | 129.34      | 122.60   |
| 1   | A     | 266 | GLY  | O-C-N       | -6.73 | 118.71      | 123.08   |
| 1   | A     | 31  | ILE  | O-C-N       | 6.70  | 129.80      | 122.36   |
| 1   | A     | 234 | ILE  | CA-C-O      | 6.69  | 128.94      | 121.18   |
| 1   | A     | 39  | HIS  | CA-CB-CG    | -6.68 | 107.12      | 113.80   |
| 1   | A     | 28  | VAL  | O-C-N       | -6.63 | 115.67      | 123.03   |
| 1   | A     | 222 | MET  | CA-C-O      | -6.63 | 111.92      | 119.41   |
| 1   | A     | 174 | VAL  | O-C-N       | -6.61 | 115.89      | 122.76   |
| 1   | A     | 113 | TRP  | CD2-CE2-CZ2 | 6.60  | 129.00      | 122.40   |
| 1   | A     | 91  | TYR  | CA-CB-CG    | -6.59 | 102.03      | 113.90   |
| 1   | A     | 197 | ASP  | N-CA-CB     | -6.59 | 100.38      | 110.07   |
| 1   | A     | 85  | ALA  | O-C-N       | 6.58  | 127.83      | 121.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 220 | THR  | CA-C-N      | -6.55 | 112.38      | 122.60   |
| 1   | A     | 220 | THR  | C-N-CA      | -6.55 | 112.38      | 122.60   |
| 1   | A     | 57  | ASN  | N-CA-C      | -6.53 | 105.06      | 113.16   |
| 1   | A     | 162 | SER  | CA-C-N      | -6.52 | 113.16      | 122.94   |
| 1   | A     | 162 | SER  | C-N-CA      | -6.52 | 113.16      | 122.94   |
| 1   | A     | 19  | GLN  | CA-C-O      | 6.50  | 126.29      | 119.14   |
| 1   | A     | 245 | GLN  | N-CA-C      | -6.48 | 103.33      | 111.11   |
| 1   | A     | 105 | SER  | CA-C-O      | -6.47 | 111.29      | 119.31   |
| 1   | A     | 255 | THR  | O-C-N       | -6.44 | 115.72      | 123.13   |
| 1   | A     | 58  | PHE  | N-CA-CB     | -6.42 | 101.88      | 111.25   |
| 1   | A     | 263 | TYR  | O-C-N       | 6.42  | 129.40      | 122.34   |
| 1   | A     | 106 | TRP  | N-CA-CB     | 6.41  | 119.74      | 110.20   |
| 1   | A     | 193 | GLY  | O-C-N       | -6.41 | 115.36      | 121.77   |
| 1   | A     | 185 | GLN  | CA-C-N      | -6.40 | 112.35      | 121.50   |
| 1   | A     | 185 | GLN  | C-N-CA      | -6.40 | 112.35      | 121.50   |
| 1   | A     | 117 | ASN  | OD1-CG-ND2  | -6.39 | 116.21      | 122.60   |
| 1   | A     | 195 | GLU  | CG-CD-OE1   | 6.38  | 133.08      | 118.40   |
| 1   | A     | 220 | THR  | N-CA-CB     | 6.37  | 121.91      | 110.32   |
| 1   | A     | 257 | LEU  | N-CA-CB     | 6.35  | 119.61      | 110.40   |
| 1   | A     | 164 | THR  | CA-CB-CG2   | -6.35 | 99.71       | 110.50   |
| 1   | A     | 123 | ASN  | CA-CB-CG    | -6.34 | 106.26      | 112.60   |
| 1   | A     | 124 | MET  | CB-CA-C     | -6.34 | 100.99      | 111.51   |
| 1   | A     | 27  | LYS  | CA-CB-CG    | -6.33 | 101.44      | 114.10   |
| 1   | A     | 148 | VAL  | CA-CB-CG2   | 6.33  | 121.16      | 110.40   |
| 1   | A     | 227 | VAL  | CA-C-N      | 6.32  | 129.61      | 120.38   |
| 1   | A     | 227 | VAL  | C-N-CA      | 6.32  | 129.61      | 120.38   |
| 1   | A     | 85  | ALA  | N-CA-C      | -6.32 | 98.78       | 110.02   |
| 1   | A     | 115 | ILE  | CB-CA-C     | 6.30  | 119.68      | 111.81   |
| 1   | A     | 119 | MET  | CB-CA-C     | 6.30  | 121.05      | 109.46   |
| 1   | A     | 28  | VAL  | CA-C-O      | -6.29 | 113.84      | 120.57   |
| 1   | A     | 172 | PRO  | CA-C-N      | -6.28 | 112.60      | 122.65   |
| 1   | A     | 172 | PRO  | C-N-CA      | -6.28 | 112.60      | 122.65   |
| 1   | A     | 199 | MET  | CA-C-N      | 6.27  | 132.29      | 122.26   |
| 1   | A     | 199 | MET  | C-N-CA      | 6.27  | 132.29      | 122.26   |
| 1   | A     | 109 | ASN  | OD1-CG-ND2  | -6.27 | 116.33      | 122.60   |
| 1   | A     | 78  | SER  | O-C-N       | 6.23  | 130.87      | 122.59   |
| 1   | A     | 72  | VAL  | N-CA-CB     | 6.22  | 117.16      | 110.62   |
| 1   | A     | 50  | MET  | O-C-N       | 6.21  | 129.99      | 122.35   |
| 1   | A     | 106 | TRP  | CH2-CZ2-CE2 | -6.20 | 109.44      | 117.50   |
| 1   | A     | 253 | THR  | O-C-N       | 6.20  | 128.85      | 122.09   |
| 1   | A     | 35  | ILE  | N-CA-CB     | 6.18  | 121.43      | 111.23   |
| 1   | A     | 123 | ASN  | CA-C-O      | 6.17  | 126.78      | 120.24   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 119 | MET  | O-C-N      | -6.17 | 115.99      | 122.96   |
| 1   | A     | 263 | TYR  | CG-CD1-CE1 | -6.15 | 111.97      | 121.20   |
| 1   | A     | 61  | ASP  | CB-CA-C    | 6.15  | 121.81      | 110.56   |
| 1   | A     | 227 | VAL  | CA-C-O     | -6.15 | 114.88      | 121.27   |
| 1   | A     | 82  | LEU  | N-CA-CB    | 6.14  | 119.34      | 110.37   |
| 1   | A     | 185 | GLN  | N-CA-C     | -6.14 | 100.50      | 110.20   |
| 1   | A     | 62  | ASN  | CB-CG-OD1  | -6.12 | 108.56      | 120.80   |
| 1   | A     | 163 | SER  | CB-CA-C    | 6.12  | 121.06      | 109.37   |
| 1   | A     | 217 | TYR  | CA-CB-CG   | -6.12 | 102.89      | 113.90   |
| 1   | A     | 180 | VAL  | CB-CA-C    | -6.11 | 102.81      | 111.19   |
| 1   | A     | 104 | TYR  | CE1-CZ-CE2 | -6.10 | 108.09      | 120.30   |
| 1   | A     | 230 | ALA  | CA-C-N     | 6.10  | 128.77      | 120.54   |
| 1   | A     | 230 | ALA  | C-N-CA     | 6.10  | 128.77      | 120.54   |
| 1   | A     | 120 | ASP  | N-CA-C     | -6.10 | 106.38      | 113.88   |
| 1   | A     | 178 | GLY  | CA-C-O     | -6.09 | 116.03      | 121.64   |
| 1   | A     | 192 | VAL  | O-C-N      | 6.08  | 129.80      | 123.05   |
| 1   | A     | 229 | GLY  | CA-C-N     | -6.08 | 111.71      | 120.82   |
| 1   | A     | 229 | GLY  | C-N-CA     | -6.08 | 111.71      | 120.82   |
| 1   | A     | 151 | ALA  | CA-C-N     | -6.06 | 112.75      | 121.42   |
| 1   | A     | 151 | ALA  | C-N-CA     | -6.06 | 112.75      | 121.42   |
| 1   | A     | 66  | THR  | CA-CB-CG2  | -6.05 | 100.21      | 110.50   |
| 1   | A     | 171 | TYR  | CA-C-N     | 6.05  | 127.41      | 119.84   |
| 1   | A     | 171 | TYR  | C-N-CA     | 6.05  | 127.41      | 119.84   |
| 1   | A     | 217 | TYR  | CA-C-O     | 6.03  | 128.05      | 121.06   |
| 1   | A     | 79  | ILE  | N-CA-C     | -6.01 | 96.83       | 109.34   |
| 1   | A     | 22  | THR  | CA-C-O     | 6.01  | 125.82      | 119.03   |
| 1   | A     | 260 | SER  | CB-CA-C    | -6.01 | 98.47       | 110.42   |
| 1   | A     | 114 | ALA  | CA-C-N     | 6.00  | 128.20      | 120.70   |
| 1   | A     | 114 | ALA  | C-N-CA     | 6.00  | 128.20      | 120.70   |
| 1   | A     | 5   | PRO  | N-CD-CG    | 5.96  | 112.14      | 103.20   |
| 1   | A     | 239 | PRO  | N-CA-C     | 5.96  | 124.75      | 112.47   |
| 1   | A     | 39  | HIS  | CB-CG-CD2  | -5.96 | 123.46      | 131.20   |
| 1   | A     | 163 | SER  | CA-C-O     | 5.95  | 127.13      | 120.70   |
| 1   | A     | 26  | VAL  | O-C-N      | 5.94  | 129.22      | 122.93   |
| 1   | A     | 131 | GLY  | N-CA-C     | 5.93  | 120.08      | 112.13   |
| 1   | A     | 38  | SER  | CA-C-O     | -5.91 | 112.64      | 119.56   |
| 1   | A     | 192 | VAL  | N-CA-C     | -5.91 | 99.70       | 108.45   |
| 1   | A     | 64  | HIS  | CA-C-N     | 5.89  | 132.96      | 121.41   |
| 1   | A     | 64  | HIS  | C-N-CA     | 5.89  | 132.96      | 121.41   |
| 1   | A     | 147 | VAL  | CA-C-O     | -5.89 | 114.00      | 121.48   |
| 1   | A     | 212 | ASN  | CB-CA-C    | -5.87 | 103.14      | 111.95   |
| 1   | A     | 82  | LEU  | CA-C-N     | -5.86 | 112.69      | 121.01   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 82  | LEU  | C-N-CA      | -5.86 | 112.69      | 121.01   |
| 1   | A     | 169 | GLY  | CA-C-N      | 5.86  | 129.97      | 120.60   |
| 1   | A     | 169 | GLY  | C-N-CA      | 5.86  | 129.97      | 120.60   |
| 1   | A     | 64  | HIS  | N-CA-CB     | -5.85 | 101.29      | 110.30   |
| 1   | A     | 68  | VAL  | CA-CB-CG1   | -5.85 | 100.46      | 110.40   |
| 1   | A     | 203 | VAL  | CA-C-N      | 5.83  | 131.10      | 122.82   |
| 1   | A     | 203 | VAL  | C-N-CA      | 5.83  | 131.10      | 122.82   |
| 1   | A     | 109 | ASN  | CA-C-O      | -5.83 | 112.43      | 119.49   |
| 1   | A     | 227 | VAL  | CA-CB-CG2   | -5.83 | 100.49      | 110.40   |
| 1   | A     | 214 | TYR  | CE1-CZ-CE2  | -5.82 | 108.66      | 120.30   |
| 1   | A     | 4   | VAL  | O-C-N       | 5.81  | 127.73      | 121.10   |
| 1   | A     | 11  | ILE  | CA-C-O      | 5.81  | 125.77      | 120.30   |
| 1   | A     | 16  | LEU  | CA-C-O      | 5.81  | 126.66      | 119.97   |
| 1   | A     | 216 | ALA  | O-C-N       | -5.81 | 115.64      | 123.19   |
| 1   | A     | 229 | GLY  | O-C-N       | 5.81  | 130.25      | 122.70   |
| 1   | A     | 71  | THR  | O-C-N       | -5.80 | 114.69      | 122.23   |
| 1   | A     | 186 | ARG  | NH1-CZ-NH2  | -5.79 | 111.78      | 119.30   |
| 1   | A     | 181 | ASP  | CA-CB-CG    | 5.79  | 118.39      | 112.60   |
| 1   | A     | 36  | ASP  | N-CA-CB     | -5.78 | 100.99      | 109.95   |
| 1   | A     | 263 | TYR  | CD1-CE1-CZ  | 5.78  | 130.01      | 119.60   |
| 1   | A     | 54  | GLU  | CB-CA-C     | 5.77  | 121.22      | 111.41   |
| 1   | A     | 155 | ASN  | N-CA-CB     | -5.77 | 100.74      | 110.49   |
| 1   | A     | 193 | GLY  | CA-C-N      | 5.76  | 125.62      | 119.28   |
| 1   | A     | 193 | GLY  | C-N-CA      | 5.76  | 125.62      | 119.28   |
| 1   | A     | 267 | LEU  | O-C-N       | 5.75  | 130.08      | 123.29   |
| 1   | A     | 91  | TYR  | N-CA-CB     | 5.73  | 119.85      | 110.39   |
| 1   | A     | 234 | ILE  | CB-CA-C     | 5.72  | 119.24      | 111.87   |
| 1   | A     | 94  | LYS  | N-CA-C      | 5.70  | 118.03      | 108.96   |
| 1   | A     | 143 | VAL  | CA-C-O      | 5.70  | 126.47      | 119.58   |
| 1   | A     | 178 | GLY  | CA-C-N      | -5.70 | 114.86      | 122.72   |
| 1   | A     | 178 | GLY  | C-N-CA      | -5.70 | 114.86      | 122.72   |
| 1   | A     | 36  | ASP  | CB-CA-C     | 5.68  | 119.10      | 109.84   |
| 1   | A     | 136 | LYS  | CA-C-O      | -5.68 | 112.40      | 119.38   |
| 1   | A     | 119 | MET  | CA-C-N      | 5.67  | 132.12      | 122.36   |
| 1   | A     | 119 | MET  | C-N-CA      | 5.67  | 132.12      | 122.36   |
| 1   | A     | 178 | GLY  | O-C-N       | 5.67  | 128.75      | 122.96   |
| 1   | A     | 155 | ASN  | CA-CB-CG    | 5.66  | 118.26      | 112.60   |
| 1   | A     | 7   | GLY  | CA-C-N      | -5.66 | 112.38      | 120.42   |
| 1   | A     | 7   | GLY  | C-N-CA      | -5.66 | 112.38      | 120.42   |
| 1   | A     | 66  | THR  | N-CA-C      | -5.65 | 104.12      | 111.02   |
| 1   | A     | 214 | TYR  | N-CA-C      | -5.65 | 99.84       | 108.76   |
| 1   | A     | 39  | HIS  | CE1-NE2-CD2 | 5.64  | 114.64      | 109.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 251 | GLN  | CA-C-O      | 5.63  | 126.50      | 120.70   |
| 1   | A     | 95  | VAL  | N-CA-CB     | -5.63 | 101.94      | 111.23   |
| 1   | A     | 3   | SER  | CB-CA-C     | -5.61 | 99.54       | 109.70   |
| 1   | A     | 86  | PRO  | O-C-N       | 5.61  | 130.22      | 122.64   |
| 1   | A     | 127 | GLY  | N-CA-C      | -5.61 | 102.57      | 110.88   |
| 1   | A     | 176 | ALA  | N-CA-CB     | -5.61 | 100.91      | 110.16   |
| 1   | A     | 129 | PRO  | O-C-N       | 5.60  | 130.19      | 122.64   |
| 1   | A     | 37  | SER  | N-CA-CB     | -5.59 | 101.69      | 110.46   |
| 1   | A     | 137 | ALA  | CA-C-N      | -5.58 | 112.80      | 120.28   |
| 1   | A     | 137 | ALA  | C-N-CA      | -5.58 | 112.80      | 120.28   |
| 1   | A     | 189 | PHE  | CG-CD1-CE1  | -5.58 | 111.22      | 120.70   |
| 1   | A     | 55  | THR  | CA-CB-OG1   | 5.57  | 117.95      | 109.60   |
| 1   | A     | 7   | GLY  | N-CA-C      | -5.57 | 107.76      | 114.66   |
| 1   | A     | 90  | LEU  | CA-C-O      | 5.57  | 126.26      | 120.30   |
| 1   | A     | 81  | VAL  | N-CA-CB     | -5.56 | 102.05      | 111.23   |
| 1   | A     | 241 | TRP  | CE3-CZ3-CH2 | 5.56  | 128.32      | 121.10   |
| 1   | A     | 141 | LYS  | CA-C-O      | 5.55  | 127.52      | 121.02   |
| 1   | A     | 214 | TYR  | N-CA-CB     | -5.55 | 101.67      | 111.39   |
| 1   | A     | 36  | ASP  | N-CA-C      | -5.55 | 100.94      | 109.76   |
| 1   | A     | 88  | SER  | N-CA-CB     | -5.55 | 101.11      | 110.49   |
| 1   | A     | 106 | TRP  | N-CA-C      | -5.54 | 104.88      | 111.69   |
| 1   | A     | 151 | ALA  | N-CA-CB     | -5.53 | 102.66      | 111.62   |
| 1   | A     | 209 | LEU  | O-C-N       | 5.53  | 127.70      | 122.06   |
| 1   | A     | 240 | ASN  | CA-CB-CG    | -5.53 | 107.07      | 112.60   |
| 1   | A     | 64  | HIS  | CG-CD2-NE2  | -5.51 | 101.69      | 107.20   |
| 1   | A     | 25  | ASN  | CA-C-O      | 5.51  | 126.36      | 119.59   |
| 1   | A     | 117 | ASN  | CA-C-N      | -5.51 | 114.41      | 122.78   |
| 1   | A     | 117 | ASN  | C-N-CA      | -5.51 | 114.41      | 122.78   |
| 1   | A     | 154 | GLY  | CA-C-O      | 5.49  | 130.12      | 120.57   |
| 1   | A     | 117 | ASN  | O-C-N       | 5.49  | 129.56      | 122.20   |
| 1   | A     | 59  | GLN  | OE1-CD-NE2  | -5.49 | 117.11      | 122.60   |
| 1   | A     | 194 | PRO  | N-CA-CB     | 5.49  | 109.32      | 103.39   |
| 1   | A     | 241 | TRP  | N-CA-C      | 5.48  | 117.97      | 110.24   |
| 1   | A     | 55  | THR  | CA-C-O      | 5.48  | 127.66      | 120.16   |
| 1   | A     | 104 | TYR  | CZ-CE2-CD2  | 5.48  | 129.46      | 119.60   |
| 1   | A     | 227 | VAL  | CB-CA-C     | -5.47 | 104.87      | 111.88   |
| 1   | A     | 109 | ASN  | N-CA-CB     | 5.46  | 119.61      | 110.32   |
| 1   | A     | 195 | GLU  | N-CA-CB     | -5.46 | 102.08      | 110.44   |
| 1   | A     | 200 | ALA  | CA-C-O      | 5.46  | 125.45      | 120.26   |
| 1   | A     | 58  | PHE  | CB-CG-CD1   | 5.45  | 129.97      | 120.70   |
| 1   | A     | 67  | HIS  | ND1-CG-CD2  | -5.45 | 100.65      | 106.10   |
| 1   | A     | 184 | ASN  | OD1-CG-ND2  | 5.42  | 128.02      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 137 | ALA  | CA-C-O     | -5.40 | 112.78      | 120.51   |
| 1   | A     | 189 | PHE  | CZ-CE2-CD2 | -5.38 | 110.31      | 120.00   |
| 1   | A     | 255 | THR  | CB-CA-C    | 5.38  | 119.21      | 110.22   |
| 1   | A     | 165 | VAL  | CB-CA-C    | 5.38  | 118.98      | 111.34   |
| 1   | A     | 186 | ARG  | CA-C-O     | 5.38  | 126.82      | 120.69   |
| 1   | A     | 257 | LEU  | CA-C-O     | -5.38 | 113.48      | 119.67   |
| 1   | A     | 29  | ALA  | O-C-N      | 5.38  | 129.35      | 123.27   |
| 1   | A     | 171 | TYR  | CA-CB-CG   | 5.38  | 123.58      | 113.90   |
| 1   | A     | 220 | THR  | CA-CB-OG1  | 5.36  | 117.65      | 109.60   |
| 1   | A     | 240 | ASN  | CB-CG-OD1  | 5.36  | 131.53      | 120.80   |
| 1   | A     | 101 | SER  | CA-C-N     | 5.36  | 131.91      | 121.41   |
| 1   | A     | 101 | SER  | C-N-CA     | 5.36  | 131.91      | 121.41   |
| 1   | A     | 72  | VAL  | O-C-N      | 5.36  | 127.74      | 121.96   |
| 1   | A     | 76  | ASN  | CB-CG-ND2  | 5.36  | 124.43      | 116.40   |
| 1   | A     | 214 | TYR  | CE1-CZ-OH  | 5.34  | 135.91      | 119.90   |
| 1   | A     | 112 | GLU  | CB-CG-CD   | -5.32 | 103.55      | 112.60   |
| 1   | A     | 121 | VAL  | CA-CB-CG1  | 5.32  | 119.44      | 110.40   |
| 1   | A     | 1   | ALA  | CB-CA-C    | -5.32 | 102.52      | 110.50   |
| 1   | A     | 273 | ALA  | O-C-N      | 5.32  | 128.44      | 122.22   |
| 1   | A     | 189 | PHE  | N-CA-C     | 5.31  | 119.39      | 113.02   |
| 1   | A     | 29  | ALA  | N-CA-C     | -5.31 | 100.58      | 109.24   |
| 1   | A     | 159 | THR  | CA-C-N     | 5.30  | 131.79      | 121.41   |
| 1   | A     | 159 | THR  | C-N-CA     | 5.30  | 131.79      | 121.41   |
| 1   | A     | 133 | ALA  | CA-C-N     | 5.28  | 127.81      | 120.63   |
| 1   | A     | 133 | ALA  | C-N-CA     | 5.28  | 127.81      | 120.63   |
| 1   | A     | 269 | ASN  | CA-C-O     | -5.28 | 114.81      | 120.46   |
| 1   | A     | 31  | ILE  | N-CA-CB    | 5.28  | 117.18      | 112.06   |
| 1   | A     | 81  | VAL  | CA-C-O     | -5.27 | 114.19      | 120.78   |
| 1   | A     | 263 | TYR  | CA-C-O     | -5.27 | 112.92      | 118.77   |
| 1   | A     | 151 | ALA  | CA-C-O     | 5.27  | 127.41      | 121.51   |
| 1   | A     | 46  | GLY  | CA-C-O     | -5.27 | 116.88      | 121.04   |
| 1   | A     | 76  | ASN  | CB-CA-C    | 5.26  | 120.89      | 110.42   |
| 1   | A     | 84  | VAL  | O-C-N      | -5.25 | 116.95      | 122.20   |
| 1   | A     | 223 | ALA  | N-CA-CB    | -5.25 | 102.38      | 110.20   |
| 1   | A     | 93  | VAL  | N-CA-C     | 5.25  | 115.33      | 107.51   |
| 1   | A     | 112 | GLU  | N-CA-C     | 5.24  | 121.97      | 110.80   |
| 1   | A     | 25  | ASN  | CA-CB-CG   | -5.24 | 107.36      | 112.60   |
| 1   | A     | 207 | SER  | O-C-N      | 5.24  | 130.83      | 122.61   |
| 1   | A     | 175 | ILE  | CA-C-O     | -5.23 | 113.90      | 120.86   |
| 1   | A     | 28  | VAL  | CA-C-N     | 5.22  | 129.93      | 122.72   |
| 1   | A     | 28  | VAL  | C-N-CA     | 5.22  | 129.93      | 122.72   |
| 1   | A     | 132 | SER  | CA-C-N     | 5.22  | 127.59      | 120.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 132 | SER  | C-N-CA      | 5.22  | 127.59      | 120.54   |
| 1   | A     | 10  | GLN  | N-CA-CB     | -5.22 | 100.83      | 110.32   |
| 1   | A     | 190 | SER  | N-CA-C      | -5.21 | 100.81      | 109.46   |
| 1   | A     | 171 | TYR  | N-CA-CB     | 5.21  | 118.02      | 109.90   |
| 1   | A     | 80  | GLY  | N-CA-C      | 5.21  | 125.52      | 113.18   |
| 1   | A     | 40  | PRO  | CA-C-O      | -5.20 | 111.14      | 120.60   |
| 1   | A     | 228 | ALA  | O-C-N       | 5.20  | 128.13      | 122.20   |
| 1   | A     | 114 | ALA  | N-CA-C      | 5.19  | 117.01      | 111.36   |
| 1   | A     | 19  | GLN  | CB-CA-C     | 5.17  | 118.70      | 109.29   |
| 1   | A     | 104 | TYR  | CD1-CE1-CZ  | 5.17  | 128.91      | 119.60   |
| 1   | A     | 180 | VAL  | O-C-N       | -5.16 | 117.55      | 122.97   |
| 1   | A     | 259 | ASP  | O-C-N       | -5.15 | 115.74      | 122.59   |
| 1   | A     | 113 | TRP  | CD1-NE1-CE2 | -5.15 | 99.63       | 108.90   |
| 1   | A     | 106 | TRP  | CE2-CD2-CG  | 5.14  | 113.37      | 107.20   |
| 1   | A     | 40  | PRO  | O-C-N       | 5.13  | 129.56      | 122.64   |
| 1   | A     | 263 | TYR  | CD1-CG-CD2  | 5.12  | 125.78      | 118.10   |
| 1   | A     | 139 | VAL  | N-CA-C      | -5.11 | 104.80      | 110.62   |
| 1   | A     | 138 | ALA  | N-CA-C      | 5.10  | 116.84      | 111.28   |
| 1   | A     | 61  | ASP  | N-CA-C      | -5.10 | 104.70      | 112.04   |
| 1   | A     | 129 | PRO  | CA-C-O      | -5.10 | 111.33      | 120.60   |
| 1   | A     | 128 | GLY  | CA-C-O      | 5.09  | 128.81      | 121.52   |
| 1   | A     | 164 | THR  | CA-CB-OG1   | 5.09  | 117.24      | 109.60   |
| 1   | A     | 169 | GLY  | CA-C-O      | -5.09 | 115.51      | 120.75   |
| 1   | A     | 180 | VAL  | N-CA-CB     | -5.09 | 106.04      | 112.60   |
| 1   | A     | 170 | LYS  | CA-CB-CG    | -5.07 | 103.96      | 114.10   |
| 1   | A     | 156 | GLU  | N-CA-CB     | 5.07  | 115.19      | 108.96   |
| 1   | A     | 28  | VAL  | N-CA-CB     | -5.07 | 104.91      | 110.99   |
| 1   | A     | 134 | ALA  | N-CA-C      | -5.07 | 105.41      | 111.03   |
| 1   | A     | 152 | ALA  | CB-CA-C     | -5.06 | 100.98      | 109.53   |
| 1   | A     | 214 | TYR  | CD1-CE1-CZ  | 5.06  | 128.70      | 119.60   |
| 1   | A     | 149 | VAL  | CB-CA-C     | 5.05  | 117.90      | 110.98   |
| 1   | A     | 214 | TYR  | O-C-N       | 5.05  | 129.14      | 123.48   |
| 1   | A     | 253 | THR  | CA-CB-OG1   | -5.04 | 102.03      | 109.60   |
| 1   | A     | 106 | TRP  | CG-CD2-CE3  | -5.04 | 128.86      | 133.90   |
| 1   | A     | 82  | LEU  | N-CA-C      | 5.03  | 116.23      | 107.49   |
| 1   | A     | 2   | GLN  | N-CA-CB     | 5.02  | 119.56      | 110.83   |
| 1   | A     | 123 | ASN  | CB-CG-OD1   | 5.02  | 130.84      | 120.80   |
| 1   | A     | 62  | ASN  | CB-CG-ND2   | -5.00 | 108.89      | 116.40   |
| 1   | A     | 217 | TYR  | CD1-CE1-CZ  | -5.00 | 110.59      | 119.60   |

There are no chirality outliers.

All (19) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group               |
|-----|-------|-----|------|---------------------|
| 1   | A     | 10  | GLN  | Mainchain           |
| 1   | A     | 109 | ASN  | Mainchain           |
| 1   | A     | 136 | LYS  | Mainchain           |
| 1   | A     | 147 | VAL  | Mainchain           |
| 1   | A     | 157 | GLY  | Mainchain           |
| 1   | A     | 196 | LEU  | Mainchain           |
| 1   | A     | 247 | ARG  | Sidechain           |
| 1   | A     | 261 | PHE  | Sidechain           |
| 1   | A     | 266 | GLY  | Mainchain           |
| 1   | A     | 39  | HIS  | Sidechain           |
| 1   | A     | 44  | VAL  | Mainchain           |
| 1   | A     | 51  | VAL  | Mainchain           |
| 1   | A     | 56  | PRO  | Mainchain           |
| 1   | A     | 62  | ASN  | Sidechain,Mainchain |
| 1   | A     | 76  | ASN  | Sidechain           |
| 1   | A     | 78  | SER  | Mainchain           |
| 1   | A     | 80  | GLY  | Mainchain           |
| 1   | A     | 84  | VAL  | Mainchain           |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1938  | 0        | 1892     | 378     | 15           |
| 2   | A     | 17    | 0        | 0        | 2       | 0            |
| All | All   | 1955  | 0        | 1892     | 378     | 15           |

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 99.

All (378) 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:60:ASP:CB  | 1:A:60:ASP:CA  | 1.75                     | 1.58              |
| 1:A:201:PRO:C  | 1:A:201:PRO:CA | 1.75                     | 1.57              |
| 1:A:84:VAL:CA  | 1:A:84:VAL:CB  | 1.76                     | 1.54              |
| 1:A:112:GLU:CB | 1:A:112:GLU:CG | 1.78                     | 1.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ILE:CA   | 1:A:111:ILE:CB   | 1.84                     | 1.51              |
| 1:A:136:LYS:CE   | 1:A:136:LYS:CD   | 1.82                     | 1.51              |
| 1:A:96:LEU:C     | 1:A:96:LEU:CA    | 1.77                     | 1.50              |
| 1:A:76:ASN:ND2   | 1:A:76:ASN:CG    | 1.71                     | 1.47              |
| 1:A:168:PRO:N    | 1:A:168:PRO:CD   | 1.70                     | 1.39              |
| 1:A:41:ASP:OD1   | 1:A:75:LEU:HG    | 1.28                     | 1.34              |
| 1:A:22:THR:CB    | 1:A:87:SER:HG    | 1.42                     | 1.32              |
| 1:A:233:LEU:HA   | 1:A:236:SER:OG   | 1.34                     | 1.25              |
| 1:A:22:THR:CB    | 1:A:87:SER:OG    | 1.81                     | 1.23              |
| 1:A:41:ASP:CG    | 1:A:75:LEU:HG    | 1.64                     | 1.22              |
| 1:A:41:ASP:HB3   | 1:A:75:LEU:CD1   | 1.70                     | 1.22              |
| 1:A:104:TYR:HE1  | 2:A:281:HOH:O    | 1.28                     | 1.14              |
| 1:A:19:GLN:NE2   | 1:A:237:LYS:HZ2  | 1.48                     | 1.12              |
| 1:A:75:LEU:CD2   | 1:A:79:ILE:O     | 1.99                     | 1.11              |
| 1:A:75:LEU:HD12  | 1:A:75:LEU:N     | 1.65                     | 1.10              |
| 1:A:274:ALA:O    | 1:A:275:GLN:HB2  | 1.45                     | 1.10              |
| 1:A:41:ASP:HB3   | 1:A:75:LEU:HD12  | 1.14                     | 1.07              |
| 1:A:253:THR:HG23 | 1:A:272:ALA:HB3  | 1.33                     | 1.07              |
| 1:A:41:ASP:CG    | 1:A:75:LEU:CG    | 2.29                     | 1.04              |
| 1:A:41:ASP:CB    | 1:A:75:LEU:CD1   | 2.35                     | 1.03              |
| 1:A:57:ASN:ND2   | 1:A:92:ALA:O     | 1.92                     | 1.03              |
| 1:A:97:GLY:HA3   | 1:A:101:SER:CB   | 1.88                     | 1.02              |
| 1:A:253:THR:HG23 | 1:A:272:ALA:CB   | 1.89                     | 1.02              |
| 1:A:253:THR:CG2  | 1:A:272:ALA:HB3  | 1.90                     | 1.02              |
| 1:A:97:GLY:HA3   | 1:A:101:SER:HB2  | 1.40                     | 1.01              |
| 1:A:56:PRO:HB2   | 1:A:59:GLN:CG    | 1.92                     | 0.99              |
| 1:A:19:GLN:HG2   | 1:A:21:TYR:CE2   | 1.97                     | 0.99              |
| 1:A:84:VAL:C     | 1:A:86:PRO:HD3   | 1.89                     | 0.98              |
| 1:A:85:ALA:CB    | 1:A:233:LEU:HD11 | 1.94                     | 0.98              |
| 1:A:84:VAL:C     | 1:A:84:VAL:HG12  | 1.90                     | 0.97              |
| 1:A:41:ASP:CG    | 1:A:75:LEU:CD1   | 2.37                     | 0.96              |
| 1:A:19:GLN:HG2   | 1:A:21:TYR:HE2   | 1.27                     | 0.96              |
| 1:A:22:THR:HB    | 1:A:87:SER:OG    | 1.64                     | 0.96              |
| 1:A:84:VAL:C     | 1:A:84:VAL:CG1   | 2.39                     | 0.96              |
| 1:A:112:GLU:CB   | 1:A:112:GLU:CD   | 2.39                     | 0.95              |
| 1:A:84:VAL:CB    | 1:A:84:VAL:C     | 2.39                     | 0.94              |
| 1:A:75:LEU:HD21  | 1:A:79:ILE:O     | 1.65                     | 0.93              |
| 1:A:97:GLY:CA    | 1:A:101:SER:HB2  | 1.98                     | 0.93              |
| 1:A:33:SER:O     | 1:A:94:LYS:HE3   | 1.68                     | 0.93              |
| 1:A:242:THR:O    | 1:A:246:VAL:HG23 | 1.69                     | 0.92              |
| 1:A:204:SER:N    | 1:A:218:ASN:OD1  | 2.00                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:THR:HG21 | 1:A:273:ALA:N    | 1.84                     | 0.92              |
| 1:A:97:GLY:HA3   | 1:A:101:SER:OG   | 1.70                     | 0.91              |
| 1:A:135:LEU:O    | 1:A:139:VAL:HG23 | 1.71                     | 0.90              |
| 1:A:41:ASP:CG    | 1:A:75:LEU:HD11  | 1.97                     | 0.89              |
| 1:A:75:LEU:CD1   | 1:A:75:LEU:N     | 2.35                     | 0.89              |
| 1:A:233:LEU:HA   | 1:A:236:SER:HG   | 1.24                     | 0.89              |
| 1:A:19:GLN:HE21  | 1:A:237:LYS:HZ2  | 1.00                     | 0.88              |
| 1:A:274:ALA:O    | 1:A:275:GLN:CB   | 2.22                     | 0.88              |
| 1:A:11:ILE:O     | 1:A:12:LYS:HB2   | 1.71                     | 0.88              |
| 1:A:22:THR:OG1   | 1:A:87:SER:OG    | 1.62                     | 0.88              |
| 1:A:14:PRO:HA    | 1:A:17:HIS:HB2   | 1.57                     | 0.87              |
| 1:A:254:THR:HG22 | 1:A:268:ILE:HA   | 1.53                     | 0.87              |
| 1:A:19:GLN:NE2   | 1:A:237:LYS:NZ   | 2.22                     | 0.87              |
| 1:A:84:VAL:CA    | 1:A:84:VAL:CG1   | 2.53                     | 0.87              |
| 1:A:16:LEU:HD22  | 1:A:270:VAL:HG12 | 1.57                     | 0.87              |
| 1:A:104:TYR:CE1  | 2:A:281:HOH:O    | 2.12                     | 0.86              |
| 1:A:233:LEU:CA   | 1:A:236:SER:OG   | 2.21                     | 0.86              |
| 1:A:16:LEU:HD21  | 1:A:274:ALA:HB2  | 1.58                     | 0.86              |
| 1:A:254:THR:HB   | 1:A:267:LEU:O    | 1.75                     | 0.86              |
| 1:A:56:PRO:HB2   | 1:A:59:GLN:HG3   | 1.60                     | 0.84              |
| 1:A:111:ILE:CA   | 1:A:111:ILE:CG2  | 2.56                     | 0.84              |
| 1:A:41:ASP:CB    | 1:A:75:LEU:HD11  | 2.06                     | 0.84              |
| 1:A:238:HIS:HB3  | 1:A:241:TRP:CD1  | 2.12                     | 0.84              |
| 1:A:75:LEU:HD23  | 1:A:79:ILE:O     | 1.75                     | 0.83              |
| 1:A:222:MET:C    | 1:A:225:PRO:HD2  | 2.03                     | 0.83              |
| 1:A:56:PRO:HB2   | 1:A:59:GLN:HG2   | 1.60                     | 0.83              |
| 1:A:122:ILE:HD12 | 1:A:147:VAL:HG11 | 1.61                     | 0.83              |
| 1:A:167:TYR:C    | 1:A:168:PRO:CD   | 2.52                     | 0.82              |
| 1:A:33:SER:O     | 1:A:94:LYS:CE    | 2.28                     | 0.82              |
| 1:A:62:ASN:OD1   | 1:A:98:ASP:HA    | 1.80                     | 0.82              |
| 1:A:96:LEU:CA    | 1:A:97:GLY:N     | 2.42                     | 0.82              |
| 1:A:97:GLY:N     | 1:A:101:SER:HB2  | 1.94                     | 0.82              |
| 1:A:84:VAL:O     | 1:A:86:PRO:HD3   | 1.80                     | 0.81              |
| 1:A:242:THR:OG1  | 1:A:245:GLN:HB2  | 1.81                     | 0.81              |
| 1:A:142:ALA:O    | 1:A:147:VAL:HB   | 1.81                     | 0.81              |
| 1:A:209:LEU:HD12 | 1:A:214:TYR:C    | 2.07                     | 0.80              |
| 1:A:76:ASN:CG    | 1:A:76:ASN:CB    | 2.55                     | 0.80              |
| 1:A:22:THR:HG1   | 1:A:87:SER:CB    | 1.95                     | 0.79              |
| 1:A:255:THR:N    | 1:A:267:LEU:O    | 2.16                     | 0.79              |
| 1:A:34:GLY:O     | 1:A:35:ILE:CG1   | 2.30                     | 0.79              |
| 1:A:199:MET:HG2  | 1:A:263:TYR:O    | 1.83                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:122:ILE:CD1  | 1:A:147:VAL:HG11 | 2.11                     | 0.78              |
| 1:A:174:VAL:O    | 1:A:247:ARG:NH1  | 2.17                     | 0.78              |
| 1:A:60:ASP:CB    | 1:A:60:ASP:N     | 2.45                     | 0.78              |
| 1:A:199:MET:CG   | 1:A:263:TYR:O    | 2.32                     | 0.78              |
| 1:A:41:ASP:OD1   | 1:A:75:LEU:CG    | 2.22                     | 0.77              |
| 1:A:254:THR:CB   | 1:A:267:LEU:O    | 2.33                     | 0.76              |
| 1:A:56:PRO:CB    | 1:A:59:GLN:HG3   | 2.15                     | 0.76              |
| 1:A:253:THR:CG2  | 1:A:272:ALA:CB   | 2.58                     | 0.76              |
| 1:A:22:THR:C     | 1:A:87:SER:OG    | 2.30                     | 0.74              |
| 1:A:111:ILE:CA   | 1:A:111:ILE:CG1  | 2.66                     | 0.74              |
| 1:A:55:THR:HB    | 1:A:56:PRO:CD    | 2.18                     | 0.74              |
| 1:A:71:THR:HG21  | 1:A:226:HIS:CE1  | 2.23                     | 0.73              |
| 1:A:75:LEU:HD12  | 1:A:75:LEU:H     | 1.51                     | 0.73              |
| 1:A:84:VAL:CA    | 1:A:84:VAL:CG2   | 2.64                     | 0.73              |
| 1:A:97:GLY:H     | 1:A:101:SER:HB2  | 1.54                     | 0.73              |
| 1:A:68:VAL:O     | 1:A:70:GLY:N     | 2.22                     | 0.72              |
| 1:A:3:SER:O      | 1:A:5:PRO:HD3    | 1.89                     | 0.72              |
| 1:A:56:PRO:HG2   | 1:A:59:GLN:HG3   | 1.72                     | 0.72              |
| 1:A:85:ALA:HA    | 1:A:233:LEU:HD11 | 1.71                     | 0.71              |
| 1:A:136:LYS:CE   | 1:A:136:LYS:CG   | 2.69                     | 0.71              |
| 1:A:201:PRO:C    | 1:A:201:PRO:N    | 2.43                     | 0.71              |
| 1:A:56:PRO:CG    | 1:A:59:GLN:HG3   | 2.20                     | 0.71              |
| 1:A:40:PRO:HB2   | 1:A:79:ILE:HD11  | 1.73                     | 0.71              |
| 1:A:13:ALA:N     | 1:A:14:PRO:HD2   | 2.05                     | 0.71              |
| 1:A:201:PRO:CA   | 1:A:202:GLY:N    | 2.52                     | 0.70              |
| 1:A:85:ALA:HB2   | 1:A:233:LEU:HD11 | 1.74                     | 0.70              |
| 1:A:238:HIS:HE1  | 1:A:275:GLN:HB2  | 1.55                     | 0.70              |
| 1:A:153:ALA:HB1  | 1:A:165:VAL:HG22 | 1.72                     | 0.70              |
| 1:A:179:ALA:HA   | 1:A:200:ALA:O    | 1.92                     | 0.69              |
| 1:A:60:ASP:CB    | 1:A:60:ASP:C     | 2.63                     | 0.69              |
| 1:A:84:VAL:O     | 1:A:86:PRO:CD    | 2.41                     | 0.69              |
| 1:A:112:GLU:CG   | 1:A:112:GLU:CA   | 2.69                     | 0.69              |
| 1:A:11:ILE:O     | 1:A:12:LYS:CB    | 2.41                     | 0.69              |
| 1:A:56:PRO:CB    | 1:A:59:GLN:CG    | 2.70                     | 0.69              |
| 1:A:49:SER:O     | 1:A:50:MET:HE2   | 1.91                     | 0.68              |
| 1:A:254:THR:HG22 | 1:A:268:ILE:CA   | 2.23                     | 0.68              |
| 1:A:233:LEU:N    | 1:A:233:LEU:HD12 | 2.07                     | 0.68              |
| 1:A:34:GLY:O     | 1:A:35:ILE:HG13  | 1.94                     | 0.68              |
| 1:A:219:GLY:C    | 1:A:221:SER:N    | 2.50                     | 0.68              |
| 1:A:48:ALA:H     | 1:A:57:ASN:ND2   | 1.92                     | 0.68              |
| 1:A:258:GLY:O    | 1:A:263:TYR:HB2  | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:34:GLY:O     | 1:A:35:ILE:HG12  | 1.93                     | 0.67              |
| 1:A:55:THR:HG22  | 1:A:56:PRO:N     | 2.10                     | 0.67              |
| 1:A:85:ALA:HB1   | 1:A:233:LEU:HD11 | 1.74                     | 0.67              |
| 1:A:103:GLN:HB3  | 1:A:106:TRP:CD2  | 2.30                     | 0.67              |
| 1:A:253:THR:HG23 | 1:A:253:THR:O    | 1.95                     | 0.67              |
| 1:A:223:ALA:C    | 1:A:225:PRO:HD2  | 2.19                     | 0.66              |
| 1:A:110:GLY:O    | 1:A:111:ILE:C    | 2.36                     | 0.66              |
| 1:A:96:LEU:C     | 1:A:96:LEU:CB    | 2.66                     | 0.66              |
| 1:A:60:ASP:CA    | 1:A:60:ASP:CG    | 2.67                     | 0.66              |
| 1:A:55:THR:CB    | 1:A:56:PRO:CD    | 2.74                     | 0.66              |
| 1:A:74:ALA:C     | 1:A:75:LEU:HD12  | 2.20                     | 0.66              |
| 1:A:60:ASP:OD1   | 1:A:63:SER:N     | 2.20                     | 0.66              |
| 1:A:167:TYR:HD2  | 1:A:171:TYR:CZ   | 2.14                     | 0.66              |
| 1:A:75:LEU:HD21  | 1:A:79:ILE:C     | 2.21                     | 0.66              |
| 1:A:254:THR:CA   | 1:A:267:LEU:O    | 2.44                     | 0.66              |
| 1:A:85:ALA:N     | 1:A:86:PRO:CD    | 2.60                     | 0.65              |
| 1:A:237:LYS:C    | 1:A:239:PRO:HD3  | 2.22                     | 0.65              |
| 1:A:67:HIS:CD2   | 1:A:217:TYR:CD2  | 2.84                     | 0.65              |
| 1:A:73:ALA:HA    | 1:A:83:GLY:HA3   | 1.79                     | 0.65              |
| 1:A:177:VAL:HG21 | 1:A:227:VAL:HG11 | 1.79                     | 0.64              |
| 1:A:68:VAL:C     | 1:A:70:GLY:H     | 2.05                     | 0.64              |
| 1:A:219:GLY:C    | 1:A:221:SER:H    | 2.04                     | 0.64              |
| 1:A:84:VAL:C     | 1:A:86:PRO:CD    | 2.67                     | 0.64              |
| 1:A:253:THR:HG23 | 1:A:272:ALA:HB1  | 1.80                     | 0.63              |
| 1:A:33:SER:HB3   | 1:A:96:LEU:HB2   | 1.80                     | 0.63              |
| 1:A:13:ALA:N     | 1:A:14:PRO:CD    | 2.61                     | 0.63              |
| 1:A:22:THR:HG1   | 1:A:87:SER:HG    | 0.63                     | 0.63              |
| 1:A:6:TYR:OH     | 1:A:203:VAL:O    | 2.12                     | 0.63              |
| 1:A:22:THR:CA    | 1:A:87:SER:OG    | 2.46                     | 0.62              |
| 1:A:174:VAL:HG12 | 1:A:175:ILE:N    | 2.13                     | 0.62              |
| 1:A:49:SER:C     | 1:A:50:MET:HE2   | 2.24                     | 0.62              |
| 1:A:238:HIS:CG   | 1:A:241:TRP:CE2  | 2.87                     | 0.62              |
| 1:A:74:ALA:HB1   | 1:A:75:LEU:HD13  | 1.81                     | 0.61              |
| 1:A:16:LEU:HD22  | 1:A:76:ASN:OD1   | 2.01                     | 0.61              |
| 1:A:232:ALA:HB3  | 1:A:233:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:253:THR:CG2  | 1:A:253:THR:O    | 2.48                     | 0.61              |
| 1:A:84:VAL:CB    | 1:A:84:VAL:N     | 2.61                     | 0.61              |
| 1:A:85:ALA:CB    | 1:A:233:LEU:CD1  | 2.75                     | 0.61              |
| 1:A:112:GLU:OE1  | 1:A:115:ILE:HD12 | 2.01                     | 0.61              |
| 1:A:237:LYS:O    | 1:A:239:PRO:CD   | 2.49                     | 0.61              |
| 1:A:253:THR:HG21 | 1:A:273:ALA:H    | 1.61                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:VAL:CG1  | 1:A:175:ILE:N    | 2.64                     | 0.61              |
| 1:A:85:ALA:HB2   | 1:A:233:LEU:CD1  | 2.31                     | 0.60              |
| 1:A:252:ASN:OD1  | 1:A:252:ASN:N    | 2.35                     | 0.60              |
| 1:A:22:THR:OG1   | 1:A:87:SER:CB    | 2.46                     | 0.60              |
| 1:A:125:SER:HB3  | 1:A:221:SER:HB2  | 1.81                     | 0.60              |
| 1:A:201:PRO:HG2  | 1:A:226:HIS:CD2  | 2.36                     | 0.60              |
| 1:A:12:LYS:NZ    | 1:A:269:ASN:CG   | 2.60                     | 0.60              |
| 1:A:74:ALA:C     | 1:A:75:LEU:CD1   | 2.74                     | 0.60              |
| 1:A:235:LEU:O    | 1:A:239:PRO:CA   | 2.49                     | 0.60              |
| 1:A:48:ALA:N     | 1:A:57:ASN:ND2   | 2.48                     | 0.60              |
| 1:A:199:MET:HG3  | 1:A:263:TYR:O    | 2.02                     | 0.60              |
| 1:A:156:GLU:HB2  | 1:A:164:THR:HB   | 1.84                     | 0.60              |
| 1:A:74:ALA:HB1   | 1:A:75:LEU:CD1   | 2.32                     | 0.60              |
| 1:A:235:LEU:O    | 1:A:239:PRO:HA   | 2.01                     | 0.60              |
| 1:A:229:GLY:O    | 1:A:230:ALA:C    | 2.44                     | 0.59              |
| 1:A:152:ALA:HB1  | 1:A:220:THR:HG23 | 1.83                     | 0.59              |
| 1:A:209:LEU:HD11 | 1:A:215:GLY:HA3  | 1.84                     | 0.59              |
| 1:A:238:HIS:HB3  | 1:A:241:TRP:CG   | 2.36                     | 0.59              |
| 1:A:154:GLY:H    | 1:A:220:THR:HG21 | 1.68                     | 0.59              |
| 1:A:232:ALA:HB3  | 1:A:233:LEU:CD1  | 2.32                     | 0.59              |
| 1:A:229:GLY:O    | 1:A:233:LEU:HD13 | 2.03                     | 0.59              |
| 1:A:12:LYS:NZ    | 1:A:269:ASN:OD1  | 2.36                     | 0.59              |
| 1:A:177:VAL:HG11 | 1:A:227:VAL:HG21 | 1.85                     | 0.59              |
| 1:A:180:VAL:HG13 | 1:A:199:MET:HB3  | 1.84                     | 0.59              |
| 1:A:111:ILE:CB   | 1:A:111:ILE:C    | 2.67                     | 0.58              |
| 1:A:211:GLY:O    | 1:A:213:LYS:HG3  | 2.03                     | 0.58              |
| 1:A:111:ILE:O    | 1:A:114:ALA:HB3  | 2.03                     | 0.58              |
| 1:A:179:ALA:HB1  | 1:A:202:GLY:HA3  | 1.85                     | 0.58              |
| 1:A:209:LEU:O    | 1:A:213:LYS:HB2  | 2.02                     | 0.58              |
| 1:A:237:LYS:O    | 1:A:239:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:80:GLY:HA3   | 1:A:214:TYR:CE2  | 2.38                     | 0.58              |
| 1:A:207:SER:O    | 1:A:215:GLY:N    | 2.31                     | 0.58              |
| 1:A:38:SER:O     | 1:A:40:PRO:HD3   | 2.03                     | 0.57              |
| 1:A:127:GLY:CA   | 1:A:167:TYR:O    | 2.53                     | 0.57              |
| 1:A:167:TYR:CD2  | 1:A:171:TYR:CZ   | 2.91                     | 0.57              |
| 1:A:34:GLY:C     | 1:A:35:ILE:HG13  | 2.28                     | 0.57              |
| 1:A:258:GLY:O    | 1:A:259:ASP:C    | 2.46                     | 0.57              |
| 1:A:122:ILE:CG1  | 1:A:147:VAL:HG11 | 2.35                     | 0.57              |
| 1:A:222:MET:O    | 1:A:225:PRO:HD2  | 2.03                     | 0.57              |
| 1:A:98:ASP:O     | 1:A:99:ALA:HB3   | 2.05                     | 0.57              |
| 1:A:237:LYS:C    | 1:A:239:PRO:CD   | 2.77                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:GLY:HA2  | 1:A:167:TYR:O    | 2.04                     | 0.56              |
| 1:A:233:LEU:N    | 1:A:233:LEU:CD1  | 2.68                     | 0.56              |
| 1:A:71:THR:HG21  | 1:A:226:HIS:ND1  | 2.20                     | 0.56              |
| 1:A:136:LYS:HB2  | 1:A:171:TYR:CE1  | 2.40                     | 0.56              |
| 1:A:136:LYS:HB2  | 1:A:171:TYR:CZ   | 2.41                     | 0.56              |
| 1:A:184:ASN:HB3  | 1:A:257:LEU:HD13 | 1.85                     | 0.56              |
| 1:A:85:ALA:N     | 1:A:86:PRO:HD3   | 2.14                     | 0.56              |
| 1:A:109:ASN:O    | 1:A:112:GLU:HB2  | 2.05                     | 0.56              |
| 1:A:189:PHE:CD1  | 1:A:189:PHE:C    | 2.83                     | 0.56              |
| 1:A:177:VAL:CG1  | 1:A:227:VAL:HG21 | 2.35                     | 0.56              |
| 1:A:253:THR:HG21 | 1:A:272:ALA:HB3  | 1.83                     | 0.56              |
| 1:A:122:ILE:HD12 | 1:A:149:VAL:HG22 | 1.88                     | 0.56              |
| 1:A:143:VAL:HA   | 1:A:147:VAL:O    | 2.06                     | 0.56              |
| 1:A:232:ALA:CB   | 1:A:233:LEU:HD12 | 2.36                     | 0.56              |
| 1:A:238:HIS:HE1  | 1:A:274:ALA:O    | 1.89                     | 0.55              |
| 1:A:119:MET:O    | 1:A:147:VAL:HG22 | 2.07                     | 0.55              |
| 1:A:136:LYS:CD   | 1:A:136:LYS:NZ   | 2.66                     | 0.55              |
| 1:A:209:LEU:CD1  | 1:A:215:GLY:HA3  | 2.35                     | 0.55              |
| 1:A:97:GLY:CA    | 1:A:101:SER:CB   | 2.69                     | 0.55              |
| 1:A:41:ASP:OD2   | 1:A:75:LEU:HD11  | 2.05                     | 0.55              |
| 1:A:75:LEU:HB3   | 1:A:77:ASN:ND2   | 2.22                     | 0.55              |
| 1:A:23:GLY:HA2   | 1:A:236:SER:HB3  | 1.89                     | 0.54              |
| 1:A:177:VAL:HG11 | 1:A:227:VAL:CG2  | 2.37                     | 0.54              |
| 1:A:27:LYS:HG2   | 1:A:89:ALA:HB3   | 1.89                     | 0.54              |
| 1:A:206:GLN:OE1  | 1:A:215:GLY:C    | 2.51                     | 0.54              |
| 1:A:268:ILE:O    | 1:A:268:ILE:HG13 | 2.06                     | 0.54              |
| 1:A:74:ALA:O     | 1:A:75:LEU:O     | 2.26                     | 0.54              |
| 1:A:16:LEU:HD11  | 1:A:271:GLN:HA   | 1.90                     | 0.53              |
| 1:A:134:ALA:O    | 1:A:137:ALA:N    | 2.41                     | 0.53              |
| 1:A:131:GLY:O    | 1:A:132:SER:HB2  | 2.07                     | 0.53              |
| 1:A:154:GLY:CA   | 1:A:220:THR:HG21 | 2.38                     | 0.53              |
| 1:A:209:LEU:HD12 | 1:A:215:GLY:N    | 2.24                     | 0.53              |
| 1:A:222:MET:C    | 1:A:225:PRO:CD   | 2.78                     | 0.53              |
| 1:A:242:THR:OG1  | 1:A:245:GLN:OE1  | 2.27                     | 0.53              |
| 1:A:33:SER:O     | 1:A:94:LYS:HE2   | 2.07                     | 0.53              |
| 1:A:244:THR:O    | 1:A:245:GLN:C    | 2.51                     | 0.53              |
| 1:A:154:GLY:N    | 1:A:220:THR:HG21 | 2.23                     | 0.53              |
| 1:A:159:THR:HG23 | 1:A:159:THR:O    | 2.08                     | 0.52              |
| 1:A:238:HIS:CB   | 1:A:241:TRP:CE2  | 2.92                     | 0.52              |
| 1:A:62:ASN:O     | 1:A:63:SER:HB3   | 2.09                     | 0.52              |
| 1:A:84:VAL:HG12  | 1:A:84:VAL:O     | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:186:ARG:HD2  | 1:A:262:TYR:HB3  | 1.90                     | 0.52              |
| 1:A:255:THR:HB   | 1:A:267:LEU:HB3  | 1.90                     | 0.52              |
| 1:A:67:HIS:CG    | 1:A:217:TYR:HD2  | 2.27                     | 0.52              |
| 1:A:136:LYS:HB2  | 1:A:171:TYR:CE2  | 2.44                     | 0.52              |
| 1:A:210:PRO:O    | 1:A:213:LYS:HD2  | 2.09                     | 0.52              |
| 1:A:23:GLY:O     | 1:A:88:SER:HA    | 2.10                     | 0.52              |
| 1:A:22:THR:C     | 1:A:233:LEU:HG   | 2.35                     | 0.52              |
| 1:A:27:LYS:HD3   | 1:A:91:TYR:CE1   | 2.45                     | 0.52              |
| 1:A:55:THR:HB    | 1:A:56:PRO:HD3   | 1.91                     | 0.52              |
| 1:A:167:TYR:CZ   | 1:A:170:LYS:HD3  | 2.45                     | 0.51              |
| 1:A:224:SER:N    | 1:A:225:PRO:CD   | 2.72                     | 0.51              |
| 1:A:134:ALA:O    | 1:A:135:LEU:C    | 2.52                     | 0.51              |
| 1:A:12:LYS:HZ1   | 1:A:269:ASN:CG   | 2.19                     | 0.51              |
| 1:A:177:VAL:O    | 1:A:220:THR:OG1  | 2.28                     | 0.51              |
| 1:A:16:LEU:CD2   | 1:A:270:VAL:HG12 | 2.34                     | 0.51              |
| 1:A:234:ILE:HD12 | 1:A:250:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:270:VAL:O    | 1:A:274:ALA:HB2  | 2.11                     | 0.51              |
| 1:A:179:ALA:CB   | 1:A:202:GLY:HA3  | 2.41                     | 0.50              |
| 1:A:249:SER:OG   | 1:A:273:ALA:O    | 2.28                     | 0.50              |
| 1:A:64:HIS:O     | 1:A:68:VAL:HG23  | 2.11                     | 0.50              |
| 1:A:41:ASP:OD1   | 1:A:79:ILE:HG13  | 2.11                     | 0.50              |
| 1:A:237:LYS:O    | 1:A:239:PRO:HD3  | 2.11                     | 0.50              |
| 1:A:125:SER:CB   | 1:A:221:SER:HB2  | 2.42                     | 0.50              |
| 1:A:19:GLN:HE22  | 1:A:237:LYS:NZ   | 2.09                     | 0.50              |
| 1:A:103:GLN:HG2  | 1:A:105:SER:OG   | 2.12                     | 0.49              |
| 1:A:141:LYS:O    | 1:A:142:ALA:C    | 2.54                     | 0.49              |
| 1:A:91:TYR:CD1   | 1:A:119:MET:HE1  | 2.47                     | 0.49              |
| 1:A:34:GLY:C     | 1:A:35:ILE:CG1   | 2.84                     | 0.49              |
| 1:A:55:THR:HB    | 1:A:56:PRO:HD2   | 1.92                     | 0.49              |
| 1:A:204:SER:CA   | 1:A:218:ASN:OD1  | 2.59                     | 0.49              |
| 1:A:186:ARG:CD   | 1:A:262:TYR:HB3  | 2.43                     | 0.49              |
| 1:A:13:ALA:HB3   | 1:A:14:PRO:HD3   | 1.95                     | 0.48              |
| 1:A:84:VAL:CG1   | 1:A:84:VAL:O     | 2.61                     | 0.48              |
| 1:A:85:ALA:C     | 1:A:87:SER:H     | 2.21                     | 0.48              |
| 1:A:55:THR:CB    | 1:A:56:PRO:HD3   | 2.42                     | 0.48              |
| 1:A:186:ARG:HH21 | 1:A:192:VAL:CG1  | 2.26                     | 0.48              |
| 1:A:47:GLY:HA3   | 1:A:92:ALA:O     | 2.14                     | 0.48              |
| 1:A:184:ASN:HB3  | 1:A:257:LEU:CD1  | 2.44                     | 0.48              |
| 1:A:57:ASN:HD21  | 1:A:92:ALA:C     | 2.11                     | 0.48              |
| 1:A:103:GLN:HB3  | 1:A:106:TRP:CE3  | 2.48                     | 0.48              |
| 1:A:238:HIS:CE1  | 1:A:274:ALA:O    | 2.66                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ILE:CB   | 1:A:111:ILE:N    | 2.69                     | 0.48              |
| 1:A:223:ALA:C    | 1:A:225:PRO:CD   | 2.87                     | 0.48              |
| 1:A:257:LEU:HD23 | 1:A:257:LEU:HA   | 1.59                     | 0.48              |
| 1:A:41:ASP:OD2   | 1:A:80:GLY:HA3   | 2.14                     | 0.47              |
| 1:A:122:ILE:HG13 | 1:A:147:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:155:ASN:OD1  | 1:A:220:THR:HG22 | 2.14                     | 0.47              |
| 1:A:39:HIS:ND1   | 1:A:39:HIS:C     | 2.72                     | 0.47              |
| 1:A:113:TRP:C    | 1:A:113:TRP:CD2  | 2.92                     | 0.47              |
| 1:A:6:TYR:CD1    | 1:A:6:TYR:C      | 2.93                     | 0.47              |
| 1:A:39:HIS:ND1   | 1:A:40:PRO:HD2   | 2.29                     | 0.47              |
| 1:A:201:PRO:HG2  | 1:A:226:HIS:CG   | 2.48                     | 0.47              |
| 1:A:235:LEU:O    | 1:A:239:PRO:N    | 2.47                     | 0.47              |
| 1:A:46:GLY:O     | 1:A:92:ALA:N     | 2.47                     | 0.47              |
| 1:A:85:ALA:CA    | 1:A:233:LEU:HD11 | 2.40                     | 0.47              |
| 1:A:139:VAL:HG12 | 1:A:173:SER:OG   | 2.14                     | 0.46              |
| 1:A:113:TRP:CD2  | 1:A:113:TRP:O    | 2.69                     | 0.46              |
| 1:A:135:LEU:C    | 1:A:139:VAL:HG23 | 2.40                     | 0.46              |
| 1:A:125:SER:HB3  | 1:A:221:SER:CB   | 2.44                     | 0.46              |
| 1:A:68:VAL:HG13  | 1:A:225:PRO:HG3  | 1.97                     | 0.46              |
| 1:A:122:ILE:HD12 | 1:A:147:VAL:CG1  | 2.41                     | 0.46              |
| 1:A:231:ALA:O    | 1:A:232:ALA:C    | 2.58                     | 0.46              |
| 1:A:17:HIS:HE2   | 1:A:86:PRO:CD    | 2.29                     | 0.46              |
| 1:A:13:ALA:O     | 1:A:17:HIS:N     | 2.49                     | 0.45              |
| 1:A:51:VAL:HA    | 1:A:52:PRO:HD2   | 1.62                     | 0.45              |
| 1:A:17:HIS:NE2   | 1:A:86:PRO:CD    | 2.80                     | 0.45              |
| 1:A:104:TYR:CD1  | 1:A:107:ILE:HD12 | 2.50                     | 0.45              |
| 1:A:201:PRO:C    | 1:A:201:PRO:CB   | 2.81                     | 0.45              |
| 1:A:138:ALA:O    | 1:A:139:VAL:C    | 2.59                     | 0.45              |
| 1:A:67:HIS:CD2   | 1:A:217:TYR:HD2  | 2.34                     | 0.45              |
| 1:A:238:HIS:HB3  | 1:A:241:TRP:CE2  | 2.51                     | 0.45              |
| 1:A:250:LEU:HD13 | 1:A:250:LEU:HA   | 1.80                     | 0.45              |
| 1:A:71:THR:O     | 1:A:84:VAL:N     | 2.44                     | 0.45              |
| 1:A:159:THR:O    | 1:A:159:THR:CG2  | 2.65                     | 0.45              |
| 1:A:177:VAL:CG1  | 1:A:200:ALA:HB3  | 2.46                     | 0.45              |
| 1:A:219:GLY:HA3  | 1:A:222:MET:SD   | 2.57                     | 0.45              |
| 1:A:47:GLY:O     | 1:A:48:ALA:HB2   | 2.17                     | 0.45              |
| 1:A:233:LEU:CD1  | 1:A:233:LEU:H    | 2.30                     | 0.45              |
| 1:A:41:ASP:O     | 1:A:75:LEU:N     | 2.42                     | 0.45              |
| 1:A:154:GLY:C    | 1:A:191:SER:OG   | 2.60                     | 0.45              |
| 1:A:26:VAL:HG21  | 1:A:232:ALA:O    | 2.16                     | 0.45              |
| 1:A:85:ALA:C     | 1:A:87:SER:N     | 2.72                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:17:HIS:HE2   | 1:A:86:PRO:HD2  | 1.81                     | 0.44              |
| 1:A:74:ALA:HB3   | 1:A:83:GLY:N    | 2.32                     | 0.44              |
| 1:A:96:LEU:C     | 1:A:96:LEU:N    | 2.64                     | 0.44              |
| 1:A:12:LYS:C     | 1:A:14:PRO:HD2  | 2.42                     | 0.44              |
| 1:A:19:GLN:HG2   | 1:A:21:TYR:CD2  | 2.51                     | 0.44              |
| 1:A:34:GLY:O     | 1:A:65:GLY:HA3  | 2.18                     | 0.44              |
| 1:A:55:THR:CG2   | 1:A:56:PRO:N    | 2.78                     | 0.44              |
| 1:A:238:HIS:ND1  | 1:A:241:TRP:CZ2 | 2.85                     | 0.44              |
| 1:A:67:HIS:CE1   | 1:A:217:TYR:HB2 | 2.53                     | 0.44              |
| 1:A:4:VAL:HA     | 1:A:5:PRO:HD2   | 1.64                     | 0.44              |
| 1:A:55:THR:CG2   | 1:A:56:PRO:HD3  | 2.48                     | 0.44              |
| 1:A:200:ALA:O    | 1:A:202:GLY:N   | 2.51                     | 0.44              |
| 1:A:209:LEU:CD1  | 1:A:215:GLY:N   | 2.81                     | 0.43              |
| 1:A:201:PRO:HB2  | 1:A:226:HIS:CE1 | 2.53                     | 0.43              |
| 1:A:19:GLN:CG    | 1:A:21:TYR:HE2  | 2.13                     | 0.43              |
| 1:A:211:GLY:O    | 1:A:212:ASN:C   | 2.61                     | 0.43              |
| 1:A:222:MET:O    | 1:A:225:PRO:HG2 | 2.18                     | 0.43              |
| 1:A:180:VAL:HG22 | 1:A:200:ALA:C   | 2.43                     | 0.43              |
| 1:A:224:SER:HB3  | 1:A:225:PRO:HD3 | 2.01                     | 0.43              |
| 1:A:84:VAL:CA    | 1:A:86:PRO:HD3  | 2.49                     | 0.42              |
| 1:A:161:SER:C    | 1:A:162:SER:O   | 2.61                     | 0.42              |
| 1:A:203:VAL:O    | 1:A:204:SER:C   | 2.62                     | 0.42              |
| 1:A:113:TRP:C    | 1:A:113:TRP:CE3 | 2.97                     | 0.42              |
| 1:A:11:ILE:O     | 1:A:12:LYS:NZ   | 2.33                     | 0.42              |
| 1:A:34:GLY:HA3   | 1:A:60:ASP:HB2  | 2.02                     | 0.42              |
| 1:A:142:ALA:O    | 1:A:147:VAL:N   | 2.44                     | 0.42              |
| 1:A:96:LEU:HD23  | 1:A:101:SER:O   | 2.20                     | 0.42              |
| 1:A:64:HIS:O     | 1:A:65:GLY:C    | 2.62                     | 0.42              |
| 1:A:12:LYS:HB2   | 1:A:12:LYS:HZ2  | 1.85                     | 0.41              |
| 1:A:238:HIS:CB   | 1:A:241:TRP:CD2 | 3.03                     | 0.41              |
| 1:A:6:TYR:CZ     | 1:A:203:VAL:O   | 2.73                     | 0.41              |
| 1:A:207:SER:O    | 1:A:214:TYR:HA  | 2.19                     | 0.41              |
| 1:A:213:LYS:C    | 1:A:214:TYR:CG  | 2.98                     | 0.41              |
| 1:A:6:TYR:CZ     | 1:A:205:ILE:CD1 | 3.03                     | 0.41              |
| 1:A:153:ALA:HB2  | 1:A:176:ALA:HB1 | 2.02                     | 0.41              |
| 1:A:199:MET:HG3  | 1:A:263:TYR:HA  | 2.02                     | 0.41              |
| 1:A:270:VAL:O    | 1:A:274:ALA:CB  | 2.69                     | 0.41              |
| 1:A:54:GLU:O     | 1:A:55:THR:C    | 2.64                     | 0.41              |
| 1:A:60:ASP:C     | 1:A:60:ASP:OD1  | 2.64                     | 0.41              |
| 1:A:84:VAL:O     | 1:A:86:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:97:GLY:O     | 1:A:98:ASP:C    | 2.64                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ILE:HG21 | 1:A:111:ILE:HD13 | 1.92                     | 0.41              |
| 1:A:135:LEU:HD12 | 1:A:135:LEU:HA   | 1.83                     | 0.41              |
| 1:A:123:ASN:HA   | 1:A:150:VAL:O    | 2.21                     | 0.40              |
| 1:A:170:LYS:NZ   | 1:A:195:GLU:OE1  | 2.48                     | 0.40              |
| 1:A:67:HIS:CG    | 1:A:217:TYR:CD2  | 3.09                     | 0.40              |

All (15) 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:6:TYR:CG    | 1:A:161:SER:OG[4_545]  | 0.90                     | 1.30              |
| 1:A:18:SER:CB   | 1:A:162:SER:OG[3_545]  | 1.11                     | 1.09              |
| 1:A:6:TYR:CB    | 1:A:161:SER:OG[4_545]  | 1.26                     | 0.94              |
| 1:A:185:GLN:OE1 | 1:A:213:LYS:CD[4_555]  | 1.37                     | 0.83              |
| 1:A:183:SER:OG  | 1:A:271:GLN:OE1[2_655] | 1.51                     | 0.69              |
| 1:A:6:TYR:CD2   | 1:A:161:SER:OG[4_545]  | 1.54                     | 0.66              |
| 1:A:55:THR:OG1  | 1:A:144:ALA:O[4_546]   | 1.55                     | 0.65              |
| 1:A:185:GLN:NE2 | 1:A:213:LYS:NZ[4_555]  | 1.61                     | 0.59              |
| 1:A:18:SER:OG   | 1:A:162:SER:OG[3_545]  | 1.70                     | 0.50              |
| 1:A:185:GLN:CD  | 1:A:213:LYS:CE[4_555]  | 1.81                     | 0.39              |
| 1:A:185:GLN:CD  | 1:A:213:LYS:CD[4_555]  | 1.88                     | 0.32              |
| 1:A:206:GLN:CB  | 1:A:262:TYR:OH[4_545]  | 1.90                     | 0.30              |
| 1:A:6:TYR:CB    | 1:A:161:SER:CB[4_545]  | 1.97                     | 0.23              |
| 1:A:6:TYR:CG    | 1:A:161:SER:CB[4_545]  | 1.97                     | 0.23              |
| 1:A:185:GLN:CD  | 1:A:213:LYS:NZ[4_555]  | 2.14                     | 0.06              |

## 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     | 273/275 (99%) | 212 (78%) | 43 (16%) | 18 (7%)  | <b>1</b> <b>1</b> |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LYS  |
| 1   | A     | 35  | ILE  |
| 1   | A     | 55  | THR  |
| 1   | A     | 69  | ALA  |
| 1   | A     | 75  | LEU  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 132 | SER  |
| 1   | A     | 48  | ALA  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 81  | VAL  |
| 1   | A     | 112 | GLU  |
| 1   | A     | 113 | TRP  |
| 1   | A     | 259 | ASP  |
| 1   | A     | 260 | SER  |
| 1   | A     | 254 | THR  |
| 1   | A     | 201 | PRO  |
| 1   | A     | 65  | GLY  |
| 1   | A     | 80  | GLY  |

### 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     | 205/205 (100%) | 183 (89%) | 22 (11%) | <b>6</b> <b>13</b> |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | TYR  |
| 1   | A     | 75  | LEU  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 87  | SER  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 126 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 130 | SER  |
| 1   | A     | 158 | SER  |
| 1   | A     | 233 | LEU  |
| 1   | A     | 235 | LEU  |
| 1   | A     | 236 | SER  |
| 1   | A     | 242 | THR  |
| 1   | A     | 243 | ASN  |
| 1   | A     | 247 | ARG  |
| 1   | A     | 250 | LEU  |
| 1   | A     | 251 | GLN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 253 | THR  |
| 1   | A     | 268 | ILE  |
| 1   | A     | 270 | VAL  |
| 1   | A     | 275 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 19  | GLN  |
| 1   | A     | 25  | ASN  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 67  | HIS  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 212 | ASN  |
| 1   | A     | 238 | HIS  |
| 1   | A     | 245 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [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     | 19               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 79:ILE    | C      | 80:GLY    | N      | 1.62         |
| 1     | A     | 265:LYS   | C      | 266:GLY   | N      | 1.20         |
| 1     | A     | 129:PRO   | C      | 130:SER   | N      | 1.19         |
| 1     | A     | 215:GLY   | C      | 216:ALA   | N      | 1.19         |
| 1     | A     | 254:THR   | C      | 255:THR   | N      | 1.19         |
| 1     | A     | 78:SER    | C      | 79:ILE    | N      | 1.18         |
| 1     | A     | 124:MET   | C      | 125:SER   | N      | 1.18         |
| 1     | A     | 147:VAL   | C      | 148:VAL   | N      | 1.18         |
| 1     | A     | 156:GLU   | C      | 157:GLY   | N      | 1.18         |
| 1     | A     | 177:VAL   | C      | 178:GLY   | N      | 1.18         |
| 1     | A     | 4:VAL     | C      | 5:PRO     | N      | 1.17         |
| 1     | A     | 182:SER   | C      | 183:SER   | N      | 1.17         |
| 1     | A     | 218:ASN   | C      | 219:GLY   | N      | 1.17         |
| 1     | A     | 158:SER   | C      | 159:THR   | N      | 1.16         |
| 1     | A     | 118:ASN   | C      | 119:MET   | N      | 1.14         |
| 1     | A     | 196:LEU   | C      | 197:ASP   | N      | 1.14         |
| 1     | A     | 263:TYR   | C      | 264:GLY   | N      | 1.14         |
| 1     | A     | 219:GLY   | C      | 220:THR   | N      | 1.12         |
| 1     | A     | 85:ALA    | C      | 86:PRO    | N      | 1.11         |

## 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.